Title 40 CFR Part 191 Subparts B and C Compliance Recertification Application for the Waste Isolation Pilot Plant

Appendix PA

United States Department of Energy
Waste Isolation Pilot Plant

Carlsbad Field Office
Carlsbad, New Mexico

Appendix PA

Table of Contents

List of Figures

List of Tables

ACRONYMS AND ABBREVIATIONS

AMG	***algebraic multi-grid solver***
CDF	***cumulative distribution function***
CCDF	***complementary cumulative distribution function***
CFR	***Code of Federal Regulations***
CH-TRU	***contact-handled transuranic (waste)***
DBR	***direct brine release***
DOE	***United States Department of Energy***
DDZ	***drilling damaged zone***
DRZ	***disturbed rock zone***
EPA	***United States Environmental Protection Agency***
FEP	***feature, event, or process***
LHS	***Latin Hypercube Sample***
LMG	***Link- algebraic multi-grid solver***
LWB	***Land Withdrawal Boundary***
MB	***Marker Bed***
PA	***performance assessment***
PAVT	***Performance Assessment Verification Test***
PCS	***panel closure system***
PDF	***probability density function***
PDE	***partial differential equations***
PRCC	***partial rank correlation coefficient***
RH-TRU	***remote-handled transuranic (waste)***
SMC	***Salado Mass Concrete***
SOR	***successive over-relaxation***
TRU	***transuranic (waste)***
TVD	***Total Variation Diminishing***
WIPP	***Waste Isolation Pilot Plan***

PA-1.0 INTRODUCTION

This appendix presents the mathematical models used to evaluate performance of the Waste Isolation Pilot Plant (WIPP) and the results of these models for the CRA-2004 Performance Assessment (PA). This appendix supplements information presented in Chapter 6 of this application.

This appendix is organized as follows. Section PA-2.0 describes the overall conceptual structure of the CRA-2004 PA. As described in Section 6.1, the WIPP PA is designed to answer the requirements of Title 40 Code of Federal Regulations (CFR) Part 191, and thus involves three basic entities: (1) A probabilistic characterization of different futures that could occur at the WIPP site over the next 10,000 years, (2) Models for the physical processes that take place at the WIPP site and for the estimation of potential radionuclide releases that may be associated with these processes, and (3) A probabilistic characterization of the uncertainty in the models and parameters that underlie the WIPP PA. Section PA-2.0 is supplemented by Attachment SCR, which documents the results of the screening process for features, events, and processes (FEPs) that are retained in the conceptual models of repository performance.

Section PA-3.0 describes the probabilistic characterization of different futures. This characterization plays an important role in the construction of the complementary cumulative distribution function (CCDF) specified in 40 CFR § 191.13. Regulatory guidance and extensive review of the WIPP site resulted in identification of exploratory drilling for natural resources and the mining of potash as the only significant disruptions at the WIPP site with the potential to affect radionuclide releases to the accessible environment (Section 6.2.5). Section PA-3.0 summarizes the stochastic variables that represent future drilling and mining events in the PA.

Section PA-4.0 presents the mathematical models for the physical processes that take place at the WIPP and for the estimation of potential radionuclide releases. The mathematical models implement the conceptual models described in Section 6.4, and permit the construction of the CCDF specified in 40 CFR § 191.13. Models presented in Section PA-4.0 include: two-phase (i.e., gas and brine) flow in the vicinity of the repository; radionuclide transport in the Salado; releases to the surface at the time of a drilling intrusion due to cuttings, cavings, spallings, and direct releases of brine; brine flow in the Culebra Dolomite Formation; and radionuclide transport in the Culebra Dolomite. Section PA-4.0 is supplemented by Attachments MASS, TFIELD, and PORSURF. Attachment MASS discusses the modeling assumptions used in the WIPP PA. Attachment TFIELD discusses the generation of the transmissivity fields used to model fluid flow in the Culebra. Attachment PORSURF presents results of modeling the effects of excavated region closure, waste consolidation, and gas generation in the repository.

Section PA-5.0 discusses the probabilistic characterization of parameter uncertainty, and summarizes the uncertain variables incorporated into the 2004 PA, the distributions assigned to these variables, and the correlations between variables. Section PA-5.0 is supplemented by Attachments PAR and SOTERM. Attachment PAR catalogs the full set of parameters used in the CRA-2004 PA. Attachment SOTERM describes the actinide source term for the WIPP performance calculations, including calculation of the mobile concentrations of actinides that may be released from the repository in brine.

Section PA-6.0 summarizes the computational procedures used in the CRA-2004 PA, including: sampling techniques (i.e., random and Latin hypercube sampling); sample size; statistical confidence for mean CCDF; generation of Latin hypercube samples (LHSs); generation of individual futures; construction of CCDFs; calculations performed with the models discussed in Section PA-4.0; construction of releases for each future; and the sensitivity analysis techniques in use.

Section PA-7.0 presents the results of the PA for an undisturbed repository. Releases from the undisturbed repository are determined by radionuclide transport in brine flowing from the repository to the land withdrawal boundary (LWB) through the marker beds (MBs) or shafts (Section 6.3.1. Releases in the undisturbed scenario are used to demonstrate compliance with the individual and groundwater protection requirements in 40 CFR Part 191 (Chapter 8).

Section PA-8.0 presents PA results for a disturbed repository. As discussed in Section 6.2.3, the only future events and processes in the analysis of disturbed performance are those associated with mining and deep drilling. Release mechanisms include direct releases at the time of the intrusion via cuttings, cavings, spallings, and direct release of brine; and radionuclide transport up abandoned boreholes to the Culebra and thence to the land withdrawal boundary. Section PA-8.0 presents results for the most significant output variables from the PA models, accompanied by sensitivity analyses to determine which subjectively uncertain parameters are most influential in the uncertainty of PA results.

Section PA-9.0 presents the set of CCDFs resulting from the CRA-2004 PA. This material supplements Section 6.5, which demonstrates compliance with the containment requirements of 40 CFR § 191.13. Section PA.9.0 includes sensitivity analyses that identify which uncertain parameters are most significant in the calculation of releases.

This appendix follows the approach used by Helton et al. (1998) to document the mathematical models used in the CCA PA and the results of that analysis. Much of the content of this appendix derives from Helton et al. (1998); these authors' contributions are gratefully acknowledged.

PA-2.0 CONCEPTUAL STRUCTURE OF THE PERFORMANCE ASSESSMENT

The conceptual structure of the CRA-2004 PA is unchanged from the CCA PA. Section 6.1 provides a general, less technical overview of the PA conceptual structure. This section of Appendix PA presents the conceptual basis for the CRA-2004 PA in a more formal manner. A corresponding presentation for the CCA PA is provided in Helton et al. (1998).

PA-2.1 Regulatory Requirements

The conceptual structure of the CRA-2004 PA derives from the regulatory requirements imposed on this facility. The primary regulation determining this structure is the Environmental Protection Agency's (EPA's) standard for the geologic disposal of radioactive waste, Environmental Radiation Protection Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes (40 CFR Part 191) (EPA 1985, 1993), which is divided into three subparts. Subpart A applies to a disposal facility prior to decommissioning and limits the annual radiation doses members of the public can be exposed to from waste management and storage operations. Subpart B applies after decommissioning and sets probabilistic limits on cumulative releases of radionuclides to the accessible environment for 10,000 years (40 CFR § 191.13) and assurance requirements to provide confidence that 40 CFR Section 191.13 will be met (40 CFR Section 191.14). Subpart B also sets limits on radiation doses to members of the public in the accessible environment for 10,000 years of undisturbed performance (40 CFR § 191.15). Subpart C limits radioactive contamination of groundwater for 10,000 years after disposal (40 CFR § 191.24). The Department of Energy (DOE) must demonstrate a reasonable expectation that the WIPP will continue to comply with the requirements of Subparts B and C of 40 CFR Part 191.

