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## Progression of performance assessment modeling for the Yucca Mountain disposal system for spent nuclear fuel and high-level radioactive waste

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### ABSTRACT

This paper summarizes the evolution of consequence modeling for a repository for spent nuclear fuel and high-level radioactive waste at Yucca Mountain in southern Nevada. The discussion includes four early performance assessments (PAs) conducted between 1982 and 1995 to support selection and to evaluate feasibility and three major PAs conducted between 1998 and 2008 to evaluate viability, recommend the site, and assess compliance. Modeling efforts in 1982 estimated dose to individuals 18 km from the site caused by volcanic eruption through the repository. Modeling in 1984 estimated releases via the groundwater pathway because of container corrosion. In combination, this early analysis supported the first environmental assessment. Analysts in 1991 evaluated cumulative release, as specified in the 1985 US radiation protection standards, via the groundwater pathway over  $10^4$  yr at a 5-km boundary by modeling waste degradation and flow/transport in the saturated and unsaturated zones. By 1992, however, the US Congress mandated a change to a dose measure. Thus, the 1993 and 1995 performance assessments improved modeling of waste container degradation to provide better estimates of radionuclide release rates out to  $10^6$  yr. The 1998 viability assessment was a major step in modeling complexity. Dose at a 20-km boundary from the repository was evaluated through  $10^6$  yr for undisturbed conditions using more elaborate modeling of flow and the addition of modules for modeling infiltration, drift seepage, the chemical environment, and biosphere transport. The 2000 assessment for the site recommendation refined the analysis. Seepage modeling was greatly improved and waste form degradation modeling included more chemical dependence. The 2008 compliance assessment for the license application incorporated the influence of the seismicity on waste package performance to evaluate dose at an ~18-km boundary.

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### 1. Introduction

In June 2008, the US Department of Energy (DOE) submitted the safety analysis report for a license application (SAR/LA) to the US Nuclear Regulatory Commission (NRC) to construct a repository at Yucca Mountain in southern Nevada for disposal of commercial spent nuclear fuel (CSNF), DOE-owned spent nuclear fuel (DSNF), and high-level radioactive waste (HLW) [1,2]. The SAR/LA was an important milestone in the effort to implement the US nuclear waste policy, which had been in place since 1983. The application is heavily dependent on the result of an engineering modeling analysis of the disposal system, called a performance assessment (PA), which is summarized in this special issue of *Reliability Engineering and System Safety*. This paper summarizes the progression of exposure pathway/consequence models used in seven PAs, starting in 1982, to provide historical context to the 2008 PA for the license application (PA-LA).<sup>1</sup> Appendix A provides a timeline of modeling events. Although the Obama Administration and the US Congress brought a *de facto* halt to the Yucca Mountain Project (YMP) by a lack of funding in 2010 and began the process of formulating new policy, much can be learned from the past technical approach used to reach this milestone.

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<sup>1</sup> This is but one approach. Other perspectives can be useful to comprehend the immense amount of information, since this paper cannot provide a detailed introduction to the models as in the 8578 page, 16 volume SAR/LA [2] or in the 4270 page Analysis Model Report (AMR) on the PA-LA [1], while, at the same time, providing an historical perspective from earlier PAs.

## 1.1. Consequence modeling

Although an analysis for characterization of a system often involves teasing a system apart into simpler components (e.g. [3]), an analysis for a PA involves synthesis of diverse components to comprehend the behavior of the system as a whole. The ultimate purpose of the PA is to build confidence that the range in behavior of the disposal system will be within safe limits in the future whatever the real situation [4]. That is, the purpose of a PA is to assess risk, not to make a precise prediction. A precise prediction requires identifying when events and processes will occur, where the events and processes will occur, and the characteristics of the particular events and processes (i.e., when, where, and how much). The usefulness of the prediction depends on its accuracy (such as the exact date, time, location, wind velocity, and precipitation for a severe thunderstorm event). In contrast, assessing the risk of events and process requires examining the record of the possible range of consequences and corresponding probabilities from these events and processes, not their precise timing in the future. For common hazards, such as severe weather, past records exist from which to estimate the range in severity and corresponding probability of the event occurring at some location (i.e., the range in “how much”). For extremely rare hazards, records do not exist. Hence, an important purpose of PA modeling is to develop a synthetic record of a range of consequences, using a system model as described in this paper, and corresponding probabilities (e.g., [5]). Furthermore, the synthetic record is constrained to those hypothetical situations of regulatory interest. Fortunately, science is more capable of estimating the range in consequences, based on the scientific knowledge identified as important during disposal system characterization, than making a precise prediction of the timing of one particular consequence sometime in the future.

The practicality of using the synthesized system for analyzing a risk measure such as mean cumulative releases  $\bar{R}$  or mean dose  $\bar{D}(t)$  for comparison to limits set by the US Environmental Protection Agency (EPA) [6] depends on the level of detail and complexity of the underlying exposure pathway/consequence model  $\mathcal{R}_j(\sim)$ , the probability model  $\mathcal{P}\{\mathcal{A}_j\}$  for scenario class  $\mathcal{A}_j$ , and the computational capabilities available at the time. Because EPA also required that uncertainty in the performance measure be evaluated, the distribution of  $R(\mathbf{e}^e, \mathbf{a})$  or  $D(t; \mathbf{e}^e, \mathbf{a})$  (i.e.,  $\mathcal{G}(R(\mathbf{e}^e, \mathbf{a}))$  and  $\mathcal{G}(D(t; \mathbf{e}^e, \mathbf{a}))$ , respectively) had to be determined along with the mean (where the parameter set  $\mathbf{p}$  is divided into a set of epistemic parameters  $\mathbf{e}$  for exposure consequence or probability models, a set of aleatoric parameters  $\mathbf{a}$ , and a set of fixed parameters  $\mathbf{f}$  (i.e.,  $\mathbf{p} = \{\mathbf{e}^e, \mathbf{e}^p, \mathbf{a}, \mathbf{f}\}$ ) but where the set of fixed parameters will normally be omitted herein [5]).

The complicated  $\mathcal{R}(\sim)$  assembled for YMP necessitated a Monte Carlo approach to evaluating  $\mathcal{G}(R(\mathbf{e}^e, \mathbf{a}))$  and  $\mathcal{G}(D(t; \mathbf{e}^e, \mathbf{a}))$  and, thus, numerous evaluations of  $R(\mathbf{e}^e, \mathbf{a})$  or  $D(t; \mathbf{e}^e, \mathbf{a})$ . Although  $\mathcal{R}(\sim)$  for a PA model could consist of one mega model, the scenario classes, the time scales, and the spatial scales are so varied over which various phenomena act that the disposal system must be divided into several submodels. An obvious division is the use of distinct models for the main scenario classes considered ( $\mathcal{A}_j$ ),  $\mathcal{R}_j(\sim)$ . In 1982 and thereafter, a distinct model was developed to evaluate the consequences of volcanic eruption through the repository,  $\mathcal{R}_{VE}(\sim)$ . Another consideration used to divide  $\mathcal{R}(\sim)$  into submodels was the spatial location  $\beta$ . In 1991 and thereafter, a distinct model was used for the waste degradation ( $\mathcal{M}^{Waste}$ ), the underlying natural barrier in the unsaturated zone ( $\mathcal{M}^{UZ}$ ), and the natural barrier in the saturated zone ( $\mathcal{M}^{SZ}$ ). Finally, another consideration used to divide  $R$  was various phenomena such as hydrologic flow and chemical species transport. The  $\mathcal{R}(\sim)$  was formed by linking the modeling modules  $\mathcal{M}_j^p$ ; in other words,  $\mathcal{R}(\sim)$  is a composite of several submodels  $\mathcal{M}_j^p$  such as the 4 modules in 1991:  $\mathcal{R}_j(\mathcal{M}_j^{SZ}(\mathcal{M}_j^{UZTrans}(\mathcal{M}_j^{UZFlow}, \mathcal{M}_j^{Waste}(\mathcal{M}_j^{UZFlow}))))$ . Herein, the evolution of  $\mathcal{R}(\sim)$  is discussed primarily by depicting the addition and linkage of computational models from the 2 modules in 1984 to 11 modules for the undisturbed groundwater scenario class by 2008 ( $\mathcal{M}_U^p$ ). That is, as computer capabilities increased so did the level of detail and complexity of  $\mathcal{R}(\sim)$ .

Presentation of some of the simplifications in  $\mathcal{R}(\sim)$  is also necessary to understand the information flowing through the linkages. Hence, some details on the modeling of disruptive scenario classes (human intrusion, igneous intrusion, and volcanic eruption) are also presented here. However, more extensive explanations of modeling simplifications for the undisturbed scenario class are discussed in companion papers [7–10].

## 1.2. Overview of PA modeling studies

Similar in concept to the iterative numerical solution of mathematical models, YMP iterated upon the overall mathematical formulation of  $\mathcal{R}(\sim)$  to obtain a better, more focused description. Four early iterations of the PAs to evaluate feasibility of the YM disposal system are discussed: (1) PA-EA, a deterministic evaluation of a volcanic eruption [11], and a deterministic evaluation of undisturbed disposal system evolution [12,13], which supported a 1984 draft and 1986 final environmental assessment [6]; (2) PA-91 [14], the first stochastic simulation; (3) PA-93 [15]; and (4) PA-95 [16]. The latter two evaluations provided guidance on repository design options. These four early PAs were followed by three PAs to support major decisions: (5) PA-VA [17], a viability assessment for Congress in 1998; (6) PA-SR [18], an analysis completed in 2000 for the site recommendation; and (7) PA-LA [1,2], the licensing application analysis completed in 2008.

## 2. Volcanic consequence and groundwater release in PA-EA

### 2.1. Doses via volcanic eruption in 1982

In 1976, DOE and NRC both funded conferences to explore modeling of geologic disposal systems for radioactive waste [5, Appendix A]. By 1978, NRC had asked Sandia National Laboratories (SNL) to develop an analysis methodology for radioactive waste repositories [19], similar to that conducted for nuclear reactors [20] (Appendix A). The analyst method abandoned complicated event trees and selected an approach using simple process modeling [5,21].<sup>2</sup> From this background, SNL evaluated the radiological consequences and probability of an igneous eruption scenario ( $\mathcal{A}_{VE}$ ) through the Yucca Mountain (YM) repository at the edge of the Nevada Nuclear Security Site (formerly Nevada Test Site or NTS) in 1982. The models for the deterministic evaluation of exposure via volcanic eruption  $\mathcal{R}_{VE}(\sim)$  consisted of a volcanic eruption model  $\mathcal{M}^{Ash}$ , a dike interaction module  $\mathcal{M}^{dike}$ , and a biosphere pathway model  $\mathcal{M}^{Bio}$ . The  $\mathcal{M}^{Ash}$  was based on a Gaussian

<sup>2</sup> However, the Electrical Power Research Institute (EPRI) has conducted PAs using a logic-tree approach since 1990 which was akin to using discrete rather than continuous parameter values in the process models [22].

plume computational code constructed for the EPA, AIRDOS-EPA [11].

$$D_{VE}^{82}(t; \mathbf{e}_{VE}^e) = \sum_{r=1}^{n_{VE}^r = 33} f_{VE,path,r}^{BCDF} \mathcal{R}_{VE,r}(t; \mathbf{e}_{VE}^e) \Big|_{x^{ae} = 18 \text{ km}} \quad (1)$$

The  $\mathcal{M}^{Dike}$  evaluated the fraction of inventory disrupted by the dike (here for the  $\mathcal{A}_{VE}$  scenario subclass but also for the  $\mathcal{A}_{VI}$  scenario subclass in later PAs<sup>3</sup>). The inventory was the product of two fractions: (1) the fraction of packages breached by an erupting dike  $f_{VE}^{br}$ , and (2) the fraction of inventory entrained per package given a package contacted a dike  $f_{VE}^{waste}$ . For the volcanic eruption, the entire contents of a package was released (i.e.,  $f_{VE}^{waste} = 1.0$ ). The mean fraction of vertically emplaced packages intersected by an erupting dike was quite small for vertically emplaced packages (i.e.,  $f_{VE}^{br} = 8 \times 10^{-5}$ ) [11, Section 4.3.2]. The  $f_{VE}^{br}$  was estimated from geometric arguments as a function of expected dike length in the repository, dike width, container diameter, and repository area (i.e.,  $f_{VE}^{br} = \bar{L}^{dike} (w^{dike} + 2r^{can}) / A^{rep}$ ).<sup>4</sup>

The  $\mathcal{M}^{Bio}$  was based on another code specifically built for EPA, AMRAW (Assessment Method for Radioactive Waste) [11, Appendix C]. The  $\mathcal{M}^{Bio}$  calculated fixed biological dose conversion factors for four pathways  $f_{VE,path,r}^{BCDF}$ : (1) inhalation during eruption and ingestion of food crops, (2) redistribution of tephra and resuspension, (3) surface exposure while hiking on the volcanic cone, and (4) use of material from the volcanic cone for buildings.<sup>5</sup>

### 2.2. Release via groundwater pathway in PA-EA

By December of 1984, SNL had completed a deterministic analysis to evaluate the feasibility of a repository at Yucca Mountain [12,13]. Based on draft EPA requirements in 40 CFR 191, proposed in 1982, and the NRC subsystem requirements of 10 CFR 60, published in 1983, SNL evaluated the normalized, cumulative release  $R_U^{84}(\mathbf{e}^e)$  over  $10^4$  yr, using fixed parameters  $\mathbf{e}^e$  for the undisturbed scenario class at a boundary 10 km away from the repository (although results at an intermediate 2-km boundary were also calculated) (Appendix B):

$$R_U^{84}(\mathbf{e}^e) = \sum_{r=1}^{n_U^r = 17} \frac{1}{L_r f_{mass}} \int_0^{10^4 \text{ yr}} \mathcal{R}_{U,r}(t; \mathbf{e}^e) \Big|_{x^{ae} = 10 \text{ km}} dt \quad (2)$$

where  $L_r$  is the limiting value specified in 40 CFR 191 for 17 radionuclides  $r$  evaluated in PA-EA for the groundwater pathway (i.e.,  $n_U^r = 17$ ) and  $f_{mass}$  is the mass fraction in the repository (metric tons of heavy metal—MTHM—divided by 1000). Because only a subset of radionuclides is of interest in 40 CFR 191, the parameters specific to each radionuclide are here conceptually represented by a separate model ( $\mathcal{R}_{U,r}(t; \mathbf{e}^e)$ ) so that the sum over the radionuclides is explicit. Although a detailed one-dimensional groundwater and transport code was under development at SNL, the Total System Performance Assessment Code (TOSPAC) [23–25], the groundwater pathway exposure model for the undisturbed scenario class ( $\mathcal{R}_{U,r}(t; \mathbf{e}^e)$ ) was based on a preliminary simple computational code, SAMPLE, for PA-EA [12]. SAMPLE modeled rudimentary UZ and SZ transport ( $\mathcal{M}_{SAMPLE}^{UZtrans}$  and  $\mathcal{M}_{SAMPLE}^{SZtrans}$  in Eq. (2)). Although Eq. (2) succinctly shows the linkage of the major modules for the stochastic calculation, often several models are necessary inside the modules to conduct the PA. Hence, this paper also depicts the linkages to these major models inside the modules as a means to introduce the discussion in companion papers [7–10] (Fig. 1).

### 3. PA-91

Between PA-EA and 1991, the use of simplified models in a PA, based on more detailed process models, had been described and adopted in the 1988 Site Characterization Plan (SCP) (“abstraction” in the parlance of YMP) [26, Section 8.3.5.13; 27]. Preliminary assessments of repository risks were conducted using literature data by the Pacific Northwest National Laboratory (PNNL) in the late 1980s [28]. Also, the Performance Assessment Calculation Exercise (PACE-90) was initiated to coordinate development of the necessary modeling capability for PAs [29]. The exercise resulted in a deterministic analysis of YM performance, the first major PA analysis in the feasibility phase of YMP (Appendix A) [30]. Yet, in their first report to Congress in March 1990, the Nuclear Waste Technical Review Board (NWTRB), formed by the Nuclear Waste Policy Amendments Act of 1987 (NWPAA) [6], noted the general lack of the improvement in PA capability since PA-EA [31]. PA-91 was conducted in the later part of 1991 to demonstrate the feasibility of the repository and the ability to conduct stochastic calculations using abstractions [14, p. ES-2]<sup>6</sup>. The progress of PA-91 was noted by the NWTRB [39].

PA-91 evaluated the total CCDF of the cumulative, normalized releases  $R^{91}$  for the undisturbed scenario class and two disruptive scenario classes, volcanic eruption and human intrusion (i.e.,  $\mathcal{A}_U$ ,  $\mathcal{A}_{VE}$ , and  $\mathcal{A}_H$ ). Although not mutually exclusive, the scenario classes were independent

<sup>3</sup> The other part of the igneous intrusive scenario, disruption of containers in the repository by a dike that does not necessarily erupt at the surface, was first included in PA-93.

<sup>4</sup> For PA-LA with packages emplaced in the drifts without backfill,  $f_{VE}^{br}$  was set at 1.0.

<sup>5</sup> A dose measure was evaluated in 1982, similar to an Environmental Impact Statement (EIS). The EPA radiation protection standards, 40 CFR 191, promulgated later in 1985, used a normalized, cumulative release measure  $R$  and considered the surface as part of the accessible environment.

<sup>6</sup> In comparison, direct use of streamlined process models in the PA was emphasized when evaluating the disposal of defense-related transuranic waste at the Waste Isolation Pilot Plant (WIPP), although simplifications such as response surfaces and impulse functions were still necessary. Two full stochastic PAs using this detailed modeling approach had been conducted for WIPP by 1991 (Appendix A). With due diligence either approach is viable; yet, when applied to specific sites one approach may offer implementation advantages [32; 33; 34, p. 3, 35–38].

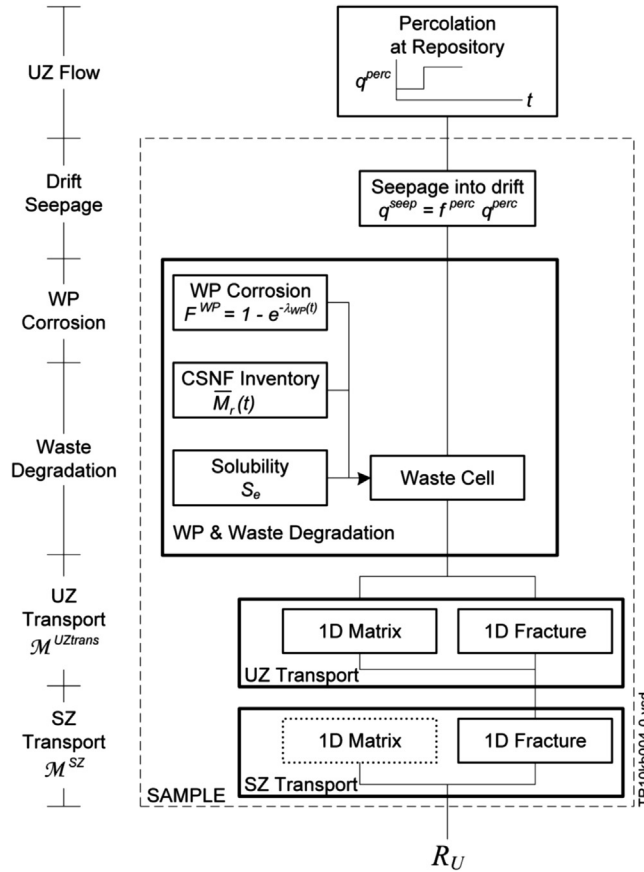


Fig. 1. PA-EA model for UZ and SZ groundwater pathway of undisturbed scenario class ( $A_U$ ).

practically; thus, the disruptive scenario classes were treated as *incremental* releases (an assumption that would be used also for PA-SR and PA-LA) [14, Fig. 8-2]. Thus, the total CCDF was the sum of the CCDFs for each scenario class (and implemented by summing random samples from the scenario class CCDFs) [14, p. 8-9]:

$$\wp\{R^{91} > R\} = 1 - G(R^{91}) = \sum_{i=1}^{n^{ndm}=10^4} \mathcal{H}\{(R_{U,i} + R_{VE,i} + R_{H,i}) - R\} = \sum_{i=1}^{n^{ndm}=10^4} \mathcal{H}\left\{\left(\sum_{j=1}^{n^S} G_j^{-1}(U_{j,i})\right) - R\right\} \quad (3)$$

where  $G_j(\sim)$  is the cumulative distribution function for  $\mathcal{R}_j$  (Eq. (2)) and  $G_j^{-1}(\sim)$ , its inverse;  $U_{j,i}$  is an independently randomly sampled value for the  $j$  scenario classes considered ( $\mathcal{A}_U$ ,  $\mathcal{A}_{VE}$ , and  $\mathcal{A}_H$ );  $\mathcal{H}\{x\}=0$  if  $x \leq 0$ ;  $\mathcal{H}\{x\}=1$  if  $x > 0$ , and  $R$  is a number  $\geq 0$ . The practical independence of the parameters for each scenario classes is assumed in Eq. (3) (i.e., the undisturbed scenario is (1) clearly independent from eruptive releases; (2) clearly independent from the cutting release brought to the surface after human intrusion; and (3) independent in a practical sense from the groundwater releases after human intrusion since the latter are so small).