The following is the central requirement in 40 CFR Part 191, Subpart B, and the primary determinant of the conceptual structure of the CRA-2004 PA (p. 38086, EPA 1985):

> ***§ 191.13 Containment requirements:***
>
> ***(a) Disposal systems for spent nuclear fuel or high-level or transuranic radioactive wastes shall be designed to provide a reasonable expectation, based upon performance assessments, that cumulative releases of radionuclides to the accessible environment for 10,000 years after disposal from all significant processes and events that may affect the disposal system shall:***
>
> > ***(1) Have a likelihood of less than one chance in 10 of exceeding the quantities calculated according to Table 1 (Appendix A); and***
> >
> > ***(2) Have a likelihood of less than one chance in 1,000 of exceeding ten times the quantities calculated according to Table 1 (Appendix A).***
>
> ***(b) Performance assessments need not provide complete assurance that the requirements of 191.13(a) will be met. Because of the long time period involved and the nature of the events and processes of interest, there will inevitably be substantial uncertainties in projecting disposal system performance. Proof of the future performance of a disposal system is not to be had in the ordinary sense of the word in situations that deal with much shorter time frames. Instead, what is required is a reasonable expectation, on the basis of the record before the implementing agency, that compliance with 191.13(a) will be achieved.***

Section 191.13(a) refers to "quantities calculated according to Table 1 (Appendix A)," which means a normalized radionuclide release to the accessible environment based on the type of waste being disposed of, the initial waste inventory, and the size of release that may occur (EPA 1985, Appendix A). Table 1 of Appendix A specifies allowable releases (i.e., release limits) for individual radionuclides and is reproduced as Table PA-1 of this appendix. The WIPP is a repository to transuranic (TRU) waste, which is defined as "waste containing more than 100 nanocuries of alpha-emitting transuranic isotopes, with half-lives greater than twenty years, per gram of waste" (p. 38084, EPA 1985). The normalized release R for transuranic waste is defined by

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

where Q_i is the cumulative release of radionuclide i to the accessible environment during the 10,000-year period following closure of the repository (curies), L_i is the release limit for radionuclide i given in Table PA-1 (curies), and C is the amount of TRU waste emplaced in the repository (curies). In the CRA-2004 PA, $C = 2.48 \times 10^6$ curies (Appendix TRU WASTE, Section TRU WASTE-2.3.1). Further, accessible environment means (1) the atmosphere, (2) land surfaces, (3) surface waters, (4) oceans, and (5) all of the lithosphere that is beyond the controlled area; and controlled area means (1) a surface location, to be identified by passive institutional controls, that encompasses no more than 100 square kilometers and extends horizontally no more than five kilometers in any direction from the outer boundary of the original location of the radioactive wastes in a disposal system and (2) the subsurface underlying such a surface location (40 CFR § 191.13).

To help clarify the intent of 40 CFR Part 191, the EPA promulgated 40 CFR Part 194, Criteria for the Certification and Re-Certification of the Waste Isolation Pilot Plant's Compliance With the 40 CFR Part 191 Disposal Regulations. There, the following elaboration on the intent of 40 CFR § 191.13 set out.

> ***§ 194.34 Results of performance assessments.***
>
> ***(a) The results of performance assessments shall be assembled into "complementary, cumulative distributions functions" (CCDFs) that represent the probability of exceeding various levels of cumulative release caused by all significant processes and events.***
>
> ***(b) Probability distributions for uncertain disposal system parameter values used in performance assessments shall be developed and documented in any compliance application.***
>
> ***(c) Computational techniques, which draw random samples from across the entire range of the probability distributions developed pursuant to paragraph (b) of this section, shall be used in generating CCDFs and shall be documented in any compliance application.***
>
> ***(d) The number of CCDFs generated shall be large enough such that, at cumulative releases of 1 and 10, the maximum CCDF generated exceeds the 99th percentile of the population of CCDFs with at least a 0.95 probability.***

Table PA-1. Release Limits for the Containment Requirements (EPA 1985, Appendix A, Table 1)

Radionuclide	Release Limit L_i per 1000 MTHM[1] or other unit of waste[2]
Americium (Am)-241 or –243	100
Carbon 14	100
Cesium-135 or -137	1,000
Iodine-129	100
Neptunium-237	100
Plutonium (Pu)-238, -239, -240, or -242	100
Radium-226	100
Strontium-90	1,000
Technetium-99	10,000
Thorium (Th)-230 or -232	10
Tin-126	1,000
Uranium (U)-233, -234, -235, -236, or -238	100
Any other alpha-emitting radionuclide with a half-life greater than 20 years	100
Any other radionuclide with a half-life greater than 20 years that does not emit alpha particles	1,000

[1] Metric tons of heavy metal exposed to a burnup between 25,000 megawatt-days per metric ton of heavy metal (MWd/MTHM) and 40,000 MWd/MTHM

[2] An amount of transuranic wastes containing one million curies of alpha-emitting transuranic radionuclides with half-lives greater than 20 years

(e) Any compliance application shall display the full range of CCDFs generated.

(f) Any compliance application shall provide information which demonstrates that there is at least a 95 percent level of statistical confidence that the mean of the population of CCDFs meets the containment requirements of § 191.13 of this chapter.

Three basic entities (EN1, EN2, EN3) underlie the results required by Sections 191.13 and § 194.34 and ultimately determine the conceptual and computational structure of the CRA-2004 PA:

EN1 - a probabilistic characterization of the likelihood of different futures occurring at the WIPP site over the next 10,000 years,

EN2 - a procedure for estimating the radionuclide releases to the accessible environment associated with each of the possible futures that could occur at the WIPP site over the next 10,000 years,

EN3 - a probabilistic characterization of the uncertainty in the parameters used in the definition of EN1 and EN2.

The preceding entities arise from an attempt to answer three questions about the WIPP:

Q1 - What events could occur at the WIPP site over the next 10,000 years?

Q2 - How likely are the different futures that could take place at the WIPP site over the next 10,000 years?

Q3 - What are the consequences of the different occurrences that could take place at the WIPP site over the next 10,000 years?

and one question about the PA:

Q4 - How much confidence can be placed in answers to these questions?

In the WIPP PA, EN1 provides answers to Q1 and Q2, EN2 provides an answer to Q3, and EN3 provides an answer to Q4. Together, EN1 and EN2 give rise to the CCDF specified in Section 191.13(a), and EN3 corresponds to the distributions specified by Section 194.34(b). The nature of EN1, EN2 and EN3, the role that they play in the CRA-2004 PA, and the method for constructing CCDFs are elaborated on in the next three sections.

PA-2.2 EN1: Probabilistic Characterization of Different Futures

The entity EN1 results from the scenario development process for the WIPP outlined in Section 6.3. The EN1 entity provides a probabilistic characterization of the likelihood of different futures that could occur at the WIPP site over the 10,000-year period specified in 40 CFR Part 191. Formally, EN1 is defined by a probability space (X_{st}, S_{st}, p_{st})*, with the sample space* X_{st} *given by Equation (2).*

$$X_{st} = \{\mathbf{x}_{st} : \mathbf{x}_{st} \text{ is a possible 10,000-year sequence of occurrences at the WIPP}\} \quad (2)$$

The subscript st refers to stochastic (i.e., aleatory) uncertainty and is used because (X_{st}, S_{st}, p_{st}) *is providing a probabilistic characterization of occurrences that may take place in the future (Helton 1997). Incorporation of stochastic uncertainty is fundamental to the DOE's methodology for performance assessment Section 6.1.2. It is this stochastic uncertainty that gives rise to the distribution of releases evident in a CCDF.*

A probability space (X, S, p) *consists of three components: a set X that contains everything that could occur for the particular "universe" under consideration, a suitably restricted set S of subsets of X and a function p defined for elements of S that actually defines probability (Feller 1971). In the terminology of probability theory, X is the sample space, the elements of X are elementary events, the subsets of X contained in S are events, and p is a probability measure. In most applied problems, the function p defined on S is replaced by a probability density function (PDF) d (e.g.,* d_{st} *in Figure PA-1).*

In the CCA PA, the scenario development process for the WIPP identified exploratory drilling for natural resources as the only disruption with sufficient likelihood and consequence for

inclusion in the definition of EN1 (CCA Appendix SCR [DOE 1996]). Reexamination of the FEPs and the scenario development process for the CRA-2004 PA did not change this conclusion (Section 6.2.6). In addition, 40 CFR Part 194 specifies that the occurrence of mining within the land withdrawal boundary must be included in the PA. As a result, the elements $\mathbf{x}_{st}$ of X_{st} are vectors of the form

$$\mathbf{x}_{st} = [\underbrace{t_1, e_1, l_1, b_1, p_1, \mathbf{a}_1}_{1^{st}\ \text{intrusion}}, \underbrace{t_2, e_2, l_2, b_2, p_2, \mathbf{a}_2}_{2^{nd}\ \text{intrusion}}, \ldots, \underbrace{t_n, e_n, l_n, b_n, p_n, \mathbf{a}_n}_{n^{th}\ \text{intrusion}}, t_{min}], \qquad (3)$$

where n is the number of drilling intrusions, t_i is the time (year) of the i^{th} $_{intrusion}$, l_i designates the location of the i^{th} intrusion, e_i designates the penetration of an excavated or nonexcavated area by the i^{th} intrusion, b_i designates whether or not the i^{th} intrusion penetrates pressurized brine in the Castile Formation, p_i designates the plugging procedure used with the i^{th} intrusion (i.e., continuous plug, two discrete plugs, three discrete plugs), $\mathbf{a}_i$ designates the type of waste penetrated by the i^{th} intrusion (i.e., no waste, contact-handled (CH-TRU) waste, remote-handled (RH-TRU) waste), and t_{min} is the time at which potash mining occurs within the land withdrawal boundary.

In the development of (X_{st}, S_{st}, p_{st}), the probabilistic characterization of n, t_i, l_i and e_i is based on the assumption that drilling intrusions will occur randomly in time and space (i.e., follow a Poisson process), the probabilistic characterization of b_i derives from assessed properties of brine pockets, the probabilistic characterization of $\mathbf{a}_i$ derives from the properties of the waste emplaced in the WIPP, and the probabilistic characterization of p_i derives from current drilling practices in the sedimentary basin (i.e., the Delaware Basin) in which the WIPP is located. A vector notation is used for $\mathbf{a}_i$ because it is possible for a given drilling intrusion to penetrate several different types of waste. Further, the probabilistic characterization for t_{min} follows from the guidance in 40 CFR Part 194 that the occurrence of potash mining within the land withdrawal boundary should be assumed to occur randomly in time (i.e., follow a Poisson process with a rate constant of $\lambda_m = 10^{-4}$ yr^{-1}), with all commercially viable potash reserves within the land withdrawal boundary being extracted at time t_{min}.

With respect to the three fundamental questions discussed about, X_{st} provides an answer to Q1, while S_{st} and p_{st} provide an answer to Q2. In practice, Q2 will be answered by specifying distributions for n, t_i, e_i, l_i, b_i, p_i, $\mathbf{a}_i$, and t_{min}, which in turn lead to definitions for S_{st} and p_{st}. The CCDF in 40 CFR Part 191 will be obtained by evaluating an integral involving (X_{st}, S_{st}, p_{st}) (Figure PA-1). The definition of (X_{st}, S_{st}, p_{st}) is discussed in more detail in Section PA-3.0.

PA-2.3 EN2: Estimation of Releases

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

The function f in Figure PA-1 is evaluated by a series of computational models shown in Figure PA-2. These computational models implement the conceptual models representing the repository system as described in Section 6.4, and the mathematical models for physical processes that are presented in Section PA-4.0. Most of the computational models involve the numerical solution of partial differential equations used to represent processes such as material deformation, fluid flow and radionuclide transport.

The models in Figure PA-2 are too complex to permit a closed form evaluation of the integral in Figure PA-1 that defines the CCDF specified in 40 CFR Part 191. Rather, a Monte Carlo procedure is used in the CRA-2004 PA. Specifically, elements $\mathbf{x}_{st,i}$, i = 1, 2, …, nS are randomly sampled from X_{st} in consistency with the definition of $\left(X_{st}, S_{st}, p_{st}\right)$. Then, the integral in Figure PA-1, and hence the associated CCDF, is approximated by

$$prob\left(Rel > R\right) = \int_{S_{st}} \delta_R\left[f\left(\mathbf{x}_{st}\right)\right] d_{st}\left(\mathbf{x}_{st}\right) dV_{st} = \sum_{i=1}^{nS} \delta_R\left[f\left(\mathbf{x}_{st,i}\right)\right] / nS, \qquad (4)$$

where $\delta_R\left[f\left(\mathbf{x}_{st}\right)\right] = 1$ if $f\left(\mathbf{x}_{st}\right) > R$ and $\delta_R\left[f\left(\mathbf{x}_{st}\right)\right] = 0$ if $f\left(\mathbf{x}_{st}\right) \le R$ (Helton and Shiver 1996). However, the models in Figure PA-2 are also too computationally intensive to permit their evaluation for every element $\mathbf{x}_{st,i}$ of X_{st} in Equation (4). Due to this constraint, the models in Figure PA-2 are evaluated for representative elements of X_{st} and the results of these evaluations are used to construct values of f for the large number of $\mathbf{x}_{st,i}$ (e.g., nS = 10,000) in Equation (4). The representative elements are the scenarios E0, E1, E2, and E1E2 defined in Section PA-3.9; the procedure for constructing a CCDF from these scenarios is described in Section PA-6.0.