### 3.1. Undisturbed release via groundwater pathway

The undisturbed scenario class was further divided into two pathways: a groundwater pathway (*gw*) and a gaseous pathway for  $^{14}\text{C}$  (*gas*), whose releases were summed prior to forming the CCDF [14, Fig. 8-2] (Fig. 2). The model for evaluating  $\mathcal{R}_{U,gw}(\sim)$  consisted of four modules: (1) a module for vertical UZ flow from 10 m above the repository and to the water table below the repository,  $\mathcal{R}_{U,gw}$  [7], (2) a source term component (a subroutine in TOSPAC) for degradation of the waste (precursor to waste package and waste degradation modules  $\mathcal{M}^{WP}$  and  $\mathcal{M}^{Waste}$ ) [8,9], (3) a module for transport in six columns in the UZ,  $\mathcal{M}^{UZtrans}$ , using TOSPAC [10], and (4) a module for horizontal flow and transport in the SZ to the 5-km boundary of the accessible environment,  $\mathcal{M}^{SZ}$ , using STAFF2D [10] (Fig. 2). Two conceptual models were evaluated in  $\mathcal{M}^{UZflow}$ : an equivalent continuum model (ECM) of the fluid flow in the tuff matrix and fractures, implemented in TOSPAC [24,25], and a conceptualization of only fracture flow implemented in WEEPSTA (i.e.,  $\mathcal{M}_{TOSPAC}^{UZflow}$  and  $\mathcal{M}_{WEEPSTA}^{UZflow}$ ) [7]. In addition, rudimentary aspects of the thermal environment (for scaling gas flow calculations), drift seepage (as a distribution), and container corrosion (as a distribution of complete failure) were also present [8] (Fig. 2). PA-91 was assembled by manually connecting  $\mathcal{M}^{UZtrans}$  and  $\mathcal{M}^{SZ}$  [14, pp. 4-51 to 4-94], but much of the analysis was automated through a Total System Analyzer (TSA) developed at SNL (Fig. 2) [40].

The evaluation of the CCDF for the undisturbed scenario class for the ECM conceptualization (Eq. (4)) and weeps conceptualization (Eq. (5)) was performed with the following linked modeling modules for 9 radionuclides  $r$  using either 300 or 1000 Latin Hypercube Samples

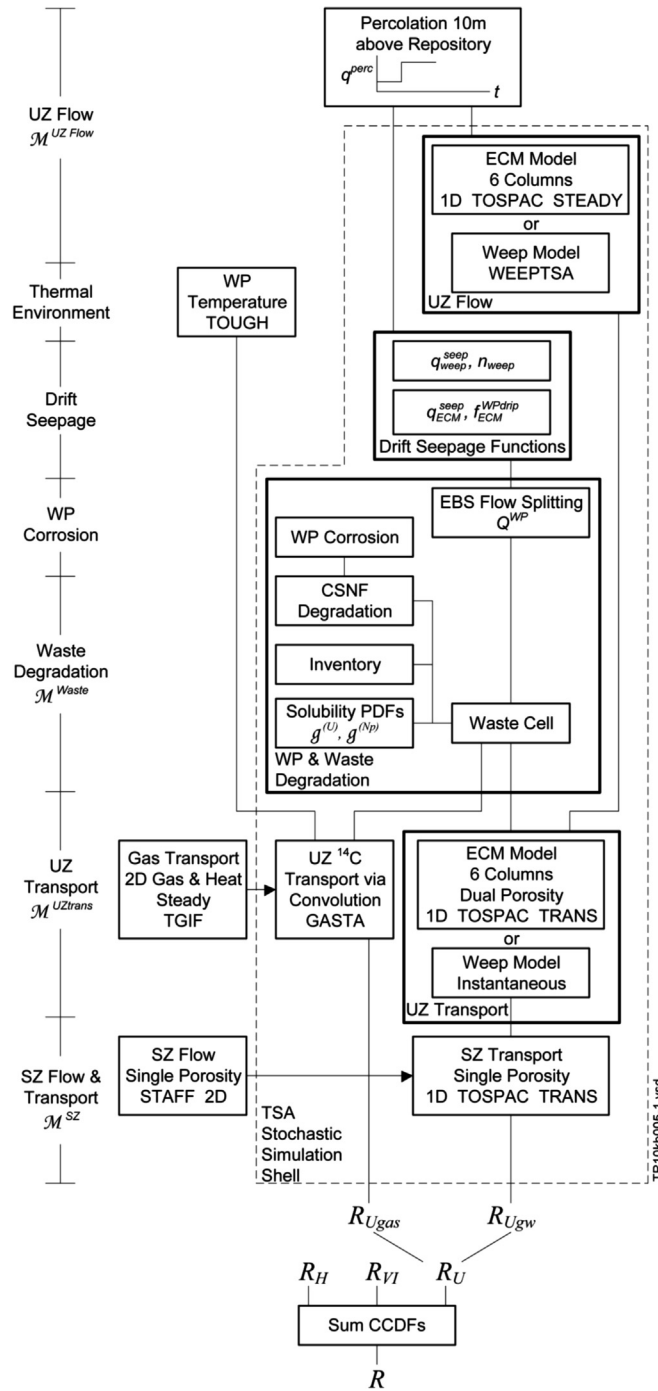


Fig. 2. PA-91 added UZ flow ( $\mathcal{M}^{UZflows}$ ) and waste degradation ( $\mathcal{M}^{Waste}$ ) modules for groundwater and gaseous pathways of the undisturbed scenario class ( $\mathcal{A}_U$ ) [14, Figs. 4–5 and 5-2]. The releases from the undisturbed scenario class ( $R_U$ ) were combined with releases from the human intrusion ( $R_H$ ) and igneous ( $R_{VI}$ ) disruptions to form the CCDF.

(LHS) (where the general form of Eqs. (4) and (5) for evaluating the CCDF of cumulative releases is discussed in Appendix B, Eq. B.9).

$$\begin{aligned}
 & \left. \begin{array}{l} \mathcal{M}_{TOSPAC}^{UZflow} \\ \mathcal{M}_{TOSPAC}^{Waste} \end{array} \right\} \rightarrow \mathcal{M}_{TOSPAC}^{UZtrans} \rightarrow \mathcal{M}_{TOSPAC, STAFF2D}^{SZ} \\
 & \varphi\{R_{U, gw, ECM}^{91} > R\} = \frac{1}{n_U^{LHS}} \sum_{l=1}^{n_U^{LHS} = 300} \mathcal{H} \left[ \left[ \sum_{r=1}^{n_U^r = 9} \frac{1}{L_{rj}^{mass}} \int_0^{10^4 yr} \mathcal{R}_{U, gw, ECM, r}(t; \mathbf{e}_l^e) \Big|_{x^{ae} = 5 km} dt \right] - R \right]
 \end{aligned} \tag{4}$$



$$\begin{array}{c}
 \mathcal{M}_{WEEPSTA}^{UZflow} \longrightarrow \mathcal{M}_{TOSPAC}^{Waste} \longrightarrow \mathcal{M}_{TOSPAC, STAFF2D}^{SZ} \\
 \downarrow \\
 \varnothing \{R_{U, gw, Weep}^{91} > R\} = \frac{1}{n_U^{LHS}} \sum_{l=1}^{n_U^{LHS} = 10^3} \mathcal{H} \left\{ \left[ \sum_{r=1}^{n_U^r = 9} \frac{1}{L_r f^{mass}} \int_0^{10^4 yr} \mathcal{R}_{U, gw, Weep, r}(t; \mathbf{e}_l^e) \Big|_{x^{ae} = 5 \text{ km}} dt \right] - R \right\} \\
 \uparrow \\
 40 \text{ CFR } 191
 \end{array} \tag{5}$$

3.2. Undisturbed release via gaseous pathway

The undisturbed scenario class also considered gaseous release of <sup>14</sup>C upward through the UZ to the surface ( $\mathcal{R}_{U, gas}$ ) in addition to aqueous release via groundwater flow,  $\mathcal{R}_{U, gw}$ . The source-term model for gaseous <sup>14</sup>C was the same as under aqueous conditions for radionuclides controlled by matrix degradation [9]. The sole purpose of the seepage abstractions and the source-term model in  $\mathcal{R}_{U, gas}$  was to determine when failure of the container occurred and released <sup>14</sup>C (Fig. 2). The release rate  $f_{CSNF, C14}^{deg}(t)$  and the estimated package temperature history from the code TOUGH by Lawrence Berkeley National Laboratory (LBNL) was then used by GASTSA as input for the convolution<sup>7</sup> of the unit gas transport estimated by a 2-D, steady-state gas and heat transport code, TGIF (Fig. 2) [14, Fig. 5-2].

$$\begin{array}{c}
 \left. \begin{array}{l} \mathcal{M}_{TOSPAC}^{UZflow} \\ \text{or} \\ \mathcal{M}_{WEEPSTA}^{UZflow} \end{array} \right\} \longrightarrow \mathcal{M}_{TOSPAC}^{Waste} \longrightarrow \mathcal{M}_{GASTSZ, TGIF, TOUGH}^{UZgastrans} \\
 \downarrow \\
 \varnothing \{R_{U, gas, acm}^{91} > R\} = \frac{1}{n_{Ugas}^{LHS}} \sum_{l=1}^{n_{Ugas}^{LHS} = 10^3} \mathcal{H} \left\{ \frac{1}{L_{C14} f^{mass}} \int_0^{10^4 yr} \mathcal{R}_{U, gw, acm, C14}(t; \mathbf{e}_l^e) dt - R \right\}
 \end{array} \tag{6}$$

In PA-91, the estimates of  $\varnothing\{(R_{U, gas, acm} > R)\}$  and  $\varnothing\{(R_{U, gw, acm} > R)\}$  used independent LHS samples. Fortunately,  $R_{U, gas, acm} \gg R_{U, gw, acm}$  and so a pragmatic method, which combined high groundwater releases with high gaseous releases, was used to combine CCDFs to calculate  $\varnothing\{R_{U, acm} > R\}$  (Fig. 2) [14, p. 8–9]. As previously mentioned, modeling assumptions in the modules of the undisturbed scenario for past PAs are discussed in companion papers [7–10], but in this paper aspects of evaluating other scenario classes are briefly discussed as follows.

3.3. Release via volcanic eruption

In 40 CFR 191, the accessible environment was defined as releases beyond the 5-km boundary or release to the surface; hence, modeling of a volcanic eruptive ash plume and its disposition for  $\mathcal{A}_{VE}$  was unnecessary in PA-91. Furthermore, since waste containers were placed in a sealed borehole in the floor of the repository, the disruption from a volcanic eruption consisted solely of the containers intersected by the igneous dike. Hence,  $\mathcal{R}_{VE}(\sim)$  consisted of one module  $\mathcal{M}^{Dike}$ , based on the computational code VOLCAN, to calculate the fraction of containers breached by the eruption, and, thereby, the inventory released (i.e., the combined product  $f_{VE}^{waste} f_{VE}^{br}$ ). The  $f_{VE}^{waste} f_{VE}^{br}$  product was estimated as the ratio of the volume intersected by the igneous dike to the repository volume from geometrical arguments as a function of dike length in repository, dike width, and depth of erosion of the host rock (based on analogous field observations), and repository area [30, Section 7.2] (i.e.,  $f_{VE}^{waste} f_{VE}^{br}(\mathbf{e}_l^e) = 2(L_{dike}^{dike} + w_{dike}^{dike})d_{erode}^{erode}/A^{rep}$ ), which differed from that assumed in PA–EA, Section 2.1, but used similar terms). The  $f_{VE}^{br}$  product for each realization  $l$  was sampled from epistemic uncertainty distributions of  $L^{dike}$ ,  $w^{dike}$ ,  $d^{erode}$ .<sup>8</sup> The CCDF for the volcanic eruption was calculated as follows:

$$\begin{array}{c}
 \varnothing \{R_{VE, acm}^{91} > R\} = \frac{1}{n_{VE}^{LHS}} \sum_{l=1}^{n_{VE}^{LHS} = 10^3} \varnothing \{ \mathcal{A}_{VE}(\mathbf{e}_l^e) \} \mathcal{H} \left\{ \left[ \sum_{r=1}^{n_r = 39} \frac{1}{L_r f^{mass}} \int_0^{10^4 yr} \mathcal{R}_{VE, r}(t; \mathbf{e}_l^e, \mathbf{a}_{VE}) \Big|_{x^{ae} = 5 \text{ km}} dt \right] - R \right\} \\
 \uparrow \\
 \mathcal{M}_{VOLCAN}^{Dike} \longrightarrow \mathcal{M}_{VE}^{Waste}
 \end{array} \tag{7}$$

3.4. Release via human intrusion

Although the initial YM site evaluation had found no economic minerals [41], EPA’s 40 CFR 191 required an estimate of the consequences and probability from inadvertent human intrusion while exploring for minerals [5]. Consequences from three mutually exclusive scenario subclasses were estimated:  $i \sim 1$  direct release to the surface,  $i \sim 2$  release through the tuff aquifer ( $\mathcal{M}^{HgwTuff}$ ), and  $i \sim 3$  release through the deeper carbonate

<sup>7</sup> By PA–VA, the convolution method would also be used for modeling transport in the SZ [10].  
<sup>8</sup> A second estimate was made from (a) observed volumes of basaltic eruptions, (b) observed portion of large fragments (xenoliths) in eruptions, (c) observed fraction of host rock in eruptions, (d) fraction of dike length represented by volcanic conduit (subjective), (e) repository height, and (f) repository area; however, the second estimate was not used since releases from the first method were somewhat larger, though still very small [30, §7.2].

aquifer below the repository ( $\mathcal{M}^{Hgwcarb}$ ).

$$\wp\{R_H > R\} = \sum_{i=1}^3 \wp\{\mathcal{A}_{Hi}|\mathcal{A}_H\} \wp\{R_{Hi} > R\} \quad (8)$$

where  $\wp\{\mathcal{A}_{Hi}|\mathcal{A}_H\}$  is the weighting for each of the mutually exclusive scenario subclasses of human intrusion and equal to 1/3rd. The distributions for the three scenario subclasses are as follows. The distribution for the release to the surface was evaluated as

$$\wp\{R_{Hdirect}^{91} > R\} = \frac{1}{n_{Hdirect}^{rdm}} \sum_{l=1}^{n_{Hdirect}^{rdm} = 2 \times 10^3} \wp\{\mathcal{A}_H(\mathbf{e}_l^p)\} \mathcal{H} \left\{ \left[ \sum_{r=1}^{n_{Hdirect}^r = 39} \frac{1}{L_{rj}^{mass}} \int_0^{10^4 \text{ yr}} \mathcal{R}_{Hdirect,r}(t; \mathbf{e}_l^e, \mathbf{a}_{Hdirect,l}) dt \right] - R \right\} \quad (9)$$

$\mathcal{M}_{Hdirect}^{Waste} \longleftarrow \mathcal{M}_{DRILL}^{Hdirect \& \text{ halo}}$

where  $\wp\{\mathcal{A}_H(\mathbf{e}_{corr}^{clad})\}$  is the probability of human intrusion [5]. The release to the surface, as calculated by DRILL, occurred both because of a direct hit of the waste package by the drill and because of a near miss of the drill that intersected radionuclides that had diffused into the halo around the package ( $\mathcal{M}_H^{Hdirect \& \text{ halo}}$ ). The diffusive halo around the waste packages was estimated from a simple diffusion equation based on the time of intrusion, as first calculated in PACE-90 [30]. The diffusive halo did not contribute much to  $R_{Hdirect}^{PA91}$  [14, Fig. 6–9].

The fraction of waste removed in direct hits was sampled from a uniform distribution between 0 and 1, but the releases were not substantially increased by assuming a fraction of one [14, Fig. 20]. The time of human intrusion ( $\tau_H$ ) was sampled from a uniform distribution between 0 and  $10^4$  yr rather than developing computational scenarios at specific times (Appendix B, Eq. (B.7)). The inventory of radionuclides in the base case was an average CSNF inventory in a package (2.1 MTHM), decayed to the simulated times of intrusion  $\mathcal{M}_{Hdirect}^{Waste}$ . However, inventories representing various types and burnups of CSNF were also modeled and shown not to influence the overall releases [14, Fig. 25]. The insensitivity to the variability of inventory for cuttings and cavings was similar to that found for the hypothetical human intrusion into defense-related transuranic waste disposed in bedded salt at the Waste Isolation Pilot Plant (WIPP) in southern New Mexico [42].

The cumulative release through the groundwater was estimated by assuming waste from one package fell directly in the tuff aquifer underlying the repository or much deeper to the carbonate aquifer, bypassing the UZ entirely.<sup>9</sup> As with the undisturbed scenario class, radionuclide transport in the SZ was based on TOSPAC TRANS [24,25] and, in turn, used aquifer water velocities estimated by STAFF2D for the tuff aquifer  $\mathcal{M}^{Hgw tuff}$ . For the deeper carbonate aquifer TOSPAC TRANS used estimates of the much higher aquifer water velocities extracted from work for the Early-Site Suitability Evaluation (ESSE) conducted for evaluating DOE site selection guidelines in 10 CFR 960, which used the PNNL code EPASTAT [43,44].

$$\wp\{R_{Hgw,path}^{91} > R\} = \frac{1}{n_{Hgw}^{LHS}} \sum_{l=1}^{n_{Hgw}^{LHS} = 10^3} \mathcal{H} \left\{ \left[ \sum_{r=1}^{n_{Hgw}^r = 9} \frac{1}{L_{rj}^{mass}} \int_0^{10^4 \text{ yr}} \mathcal{R}_{Hgw,path,r}(t; \mathbf{e}_l^e, \mathbf{a}_{Hgw tuff,l}) \Big|_{x,ae=5 \text{ km}} dt \right] - R \right\} \quad (10)$$

$\mathcal{M}_{TOSPAC, STAFF2D}^{Hgw tuff} \text{ or } \mathcal{M}_{TOSPAC, EPASTAT}^{Hgw carb} \longleftarrow \mathcal{M}_{DRILL}^{Hgw} \longleftarrow \mathcal{M}_{Hgw}^{Waste}$

where the pathway in Eq. (10) is either the tuff aquifer or the carbonate aquifer ( $path \sim tuff, carb$ ). The groundwater releases from the carbonate aquifer ( $\mathcal{M}^{Hgw carb}$ ) were  $\sim 3$  orders of magnitude larger than from the tuff aquifer, but direct releases still dominated (i.e.,  $R_{Hdirect} \gg R_{Hgw}$ ).

#### 4. PA-93

After completing PA-91, PA-93 was started to provide guidance on several design options and the importance of site characterization data in relation to [15, Fig. ES-2] (1) the cumulative release measure in 40 CFR 191, and (2) the future individual dose measure mandated in the Energy Policy Act of 1992 [6]. Prior to and during work for PA-93, (a) PNNL completed their PA of YM disposal system using complex process codes (PA-PNNL-91) [45,46], (b) Electrical Power Research Institute (EPRI) completed their second PA [47], and (c) NRC completed their own PA to develop understanding of the modeling issues related to a repository in the UZ at Yucca Mountain [48] (Appendix A).

Similar to PA-91, cumulative releases were evaluated from  $\mathcal{A}_{U+EF}$ ,  $\mathcal{A}_H$ , and  $\mathcal{A}_V$  for PA-93 [15]. However, early failure of the container was evaluated for the undisturbed scenario and two subclasses were evaluated for  $\mathcal{A}_V$ : igneous eruption ( $\mathcal{A}_{VE}$ ) and igneous intrusion followed by groundwater flow ( $\mathcal{A}_{VI}$ ). The effects of seismic damage events and direct contact of magma with waste in igneous intrusive events were not modeled, which was a reasonable assumption for vertical emplacement and even for in-drift emplacement provided the drifts were backfilled as specified for PA-93. However, in June 1994, DOE decided to not backfill because of operational concerns [49, Appendix A], and, thus, PA-VA and PA-SR examined some implications of seismicity and PA-LA included the seismic event.

##### 4.1. Release via undisturbed and early container failure

The thermal environment module  $\mathcal{M}^T$ , consisting of 5 models, was developed for  $\mathcal{A}_U$  and  $\mathcal{A}_{VI}$  to evaluate two repository design options ( $Q_{option}^{heat} \sim$  hot 28 W/m<sup>2</sup> and cool 14 W/m<sup>2</sup> repository layouts) and two WP placement design options: a thin-walled,

<sup>9</sup> EPA and NRC later specified similar guidance for the site specific Yucca Mountain regulations [6].

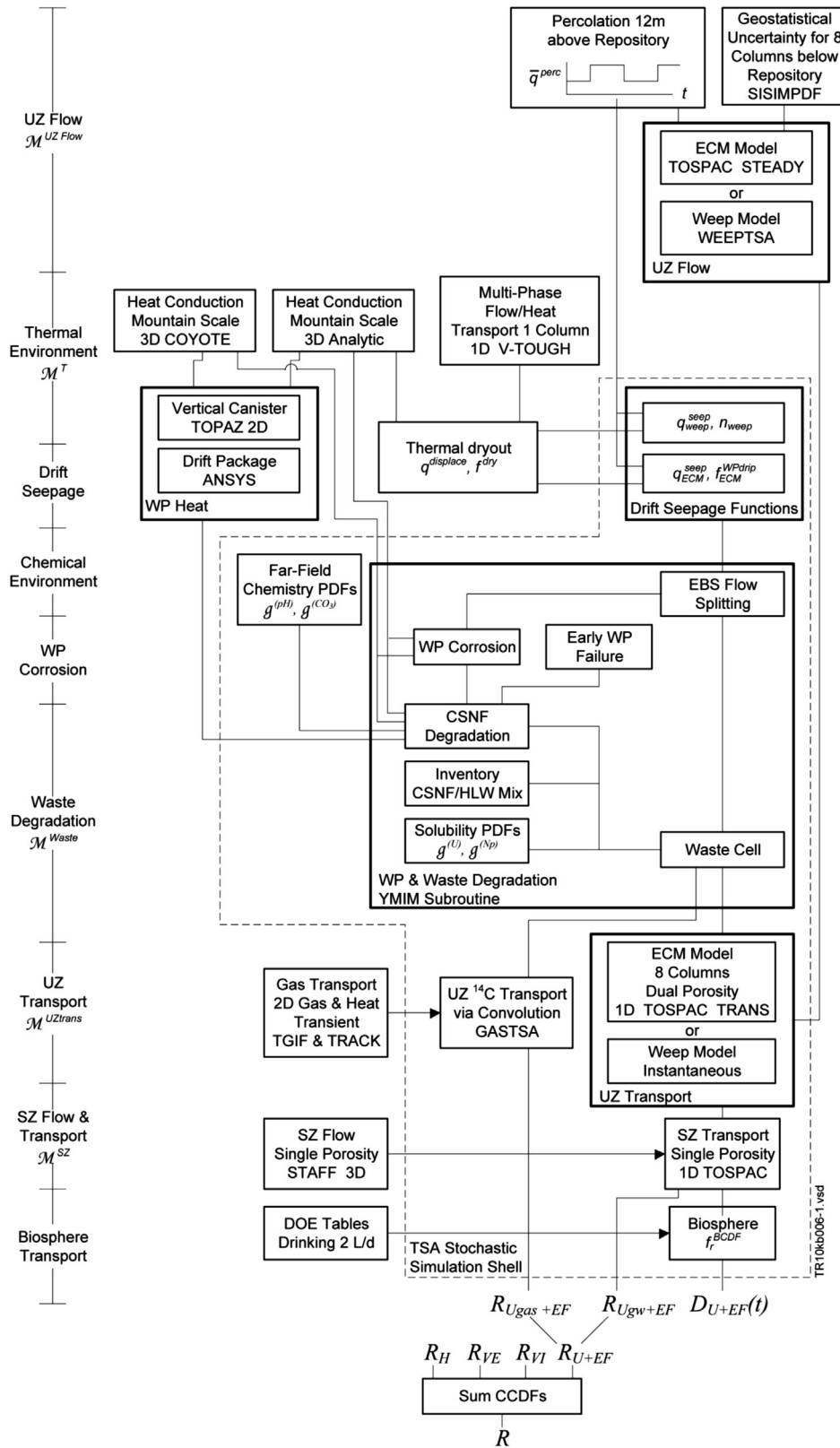


Fig. 3. PA-93 added a thermal module to compare the performance of a hotter and cooler repository design option for the combined undisturbed and early failure scenario class ( $\mathcal{A}_{U+EF}$ ) [15, Figs. 3–6, 3–7, 3–8]. Both cumulative release and dose were evaluated.

small vertical borehole container and a thick-walled, large in-drift container (with results for each option presented in a companion paper [50]) (Fig. 3). Also for PA-93, container breach was based on material corrosion rates, rather than a distribution of failure times, although still part of the waste module  $\mathcal{M}^{Waste}$  (Fig. 3). Both the ECM and weeps formulations were of continued interest in PA-93



(Appendix B, Eq. (B.9)).

$$\begin{array}{c}
 \mathcal{M}_{COYOTE, TOPAZ, ANSYS}^T \xrightarrow{\quad} \left. \begin{array}{l} \mathcal{M}_{TOSPAC}^{UZflow} \longrightarrow \\ \mathcal{M}_{YMIM}^{Waste} \longrightarrow \end{array} \right\} \longrightarrow \mathcal{M}_{TOSPAC}^{UZtrans} \longrightarrow \mathcal{M}_{TOSPAC, STAFF3D}^{SZ} \\
 \varphi \{ R_{U+EF, gw, ECM}^{93} > R \} = \frac{1}{n_{U, Weep}^{LHS}} \sum_{\ell=1}^{n_{U, ECM}^{LHS}=300} \mathcal{H} \left\{ \left[ \sum_{r=1}^{n_{U, gw}^r=7} \frac{1}{L_{r, f^{mass}}} \int_0^{10^4 \text{ yr}} \mathcal{R}_{U+EF, gw, ECM, r}(t; \mathbf{e}_\ell^e) \Big|_{x^{ae}=5 \text{ km}} dt \right] - R \right\}
 \end{array} \quad (11)$$

$$\begin{array}{c}
 \mathcal{M}_{V-TOUGH}^T \xrightarrow{\quad} \mathcal{M}_{WEEPSTA}^{UZflow} \\
 \mathcal{M}_{COYOTE, TOPAZ, ANSYS}^T \xrightarrow{\quad} \mathcal{M}_{YMIM}^{Waste} \longrightarrow \mathcal{M}_{TOSPAC, STAFF3D}^{SZ} \\
 \varphi \{ R_{U+EF, gw, Weep}^{93} > R \} = \frac{1}{n_{U, Weep}^{LHS}} \sum_{\ell=1}^{n_{U, Weep}^{LHS}=10^3} \mathcal{H} \left\{ \left[ \sum_{r=1}^{n_{U, gw}^r=7} \frac{1}{L_{r, f^{mass}}} \int_0^{10^4 \text{ yr}} \mathcal{R}_{U+EF, gw, Weep, r}(t; \mathbf{e}_\ell^e) \Big|_{x^{ae}=5 \text{ km}} dt \right] - R \right\}
 \end{array} \quad (12)$$

For PA-93, a CCDF of the maximum expected doses  $\max D_{U+EF, gw}$  was also calculated at the 5-km boundary of accessible environment for  $t < 10^6$  yr as

$$\varphi \{ \max D_{U+EF, gw, acm}^{93} > D \} = \frac{1}{n_{U, acm}^{LHS}} \sum_{\ell=1}^{n_{U, acm}^{LHS}} \mathcal{H} \left\{ \left[ \sum_{r=1}^{n_{U, gw}^r=7} \frac{f_{U, \ell, r}^{BDCF}}{Q_{93}^{indv}} \mathcal{R}_{U+EF, gw, acm, r}(t; \mathbf{e}_\ell^e) \Big|_{x^{ae}=5 \text{ km}} - D \right] \right\} \quad (13)$$

where  $\mathcal{R}_{U+EF, gw, acm, r}(t; \mathbf{e}_\ell^e)$  was as calculated for the cumulative releases and approximately equal to the mass injection rates from the UZ for both the ECM and weeps models ( $acm \sim ECM, Weeps$ ) since the SZ did not substantially reduce releases. Fixed drinking water dose conversion factors  $f_{U, r}^{BDCF}$  recommended by DOE were used [15, Table 14-1].

The mass release from the transport calculations was mixed with the dilution volume of the SZ  $Q_{93}^{indv}$  to calculate the mass concentration. The dilution volume was estimated as the product of the maximum velocity range ( $5.5 < v_{path}^{SZ} < 12.5$  m/yr), SZ porosity ( $\phi^{SZ} = 0.2$ ), and cross-sectional area of a contaminate plume after traveling 5 km [15, Tables 11-7 & 11-14-11]. The cross-sectional area ( $h^{SZ} w^{re}$ ), which was an important parameter in PA-93 [50, Table 2], was assumed to range loguniformly between  $2 \times 10^4$  and  $2 \times 10^6$  m<sup>2</sup>, based on an estimated width (3400–4400 m from original 3000 m repository width) and depth (50–500 m) [15, Section 11.6.2, Tables 11-7 and 14-11]. Hence,  $Q_{93}^{indv}$  in Eq. (13) ranged between  $2 \times 10^4$  and  $5 \times 10^6$  m<sup>3</sup>/yr for PA-93 (i.e.,  $Q_{93}^{indv} = \phi^{SZ} v_{path}^{SZ} h^{SZ} w^{re}$ ).

#### 4.2. Release via igneous intrusion

As already mentioned, releases from igneous disruptive scenario class included two subclasses for PA-93:  $\mathcal{A}_{VE}$  (which used the results of PA-91) and  $\mathcal{A}_{VI}$  (whereby the lifetime of containers near a dike was shortened by heat and magma volatiles and thereby the radionuclide source-term was enhanced). The summed normalized release for igneous intrusion was calculated as follows:

$$\begin{array}{c}
 \mathcal{M}_{COYOTE, TOPAZ, ANSYS}^T \xrightarrow{\quad} \left. \begin{array}{l} \mathcal{M}_{VOLCAN}^{Dike} \longrightarrow \\ \mathcal{M}_{ROCKTEMP}^T \longrightarrow \end{array} \right\} \left. \begin{array}{l} \mathcal{M}_{YMIM}^{WP \& Waste} \longrightarrow \\ \mathcal{M}_{TOSPAC}^{UZflow} \longrightarrow \end{array} \right\} \longrightarrow \mathcal{M}_{TOSPAC}^{UZtrans} \longrightarrow \mathcal{M}_{TOSPAC, STAFFED3D}^{SZ} \\
 \varphi \{ (R_{VI, ECM}^{93} > R) \} = \frac{1}{n_{U, ECM}^{LHS}} \sum_{\ell=1}^{n_{U, ECM}^{LHS}=300} \mathcal{H} \left\{ \left[ \sum_{r=1}^{n_{U, gw}^r=7} \frac{1}{L_{r, f^{mass}}} \int_0^{10^4 \text{ yr}} \mathcal{R}_{VI, ECM, r}(t; \mathbf{e}_{VI, \ell}^e, \mathbf{a}_{VI}) dt \right] - R \right\}
 \end{array} \quad (14)$$

where igneous releases were evaluated using only the ECM conceptual model.

As in PA-91, VOLCAN estimated the number of disposal drifts potentially intersected by igneous disruption. Because disposal drifts were backfilled after 75 years of ventilation thereby preventing magma from flowing down a disposal drift, only one package on either side of an intrusive dike was assumed affected by elevated temperatures and magma volatiles. However, the igneous intrusion consequence analysis calculated an analytical, time-dependent temperature excursion for a package on either side of a dike ( $T_{VI}^{WP}(t)$ ), using ROCKTEMP (Eq. (14)) during which enhanced corrosion could occur, rather than merely assuming containers on either side of dike were breached (as would be assumed for PA-SR). The temperature excursion was based on three uncertain thermal properties for the dike and tuff: thermal conductivity, bulk density, and specific heat (i.e.,  $\mathbf{e}_{VI}^e = \{k_{tuff}^{therm}, k_{dike}^{therm}, \rho_{tuff}^{bulk}, \rho_{dike}^{bulk}, \alpha_{tuff}^{therm}, \alpha_{dike}^{therm}\}$ ). The  $T_{VI}^{WP}(t)$  was superimposed upon the undisturbed temperature history of the CSNF fuel rods  $T_{U}^{CSNF}(t)$  from  $\mathcal{M}^T$ , which was not recalculated for the igneous intrusion scenario (Eq. (14) and Fig. 3)). The Arrhenius degradation coefficients of the container layers (i.e.,  $\kappa_1^{A825}, \kappa_2^{A825}, \kappa_1^{steel}$  and  $\kappa_2^{steel}$ ), but not the coefficients of

the fuel matrix degradation rate (i.e., coefficients of  $\dot{a}_{CSNF}$  [9, Eq. 11]), were increased in the source term code, Yucca Mountain integrating model or YMIM (Fig. 3), during the period of  $T_{VI}^{WP}(t)$  to account for the possible presence of aggressive sulfide volatiles in the magma.

4.3. Release via human intrusion

For human intrusion, PA-93 had three similarities to PA-91: (1) both release from a direct package hit ( $\mathcal{M}_H^{direct}$ ) and release from removing waste that had diffused into the tuff ( $\mathcal{M}^{Hdirect \& \text{halo}}$ ) were considered in the code DRILL; (2) the time of human intrusion ( $\tau_H$ ) was simulated, based on 20,000 Monte Carlo samples, rather than developing computational scenarios at specific times (Appendix B); and (3) only cumulative release was evaluated, not dose.

Yet, PA-93 made several changes. PA-93 only considered direct releases to the surface, not groundwater releases from waste falling to the bottom of the hole, since the latter releases were so small in PA-91 (i.e.,  $\mathcal{M}^{Hgw\text{tuff}}$  and  $\mathcal{M}^{Hgw\text{carb}}$  were not calculated in PA-93). For human intrusion, PA-93 considered the four design choices (hot and cold vertical borehole disposal, and hot and cold in-drift disposal); hence, the number of drill holes varied between 7 and 14 as the repository area changed with the hot or cool repository). In addition, several waste types in vertical and in-drift packages were considered that included HLW explicitly (unlike the undisturbed scenario in PA-93): four waste types in vertical packages (hybrid, pressurized water reactor, boiling water reactor, and HLW) [49, Fig. 4] and three waste types of in-drift packages (pressurized water reactor, boiling water reactor, and HLW). In the repository layout, HLW was placed in between CSNF packages. The time of container breach varied, which required developing distributions of container lifetime, and the resulting diffusive release into the halo about the package varied greatly. Because of the larger size, releases from in-drift packages were 3 times as large as borehole disposal except in those analyses that assumed less than the entire container contents were disrupted [15, Figs. 16–26 and 16–27]. Differences in releases from packages at the two repository heat loads were not great [15, Fig. 16–20].

4.4. PA-M&O-93 model

The newly assigned management and operator (M&O) contractor team (TRW Environmental Safety Systems, INTERA, Duke Engineering & Services, B&W Fuel Company, Fluor Daniel, Morrison-Knudsen, Woodward-Clyde, Logicon RDA, ER Johnson Associates, and JK Research Associates) also conducted a PA in 1993 (PA-M&O-93) [51]. PA-M&O-93 used the Repository Integration Program (RIP) computational platform for personal computers, which was intended to rapidly simulate disposal system behavior for system evaluation using simple models, which, in turn, was the basis of the GoldSim platform used for PA-SR and PA-LA [52]. RIP only tracked the radioactive mass and ignored water balance. Modeling of container and waste form degradation included only wet corrosion (no humid air corrosion) and no corrosion was assumed to occur when temperature on the package surface was above boiling [51]. A separate wet degradation rate for HLW was included (i.e., two package types:  $p \sim CSNF, HLW$ ).

5. PA-95

Only one PA was conducted under the supervision of the M&O in 1995. PA-95, building upon the modeling concepts in PA-M&O-93, used the RIP v3.21c computational platform. Parameter distributions developed for PA-93 were usually used in PA-95. Based on the recommendations of PA-M&O-93 [16, p. ES-2], PA-95 included 3 new modeling modules, for a total of 7 modules (Fig. 4). Specifically, PA-95 sought to (1) improve modeling of the environment adjacent to the package by using results from a coupled thermal-hydrology process model ( $\mathcal{M}^{TH}$ ), (2) improve modeling of waste package (WP) degradation by using results from a new model that included variability in spatial location of corrosion ( $\mathcal{M}^{WP}$ ), and (3) improve modeling of waste mobilization by exploring three conceptual models of flow and transport about the in-drift package ( $\mathcal{M}^{EBstrans}$ ). In addition, PA-95 improved estimation of drift seepage by including uncertainty through sampling of distributions (precursor of  $\mathcal{M}^{Seep}$ ). PA-95 also switched to the TOUGH2 process model, which was capable of 2 and 3-D modeling of UZ flow above and below the repository, to improve modeling of UZ flow and transport in future PAs ( $\mathcal{M}^{UZ}$ ). Because of the small releases in PA-93 from  $\mathcal{A}_V$  and  $\mathcal{A}_H$ , only  $\mathcal{A}_U$  via the groundwater pathway was modeled in PA-95.

Four design options were considered in PA-95: a hot and cold repository design ( $Q_{option}^{heat} \sim 20$  and  $6 \text{ W/m}^2$ ) with and without disposal drift backfill ( $\mathcal{B}_{option}^{backfill}$ ). Also, two conceptual models of infiltration were considered. For PA-95, both the summed normalized release and the expected dose were calculated; however, the summed normalized release was primarily for comparison with past PAs. The undisturbed expected total dose  $\bar{D}_U^{PA95}(t)$  was calculated at the 5 km boundary of the accessible environment for  $t < 10^6 \text{ yr}$  [16, Section 7.6.2] (where the general form of Eq. (15) for evaluating doses is described in Appendix B, Eq. (B.14)) (Fig. 4):

$$\begin{array}{c}
 \mathcal{M}_{FEHM}^{TH} \searrow \\
 \mathcal{M}_{WAPDEG}^{WP} \xrightarrow{\quad} \mathcal{M}_{RIP}^{Waste} \xrightarrow{\quad} \mathcal{M}_{RIP}^{EBstrans} \xrightarrow{\quad} \mathcal{M}_{RIP}^{UZtrans} \xrightarrow{\quad} \mathcal{M}_{RIP, STAFF2D}^{SZ} \\
 \mathcal{M}_{TOUGH2D}^{UZflow} \searrow \\
 \mathcal{M}_{EPAtables}^{Bio} \nearrow \\
 \bar{D}_U^{95}(t) = \frac{1}{n_U^{LHS}} \sum_{l=1}^{n_U^{LHS}=100} \sum_{r=1}^{n_U^r=39} f_{U,l,r}^{BDCF} \frac{1}{Q_{95}^{m\dot{v}}} \mathcal{R}_{U,r}(t; \mathbf{e}_l)_{x^{ae}=5 \text{ km}}
 \end{array} \tag{15}$$

6. PA-VA

In 1997, Congress asked for a viability assessment (PA-VA), which was completed the next year [6]. For PA-VA, the emphasis was on the undisturbed release scenario class via a groundwater pathway. Similar to PA-93, an early WP failure scenario class ( $\mathcal{A}_{EF}$ ) was evaluated and