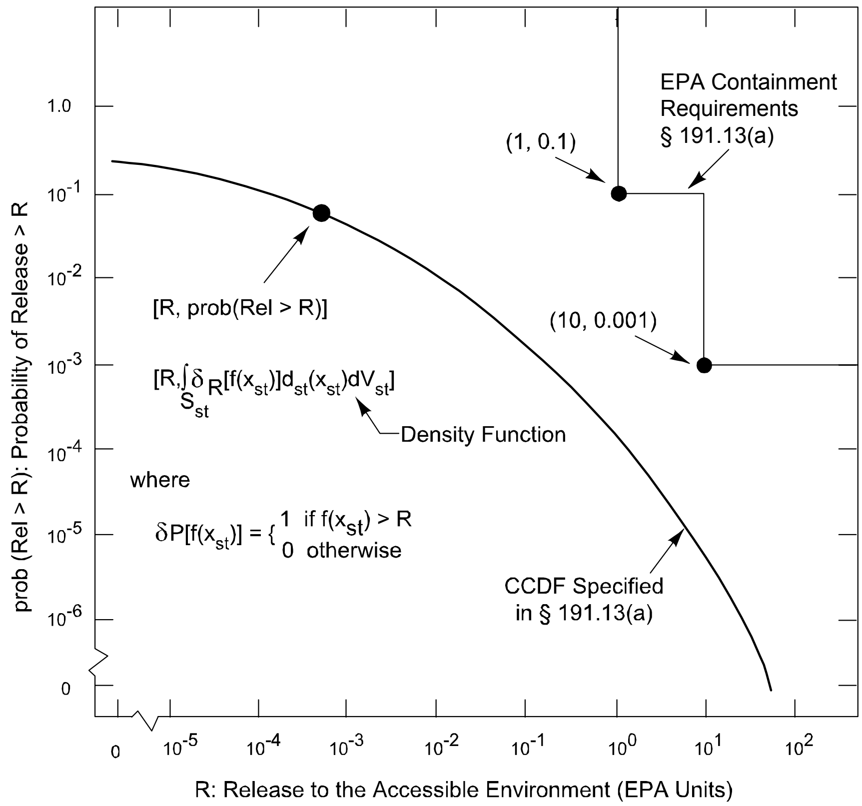


Figure PA-1. Construction of the CCDF Specified in 40 CFR Part 191, Subpart B.

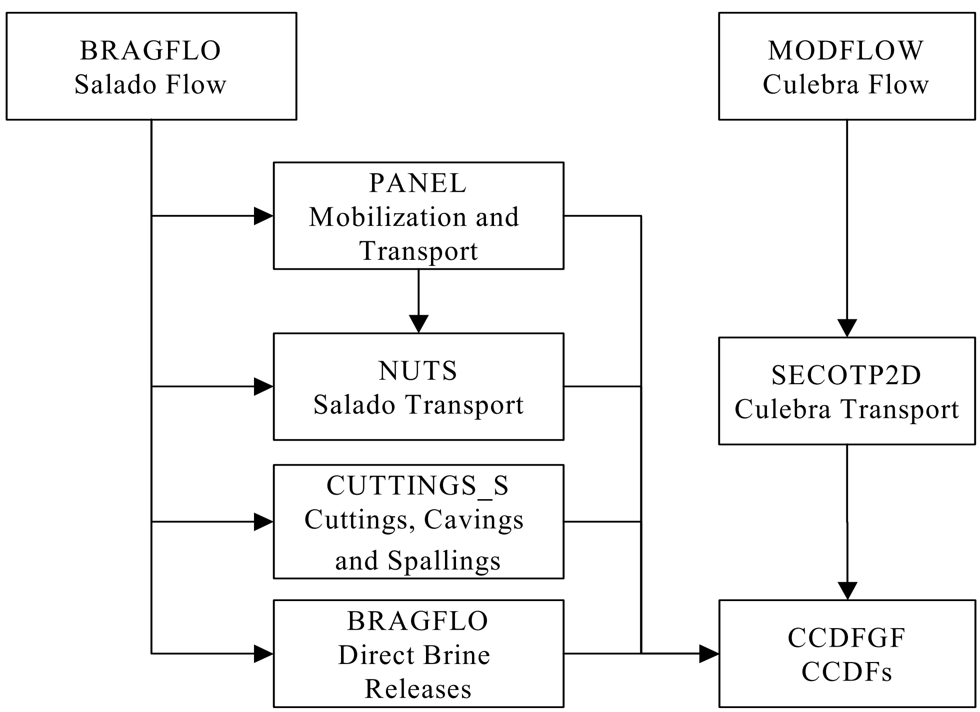


Figure PA-2. Computational Models Used in the CRA-2004 PA.

PA-2.4 EN3: Probabilistic Characterization of Parameter Uncertainty

The entity EN3 is the outcome of the data development effort for the WIPP (summarized in Chapter 2) and provides a probabilistic characterization of the uncertainty in the parameters that underlie the CRA-2004 PA. When viewed formally, EN3 is defined by a probability space (X_{su}, S_{su}, p_{su}), with the sample space X_{su} given by Equation (5).

$$X_{su} = \{\mathbf{x}_{su} : \mathbf{x}_{su} \text{ is a possible vector of parameter values for the WIPP PA models}\} \quad (5)$$

The subscript su refers to subjective (i.e., epistemic) uncertainty and is used because (X_{su}, S_{su}, p_{su}) is providing a probabilistic characterization of the possible inputs to the WIPP PA (Helton 1997). In practice, some elements of $\mathbf{x}_{su}$ could affect the definition of (X_{st}, S_{st}, p_{st}) (e.g., the rate constant λ used to define the Poisson process for drilling intrusions) and other elements could relate to the models in Figure PA-2 that determine the function f in Figure PA-1 (e.g., radionuclide solubilities in Castile brine). Incorporation of subjective uncertainty is fundamental to the DOE's methodology for PA (Section 6.1.2).

If the value for $\mathbf{x}_{su}$ was precisely known, the CCDF in Figure PA-1 could be determined with certainty and compared with the boundary line specified in 40 CFR Part 191. However, given the complexity of the WIPP site and the 10,000-year time period under consideration, $\mathbf{x}_{su}$ can never be known with certainty. Rather, uncertainty in $\mathbf{x}_{su}$ as characterized by (X_{su}, S_{su}, p_{su}) will lead to a distribution of CCDFs (Figure PA-3), with a different CCDF resulting for each possible value that $\mathbf{x}_{su}$ can take on. The proximity of this distribution to the boundary line in Figure PA-1 provides an indication of the confidence with which 40 CFR Part 191 will be met.

The distribution of CCDFs in Figure PA-3 can be summarized by distributions of exceedance probabilities conditional on individual release values (Figure PA-4). For a given release value R, this distribution is defined by a double integral over X_{su} and X_{st} (Helton 1996, 1997). In practice, this integral is too complex to permit a closed-form evaluation. Instead, the WIPP PA uses Latin hypercube sampling (McKay et al. 1979) to evaluate the integral over S_{su} and, as indicated in Equation (4), simple random sampling to evaluate the integral over X_{st}.

Specifically, a LHS $\mathbf{x}_{su,k}$, k = 1, 2, …, nLHS, is generated from S_{su} in consistency with the definition of (X_{su}, S_{su}, p_{su}) and a random sample $\mathbf{x}_{st,i}$, i = 1, 2, …, nS, is generated from X_{st} in consistency with the definition of (X_{st}, S_{st}, p_{st}). The probability $prob(p \le P|R)$ is approximated by

$$prob(p \le P \mid R) \cong 1 - \sum_{k=1}^{nLHS} \delta_P \left[\sum_{i=1}^{nS} \delta_R \left[f\left(\mathbf{x}_{st,i}, \mathbf{x}_{su,k}\right) \right] / nS \right] / nLHS \quad (6)$$