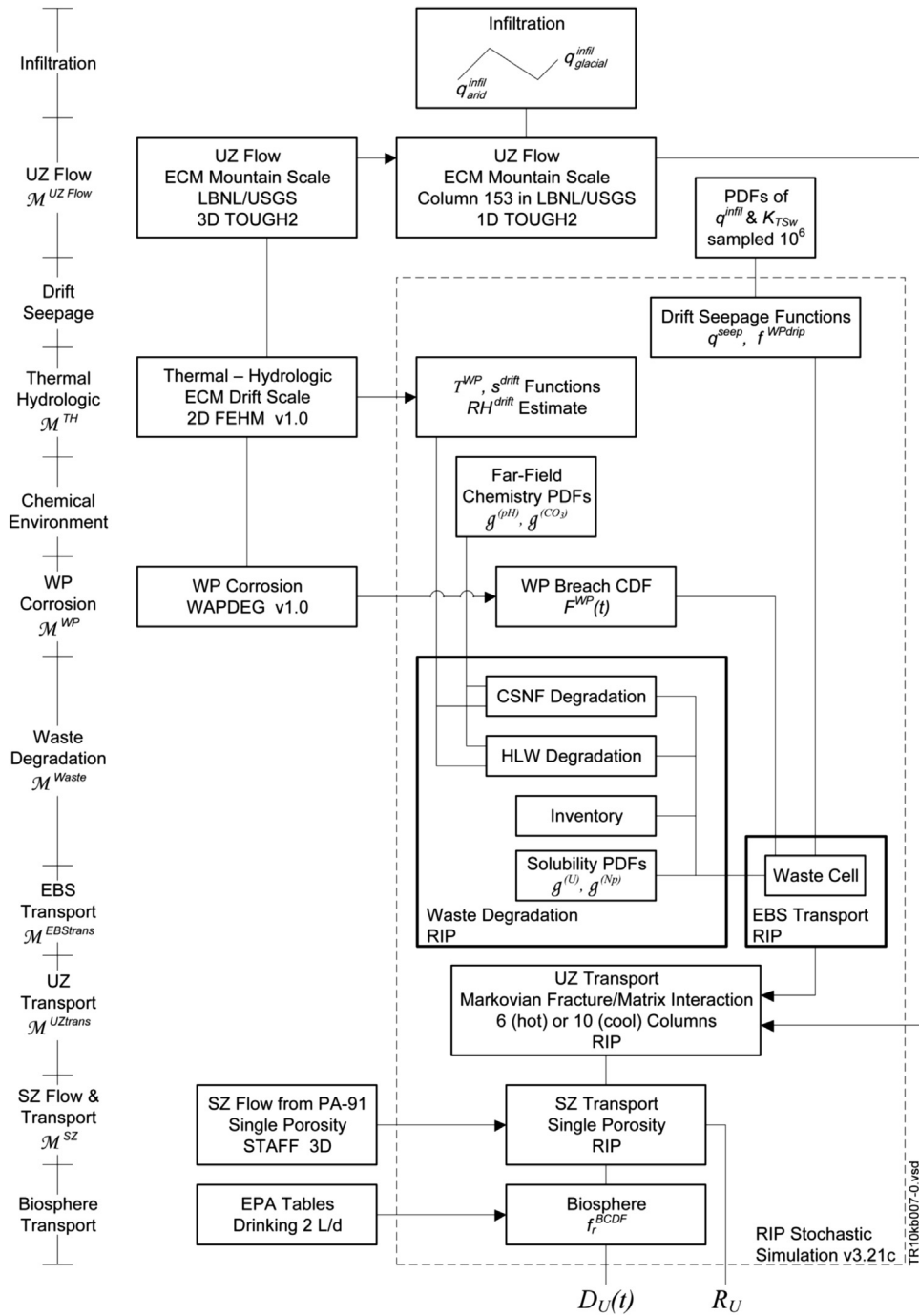


Fig. 4. PA-95 coupled hydrologic processes to the thermal module, added a separate container degradation module, and added the beginnings of the EBS transport module for undisturbed scenario class ( $\mathcal{A}_U$ ) [16, Fig. ES.3-3].

included with the undisturbed scenario ( $\mathcal{A}_U$ ) in modeling  $\mathcal{R}_{U+EF}(\sim)$ . A gaseous pathway for  $^{14}\text{C}$  (and possibly  $^{36}\text{Cl}_2$  and  $^{129}\text{I}_2$ ) was not included because of the proposed change to a dose standard at a point 20 km from the repository such that gaseous doses were inconsequential [6]. Similar to PA-95 [16], the stochastic analysis was conducted with RIP v5.19.01 [52; 53, Table 7–2; 54, Table 11–2].

6.1. Doses via undisturbed and early container failure

For PA-VA, the dose at a 20 km boundary for the combined undisturbed and early failure scenario class ( $D_{U+EF}(t)$ ) was calculated from 9 radionuclides ( $n_r=9$ ). The stochastic integral for 177 epistemic uncertain parameters  $e_i^e$  of  $\mathcal{R}_{U+EF,r}(\sim)$  was evaluated using 100 LHS samples ( $n_N^{\text{LHS}} = 100$ ) (Appendix B, Eq. (B.13)). The  $\mathcal{R}_{U+EF,r}(\sim)$  consisted of all 11 modules that would be present in PA-LA (Fig. 5): (1) a new infiltration module based on INFIL [7]  $\mathcal{M}_{\text{INFIL}}^{\text{Infil}}$ ; (2) the UZ flow module, based on TOUGH2, which included model calibration, based on iTOUGH2 [7]  $\mathcal{M}_{\text{TOUGH2},\text{iTOUGH2}}^{\text{UZflow}}$ , both developed by LBNL; (3) a new numerical model of drift seepage, based on iTOUGH2 and the geostatistical simulator SGSIM

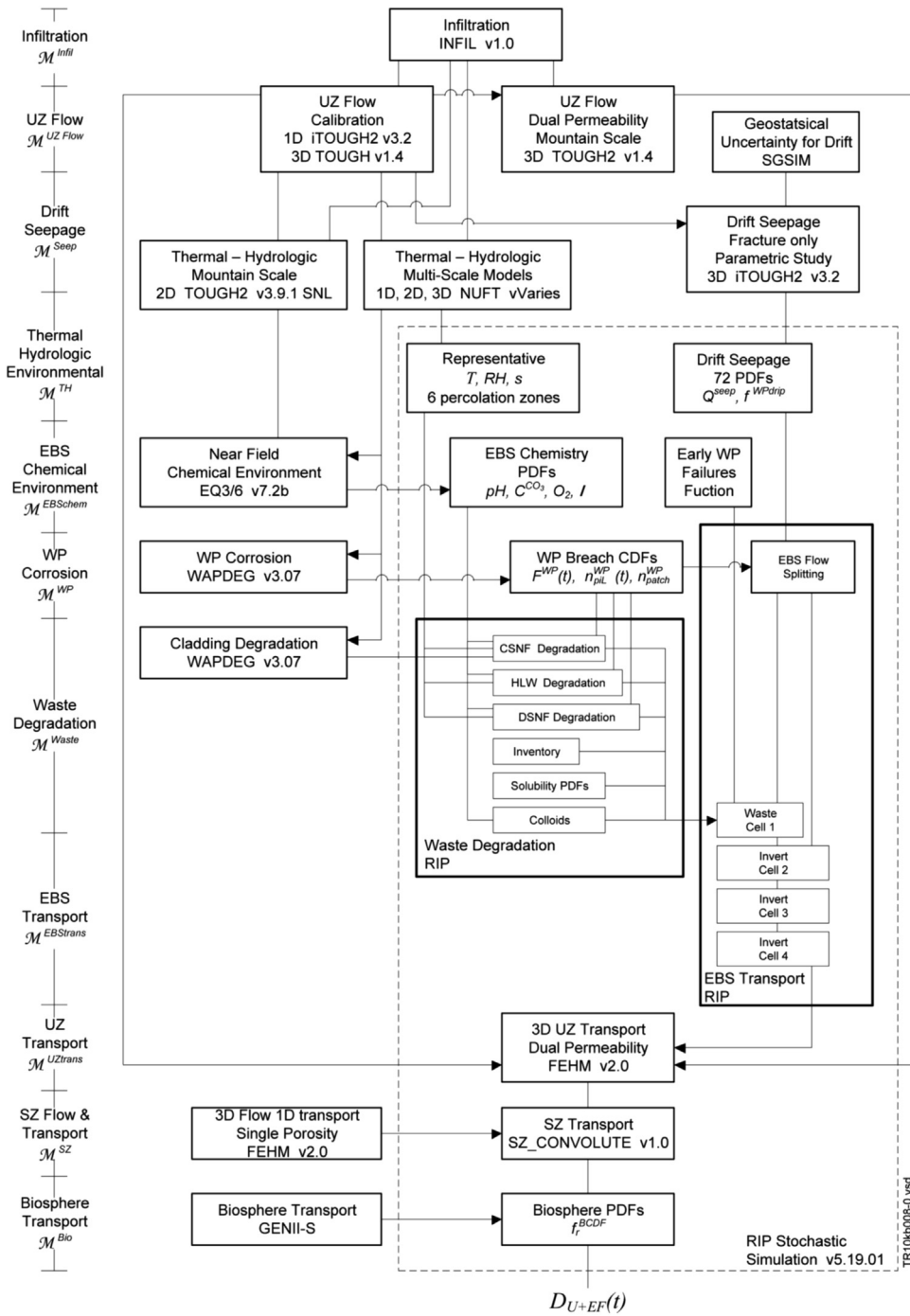
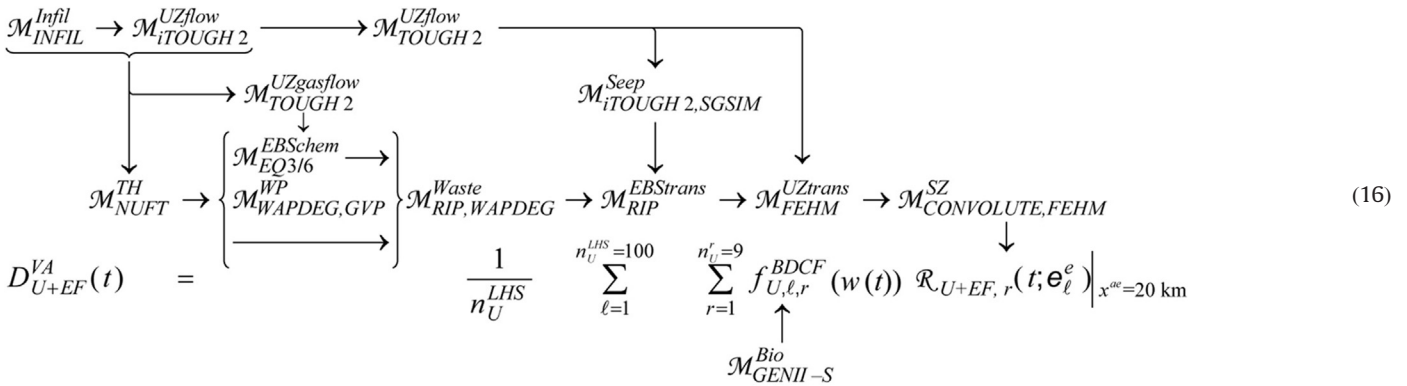


Fig. 5. PA–VA added four new modules for infiltration, seepage, EBS chemistry, and biosphere transport for the combined undisturbed and early failure scenario class ( $A_{U+EF}$ ) [17, Fig. 2-13].

[7]  $M_{\text{TOUGH2,SGSIM}}^{\text{Seep}}$ ; (4) a thermal-hydrologic module, now based on NUFT [8]  $M_{\text{NUFT}}^{\text{TH}}$ , developed by Lawrence Livermore National Laboratory (LLNL); (5) a new model of the chemical environment around the drift based on EQ3/6 developed by LLNL  $M_{\text{EQ3/6}}^{\text{EBSchem}}$ , which used estimates of  $O_2$  and  $CO_2$  concentrations from TOUGH2 [8]  $M_{\text{TOUGH2}}^{\text{UZgasflow}}$ ; (6) a model of WP degradation, based on WAPDEG, and a new Gaussian variance partitioning (GVP) model to partition uncertainty between spatial aleatoric variability and epistemic parameter uncertainty [8]  $M_{\text{WAPDEG,GVP}}^{\text{WP}}$ ; (7) the waste degradation model [9], based on RIP, that added cladding degradation (using WAPDEG) and the influence of colloids (because of the recent discovery of Pu colloids far from the Benham explosion at NTS [3, Appendix A; 55]  $M_{\text{RIP,WAPDEG}}^{\text{Waste}}$ ; (8) an engineered barrier system (EBS) transport model, based on RIP, that added more mixing cells for modeling radionuclide movement through the invert [9]  $M_{\text{RIP}}^{\text{EBStrans}}$ ; (9) a new UZ transport model based on particle tracking in finite element heat and mass (FEHM) transfer code developed by Los Alamos National Laboratory (LANL) [10]  $M_{\text{FEHM}}^{\text{UZtrans}}$ ; (10) an SZ flow and transport model based on FEHM and a transport simplification based on convolution that included colloid transport [10]  $M_{\text{CONVOLUTE,FEHM}}^{\text{SZ}}$ ; and (11) a new biosphere transport model, based on GENII-S developed by Pacific Northwest National Laboratory (PNNL), that calculated uncertain biological dose conversion factors ( $f^{\text{BDCF}}$ ) specific to potential water use at Amargosa Valley near Yucca Mountain [10]

$\mathcal{M}_{GENII-S}^{Bio}$  (Fig. 5, Eq. (16)).<sup>10</sup>



6.2. Consequences via igneous disruption

Three igneous disruptive scenario subclasses were analyzed in PA–VA [17, vol. 3 Section 4.4]: (1) the direct effect of a volcanic eruption ( $\mathcal{A}_{VE}$ ), (2) the direct effect of an igneous dike intrusion disrupting the waste packages and enhancing the source-term for a short time ( $\mathcal{A}_{VI}$ ), and (3) the indirect effect of an igneous dike altering the SZ permeability, and thereby, altering groundwater flow paths to the accessible environment ( $\mathcal{A}_{V Dike}$ ). However, a mean dose over time (e.g.,  $\bar{D}_{VI}(t)$ ) was not calculated. Rather, the peak doses from the igneous class were calculated and then compared with undisturbed and early failure (nominal) peak doses to argue doses from the igneous scenario class would not change the peak doses calculated and, thereby, the overall conclusion of the PA–VA (i.e.,  $\max D_{U+EF,\ell} \gg \max D_{VE,\ell}$  and  $\max D_{VI,\ell}$ ). Therefore, the calculations were similar to a scenario class screening analysis; however, the purpose was not to exclude the igneous scenario class from the PA–VA, since the mean probability of the igneous event ( $1.5 \times 10^{-4}$  for PA–VA) was slightly larger than the regulatory screening limit of  $10^{-4}$  per  $10^4$  yr [5].

6.2.1. Consequences from eruption

With the change in performance measure from cumulative release at the surface in 40 CFR 191 to dose as proposed by the National Academy of Sciences (NAS) in 1995 [6], the model for the volcanic eruption scenario class ( $\mathcal{R}_{VE}(\sim)$ ) had to include dispersion and deposition of the volcanic plume, similar to PA–EA. To determine the conditions of the repository at the time of volcanic eruption, aleatoric and epistemic parameters pertinent to  $\mathcal{A}_{VE}$  were randomly sampled 300 times [56, Section 10.4.2.8]. From the Monte Carlo simulation, 17 cases (5.7%) resulted in conditions favorable to a volcanic eruption within the repository footprint that also intersected one or more waste packages. A volcanic peak dose  $\max D_{VE}$  for  $t < 10^6$  yr from deposition of volcanic ash at the receptor of the 17 eruptive cases was determined as follows:

$$D_{VE,\ell}^{VE} = \sum_{r=1}^{n_{VE}^{r=39}} f_{VE,\ell,r}^{BDCF} \mathcal{R}_{VE,r}(\mathbf{a}_{VE,\ell}, \mathbf{e}_{VE,\ell}^e) \Big|_{x_{VA}^{ae} = 20 \text{ km}} \tag{17}$$

where  $f_{VE,\ell,r}^{BDCF}$  was the biological dose conversion factor for radionuclide  $r$  in contaminated soil, as evaluated by  $\mathcal{M}_{VE,GENII-S}^{Bio}$  for all 39 radionuclides considered in  $\mathcal{M}_{Waste}$  [9]. The  $\mathcal{M}_{VE,GENII-S}^{Bio}$  considered exposure to an average Amargosa Valley resident from external exposure by soil contaminated with ash, inhalation of ash, ingestion of ash, ingestion of food crops, and ingestion of food and animal products grown in the contaminated soil. Use of contaminated water was not considered, since it was already considered in  $\mathcal{A}_{U+EF}$  (Eq. (16)). Consumption of leafy vegetables dominated  $f_{VE,\ell,r}^{BDCF}$  [56, Section 10.4.2.10.1]. The  $\mathcal{R}_{VE}(\sim)$  was

$$\mathcal{R}_{VE,r}(\mathbf{a}_{VE,\ell}, \mathbf{e}_{VE,\ell}^e) = N^{WP} I_{CSNF,r}(\tau_{V,\ell}) f_{VE,\ell}^{waste} f_{VE,\ell}^{br} \cdot C^{Ash}(\mathbf{a}_{VE,\ell}, \mathbf{e}_{VE,\ell}^e) \Big|_{x_{VA}^{ae} = 20 \text{ km}} \tag{18}$$

where  $N^{WP}$  was the total number of waste packages,  $I_{CSNF,r}(\tau_{V,\ell})$  was the inventory of radionuclide  $r$  in CSNF packages at the sampled intrusion time  $\tau_{V,\ell}$ ,  $f_{VE,\ell}^{br}$  was the fraction of containers breached, and  $f_{VE,\ell}^{waste}$  was the fraction of container contents ejected in the volcanic eruption. The  $f_{VE,\ell}^{br}$  was calculated through a combination of (a) distributions that specified the probability of vent diameter and probability of number of vents, and (b) functions for the number of packages hit per vent diameter and number of drifts hit per vent diameter as in PA-91. The  $f_{VE,\ell}^{waste}$  incorporated factors expressing the potential of the eruption to breach the waste container and entrain waste. The combined fraction  $f_{VE,\ell}^{br} f_{VE,\ell}^{waste}$  was  $\sim 0.001$  for PA–VA [17, vol. 3 Section 4.4.2.4; 56, Table 10-16d].

The  $C^{Ash}(\mathbf{a}_{VE,\ell}, \mathbf{e}_{VE,\ell}^e)$  of Eq. (18) was the ash concentration deposited 20 km from the repository in the Amargosa Valley using the volcanic eruption module ( $\mathcal{M}_{VE}^{Ash}$ ), based on the code ASHPPLUME developed for NRC [56, Section 10.4.2; 57]. The model parameters of ASHPPLUME were (a) eruptive characteristics (such as volcanic duration, column height, eruptive velocity, eruptive power, eruptive volume); (b) atmospheric characteristics (such as wind speed, wind direction, air density, air viscosity, and eddy-diffusivity constant); and (c) ash characteristics (such as ash-particle shape factor, ash-particle size, waste-particle size, ratio of waste to ash, maximum ash size transported, and the total mass of waste  $m_{total}^{waste}(f_{VE}^{br})$ ) [56, Section 10.4.2.7]. The parameters of ASHPPLUME are a mixture of aleatoric  $\mathbf{a}_{VE}$  and epistemic parameters  $\mathbf{e}_{VE,\ell}^e$ . For example, the two atmospheric characteristics (wind speed and wind direction) are members of  $\mathbf{a}_{VE}$  and typically define scenario subclasses in analysis of nuclear reactor accidents. The eruptive characteristics are also members of  $\mathbf{a}_{VE}$ .

<sup>10</sup> This taxonomy of modules is the “common denominator” of two other model groupings: the SAR/LA uses 9 groups of models for the nominal scenario where modules 2 and 4 of this paper are grouped together, modules 7 and 8 are grouped together (and models for the seismic and igneous scenarios formed another 2 groups for the SAR/LA) [2]. In previous documentation of PA–SR and PA–LA, 9 groups of models are discussed where modules 1, 2, and 3 are grouped together, modules 4 and 5 are grouped together, and models for the seismic and igneous scenarios are grouped together for a 9th group [1, Fig. ES-9].



Nonetheless, all the aleatoric parameters were sampled along with the epistemic parameters for  $\mathcal{A}_{VE}$  in PA–VA since  $D_{VE}$  was so small and, thus, of limited interest. The  $\max D_{VE}$  of  $1.75 \times 10^{-5}$  mSv/yr, as calculated by Eq. (17), was  $10^6$  times smaller than the nominal peak dose of  $4 \times 10^1$  mSv/yr (i.e.,  $\max D_{VE,\ell}(t) \ll \max D_{U+EF,\ell}(t)$ ,  $\ell = 1, \dots, 17$ ) [17, vol. 3 Fig. 4–26; 56, Fig. 10–41 Table 10–19]. The median dose of  $10^{-6}$  mSv/yr was similar to the expected dose estimated in PA–EA and PA–LA [17, vol. 3 Fig. 4–44].