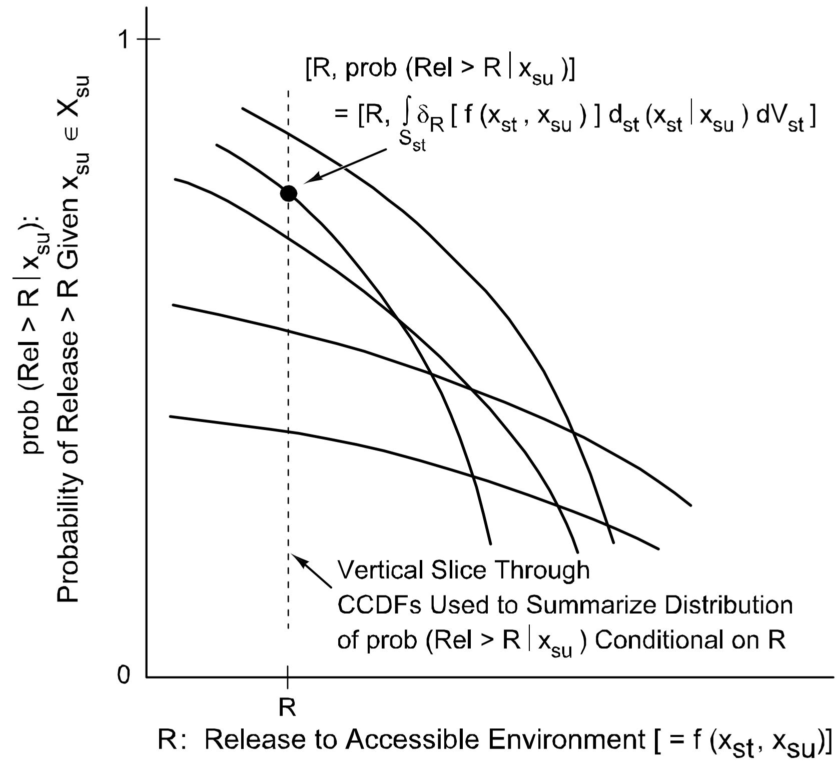


Figure PA-3. Distribution of CCDFs Resulting from Possible Values for $\mathbf{x}_{su} \in X_{su}$.

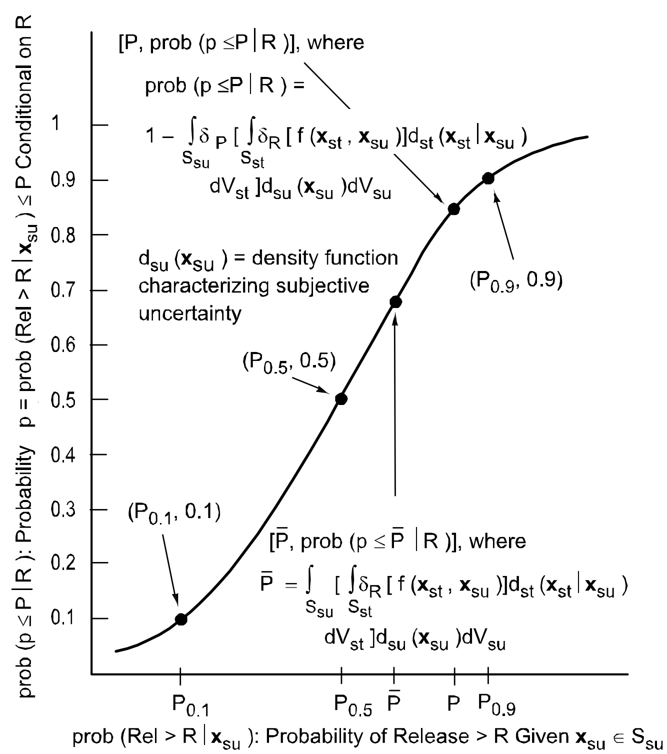


Figure PA-4. Distribution of Exceedance Probabilities Due to Subjective Uncertainty.

The result of the preceding calculation is typically displayed by plotting percentile values (e.g., $P_{0.1}$, $P_{0.5}$, $P_{0.9}$ in Figure PA-4) and also mean values for exceedance probabilities above the corresponding release values (i.e., R) and then connecting these points to form continuous curves (Figure PA-5). The proximity of these curves to the indicated boundary line provides an indication of the confidence with which 40 CFR Part 191 will be met.

With respect to the previously indicated questions, (X_{su}, S_{su}, p_{su}) and results derived from (X_{su}, S_{su}, p_{su}) (e.g., the distributions in Figure PA-3 and Figure PA-5) provide an answer to Q4. The definition of (X_{su}, S_{su}, p_{su}) is discussed in more detail in Section PA-5.0.

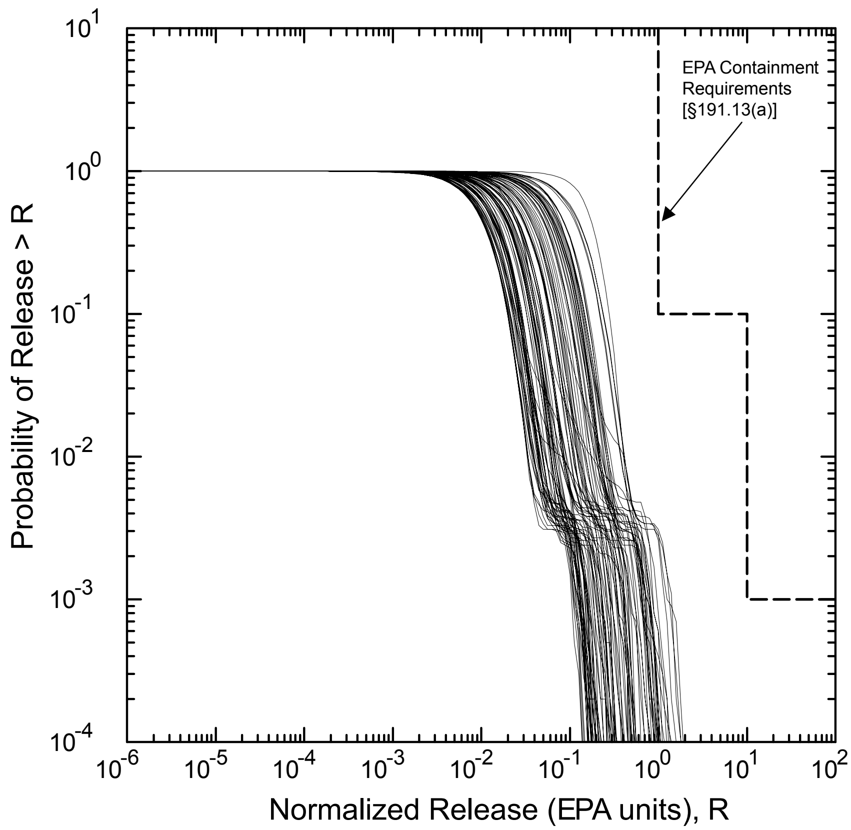


Figure PA-5. Example CCDF Distribution From CRA-2004 PA.

PA-3.0 PROBABILISTIC CHARACTERIZATION OF FUTURES

This section describes how stochastic uncertainty is implemented in PA. Screening analyses of possible future events concluded that the only significant events with potential to affect radionuclide releases to the accessible environment are drilling and mining within the land withdrawal boundary (Section 6.2.6). Consequently, modeling the future states of the repository focuses on representing the occurrences and effects of these two events.