### 6.2.2. Consequences from groundwater releases

About 65% ( $\sim 195$ ) of the Monte Carlo cases studied for the igneous intrusion scenario resulted in conditions favorable to magmatic disruption of the waste container and, thereby, enhancing the source-term for a short time. The  $\mathcal{M}_{RIP}^{Waste}$  and  $\mathcal{M}_{RIP}^{EBStrans}$  were modified for evaluating the peak dose from igneous disrupted packages. The modifications to  $\mathcal{M}_{V_{RIP}}^{Waste}$  consisted of (1) complete failure of 2 packages per intersected drift, which resulted in a rough average of  $\sim 52$  packages per intrusion (i.e.,  $\bar{f}_{VI}^{dr} = \sim 0.005$  [56, Table 10–22b]), and (2) enhanced degradation rates for the CSNF and increased surface areas. Separate source-cells were added with disrupted packages in the modified  $\mathcal{M}_{V_{RIP}}^{EBStrans}$ . The sampled parameters from the 195 Monte Carlo cases were manually inserted into the simulation [56, Section 10.4.3.6.1]. The simulation instantaneously introduced the igneous event at the sampled time of the intrusion and transported 9 radionuclides (same as  $\mathcal{A}_U$ ) through the UZ and SZ. With this approach, the initial conditions for the disposal system including UZ percolation, drift seepage, WP corrosion were established prior to the time of the igneous event. Container corrosion would be neglected in the approach for PA–SR and PA–LA.

The maximum peak dose observed in the 195 igneous simulations was 30% less than the maximum peak dose observed in the 100 nominal scenario simulations (i.e., peak doses observed after the event were typically between 2 and 10 mSv/yr) ( $\max D_{VI,\ell}(t)$   $\ell = 1, \dots, 195 < \max D_{U+EF,\ell}(t)$ ,  $\ell = 1, \dots, 100$ ). Furthermore, the simulation conditional probability (1/195) and the peak doses for the igneous simulations were multiplied by  $\phi\{\mathcal{A}_V\}$  [5] to show that expected peak doses from  $\mathcal{A}_{VI}$  would be much smaller [17, vol. 3 Fig. 4–46].

### 6.2.3. Consequences from igneous dike in far field

The effect of an igneous dike altering the SZ permeability, and thereby, altering groundwater flow paths to the accessible environment ( $\mathcal{A}_{VDike}$ ) was evaluated through analysis based on STAFF3D from PA-93 [10]. Placing highly transmissive dikes down gradient of the repository moved flow patterns to the east rather than south and tended to reduce average groundwater velocities compared to the nominal scenario class ( $\mathcal{A}_{U+EF}$ ). These example results suggested that igneous intrusion in the far field would cause radionuclide transport to be slower and directed away from residents in Amargosa Valley (i.e.,  $\bar{D}_{U+EF+VDike}(t) < \bar{D}_{U+EF}(t)$ ) [17, vol. 3 Section 4.4.2.4]. By the time of PA–LA, the EPA radiation protection standard regulations would clarify that the situation described by this FEP was not of regulatory interest [58, Section 197.36].

### 6.2.4. Consequences via seismic events

PA–VA considered, for the first time, a seismic scenario class. The two seismic scenario subclasses considered were (1) ground motion causing rockfall on the package ( $\mathcal{A}_{SG}$ ),<sup>11</sup> and (2) faults altering SZ permeability ( $\mathcal{A}_{SF}$ ). The latter influence was assumed similar to that of an igneous dike; hence,  $\bar{D}_{U+EF+SF}(t) \approx \bar{D}_{U+EF+VI}(t) < \bar{D}_{U+EF}(t)$ .

The analysis of seismic rockfall considered the seismic event in combination with the undisturbed scenario (i.e.,  $\bar{D}_{U+EF+SG}(t)$ ). For the rockfall analysis, the WP module, based on WAPDEG v3.09, was modified to include rockfall causing either container breaches or enhanced localized corrosion in a dripping environment ( $\mathcal{M}_{SG,WAPDEG}^{WP}$ ). An uncertain  $v_{\ell}^{peak}$  was sampled from a constructed normal distribution, based on the Probabilistic Seismic Hazard Analysis (PSHA), completed in September 1988 [5]. The sampled  $v_{\ell}^{peak}$  was used to qualitatively estimate drift damage from a qualitative description of rock integrity (but PA–LA would later quantitatively estimate drift damage). The maximum rock diameter was then determined from a probabilistic description of fracture spacing  $B_f$ . The time of a seismic event  $\tau_{SG}$  was used to determine the remaining thickness of the steel and nickel Alloy 22. A comparison of the rock size and limited modeling of the container strength, based on the steel and Alloy 22 thickness, was used to determine whether the container breached, dented, or was unharmed. Later, PA–LA would greatly improve the modeling of the container failure by seismic damage. The rock diameter was also used to determine the number of patches failed or dented. For dented patches, enhanced localized corrosion was assumed in the WAPDEG analysis.

The analysis was repeated 500 times for each of four periods (0– $10^3$  yr, 0– $10^4$  yr, 0– $10^5$  yr, and 0– $10^6$  yr), to estimate the cumulative distribution for container failures for rockfall, enhanced localized corrosion, and long-term corrosion for the four periods (i.e.,  $F_{patch,drip}^{WP}(t) + F_{patch,drip}^{WP}(t)$ ). Except for the modified container module  $\mathcal{M}_{SG,WAPDEG}^{WP}$ , the dose calculation proceeded as with the undisturbed scenario (Eq. (16), Fig. 5). PA–VA did not accumulate damage from multiple events but PA–LA would. The dose was similar to the dose of nominal scenario class alone (i.e.,  $\bar{D}_{U+EF+SG}(t) \approx \bar{D}_{U+EF}(t)$ ) [56, Fig. 10–72]. This result was used to argue that inclusion of  $\mathcal{A}_{SG}$  would not substantially alter the finding of repository viability based on  $\mathcal{A}_{U+EF}$  [17, Section 4.4.3.3].

## 7. PA–SR

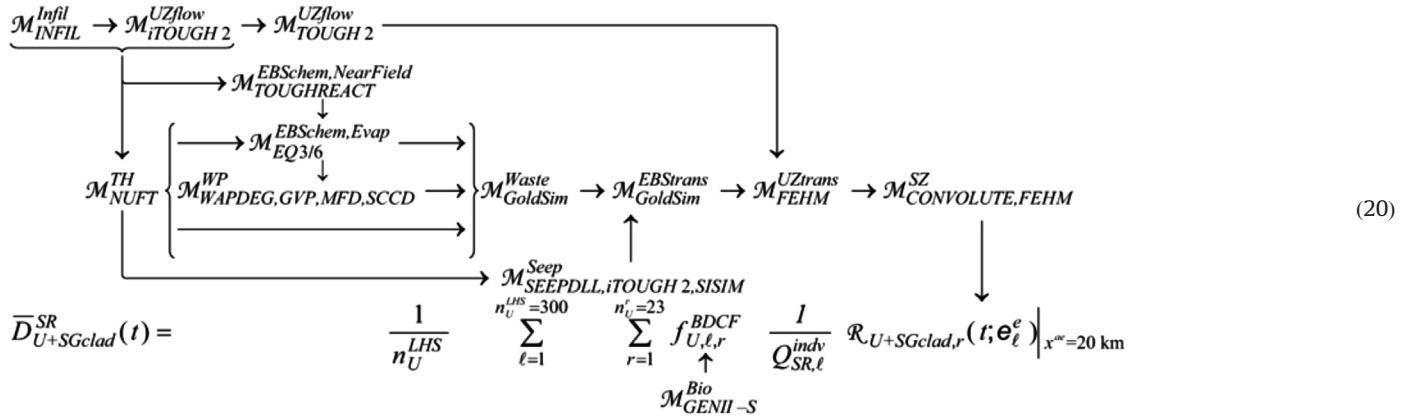
PA–SR was concluded in late 2000 to support the site recommendation [18,59]. The emphasis in PA–SR was on the scenario class that combined undisturbed and seismic events for cladding degradation ( $\mathcal{A}_{U+SGclad}$ ). In addition, the igneous scenario class received much more attention and the total dose  $\bar{D}(t)$  included the contribution of volcanic eruptive ( $\mathcal{A}_{VE}$ ) and igneous dike intrusive ( $\mathcal{A}_{VI}$ ) releases for the first time since PA-93. The  $\bar{D}(t)$  was the sum of the incremental dose from the 3 retained scenario classes— $\mathcal{A}_{U+SGclad}$ ,  $\mathcal{A}_{VE}$ , and  $\mathcal{A}_{VI}$ :

$$\bar{D}^{SR}(t) = \sum_{j=1}^3 \bar{D}_j(t; \mathbf{e}^e) = \bar{D}_{U+SGclad}(t) + \bar{D}_{VE}(t) + \bar{D}_{VI}(t) \quad (19)$$

<sup>11</sup> PA–LA would evaluate packages bouncing up and down and into each other underneath a drip shield. For PA–VA, rockfall was assumed to limit package movement since a drip shield was not yet included in the PA–VA design.



was more fully embedded into the PA (Fig. 6, Eq. (20)). Also, the stochastic analysis for PA–SR was conducted with the new Windows<sup>®</sup>-based RIP, Goldsim<sup>®</sup> v6.04.007 [60, Section 3.1]. The evaluation of the undisturbed dose consisted of the summation of the doses from 23 radionuclides using uncertain  $f_{U,\ell,r}^{BCDF}$  and  $Q_{SR,\ell}^{indv}$  sampled 300 times along with the numerous epistemic parameters  $\mathbf{e}_{U,\ell}^e$  (Eq. (20)).



## 7.2. Doses via volcanic eruption and igneous intrusion

For the PA–SR, the incremental mean dose from the igneous scenario class was the sum of the mean dose from volcanic eruption ( $\bar{D}_{VE}(t)$ ) and igneous dike intrusion ( $\bar{D}_{VI}(t)$ ). Because  $\mathcal{R}_{VE,r}$  was easy to evaluate, the aleatoric stochastic integral over the time of igneous eruption (where the time of eruption defines computational scenarios) was integrated numerically with an eruption in each time step ( $\Delta\tau_V$ ) of 31.25 yr out to  $5 \times 10^4$  yr rather than with a Monte Carlo scheme; that is

$$\bar{D}_{VE}^{SR}(t) = \frac{1}{n_{VE}^{LHS}} \sum_{\ell=1}^{n_{VE}^{LHS}=5000} \varphi\{\mathcal{A}_{VE}(\lambda_{V,\ell})\} \sum_{r=1}^{n_r^{BCDF}=12} f_{VE,r}^{BCDF} \sum_{n=1}^{n_{\Delta t}=1600} \mathcal{R}_{VE,r}(t_n; \tau_{V,n}, \mathbf{a}_{VE,\ell}, \mathbf{e}_{VE,\ell}^e) \Delta\tau_V \quad (21)$$

where  $\varphi\{\mathcal{A}_{VE}(\lambda_{V,\ell})\}$  is the product of sampled event probability  $\varphi\{\mathcal{A}_{VE}\}$ , the probability that a vent within the repository intersects waste  $\varphi\{E_{WP}^{hit}|\mathcal{A}_V\}$  [5]. The  $f_{VE,r}^{BCDF}$  for 12 radionuclides were evaluated as in PA–VA.

The consequence model of volcanic eruption ( $\mathcal{R}_{VE}(\sim)$ ) in Eq. (21) was [60, Section 6.3.9.1]

$$\mathcal{R}_{VE,r} = \sum_{p=1}^2 f_p^{WP} N_p^{WP} I_{p,r}(t_n) \exp\{\lambda_r(t_n - t_1)\} f_{VE,\ell}^{br} f_{VE}^{waste} \cdot C^{Ash}(m_{total}^{waste}(f_{VE,\ell}^{br}); \mathbf{a}_{VE,\ell}, \mathbf{e}_{VE,\ell}^e) \bullet \sum_{m=1}^n \exp\{-k_{soil}(t_n - t_m)\} \Big|_{x_{SR}^e = 20 \text{ km}} \quad (22)$$

where the first group of terms is the inventory of radionuclide  $r$  in the packages ( $p=1 \sim \text{CSNF}$  or  $p=2 \sim \text{CoWP}$  where the co-disposal package tracked the inventory of DSNF and HLW separately) based on the fraction of each type of package in the repository ( $f_p^{WP}$ ), the total number of packages ( $N_p^{WP}$ ), inventory over time of each package ( $I_{p,r}(t_n)$ ) adjusted for radioactive decay  $\exp\{\lambda_r(t_n - t_1)\}$ , and fraction of containers breached ( $f_{VE,\ell}^{br}$ ). The  $f_{VE}^{waste}$  was calculated as in PA–VA [60, Fig. 6–189]. However, 100% of the contents of a container intersected by a conduit were assumed ejected by the eruption for PA–SR and PA–LA (i.e.,  $f_{VE}^{waste} = 1$  rather than a small fraction as in PA–VA, Eq. (18)).

The second group of terms of  $\mathcal{R}_{VE,r}$  was the peak concentration ( $C^{Ash}(m_{total}^{waste}(f_{VE,\ell}^{br}); \mathbf{e}_{VE,\ell}^e)$ ), calculated by  $\mathcal{M}^{Ash}$ . The  $\mathcal{M}^{Ash}$  was again based on ASHPUME v1.4LV but with revised parameters  $\mathbf{e}_{VE}^e$  (in particular, the generic waste particle size diameter for CSNF, DSNF, and HLW was greatly decreased, which greatly increased the amount of entrainment and transport in the ash plume). Also, the wind direction was fixed toward the critical group in Amargosa Valley rather than sampled [61]. The  $\mathcal{R}_{VE}(\sim)$  also calculated the loss of contaminants via soil erosion, since long-lived radionuclides build up in the soil. Soil erosion was modeled as exponential decay with a constant decay rate ( $k_{soil}$ ); specifically,  $\sum_{m=1}^n \exp\{-k_{soil}(t_n - t_m)\}$ , using SOILEXP v1.0 [60, p. 467, Table 3-1]. For PA–LA, YMP would develop a new biosphere process model that avoided this external calculation of soil erosion.

The consequence model of igneous dike intrusion ( $\mathcal{R}_{VI}(\sim)$ ) consisted of only a modified source-term module ( $\mathcal{M}_V^{Waste}$ ). Beyond the source term module, radionuclides were transported through the UZ and SZ as in the undisturbed scenario. To calculate the fracture of containers breached by the dike intrusion ( $f_{VE}^{br}$ ), the area around an intrusion dike was divided into two zones in  $\mathcal{M}_V^{Waste}$  [62]. Zone 1 consisted of 3 packages on either size of the dike that completely failed. Container failure in Zone 2 depended upon whether drift backfill was or was not present. If backfill was present, no container failure occurred in the remainder of an intersected drift. The mean fraction of containers breached  $\bar{f}_{VE,back}^{br}$  was 0.027 (i.e., failure in Zone 1). If backfill was absent (the base case),  $\mathcal{M}_V^{Waste}$  removed the drip shield, completely failed the waste container, and perforated all the cladding in the remainder of an intersected drift (Zone 2). For no backfill,  $\bar{f}_{VE,no-back}^{br}$  was 0.21 (an order of magnitude larger) [63, Fig. 7]. For failed containers in either Zone 1 or 2, the Package Chemistry Component of  $\mathcal{M}_V^{Waste}$  [9] defaulted to the pH and ionic strength (I) of the drift, as evaluated by  $\mathcal{M}^{EBSchem}$  [8]. Also, for those regions with failed containers, the drift was assumed filled such that percolation in the undisturbed mountain ( $q^{perc}$ , as determined from  $\mathcal{M}^{TH}$ ) was set equal to the advective flow through the engineered barrier (i.e.,  $\mathcal{M}^{Seep}$  was not used to evaluate the influence of capillary forces on flow into an open drift). These modifications were implemented in  $\mathcal{M}_V^{Waste}$  by adding a new WP type to the always drip environment of each bin.

The time of one igneous dike intrusion ( $\tau_{V,\ell}$ ) was sampled along with the epistemic parameters  $\mathbf{e}_{V,\ell}^e$  using the LHS scheme for  $t < 5 \times 10^4$  yr:

$$\bar{D}_{V\ell}^{SR}(t) = \frac{1}{n_{V\ell}^{LHS}} \sum_{\ell=1}^{n_{V\ell}^{LHS}=5000} \wp\{\mathcal{A}_V(\lambda_{V,\ell})\} \sum_{r=1}^{n_{U,\ell}^{BDCF}=23} \frac{f_{U,\ell,r}^{BDCF}}{Q_{\ell}^{indv}} \mathcal{R}_{V\ell,r}(t; \mathbf{e}_{V,\ell}^e, \tau_{V,\ell}) \Big|_{x_{SR}^{se} = 20 \text{ km}} \quad (23)$$

**8. PA-LA**

In response to a request by NWTRB [64], YMP conducted the July 2001 Supplemental Science Performance Analysis (SSPA) using more realistic parameter values and more realistic models to better elucidate the relative importance of included features, events, and processes. The SSPA also evaluated an alternative cooler repository design [65]. Within 8 months, another analysis was made for the February 2002 final EIS on site suitability (PA-EIS) [66], which built upon SSPA. Because of the EPA requirement in 40 CFR 197 that the EIS would evaluate performance over  $10^6$ -yr, a climate change beyond  $10^4$  yr was added to the PA-EIS. Furthermore, the  $\mathcal{M}^{WP}$  module was updated; the  $\mathcal{M}^{TH}$  module was rerun for the cooler repository (rather than make manual adjustments as in SSPA); Np solubility was reduced in  $\mathcal{M}^{Waste}$  [9] and the colloidal transport model in  $\mathcal{M}^{SZ}$  was improved [50, Section 2.6.2 and Table 1].

An unpublished interim PA was conducted in 2004, but the DOE did not proceed to submit an SAR/LA because the licensing support network (LSN) containing documents supporting NRC hearings on the SAR/LA was not certified as complete (Appendix A). Most of the major modeling changes between PA-SR and PA-LA (such as inclusion of the seismic disruptive scenario class), as mentioned in companion papers [7–10] and summarized in the EIS [67, Table 5-1], occurred for this first interim PA.

Another unpublished interim PA was conducted in 2005 that included a more realistic seismic hazard curve; revision of waste inventory to include conversion of excess Pu to mixed-oxide (MOX) fuel and encapsulation in HLW glass [9,68]; revision of irreversible sorption of radionuclides on rust ( $\text{Fe}_2\text{O}_3$ ) to avoid excessive sorption that had occurred with the 2004 interim PA; addition of localized corrosion of the container from early failure of drip shield; and revision of the biological dose conversion factors to conform with the revised calculation method specified in the proposed 10 CFR 63 [6,10]. Although the LSN was now certified complete, DOE did not proceed to submit an SAR/LA in order to adopt a new transportation, aging, and disposal (TAD) handling canister to facilitate operations at the site [49], redesign the waste handling facility, improve modularity of surface and underground [49], adhere to the EPA and NRC proposed  $10^6$  yr regulatory period [6], remove the magma bulkheads in the design, replace the infiltration model [7,69], allow time to incorporate new technical information, and continue to improve the documentation.

A third iteration became the basis for SAR/LA submitted to NRC in June 2008 [1,2]. Both a licensing case (PA-LA), discussed here, and an unqualified case (PA-PMA) to evaluate the influence of conservatism in for the seismic scenario class were conducted, somewhat similar to the situation in 2000 with PA-SR and SSPA.

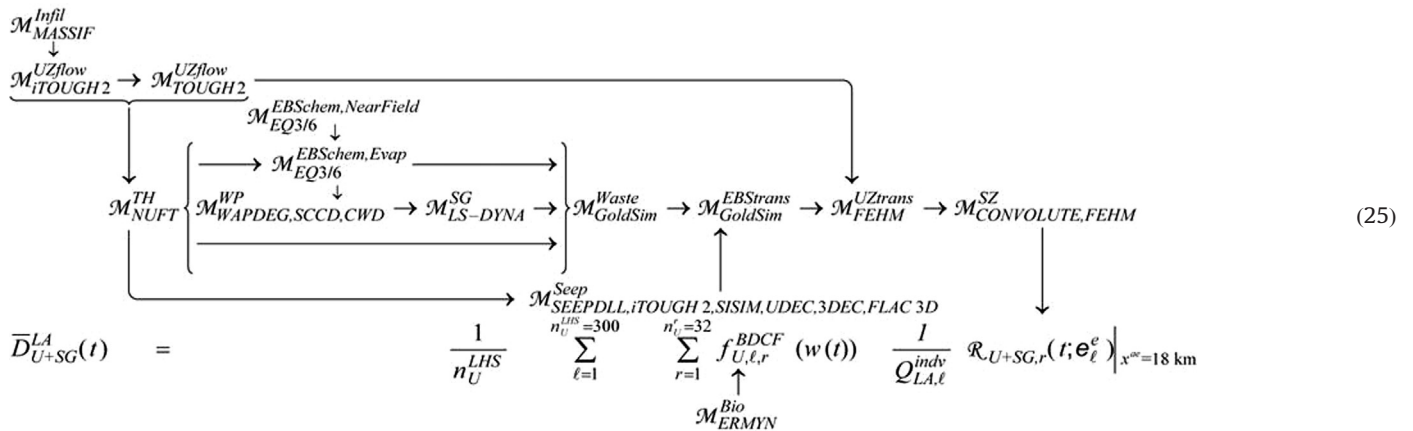
A major emphasis was on the potential doses from seismic ground motion not included in PA-SR. Beyond  $10^4$  yr, the consequences of seismic ground motion were closely dependent upon the state of the repository at the time of the seismic event and so it was not possible to separate the undisturbed from the seismic ground motion (i.e.,  $\mathcal{A}_{U+SG}$ ) [1, Eq. (6.1.2–24)].<sup>12</sup> Hence, the total dose was evaluated as the sum of 6 incremental doses beyond  $10^4$  yr as [70,154]

$$\bar{D}_{U+SG}^{LA}(t) = \sum_{j=1}^{n_s} \bar{D}_j(t; \mathbf{e}^e) = \bar{D}_{U+SG}(t) + \bar{D}_{SF}(t) + \bar{D}_{VE}(t) + \bar{D}_{V\ell}(t) + \bar{D}_{EW}(t) + \bar{D}_{ED}(t) \quad (24)$$

from four retained scenario classes: (1) undisturbed, (2) seismic disruption—new for PA-LA (with seismic ground motion and seismic fault displacement subclasses), (3) igneous disruption (with volcanic eruption and igneous intrusion subclasses), and (4) early EBS failure (with an early waste container subclass and an early drip shield failure subclass—new for PA-LA) [71].

**8.1. Doses via undisturbed and seismic disruption**

The evaluation of  $\bar{D}_{U+SG}(t)$  consisted of summing doses from 32 radionuclides based on 300 samples of 392 uncertain epistemic parameters  $\mathbf{e}_{U,\ell}^e$  of  $\mathcal{R}_{U+SG,r}(\sim)$  (Eq. (25), Fig. 7).



<sup>12</sup> Prior to  $10^4$  yr, the calculation of the undisturbed and seismic scenario classes was separated since packages were mostly intact, but, in turn, the undisturbed scenario had no releases since packages were mostly intact. The calculation method for the seismic scenario class prior to  $10^4$  yr is described elsewhere [1, Appendix J; 155].

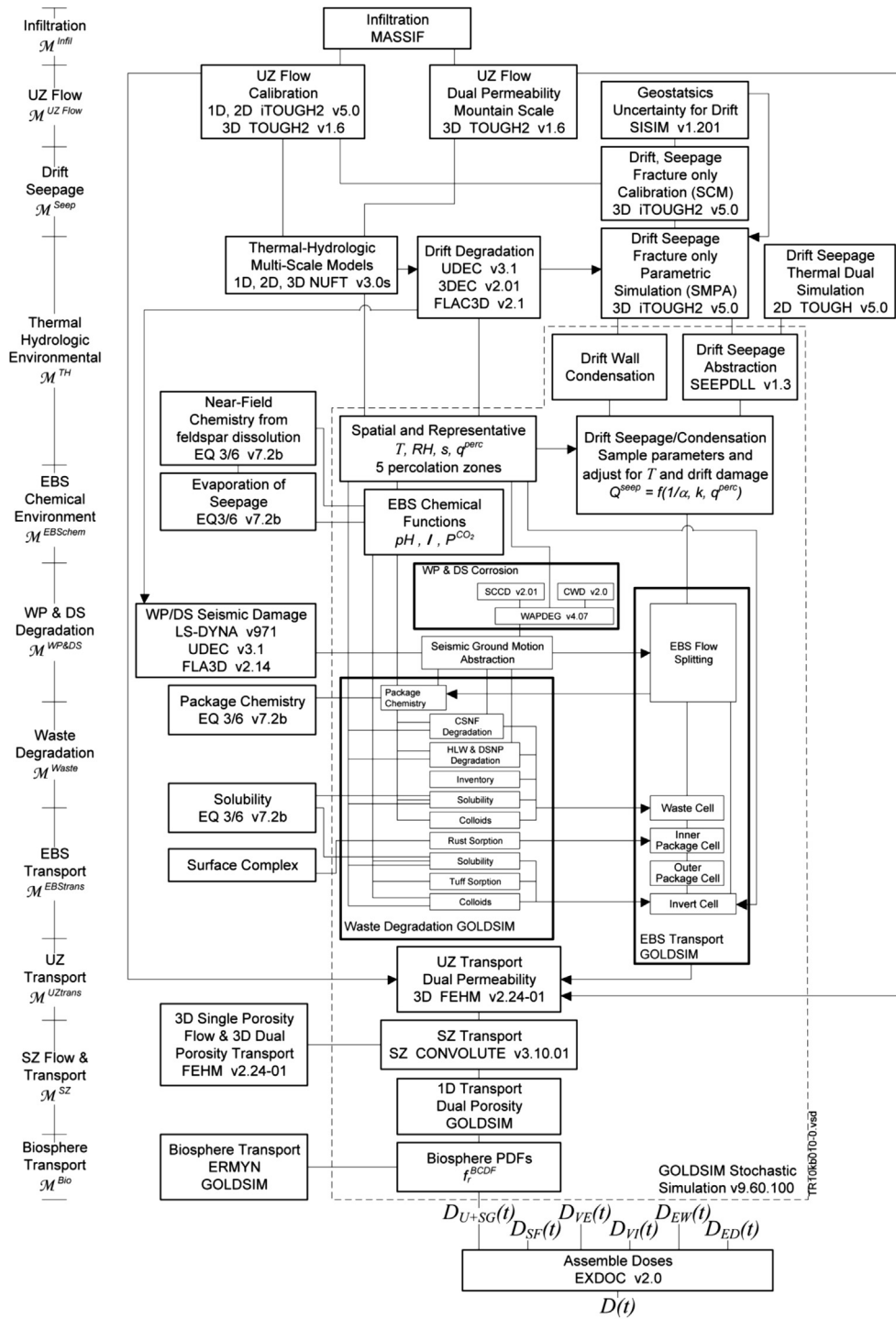


Fig. 7. PA-LA modules included seismic disruption for the combined undisturbed and seismic scenario class beyond  $10^4$  yr ( $\mathcal{A}_{U+SG}$ ) [153, Fig. 2].

### 8.2. Doses via igneous intrusion

Changes were made to the consequence model for a volcanic eruption (such as an update of ASHPLUME to v2.0 [72] and modeling redistribution of volcanic ash deposited in alluvial areas around Yucca Mountain [73]); however, the most important change was greatly reducing the event probability  $\varphi\{E_{WPhit}|\mathcal{A}_V\}$  by including the probability of a volcanic vent intersecting a waste package  $\varphi\{E_{WPhit}|\mathcal{A}_{Vvent}\}$  such the overall probability was similar to that used in PA-VA [5]; hence, volcanic eruption did not contribute substantially to total dose.

The consequence model of igneous dike intrusion ( $\mathcal{R}_{VI}(\sim)$ ) consisted of modifications to the following 3 modules of  $\mathcal{R}_U(\sim)$ : for  $\mathcal{M}_{VI}^{WP&DS}$ , the magma was assumed to completely fail all drip shields and waste containers throughout the repository in PA-LA [74,75], and provide no resistance to magma flow. For  $\mathcal{M}_{VI}^{Waste}$ , the waste form was completely degraded such that radionuclides of CSNF, DSNP, and HLW were exposed and immediately available for transport. Also, the solubility of uranium in CSNF packages was determined by a silica rich environment for the co-disposal packages with the borosilicate glass HLW [9, Fig. 7; 76]. Radionuclides were transported through the UZ and SZ as in the undisturbed



scenario:

$$\bar{D}_{VI}(t) = \frac{1}{n_{VI}^{LHS}} \sum_{\ell=1}^{n_{VI}^{HS}=300} \wp\{\mathcal{A}_V(\lambda_{V,\ell})\} \frac{1}{n_{V}^{CS}} \sum_{k=1}^{n_{V}^{CS}=10} \sum_{r=1}^{n_r=23} \frac{f_{U,\ell,r}^{BDCF}}{Q_{indv}} \mathcal{R}_{VI,r}(t; \mathbf{e}_{VI,\ell}^e, \tau_{V,k}) \quad (26)$$

where the time of one igneous dike intrusion was used to define computational scenarios at  $\tau_{V,k} = \{2.5 \times 10^2, 6 \times 10^2, 10^3, 4 \times 10^3, 10^4, 4 \times 10^4, 10^5, 2 \times 10^5, 4 \times 10^5 \text{ and } 8 \times 10^5\}$  for the  $10^6$  yr simulation (but solved through numerical quadrature rather than by Monte Carlo simulation as implied in Eq. (26) (Appendix B, Eq. (B.14)) [156].

## 9. Summary

The construction of the consequence model  $\mathcal{R}(\sim)$  to simulate the relevant physical phenomena that could influence repository performance is the nuts and bolts of a PA. By the time of PA-LA,  $\mathcal{R}(\sim)$  was complicated, but it is perhaps less difficult to comprehend if the incremental changes are presented. Hence, the evolution of the mathematical formulation for the undisturbed consequence model  $\mathcal{R}_U(\sim)$  that occurred in seven iterations between 1982 and 2008 is discussed by noting the addition and linkage of computational modules  $\mathcal{M}_U^\beta$  that made up  $\mathcal{R}(\sim)$ . The consequence model of the undisturbed scenario class for PA-EA ( $\mathcal{R}_{U+EA}^A(\sim)$ ) consisted primarily of transport in the underlying UZ ( $\mathcal{M}^{UZtrans}$ ) and SZ ( $\mathcal{M}^{SZ}$ ). PA-91 demonstrated a full stochastic analysis of cumulative release 5 km from the repository [14]. The undisturbed consequence model for PA-91  $\mathcal{R}_{U+EA}^{91}(\sim)$  consisted of 4 modules: (1) flow in the UZ ( $\mathcal{M}^{UZflow}$ ) [7], (2) waste degradation in the EBS ( $\mathcal{M}^{Waste}$ ) [9], (3) transport in the UZ ( $\mathcal{M}^{UZtrans}$ ) [10], and (4) flow/transport in the SZ ( $\mathcal{M}^{SZ}$ ) [10].

PA-93 provided guidance on characterizing the site, on heat load options for the repository, and floor and in-drift package placement options [15,49]. A heat load of either 14 W/m<sup>2</sup> (as used in PA-EA and PA-91) and a hotter 28 W/m<sup>2</sup> were evaluated. The higher heat load necessitated the addition of a thermal module ( $\mathcal{M}^T$ ) to the consequence model for undisturbed conditions with early WP failure,  $\mathcal{R}_{U+EF}^{93}(\sim)$  [8].

Partially in response to the change to a dose performance measure, PA-95 improved modeling of the EBS for  $\mathcal{R}_{U+EF}^{95}(\sim)$  by [16] (1) developing an empirical PA model of degradation that including variability of corrosion between containers ( $\mathcal{R}^{WP}$ ) [8], and (2) developing a new module that evaluated 3 modes of transport of radionuclides out of the container ( $\mathcal{M}^{EBstrans}$ ) [9]. PA-95 also transitioned to using results from a process model of UZ flow above the repository [7].

A major step in modeling complexity occurred in PA-VA. The  $\mathcal{R}_{U+EF}^{VA}(\sim)$  included more elaborate modeling of the UZ flow and the addition of modules for infiltration ( $\mathcal{M}^{infil}$ ) [7], drift seepage ( $\mathcal{M}^{Seep}$ ) [7], the EBS chemical environment ( $\mathcal{M}^{EBSchem}$ ) [8], and biosphere transport ( $\mathcal{M}^{Bio}$ ) [10].

For PA-SR, the drift seepage module  $\mathcal{M}^{Seep}$  of the undisturbed consequence model with seismic cladding disruption,  $\mathcal{R}_{U+SGclad}^{SR}(\sim)$ , was more elaborate. Also,  $\mathcal{M}^{Seep}$  used estimates of flow above the repository from  $\mathcal{M}^{TH}$  such that  $\mathcal{M}^{TH}$  was more fully embedded into the PA [7]. However, seepage was less important because container corrosion no longer differed between dripping and no dripping environments. In addition, the WP corrosion module ( $\mathcal{M}^{WP\&DS}$ ) was moved directly into the stochastic calculation and included breach of the newly added drip shield [8; 50, Table 1].

For PA-LA, the potential for WP damage from drift degradation and package movement during a seismic event scenario class was included with the undisturbed class beyond  $10^4$  yr ( $\mathcal{R}_{U+SG}^{LA}(\sim)$ ) [77], which, in turn, required the addition of seismic damage process codes in  $\mathcal{M}^{TH}$  and  $\mathcal{M}^{WP\&DS}$  [8,78]. Also, the temperature dependence of general corrosion was reintroduced [8,79] and the stress corrosion cracking (SCC) model for outer Alloy 22 layer of the container updated [8,80].

The details of the linkage of the modules of  $\mathcal{R}_U(\sim)$  help the reader get a glimpse of the complexity and the challenge of using numerous model simplifications in a PA simulation for the YM disposal system. While advantages can accrue in the faster run time for the PA itself, the numerous process model simulations required for developing simplifications for  $\mathcal{M}_U^\beta$ , the analyst effort required for maintaining consistency between the simplifications and spatial averaging, and the analyst burden in describing the simplifications and linkages were substantial for YMP. As various other geologic media are examined in the future in the US, the flexibility provided by incorporating streamlined process models directly in the PA simulation (as demonstrated when using the WIPP PA modeling system to evaluate DSNF disposal in salt, granite, and tuff [36–38]) warrants further consideration.

## Acknowledgments

Sandia National Laboratories (SNL) is a multi-program laboratory operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the DOE National Nuclear Security Administration under contract DE-AC04-94AL85000. The authors wish to thank L.A. Connolly, SNL, for help with references, and S.K. Best, Raytheon, for illustration support. The historical perspective and opinions presented are those of the authors and are not necessarily those held by reviewers, SNL, or DOE. As a historical perspective, the authors are reporting on the work of others; however, any interpretative errors of documentation are those of the authors alone. Each performance assessment discussed in this paper required numerous participants with expertise in many areas of science and technology. The most complete listing of these participants is made by examining the extensive reference list. However, many of references are corporate documents without authors. Also, the extensive time some scientists and engineers devoted to PA modeling and the handoff between different scientists and engineers as YMP transitioned through four study phases (site identification, feasibility analysis, suitability analysis, and compliance analysis [3, Table 1]) is more evident if some of the organizations and persons are acknowledged here in somewhat chronological order. SNL had a prominent role in the PA methodology in the 1980s and early 1990s and contributors to the progression of PA modeling include Y.T. Lin, SNL and J.P. Brannen, SNL (development of SAMPLE and transport modeling for PA-EA [12]); R. R. Peters (transport comparisons for PA-EA [23] and TOSPAC development for PA-91 [24]); M.S. Tierney, SNL (TOSPAC mathematical basis [24] and PA methodology in SCP [26, Section 8.3.5.13]); J.H. Gauthier, SNL (PA-EA [23], PA-91 [14], PA-93 [15], PA-VA, and PA-SR); R.W. Barnard (PA-91 [14], PA-93 [15], and disruptive events for PA-VA); M.L. Wilson, SNL (design of PA-91 [40] and PA-93 [15], seepage for PA-VA and PA-SR). PNNL contributors included PW Eslinger (preliminary PAs in late 1980s [28] and PA-PNNL-91 [45]); and P.G. Doctor (preliminary PAs [46]). By the mid 1990s, the M&O Contractor to DOE had responsibility for the PA and contributors included S.D. Sevougian, Intera/Duke/Areva/SNL (RIP programming lead for PA-95 [16] and technical lead for PA modeling for PA-VA [17], PA-SR [59],

**1972** Chairman Schlesinger of Atomic Energy Commission (AEC), precursor to Department of Energy (DOE) asks for probabilistic risk assessment (PRA) of core meltdown of a nuclear reactor [81].



**1975 Oct:** 60 member team finishes PRA for 2 reactors for Nuclear Regulatory Commission (NRC) [81].

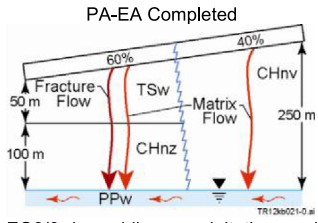
**1978** NRC funds Sandia Nat Labs (SNL) to develop performance assessment (PA) for high-level waste (HLW) and commercial spent nuclear fuel (CSNF) repositories [82].

**1981** SNL completes draft reports to NRC on PA methodology and PA of hypothetical bedded salt repository [19; 21].



**1982 Apr:** SNL evaluates dose from HLW after volcanic eruption (part of PA-EA) [11].

**1983 Mar:** SNL reports on codes necessary for repository design, evaluation of experiments, and PA [83]. **Apr:** Lawrence Livermore Nat Lab (LLNL) documents EQ3/6 geochemical equilibrium code system, first described in 1979 [84].



**1984** Pacific Northwest Nat. Lab. (PNNL) develops two-dimensional (2-D) model of repository that includes evapo-transpiration [85]. SNL starts work on TOSPAC [24]. **Feb:** LLNL reports on 2-D and 3-D thermal modeling of vertical and horizontal waste emplacement [86]. **May:** LLNL improves

EQ3/6 by adding precipitation and fixed partial gas pressures to evaluate chemistry in unsaturated zone (UZ) [84]. **Aug:** Los Alamos Nat Lab (LANL) reports on TRACR3D, a code for flow/transport in porous and fractured media [87]. **Dec:** SNL completes deterministic ground water flow portion of PA-EA for CSNF repository at Yucca Mt (YM) that shows compliance with Environmental Protection Agency (EPA) 1982 draft 40 CFR 191. The <sup>129</sup>I important when <1 mm/yr percolation (matrix flow); <sup>239</sup>Pu important when >1 mm/yr percolation (fracture flow) [13].

**1985** Two SNL codes are complete: NORIA [88], for 2-D, multiphase, porous-media and FEMTRAN [89], for nuclide transport.

**1986 Jul:** US Geological Survey/Lawrence Berkeley Nat Lab (USGS/LBNL) develop 2-D, ECM, site-scale model [90]. SNL develops equivalent continuum model (ECM) for isothermal conditions for a single phase based on Richard's equation in TOSPAC (flow mostly in matrix) [91]. **Aug:** SNL estimates travel time to accessible boundary to compare with 10<sup>3</sup>-yr requirement in 10 CFR 60 [92]. Travel time is sensitive to fracture flow in UZ, which is sensitive to percolation rate.

**1987** SNL develops 2-D, site-scale model, based on STAFF2D [93]. Model calibrated by hand to investigate effect on saturated zone (SZ) transport of permeability change from (1) igneous/seismic activity, and (2) leakage from surface or carbonate aquifer [94].

**1988 Dec:** Site Characterization Plan (SCP) describes PA methodology [26]. SNL documents TOSPAC [24]; use demonstrated in March for flow in UZ [95]. Sub-seabed Disposal Program led by SNL since 1974 along with Seabed Working Group of Nuclear Energy Agency (NEA) publish favorable final PA on concept [96].

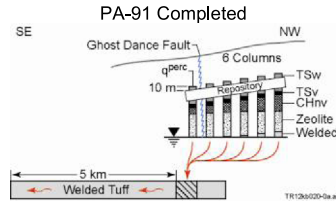
**1989 Jun:** SNL conducts PA on hypothetical basalt site [97]. **Oct:** PNNL presents deterministic risk assessment of YM repository using IPA-EA data, 0.5 to 0.75 mm/yr percolation, and 1982 SNL eruptive doses [28]. **Dec:** SNL demonstrates PA for disposal of transuranic (TRU) waste in salt at Waste Isolation Pilot Plant (WIPP) in southern New Mexico [98].

**1990** LBNL extends ECM formulation to multiphase, non-isothermal conditions in TOUGH [99]. LBNL compares results with discrete fractures [100]. Electrical Power Research Institute (EPRI) completes 1<sup>st</sup> PA using logic-tree approach [22]. SNL finishes large-scale analysis of water movement through UZ using NORIA for NEA code comparison study [88; 101]. **Jul:** SNL reports to NRC on PA for low-level waste (LLW) disposal [102]. **Sep:** DOE decides to use conservative approach for PAs with no sorption in fractures and smallest measured sorption for

matrix. LANL finds that Am, Pu and other nuclides with sorption coefficients >0.5 m<sup>3</sup>/kg will comply (retardation of 200-500); only Tc, I, U, Np adsorb poorly [103]. **Dec:** SNL conducts 1<sup>st</sup> PA of WIPP [104].