PA-3.1 Probability Space

The first entity that underlies the CRA-2004 PA is a probabilistic characterization of the likelihood of different futures occurring at the WIPP site over the next 10,000 years. As discussed in Section PA-2.2, this entity is defined by a probability space $\left(X_{st}, S_{st}, p_{st}\right)$ that characterizes stochastic uncertainty. The individual elements $\mathbf{x}_{st}$ of X_{st} are vectors of the form shown in Equation (3). Sections PA-3.2 through PA-3.8 describe the individual components t_i, e_i, l_i, b_i, p_i, $\mathbf{a}_i$, and t_{min} of $\mathbf{x}_{st}$, and their associated probability distributions. These components and their associated distributions give rise to the probability space $\left(X_{st}, S_{st}, p_{st}\right)$ for stochastic uncertainty. The concept of a scenario as a subset of the sample space X_{st} for stochastic uncertainty is discussed in Section PA-3.9. Further, the procedure used to sample the individual elements $\mathbf{x}_{st,i}$ of X_{st} indicated in Equation (4) is described in Section PA-6.5.

PA-3.2 Drilling Intrusion

As described in Section 6.3.2, drilling intrusions in the CRA-2004 PA are assumed to occur randomly in time and space (i.e., follow a Poisson process). Specifically, the drilling rate considered within the area marked by a berm as part of the system for passive institutional controls (Figure PA-6) is 5.25×10^{-3} intrusions per km $^{-2}$ yr $^{-1}$ (Section 6.4.12.2). Active institutional controls are assumed to prevent any drilling intrusions for the first 100 years after the decommissioning of the WIPP (Section 7.1). Unlike in the CCA PA, passive institutional controls are not assumed to reduce the drilling rate after decommissioning (Section 7.3).

For the computational implementation of the CRA-2004 PA, it is convenient to represent the Poisson process for drilling intrusions by its corresponding rate term $\lambda_d\left(t\right)$ for intrusions into the area marked by the berm. Specifically,

$$\lambda_d\left(t\right) = \begin{cases} 0 & 0 \le t \le 100\,yr \\ (0.6285\ km^2)(52.5\ km^{-2}\,10^{-4}\ yr) = 3.3 \times 10^{-3}\ yr^{-1} & 100 \le t \le 10{,}000\,yr \end{cases} \qquad (7)$$

where 0.6285 km^2 is the area of the berm Attachment PAR, Table PAR-45 and t is elapsed time since decommissioning of the WIPP.

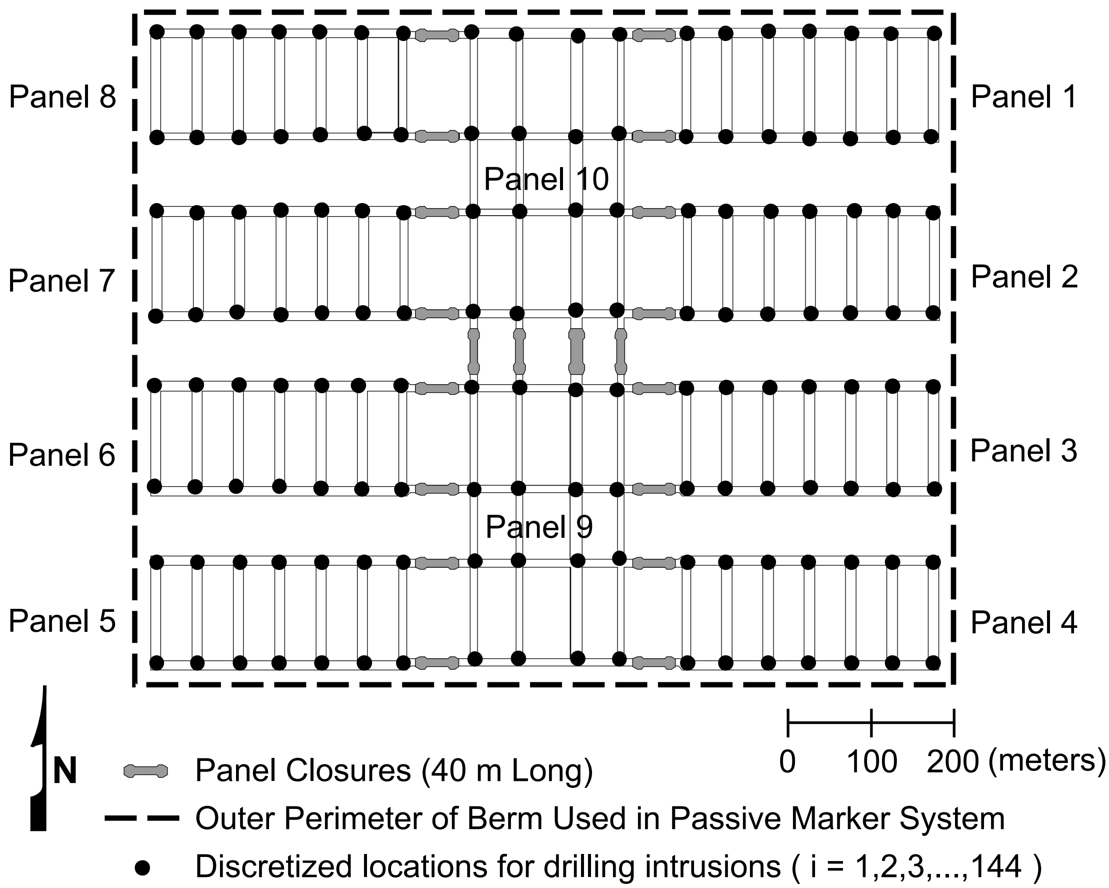


Figure PA-6. Location of Berm Used in Passive Marker System.

The function $\lambda_d(t)$ defines the part of the probability space (X_{st}, S_{st}, p_{st}) in Section PA-2.2 that corresponds to t_i. In the computational implementation of the analysis, $\lambda_d(t)$ is used to define the distribution of time between drilling intrusions (Figure PA-7). As a reminder, the occurrence of one event in a Poisson process has no effect on the occurrence of the next event. Thus, the cumulative distributions in Figure PA-7 can be used to define the time from one drilling event to the next (Section PA-6.5). Due to the 10,000-year regulatory period specified in 40 CFR § 191.13, t_i is assumed to be bounded above by 10,000 years in the definition of X_{st}. Further, t_i is bounded below by 100 years as defined in Equation (7).

The function $\lambda_d(t)$ also determines the probability $prob(nBH = n|[a,b])$ that a future will have exactly n drilling intrusions in the time interval [a, b] (Helton 1993), where

$$prob(nBH = n\,|\,[a,b]) = \left[\left(\int_a^b \lambda_d(t)dt\right)^n / n!\right] \exp\left(-\int_a^b \lambda_d(t)dt\right). \qquad (8)$$

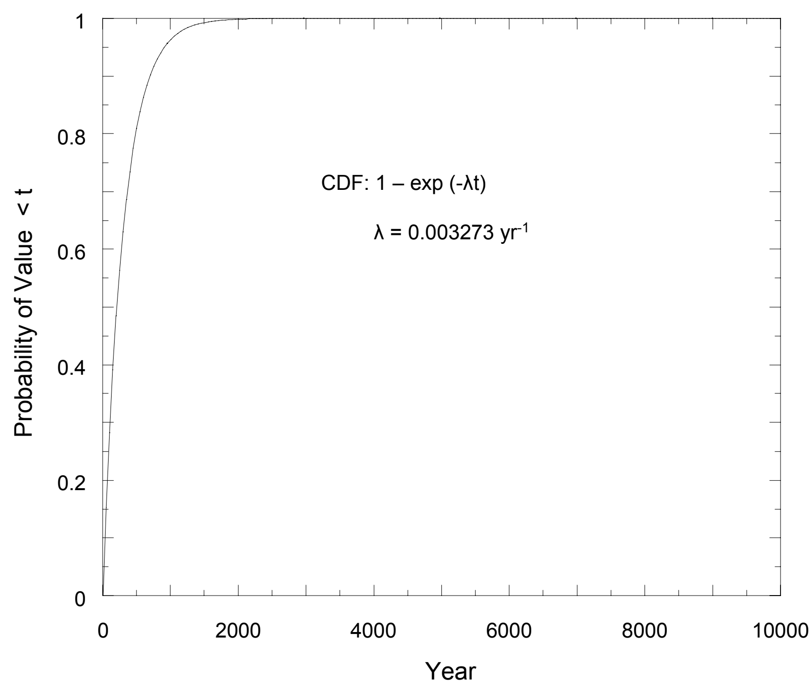


Figure PA-7. Cumulative Distribution Function (CDF) for Time Between Drilling Intrusions.