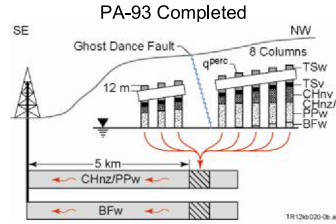
**1991 Jan:** LLNL shows reasonable agreement of ECM with G-tunnel heater tests [105]; 1<sup>st</sup> report by Nuclear Waste Technical Review Board (NWTRB) notes lack of improvement in PA capability since PA-EA [31]. **Jun:** Deterministic calculations (PACE-90) with best estimates for model parameters completed by SNL, PNNL, and LANL. Little nuclide movement in UZ over 10<sup>4</sup> yr with 0.01 mm/yr percolation at repository level [30, §3.4.5]. DOE asks SNL to complete stochastic PA by end of year [14, §1.3]. **Jul:** SNL demonstrates PA methodology for tuff for NRC [106]. **Oct:** LLNL uses discrete fractures to model episodic nonequilibrium percolation [107, pp. 316-321]. **Dec:** SNL completes 2<sup>nd</sup> PA of WIPP [14; 108].



**1992 May:** NRC completes iterative PA (IPA-1) to demonstrate capability [109]. ERPI completes 2<sup>nd</sup> PA [47]. **Jul:** SNL completes 1<sup>st</sup> stochastic PA-91 to demonstrate capability and feasibility of CSNF repository at YM [14, §4]. Progress noted by NWTRB [39]. Summed

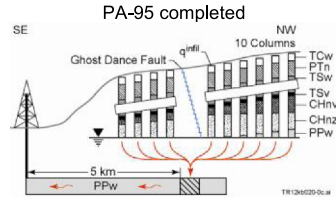
releases to 5-km boundary evaluated for undisturbed and 2 disruptive (volcanic eruption and human intrusion) scenario classes. SNL uses 2 conceptual models of UZ flow: ECM and Weeps [110]. Both disruptive scenarios and undisturbed release via groundwater meet 40 CFR 191. Undisturbed release of gaseous <sup>14</sup>C with ECM slightly exceeds 40 CFR 191. **Dec:** SNL completes 3<sup>rd</sup> PA of WIPP [111].

**1993** PNNL completes PA-PNNL-91 started in 1991 [45, §10.3]. PNNL uses same scenarios, but more complex models and fewer calculations than PA-91. PNNL uses generic site data with tuff permeability factor of 10<sup>3</sup> less than PA-91; thus, <sup>14</sup>C releases small. PNNL assumes percolation between 0 and 0.5 mm/yr; hence, no nuclides reach the SZ in 10<sup>5</sup> yr. Highest exposure is from volcanic eruption followed by drill cuttings during human intrusion [45, Ch. 10]. LLNL models environment that develops around drifts and water that contacts packages and waste [112]. **Jun:** SNL completes 1<sup>st</sup> PA on disposal of LLW tritium, sealed sources, and classified TRU at Greater Confinement Disposal (GCD) facility in 36 m deep boreholes in tuff alluvium at NTS [113]. **Dec:** SNL completes PA of waste form options for DOE-owned spent nuclear fuel (DSNF) in salt and granite showing repository mitigates differences in waste behavior [36]. Estimated degradation of DSNF used in PA-95.



**1994 Apr:** SNL completes PA-93 to provide guidance on design options [15]. Summed releases over 10<sup>4</sup> yr and dose over 10<sup>6</sup> yr calculated at 5 km boundary. Igneous intrusion scenario subclass added. Because of 10<sup>6</sup> yr period, climate change added. A thermal module added and container and waste

degradation models improved to evaluate hot repository. Flow/transport process model is 3-D to better evaluate SZ dilution for dose. PA-93 finds gaseous <sup>14</sup>C dominates release and <sup>237</sup>Np dominates groundwater releases and doses. Newly assigned DOE management and operator (M&O) also conducts PA (PA-M&O-93) [51] using PC-based Repository Integration Program (RIP) to simulate behavior with simple models [52]. RIP only tracks nuclide mass; RIP ignores water balance. Parameter values from PA-93. SNL completes 2<sup>nd</sup> PA on GCD at NTS [114].



**1995** USGS/LBNL develop 1<sup>st</sup> 3-D UZ model (UZ-95) using ECM [115, p. 8]. One column of UZ-95 mesh is used for PA-95 [16]. **Feb:** SNL shows feasibility of direct disposal without treatment of DSNF at YM (PA-SNL-95) [37]. Analysis includes cladding to

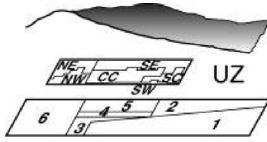
Fig. A1. Evaluation of feasibility, viability, and compliance of Yucca Mountain disposal system [81, 83–148].

distinguish ~250 types of DSNF. **Oct:** NRC completes 2<sup>nd</sup> PA (IPA-2) showing importance of waste container corrosion and infiltration [109]. **Nov:** Yucca Mt Project (YMP) completes PA-95 using RIP to evaluate summed release and doses to  $10^5$  yr at 5 km boundary for undisturbed scenario [16]. PA-95 uses (1) results from thermal-hydrology model, (2) new container degradation model that includes corrosion variability, and (3) 3 alternative transport models around package. PA-95 finds (1)  $^{14}\text{C}$ ,  $^{99}\text{Tc}$ ,  $^{129}\text{I}$  dominate releases in 1<sup>st</sup>  $10^4$  yr; and (2) peak dose from  $^{237}\text{Np}$ .

**1996** LANL develops 3-D site-scale model using dual-permeability model (DKM) in FEHM nuclide transport code [116, pp. 67–9]. YMP attempts to allocate performance among disposal system components using PA [117]. Environment Management Office of DOE (DOE-EM) supports YMP for sensitivity study (PA-96) on disposal of excess weapon Pu using parameter distributions reported in PA-93 [118]. EPRI completes 3<sup>rd</sup> PA [119]. **Sep:** Based on infiltration tests on large block test (LBT) located at Fran Ridge near YM, SNL concludes DKM more accurately models rapid percolation of blue dye than ECM [120].

**1997** LBNL completes integrated finite difference (FD) model to simulate steady-flow in SZ over 150-km<sup>2</sup> area near YM [121]. LANL completes documentation of FEHM [122]. USGS uses FEHM to model steady flow in SZ at site scale, using 16 zones, one no-flow fault, and minor recharge from Forty-Mile Wash [123]. YMP conducts PA-97 using PA-93 parameter distributions, to evaluate various design options [124]. **Oct:** SNL completes PA for Compliance Certification Application for WIPP using generic EPA standards 40 CFR 191 [33].

#### PA-VA Completed

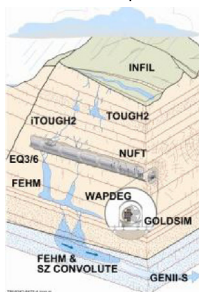


**1998** DKM applied in thermal-hydrologic models supporting PA-VA [17, Vol. 3 §3.2.1] to predict conditions in near-field, altered zone. **Sep:** For DOE-EM, SNL updates PA to examine SZ viability of direct disposal of DSNF at YM (PA-SNL-97) [38].

**Nov:** EPRI completes 4<sup>th</sup> PA of YM [125]. **Dec:** In 5 volume report to Congress, DOE concludes that YM remains a viable site based on PA-VA using a dose measure [17]. Doses from igneous and seismic disruptive events very small [17, Vol. 3 §4.4.3]. DOE-EM supports YMP so that DSNF is included in PA-VA. Assuming metallic degradation rate and no cladding, DSNF contributes about same dose as HLW; both less than CSNF [17, Vol. 3 Fig. 4-22].

**1999** USGS uses 3-D, FD model developed in 1997 to evaluate effect of full-glacial and global-warming climates on regional flow at Death Valley [126]. Results set boundary conditions for site-scale SZ model. **Feb:** PA Peer Review (PAPR) panel of PA-VA suggests using simple models, sensitivity studies, bounding analysis, and design changes to move into regime of known behavior [127]. Bounding analysis inconsistent with “reasonable expectation” using realistic analysis proposed in 40 CFR 197 [6]. **Apr:** YMP completes licensing application design selection (LADS) study of options to add to repository design; Ti drip shield added; drift spacing increased to 81 m, Alloy 22 switched to outer layer of container; and drift support switched to steel mesh [128]. **Aug:** Revisions to LADS completed [128]. **Nov:** YMP decides to conservatively estimate uncertainty in models and parameters (a) to follow PAPR suggestion, (b) to lessen onerous 1<sup>st</sup>-time qualification of data, and (c) to be consistent with the “reasonable assurance” approach in 10 CFR 60 and proposed in 10 CFR 63 [129].

#### PA-SR Completed



**2000 Mar-Apr:** YMP completes process model reports (PMRs) that summarize various aspects of the YM disposal system for the site recommendation (PA-SR) [130]. **Apr:** NWTRB states improvements needed for PA-SR: (a) better inclusion of uncertainty in PA, (b) more study of corrosion of Alloy 22, (c) evaluation of hot repository design [64]. **May-Sep:** Detailed AMRs, which provide details summarized in the PMRs, are completed during the summer. **Nov:** YMP completes PA-SR for  $10^4$ -yr regulatory period. EPRI completes 5<sup>th</sup>

PA of YM [131]. **Dec:** PA-SR is finalized based on DOE comments [59].

**2001 May:** DOE issues Science and Engineering Report (S&ER) [18; 132], which summarizes the current design and results from PA-SR. DOE also issues draft Supplement to EIS using results from PA-SR [133]. **Jun:** SSPA completed to address critique by NWTRB that

conservative bias in models and parameters of PA-SR complicates understating. SSPA includes more consistent, unbiased treatment of parameter uncertainty and modeling changes to approximate a cooler repository where drift wall temperatures do not exceed boiling [134]. **Sep:** SNL completes PA for GCD facility on NTS in tuff alluvium and shows compliance with 40 CFR 191 for self-regulating DOE for classified TRU waste [135]. **Dec:** PA-EIS completed for siting EIS based on updated SSPA parameters and models that analyze the hot and cool repository designs [66]. Joint IAEA-NEA (International Atomic Energy Agency and Nuclear Energy Agency) international review team completes review of PA-SR [136] and suggests developing a safety case (i.e., high level document that describes the strategy used to achieve safety as distinct from the PA-SR showing compliance with EPA and NRC regulations). IAEA completes review of biosphere model, which suggests updating biosphere model for LA [137].

**2002** USGS revises regional groundwater flow model of Death Valley Basin [138]. **Feb:** DOE issues final EIS on YM and recommends site to President [66]. EPRI completes 6<sup>th</sup> PA of YM, showing capability of natural barrier alone to meet limits of 40 CFR 197 [139]. **Sep:** DOE decides to submit license by Dec 2004 (under “Plan B”) and conduct PA for only  $10^3$  yr regulatory period [140]. **Dec:** EPRI completes 7<sup>th</sup> PA of YM [141].

**2003** Most AMRs completed for PA-04-LA that includes seismic scenario class; better calibration of seepage model; updated near field chemistry model to better evaluate pH, NO<sub>3</sub>, Cl<sup>-</sup> concentration in seepage water to determine localized corrosion on container; updated package chemistry model to simulate when only water vapor available and include sorption of H<sup>+</sup> and OH<sup>-</sup> on rust to constrain pH; and replaced GENII-S with ERMIL to calculate dose factors.

**2004 Mar:** Based on NRC audit [142], YMP reorganizes to form Repository Integration Teams (RITs) and initiates a 6-month, \$20 million review of most AMRs to improve justification and traceability to sources of information for PA-04-LA [143]. ~150 personnel from DOE, USGS, SNL, LANL, LBNL, and LLNL examine ~110 AMRs completed in 2003 and focuses on 89 that need more work (10 found acceptable and 11 cancelled and important aspects moved to other AMRs). SNL completes 1<sup>st</sup> recertification PA of WIPP [144]. **Dec:** YMP completes Rev 0, draft I of PA-04-LA for  $10^4$ -yr regulatory period, but work stops because certification of LSN of documents for use in hearings not accepted by NRC [6, App. B].

**2005 Jan:** While waiting for LSN certification, DOE asks for another interim PA-05-LA to improve various submodels in response to comments by Independent Validation Review Team (IVRT) and others. **Jan-Jun:** YMP updates AMRs that support PA-05-LA; seismic model uses revised hazard curve with maximum peak ground velocity of 4 rather than 12 m/s to eliminate unrealistic behavior [145]; inventory revised to include excess Pu in either MOX fuel or HLW glass; and near field chemistry model revised again.

**2006 Jan:** Acting Director Golan announces a new path: (a) implement transportation, aging, and disposal (TAD handling canister for CSNF; and (b) designate SNL as lead laboratory to coordinate repository science and provide license defense during NRC hearings [146]. **May:** YMP completes most documentation for PA-05-LA, but work stops to prepare a PA-LA to submit in June 2008 that addresses remaining IVRT comments; includes analysis out to  $10^6$  yr, consistent with EPA and NRC rules; replaces near-field chemistry model; replaces USGS INFIL with SNL MASSIF infiltration model; and models TAD inside CSNF package.

#### PA-LA Completed



**2008** NRC completes another iterative PA on YM [147]. **Jan:** SNL completes documentation on PA-LA [59]. Maximum dose of 0.02 mSv/yr at  $10^6$  yr from advectively released  $^{239}\text{Pu}$ ,  $^{242}\text{Pu}$ ,  $^{237}\text{Np}$  in combined seismic and undisturbed scenario class (breach of ~10% of containers by general corrosion in undisturbed). **Mar:** M&O completes SAR chapters on repository design and analysis of pre-closure behavior (4246 pp., 8 vol.) and most of 1<sup>st</sup> volume on General Information (GI) (344 p.). SNL completes addendum to PA-LA correcting errors found during review [59]. **Apr:** SNL completes SAR sections on site characterization (§GI-5), analysis of post-closure behavior (Ch 2—3634 pp., 1588 references, 6 vol.), and last volume on performance confirmation tests (Ch 3-5—354 pages, 147 references). **Jun:** Moving van delivers 15 copies of 41 kg, 3 million word, 8578 page, 16 volume SAR for LA to NRC [2].

**2009** Update to SAR submitted to NRC [148]

Fig. A1. (continued)



and PA–LA [2]); J.A. McNeish, Intera/Duke/Areva/SNL (technical lead for PA–M&O-93 [51] and PA-95 [16], and managerial oversight for PA–VA [17], PA–SR [59], and PA–LA [2]). Implementers of these later PAs were V. Vallikat, Intera/Duke (RIP programming lead for PA–VA), E. Devenoc, Duke (simulation run management for PA–VA); P. Mattie, Intera/SNL (Goldsim programming lead for PA–SR [60]); D. Kalinich, Areva now at SNL (Goldsim programming for SR seepage, lead for SSPA [65] and PA-EIS [66]); K.P. Lee, Areva (Goldsim programming lead for PA–LA); S. Mehta, Areva (Goldsim programming for PA–LA). Contributors to specific analysis include P.N. Swift, SNL (oversight of igneous disruption for PA–SR); M. Sauer, SNL (parameters for volcanic eruption in ASHP LUME for PA–SR); D. Krier, LANL (characteristics of eruptive process for PA–LA [61]); G. Kerring and C. Harrington, LANL (analysis of volcanic eruptions with ASHP LUME for PA–LA [72]); ES Gaffney (analysis of interaction of magma dike with repository drift for PA–LA [74]). Also, the task of translating the results of process models for PA included GA Behie, Areva (waste package and seepage PA modeling in engineered barrier system for PA–LA) and B Lester (PA modeling of the natural barrier system in PA–LA). Additional contributors for PA–LA include J.C. Helton, ASU (design of PA–LA [2, App. J; 70]); C.J. Sallaberry, SNL (implementation and sensitivity analysis of PA–LA [2, App. K; 70]); and C.W. Hansen, SNL (design and implementation of PA–LA analysis [2, App. K; 70]). PA managerial oversight during the iterations were S. Sinnock, SNL (PA–EA); F.W. Bingham, SNL (SCP, PA-91, and PA-93); A.E. Van Luik, PNNL/Intera now DOE (preliminary PAs in late 1980s [28], and PA-M&O-93); H.A. Dockery, SNL (PA-93 and PA-VA); R.W. Andrews, Intera/Duke/BSC now Intera (PA-95, PA-VA, and PA-SR); M.K. Knowles, SNL (PA–LA). Many of these contributors were also involved with the analysis of results and are also acknowledged along with others in a companion paper [50]. Furthermore, contributors to the development of specific PA modules such as igneous intrusion, UZ flow, waste container, waste form, and transport have been acknowledged in those companion papers [5,7–10]. Because so many scientists and engineers were involved in conducting the PAs at YMP, the authors recognize that this list is unavoidably incomplete, and we apologize for omissions and oversights.

## Appendix A. Progression of performance assessments

Please see Appendix Fig. A1.

## Appendix B. Evaluation of expected distribution of cumulative release and expected dose

Appendix B derives expressions for evaluating the expected distribution of the normalized cumulative releases (Eq. (B.7)) and the expected dose (Eq. (B.14)). The expressions are similar except for the factors applied at the end to normalize the releases or evaluate dose. The two expressions are simpler than required in many instances, but they serve to identify the assembly of the various model components for a PA as described in the main text. The papers in this special issue provide a more complete description of the mathematical expressions necessary for evaluating dose for PA-LA (e.g., [154–156]).

### B.1 Evaluation of expected distribution of cumulative release in PA-91, PA-93, and PA-95

For PA-91, PA-93, and PA-95, it was necessary to construct a CCDF ( $\phi\{R(\mathbf{p}) > R\}$ ) of the cumulative release  $R(\mathbf{p})$  from a stochastic simulation for comparison with the probabilistic limits of the Containment Requirements in Section 191.13 of the 1985 EPA radiation protection standards, 40 CFR 191 as described elsewhere [6]. The cumulative release  $R(\mathbf{p})$  is

$$R(\mathbf{p}) = \sum_{r=1}^{n_r} \frac{1}{f_{mass} L_r} \int_0^{10^4 \text{yr}} \oint_{x^{ae}=5\text{km}} \mathcal{R}_r(t, \mathbf{x}; \mathbf{p}) dx dt \quad (\text{B.1})$$

where  $f_{mass}$  is the mass fraction of MTHM in the repository (MTHM divided by  $10^3$  MT);  $L_r$  is the limiting value specified in 40 CFR 191 for radionuclide  $r$ ;  $\mathcal{R}_r(\sim)$  is the exposure consequence model that calculates the flux across a boundary for radionuclide  $r$ ; and  $\mathbf{p}$  is an ordered  $n_P$ -tuple of parameters,  $\mathbf{p} = \{\varphi_1, \dots, \varphi_n, \dots, \varphi_{n_P}\}$ .

The elements of  $\mathbf{p}$  can be conceptually divided into three disjoint sets [34, Appendix A; 70; 149; 150]: (1) a set, designated fixed, ( $\mathbf{f} = \{\phi_1^f, \dots, \phi_n^f, \dots, \phi_{n_P}^f\}$ ); whose elements represent fixed quantities (2) a set, designated aleatoric parameters ( $\mathbf{a} = \{\phi_1^a, \dots, \phi_n^a, \dots, \phi_{n_P}^a\}$ ), whose elements represent those aspects of the disposal system assumed to have a random character for which EPA, NRC, or PA Analysts are particularly interested (specifically, future events such as human intrusion, igneous activity, and seismic activity) and for which a probability model could be constructed to estimate the probability of occurrence; and (3) a remaining set, designated epistemic parameters ( $\mathbf{e} = \{\phi_1^e, \dots, \phi_n^e, \dots, \phi_{n_P}^e\}$ ), whose elements represent uncertainty about our knowledge in the parameter values of the models. In this paper, the epistemic set is further divided in a set of parameters for the exposure pathway/consequence model  $\mathbf{e}^e$  and a set of parameters for the probability model  $\mathbf{e}^p$  to facilitate notation since often there is epistemic uncertainty in parameter values that make up probability model (i.e.,  $\mathbf{p} = \{\mathbf{f}, \mathbf{e}^e, \mathbf{e}^p, \mathbf{a}\}$ ).