Further, the probability $prob\left(nBH \geq n \left| \left[a,b\right]\right.\right)$ that a future will have greater than or equal to n drilling intrusions in the time interval [a, b] is given by

$$prob(nBH \geq n\,|\,[a,b]) = \begin{cases} 1 & n = 0 \\ 1 - \sum_{m=0}^{n-1} prob(nBH = m\,|\,[a,b]) & n > 0 \end{cases} \tag{9}$$

PA-3.3 Penetration of Excavated/Nonexcavated Area

The variable e_i is a designator for whether or not the i^{th} drilling intrusion penetrates an excavated, waste-filled area of the repository (i.e., e_i = 0, 1 implies penetration of nonexcavated, excavated area, respectively). The corresponding probabilities pE_0 and pE_1 for $e_i = 0$ and $e_i = 1$ are

$$pE_1 = 0.1273\ km^2 / 0.6285\ km^2 = 0.203 \tag{10}$$

$$pE_0 = 1 - pE_1 = 0.797\,, \tag{11}$$

where 0.1273 km² and 0.6285 km² are the excavated area of the repository filled with waste and the area of the berm, respectively (Attachment PAR, Table PAR-45). The probabilities pE_0 and pE_1 define the part of $\left(X_{st}, S_{st}, p_{st}\right)$ in Section PA.2.2 associated with e_i.

PA-3.4 Drilling Location

Locations of drilling intrusions through the excavated, waste-filled area of the repository are discretized to the 144 locations in Figure PA-6. Assuming that a drilling intrusion occurs within the excavated area, it is assumed to be equally likely to occur at each of these 144 locations. Thus, the (conditional) probability pL_j that drilling intrusion i will occur at location L_j, j = 1, 2, …, 144, in Figure PA-6 is

$$pL_j = 1/144 = 6.94 \times 10^{-3}. \qquad (12)$$

The probabilities pL_j define the part of (X_{st}, S_{st}, p_{st}) in Section PA.2.2 associated with l_i.

PA-3.5 Penetration of Pressurized Brine

The conceptual models for the Castile Formation include the possibility that pressurized brine reservoirs underlie the repository (Section 6.4.8). The variable b_i is a designator for whether or not the i^{th} drilling intrusion penetrates pressurized brine, where $b_i = 0$ signifies nonpenetration and $b_i = 1$ signifies penetration of pressurized brine. In the CCA PA, the probabilities pB_0 and pB_1 for $b_i = 0$ and $b_i = 1$ were 0.92 and 0.08, respectively (see CCA *Section 6.4.12.6). In the CRA-2004 PA, the probability pB_1 is sampled from a uniform distribution ranging from 0.01 to 0.60 (Section 6.4.12.6*; see also *PBRINE in Table PA-17). The probabilities pB_0 and pB_1 define the part of (X_{st}, S_{st}, p_{st}) in Section PA-2.2 that corresponds to b_i.*

PA-3.6 Plugging Pattern

As presented in Section 6.4.7.2, three borehole plugging patterns are considered in the 2004 PA: (1) p_1, a full concrete plug through Salado Formation to the Bell Canyon Formation, (2) p_2, a two plug configuration with concrete plugs at Rustler/Salado interface and Castile/Bell Canyon interface, and (3) p_3, a three plug configuration with concrete plugs at the Rustler/Salado, Salado/Castile and Castile/Bell Canyon interfaces. The probability that a given drilling intrusion will be sealed with plugging pattern p_j, j = 1, 2, 3, is given by pPL_j, where $pPL_1 = 0.015$, $pPL_2 = 0.696$ and $pPL_3 = 0.289$ (Section 6.4.12.7). The probabilities pPL_j define the part of (X_{st}, S_{st}, p_{st}) in Section PA-2.2 that corresponds to p_i.

PA-3.7 Activity Level

The waste intended for disposal at the WIPP is represented by 779 distinct waste streams with 693 of these waste streams designated as CH-TRU waste and 86 designated as RH-TRU waste. For the CRA-2004 PA, the 86 separate RH-TRU waste streams are represented by a single, combined RH-TRU waste stream. The activity levels for the waste streams are given in Attachment PAR, Table PAR-50. Each waste container emplaced in the repository contains waste from a single CH-TRU waste stream. Waste packaged in 55-gallon drums is stacked

three drums high within the repository. Although waste in other packages (e.g., standard waste boxes, 10 drum overpacks, etc.) may not be stacked three high, the CRA-2004 PA assumes that each drilling intrusion into CH-TRU waste might intersect three different waste streams. In contrast, all RH-TRU waste is represented by a single waste stream, and so each drilling intrusion through RH-TRU waste is assumed to intersect this single waste stream. Attachment MASS (Section MASS.21) examines the sensitivity of PA results to the assumption that three waste streams are intersected by each drilling intrusion into CH-TRU waste.

The vector $\mathbf{a}_i$ characterizes the type of waste penetrated by the i^{th} drilling intrusion. Specifically,

$$\mathbf{a}_i = 0 \text{ if } e_i = 0 \tag{13}$$

(i.e., if the i^{th} drilling intrusion does not penetrate an excavated area of the repository);

$$\mathbf{a}_i = 1 \text{ if } e_i = 1 \text{ and RH-TRU is penetrated;} \tag{14}$$

and

$$\mathbf{a}_i = [iCH_{i1}, CH_{i2}, iCH_{i3}] \text{ if } e_i = 1 \text{ and CH-TRU is penetrated ,} \tag{15}$$

where iCH_{i1}, iCH_{i2} and iCH_{i3} are integer designators for the CH-TRU waste streams intersected by the i^{th} drilling intrusion (i.e., each of iCH_{i1}, iCH_{i2} and iCH_{i3} is an integer between 1 and 693).

Whether the i^{th} intrusion penetrates a nonexcavated or excavated area is determined by the probabilities pE_0 and pE_1 discussed in Section PA-3.4. The type of waste penetrated is determined by the probabilities pCH and pRH. The excavated area used for disposal of CH-TRU waste is 1.115×105 m^2 and the area used for disposal of RH-TRU waste is 1.576×10^4 m^2 (Attachment PAR, Table PAR-43), for a total disposal area of $aEX = aCH + aRH = 1.273 \times 10^5$ m^2. Given that the i^{th} intrusion penetrates an excavated area, the probabilities pCH and pRH of penetrating CH- and RH-TRU waste are given by

$$pCH = aCH / aEX = \left(1.115 \times 10^5 \ m^2\right) / \left(1.273 \times 10^5 \ m^2\right) = 0.876 \tag{16}$$

$$pCH = aCH / aEX = \left(1.576 \times 10^4 \ m^2\right) / \left(1.273 \times 10^5 \ m^2\right) = 0.124 . \tag{17}$$

As indicated in this section, the probabilistic characterization of $\mathbf{a}_i$ in $\left(\mathcal{X}_{st}, \mathcal{S}_{st}, p_{st}\right)$ depends on a number of individual probabilities. Specifically, pE_0 and pE_1 determine whether a nonexcavated or excavated area is penetrated (Section PA-3.4); pCH and pRH determine whether CH- or RH-TRU waste is encountered given penetration of an excavated area; and the individual waste stream probabilities in Attachment PAR, Table PAR-50 determine the

specific waste streams iCH_{i1}, iCH_{i2}, and iCH_{i3} encountered given a penetration of CH-TRU waste.