Typically, the largest set in YMP PAs is the set of fixed parameters, and the smallest set the set of aleatoric parameters. The fixed set represent a plethora of parameters types [35, Fig. 3]: (a) well known physical constants, conversion factors, and reference values based on repository design, (b) code-control parameters; (c) geometrical or model-domain parameters, (d) choice parameters selecting various design options, and (e), parameters from the aleatoric or epistemic sets not of significant influence to the modeling results. We will focus on the second and third uncertain parameters sets and omit the fixed parameter set  $\mathbf{f}$  for simplicity (i.e.,  $\mathbf{e}^e, \mathbf{e}^p, \mathbf{a}$ ).

Probability theory is used to describe the uncertainty in both the latter sets. Because aleatoric parameters describe the frequency of random agents on the disposal system such as igneous or seismic activity, the use of probability theory to represent aleatoric uncertainty is closely related to the frequentist use of probability theory.<sup>13</sup> They are called “aleatoric” parameters because uncertainty of future events

<sup>13</sup> However, this similarity only relates to its use in theory because data to determine frequencies is still fairly rare and thus requires substantial subjective interpretation (e.g., the expert elicitation for igneous and seismic frequency [5]).

is deemed irreducible. For the first probabilistic risk assessment (PRA) of a nuclear reactor in 1975, the scenarios (expressing aleatoric uncertainty) were the sequence of events in an event tree [4].

Epistemic parameters, on the other hand, usually represent physical material property quantities of exposure pathway/consequence models, probability model parameters, or indices selecting alternative conceptual models of either exposure or probability models that are currently imprecisely known, but in principle can be rendered more precise by further observation or experiment. Hence, the use of probability theory to represent epistemic uncertainty is related to the Bayesian use of probability theory [149]. One criticism of the first PRA in 1975 was that it did not include epistemic uncertainty when evaluating the expected behavior [4].

The mean CCDF of releases from the exposure consequence model  $\mathcal{R}(\mathbf{p})$  with respect to uncertain parameters  $\mathbf{p}$  is conceptually defined using an indicator function  $\mathcal{H}(\sim)$  and expectation operator,  $\mathbb{E}\{\sim\}$  [151, p. 17]:

$$\overline{\phi}\{R > R\} = 1 - \overline{G}(R) = \mathbb{E}\{\mathcal{H}\{R - R\}\} = \int_{\Omega^p} \mathcal{H}\{R(\mathbf{p}) - R\} h(\mathbf{p}) d\mathbf{p} \quad (\text{B.2})$$

$$= \int_{\Omega^e} \int_{\Omega^a} \mathcal{H}\{R(\mathbf{e}^e, \mathbf{a}) - R\} g(\mathbf{e}^e, \mathbf{a}) d\mathbf{a} g(\mathbf{e}^e) d\mathbf{e} \quad (\text{B.3})$$

where  $\overline{G}(R)$  is the expected cumulative distribution function,  $\mathcal{H}\{x\} = 0$  if  $x \leq 0$ ;  $\mathcal{H}\{x\} = 1$  if  $x > 0$ , and  $R$  is a number  $\geq 0$ . The expression using the indicator function  $\mathcal{H}\{\sim\}$  is algorithmically implemented by ordering the results from smallest to largest and then plotting.

Eq. (B.3) is based on the reasonable assumption that aleatoric parameters are independent of epistemic parameters  $\mathbf{e}$  such that joint probability distribution of parameters ( $h(\mathbf{p})$ ) is the product of the joint probability distributions of  $\mathbf{a}$  and  $\mathbf{e}$  (i.e.,  $h(\mathbf{p}) = (\mathbf{e}^e) g(\mathbf{a}, \mathbf{e}^e)$ ) and  $g(\sim)$  is a probability density function (PDF) (a type of probability model). The specification of the joint density as the product of individual PDFs was not always possible for the complex YM disposal system. Rather, the probabilistic dependence was expressed algorithmically (e.g., in the Monte Carlo sampling scheme described later).

The inner stochastic integration of Eq. (B.3) is concerned with the space of aleatoric uncertainty ( $\mathbf{a}$ ). Given a mathematical model of the disposal system ( $\mathcal{R}_r(\sim)$ ), a future or a scenario is one point in the parameter space  $\mathcal{R}_r(t, \mathbf{x}; \mathbf{e}^e, \mathbf{a})$ . For all YM PAs, the aleatoric space was discretized by developing scenario classes (i.e., groups of futures or scenarios) representing subsets of  $\mathbf{a}$  of what could happen in the future and denoted by  $\mathcal{A}_j$  where  $\mathcal{A}_j \subset \mathbf{a}$ .

From Eq. (B.3), it is apparent that the stochastic integration to determine the expected CCDF does not depend upon our classification of the uncertain parameters into aleatoric and epistemic subsets; however, the separation can facilitate analysis and understanding. Although the order of integration is immaterial here, the order of integration did matter for the complex YM disposal system since parameters in the aleatoric set had epistemic uncertainty and thus were dependent upon the epistemic integral.

The scenario classes were assumed to be independent such that there were no synergisms between scenario classes. To elaborate by expanding Eq. (B.3) by assuming  $n^s$  coarse scenario classes and leaving an aleatoric subset  $\mathcal{A}'$ .

$$\mathcal{P}\{R > R\} = \int_{\Omega^e} \sum_{j=1}^{n^s} \int_{\Omega^a} \mathcal{H}\{R_j(\mathbf{e}_j^e, \mathbf{a}_j) - R\} g(\mathbf{e}_j^e, \mathbf{a}_j) d\mathbf{a}_j g(\mathbf{e}_j^e) d\mathbf{e} \quad (\text{B.4})$$

$$= \frac{1}{n^{LHS}} \sum_{\ell=1}^{n^{LHS}} \sum_{j=1}^{n^s} \frac{1}{n_j^{CS}} \sum_{k=1}^{n_j^{CS}} \mathcal{H}\{R_j(\mathbf{e}_{j,\ell}^e, \mathbf{a}_{j,k,\ell}) - R\} \quad (\text{B.5})$$

where the scenario class subscript  $j$  on  $R_j$  in Eq. (B.4) hints at the common situation where a specific exposure consequence model  $\mathcal{R}_j(\sim)$  is constructed for each scenario class  $\mathcal{A}_j$ .

The equivalence to Eq. (B.5) is explained as follows. If  $n^s$  coarse scenario classes are used [5], then the coarse scenario class divisions may be further refined for modeling through specification of the time, number, and order of occurrence of phenomena that make up  $\mathcal{A}_j$  as in Eq. (B.5). These  $n^{CS}$  sub-scenario classes are called computational scenarios here as at WIPP. There is no sharp distinction between computational scenarios and scenario classes as expressed by Eq. (B.5); rather a continuum exists. Herein the terms distinguish between fine groupings of futures useful for numerical computations and broad categories of futures useful for organizing the analysis.<sup>14</sup> For example, the coarse scenario class might be one or more igneous intrusion events into the repository ( $n_V > 0$ ) as used in PA-EA and thereafter and the computational scenarios the possible times of an intrusion ( $\tau_V$ ) as used for PA-SR and PA-LA (i.e.,  $\mathbf{a} = \{n_V, \tau_V\}$ ,  $\mathcal{A}_V$  defined by  $n_V > 0$  and  $\mathbf{a}_{V,k} = \tau_V$ ).

Because of the complexity of the model to calculate  $R_j(\mathbf{e}_{j,\ell}^e, \mathbf{a}_{j,k,\ell})$ , numerical techniques were used to evaluate the computational scenarios in Eq. (B.5) starting with PA-91, the first stochastic simulation. Eq. (B.5) assumes that a Monte Carlo technique is used whereby each scenario configuration of the model,  $\mathcal{R}_{j,r}(\sim)$ , is run using  $n^{CS}$  samples from the aleatoric distribution  $g(\mathbf{a}, \mathbf{e}^e)$  with corresponding probability of  $1/n^{CS}$ . However, numerical quadrature was also used for PA-LA [70, Table 4].

The first integration of Eq. (B.4) deals with the epistemic parameter uncertainty for the exposure models  $\mathbf{e}^e$  and probability models  $\mathbf{e}^p$ . For PA-91 and thereafter, the integration was approximated using Latin Hypercube Sampling (LHS) in Eq. (B.5), which is a stratified Monte Carlo sampling scheme developed for PRAs of reactors in 1975, first proposed for PAs of geologic repositories in 1978, and first applied for PAs in 1980 [32,82,152].

For scenario classes that have low probability, general sampling over the entire sample space of  $\mathbf{a}$  is inefficient. Consequently, YM PAs after PA-91 would sample over a reduced set  $\mathbf{a}_j \subset \mathbf{a}$  and multiply the results by the scenario class probability  $\phi\{\mathcal{A}_j(\mathbf{e}^p)\}$ . Hence,

$$\phi\{R > R\} = \frac{1}{n^{LHS}} \sum_{\ell=1}^{n^{LHS}} \sum_{j=1}^{n^s} \phi\{\mathcal{A}_j(\mathbf{e}_{j,\ell}^p)\} \frac{1}{n_j^{CS}} \sum_{k=1}^{n_j^{CS}} \mathcal{H}\{R_j(\mathbf{e}_{j,\ell}^e, \mathbf{a}_{j,k,\ell}) - R\} \quad (\text{B.6})$$

<sup>14</sup> Within the YMP, the term "modeling cases" was used to provide a semantic distinction for the hypothetical analysis of the total scenario class dose and the incremental scenario class dose calculated here. The term is not used here since it does not convey the sense of a continuum between scenario classes, computational scenarios, and scenarios that is being emphasized.



Eq. (B.6) states that the complete CCDF is the sum of the scenario conditional CCDFs weighted by the course scenario class probability. For PA-EA and afterwards, the probability model for igneous intrusion was a Poisson process with one or more igneous intrusive events ( $n_V > 0$ ) over a period  $\mathfrak{Z}$  (i.e.,  $\wp\{\mathcal{A}_V(\mathbf{e}_V^p)\} = \wp\{n_V > 0; \lambda_V \mathfrak{Z}\} = 1 - \exp\{-\lambda_V \mathfrak{Z}\}$ ) where the frequency parameter was not precisely known and, thus, had epistemic uncertainty such that  $\mathbf{e}_V^p = \{\lambda_V\}$  [5, Section 3.1].

After substituting the expression for  $R_j(\mathbf{e}_j^p, \mathbf{a}_{j,k})$  from Eq. (B.1), the expected release CCDF is

$$\wp\{R > R\} = \frac{1}{n^{LHS}} \sum_{\ell=1}^{n^{LHS}} \sum_{j=1}^{n^S} \wp\{\mathcal{A}_j(\mathbf{e}_{j,\ell}^p)\} \frac{1}{n_j^{CS}} \sum_{k=1}^{n_j^{CS}} \mathcal{H} \left[ \left[ \sum_{r=1}^{n^r} \frac{1}{f_{mass} L_r} \int_0^{10^4 \text{yr}} \int_{x^{ae}=5 \text{ km}} \mathcal{R}_{j,r}(t, \mathbf{x}; \mathbf{e}_{j,\ell}^p, \mathbf{a}_{j,k,\ell}) d\mathbf{x} dt \right] - R \right] \quad (B.7)$$

Obviously, the time integral and the surface integral must also be approximated numerically. However, the numerical solutions of the differential equations of  $\mathcal{R}_{j,r}(\sim)$  are not the primary topic of this paper and, thus, will remain integrals.

### B.2. Evaluation of expected dose in PA-93, PA-95, and later PAs

As required by Congress, EPA promulgated site-specific radiation protection standards, 40 CFR 197 for Yucca Mountain in 2001 with dose as a health indicator. For PA-93, PA-95, and later PAs, the total individual dose ( $D(t; \mathbf{e}^e, \mathbf{e}^p, \mathbf{a})$ ) was the sum of doses from radionuclides  $r$  and calculated as

$$D(t; \mathbf{e}^e, \mathbf{e}^p, \mathbf{a}) = \sum_{r=1}^{n^r} f_r^{BCDF}(\mathbf{e}^e, \mathbf{e}^p, \mathbf{a}) C_r(t; \mathbf{e}^e, \mathbf{e}^p, \mathbf{a})|_{x^{ae}} \quad (B.8)$$

$$= \sum_{r=1}^{n^r} f_r^{BCDF}(\mathbf{e}^e, \mathbf{e}^p, \mathbf{a}) \frac{1}{Q^{indv}} \oint_{x^{ae}} \mathcal{R}_r(t, \mathbf{x}; \mathbf{e}^e, \mathbf{e}^p, \mathbf{a}) \Delta z dx \quad (B.9)$$

where  $C_r(t; \mathbf{e}^e, \mathbf{e}^p, \mathbf{a})|_{x^{ae}}$  is the activity concentration in a well withdrawing from a contaminant plume for radionuclide  $r$  at a point of compliance in the accessible environment ( $x^{ae} = \sim 18 \text{ km}$  from the repository by 2001 [6, Table 4]), and  $f_r^{BCDF}(\mathbf{e}^e, \mathbf{e}^p, \mathbf{a})$  is the biological dose conversion factor for radionuclide  $r$ , assuming local food consumption and EPA guidance to assume residents drink 2 L/day. YMP PAs assumed the entire contaminant plume was captured by a drinking water well; thus, the concentration was the mass crossing the accessible boundary  $\oint_{x^{ae}} \mathcal{R}_r(t, \mathbf{x}; \mathbf{e}^e, \mathbf{e}^p, \mathbf{a}) \Delta z dx$  (as represented by the boundary integral) divided by dilution at the withdrawal point ( $Q^{indv}$ ) as noted in Eq. (B.9).

Evaluation of expected dose  $\bar{D}(t)$  was similar to the evaluation of expected cumulative release:

$$\bar{D}(t) = \mathbb{E}\{D(t; \mathbf{e}^e, \mathbf{e}^p, \mathbf{a})\} = \int_{\Omega^E} \int_{\Omega^A} D(t; \mathbf{e}^e, \mathbf{a}) g(\mathbf{e}^p, \mathbf{a}) d\mathbf{a} g(\mathbf{e}^e) d\mathbf{e} = \sum_{j=1}^{n^S} \int_{\Omega^E} \int_{\Omega^A} D_j(t; \mathbf{e}^e, \mathbf{a}) g(\mathbf{e}^p, \mathbf{a}) d\mathbf{a} g(\mathbf{e}^e) d\mathbf{e} \quad (B.10)$$

$$= \sum_{j=1}^{n^S} \frac{1}{n^{LHS}} \sum_{\ell=1}^{n^{LHS}} \frac{1}{n_j^{CS}} \sum_{k=1}^{n_j^{CS}} D_j(t; \mathbf{e}_{j,\ell}^e, \mathbf{a}_{j,k,\ell}) \quad (B.11)$$

In Eq. (B.10), the aleatoric parameter space is decomposed into coarse scenario classes, based on disruptive events. As before, the usual coarseness of the  $n^S$  scenario classes required further refinement into  $n^{CS}$  computational scenarios. Hence, the evaluation of  $D_j(t; \mathbf{e}_{j,\ell}^e, \mathbf{a}_{j,k,\ell})$  involves another integration of the computational scenarios approximated numerically through Monte Carlo techniques as noted in Eq. (B.11) or quadrature as done for evaluating the volcanic scenario class for the license application (PA-LA) [1, Appendix J; 154]. As before, the notation  $D_j(\sim)$  suggests that a separate system model was often constructed for each scenario class  $\mathcal{A}_j$ . For YMP PAs, the expectation with respect to the epistemic parameters again used LHS integration [152]. Alternative expressions for Eq. (B.10) are

$$\bar{D}(t) = \sum_{j=1}^{n^S} \int_{\Omega^E} \int_{\Omega^A} D_j(t; \mathbf{e}^e, \mathbf{a}) g(\mathbf{e}^p, \mathbf{a}) d\mathbf{a} g(\mathbf{e}^e) d\mathbf{e} = \sum_{j=1}^{n^S} \int_{\Omega^E} \bar{D}_j^A(t; \mathbf{e}_j^e) g(\mathbf{e}^e) d\mathbf{e} = \sum_{j=1}^{n^S} \bar{D}_j(t; \mathbf{e}_j^e) \quad (B.12)$$

where the notation  $\bar{D}_j^A(t; \mathbf{e}^e)$  expresses the evaluation of the expectation  $\mathbb{E}^A\{\sim\}$  over the aleatoric subset  $\mathbf{a}$ . It is evident from Eq. (B.12) that the expected dose  $\bar{D}(t)$  is the sum of the incremental doses from the scenario classes.

The low probability of some scenario classes, such as igneous disruption, made general sampling of  $\mathbf{a}$  inefficient; thus, the probability of the scenario class, as estimated by a Poisson process, was used after PA-91 and Eq. (B.11) became [1, Appendix J Eq. J4.5–19]:

$$\bar{D}(t) = \sum_{j=1}^{n^S} \frac{1}{n^{LHS}} \sum_{\ell=1}^{n^{LHS}} \wp\{\mathcal{A}_j(\mathbf{e}_{j,\ell}^p)\} \frac{1}{n_j^{CS}} \sum_{k=1}^{n_j^{CS}} D(t; \mathbf{e}_{j,\ell}^e, \mathbf{a}_{j,k,\ell}) \quad (B.13)$$

Combining Eqs. (B.8) and B.13), the expected total dose as required by 40 CFR 197 was calculated conceptually in PA-VA, PA-SR, and PA-LA for  $t < 10^6 \text{ yr}$  as

$$\bar{D}(t) = \sum_{j=1}^{n^S} \frac{1}{n^{LHS}} \sum_{\ell=1}^{n^{LHS}} \wp\{\mathcal{A}_j(\mathbf{e}_{j,\ell}^p)\} \frac{1}{n_j^{CS}} \sum_{k=1}^{n_j^{CS}} \sum_{r=1}^{n^r} \frac{f_{j,r}^{BCDF}(\mathbf{e}_{j,\ell}^e)}{Q^{indv}} \int_{x^{ae}} \mathcal{R}_{j,r}(t, \mathbf{x}; \mathbf{e}_{j,\ell}^e, \mathbf{a}_{j,k,\ell}) d\mathbf{x} \quad (B.14)$$

However, PA-VA only evaluated dose from the undisturbed scenario class. Instead, the maximum probability weighted doses from igneous and seismic events were simply compared to the the maximum dose from the undisturbed scanrio class. Although the igneous event was reasonably independent of the evolution of the disposal system (specifically, degradation of the waste container) [156], seismic ground motion was not, and so the more general Eq. (B.10) was used for the seismic scenario class when introduced in PA-LA [155].

### B.3. Use of computational scenarios

Although the formulation for Eqs. (B.7) and B.14) includes computational scenarios ( $n^{CS}$ ) for notational generality and comparison, the numerical integration over computational scenarios was only used in PA–LA and to a limited extent in PA–SR. Rather the integration for epistemic and aleatoric parameters (except those defining the coarse scenario classes such as occurrence of an igneous intrusion) were combined and integrated using the LHS technique even though a combined integration complicates sensitivity analysis, as noted in PA–91 [14, Section 8.1].

Specifically, consider two important aleatoric parameters for igneous intrusion: the time and number of igneous intrusions (i.e.,  $\mathbf{a} = \{\tau_V, n_V\}$ ). PA–EA, PA–91, PA–93, PA–SR, and PA–LA had coarse scenario subclasses based on whether or not igneous intrusion occurs (i.e.,  $n_V = 0$  and  $n_V > 0$ ). However, in PA–91 and PA–93, the time of intrusion ( $\tau_V$ ) was grouped with epistemic parameters and sampled randomly (to be consistent with the assumption that igneous intrusion is a Poisson process) rather than used to define computational scenarios. The difficulty in this approach is that  $\tau_V$  has a significant influence on the igneous release prior to substantial degradation of the waste container. The variation of  $\tau_V$  can easily dominate the observed variance in  $D(t)$  at early times. Yet, this result is intuitively obvious. Furthermore, additional characterization of the repository system cannot make  $\tau_V$  more precise. Therefore, it is more useful to perform a sensitivity analysis on  $\mathcal{R}_{V,r}(\sim)$  at discrete times of  $\tau_V$  to be able to elicit the importance of other parameters of the model where further characterization might be able to provide more enlightenment. Using computational scenarios based on  $\tau_V$  ensures that replicates of  $\mathcal{R}_{V,r}(\sim)$  occur at fixed times of  $\tau_V$ . Yet, the stochastic integration can still be performed by combining the individual results of  $\mathcal{R}_{V,r}(\sim)$  as shown conceptually in Eqs. (B.7) and (B.14) for the computational scenarios (i.e.,  $(1/n_j^{CS}) \sum_{k=1}^{n_j^{CS}}$ ).

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