PA-3.8 Mining Time

As presented in Section 6.2.5.2, full mining of known potash reserves within the land withdrawal boundary is assumed to occur at time t_{min}. The occurrence of mining within the land withdrawal boundary in the absence of institutional controls is specified as following a Poisson process with a rate of $\lambda_m = 1 \times 10^{-4}\ yr^{-1}$. However, this rate can be reduced by active and passive institutional controls. Specifically, active institutional controls are assumed to result in no possibility of mining for the first 100 years after decommissioning of the WIPP (Section 7.1.4). In the CCA PA, passive institutional controls were assumed to reduce the base mining rate by two orders of magnitude between 100 and 700 years after decommissioning (CCA Section 7.3.4). In the CRA-2004 PA, passive institutional controls do not affect the mining rate (Section 7.3.4). Thus, the mining rate $\lambda_m(t)$ is:

$$\lambda_m(t) = 0\ yr^{-1} \quad \text{for } 0 \le t \le 100\ yrs \tag{18}$$

$$\lambda_m(t) = 1 \times 10^{-4}\ yr^{-1} \quad \text{for } 100 \le t \le 10{,}000\ yrs, \tag{19}$$

where t is elapsed time since decommissioning of the WIPP. The function $\lambda_m(t)$ defines the part of (X_{st}, S_{st}, p_{st}) that corresponds to t_{min}.

In the computational implementation of the analysis, $\lambda_m(t)$ is used to define the distribution of time to mining. The use of $\lambda_m(t)$ to characterize t_{min} is analogous to the use of λ_d to characterize the t_i except that only one mining event is assumed to occur (i.e., $\mathbf{x}_{st}$ contains only one value for t_{min}) in consistency with guidance given in 40 CFR Part 194 that mining within the land withdrawal boundary should be assumed to remove all economically viable potash reserves. Due to the 10,000-year regulatory period specified in 40 CFR § 191.13, t_{min} is assumed to be bounded above by 10,000 years in the definition of X_{st}.

PA-3.9 Scenarios and Scenario Probabilities

A scenario is a subset $\mathcal{S}$ of the sample space X_{st} for stochastic uncertainty. More specifically, a scenario is an element $\mathcal{S}$ of the set S_{st} in the probability space (X_{st}, S_{st}, p_{st}) for stochastic uncertainty, and the probability of $\mathcal{S}$ is given by $p_{st}(\mathcal{S})$. Thus, a scenario is what is called an event in the usual terminology of probability theory.

Given the complexity of the elements $\mathbf{x}_{st}$ of X_{st} (see Equation (3)), many different scenarios can be defined. The computational complexity of the function f in Figure PA-1 limits evaluation to only a few scenarios. As presented in Section 6.3, the CRA-2004 PA considers four fundamental scenarios:

E0 $=$ ***{$\mathbf{x}_{st}$: $\mathbf{x}_{st}$ involves no drilling intrusion through an excavated area of the repository (i.e., $n = 0$ or $e_i = 0$ in Equation (3) for $i = 1, 2, \ldots, n > 0$)};***

E1 $=$ ***{$\mathbf{x}_{st}$: $\mathbf{x}_{st}$ involves one drilling intrusion through an excavated area of the repository with this intrusion penetrating pressurized brine in the Castile Formation (i.e., $n > 0$ in Equation (3) and there exists exactly one integer i such that $1 \le i \le n$, $e_i = 1$, $b_i = 1$, and $e_j = 0$ for $j \ne i$ and $1 \le j \le n$)};***

E2 $=$ ***{$\mathbf{x}_{st}$: $\mathbf{x}_{st}$ involves one drilling intrusion through an excavated area of the repository, with this intrusion not penetrating pressurized brine in the Castile Formation (i.e., $n > 0$ in Equation (3) and there exists exactly one integer i such that $1 \le i \le n$, $e_i = 1$, $b_i = 0$, and $e_j = 0$ for $j \ne i$ and $1 \le j \le n$)};***

E1E2 $=$ ***{$\mathbf{x}_{st}$: $\mathbf{x}_{st}$ involves two drilling intrusions through excavated areas of the repository, with the first intrusion not penetrating pressurized brine and the second intrusion penetrating pressurized brine (i.e., $n \ge 2$ in Equation (3) and there exist two integers i, j such that $1 \le i < j \le n$, $e_i = 1$, $b_i = 0$, $e_j = 1$, $b_j = 1$, and $e_k = 0$ for $k \ne i, j$ and $1 \le k \le n$)}.***

The definitions of the preceding four scenarios are quite simple. In general, scenarios can be defined on the basis of any possible characterization of the properties of the individual elements of $\mathbf{x}_{st}$, which can lead to very complex scenario definitions.

The scenarios E0, E1, E2, and E1E2 are elements of S_{st}, and their probabilities are formally represented by $p_{st}(E0)$, $p_{st}(E1)$, $p_{st}(E2)$, and $p_{st}(E1E2)$, with these probabilities deriving from the probability distributions assigned to the individual elements of $\mathbf{x}_{st}$. For example, assume that pB_1 takes on its mean value of 0.305 (see Section PA-3.5), the probabilities of the first three scenarios can be calculated exactly:

$$p_{st}(E0) = \exp\left(-\int_a^b pE_1 \lambda_d(t)\,dt\right) = 1.3 \times 10^{-3} \qquad (20)$$

$$p_{st}(E1) = \left[\left(\int_a^b pE_1 \lambda_d(t)\,dt\right)^1 \Big/ 1!\right]\left[\exp\left(-\int_a^b pE_1 \lambda_d(t)\,dt\right)\right]\left[pB_1\right] = 2.6 \times 10^{-3} \qquad (21)$$

$$p_{st}(E2) = \left[\left(\int_a^b pE_1 \lambda_d(t)\,dt\right)^1 \Big/ 1!\right]\left[\exp\left(-\int_a^b pE_1 \lambda_d(t)\,dt\right)\right]\left[pB_0\right] = 6.0 \times 10^{-3}, \qquad (22)$$

where $[a,b] = [100,\ 10{,}000\ \text{yrs}]$, $pE_1 = 0.203$ (see Section PA-3.4), $\lambda_d(t)$ is defined in Equation (7), and the probabilities in Equation (21) and Equation (22) are based on the relationship in Equation (8).

The expressions defining $p_{st}(E0)$, $p_{st}(E1)$, and $p_{st}(E2)$ are relatively simple because the scenarios E0, E1, and E2 are relatively simple. The scenario E1E2 is more complex and, as a result, $p_{st}(E1E2)$ is also more complex. Closed-form formulas for the probabilities of quite complex scenarios can be derived but they are very complicated and involve large numbers of iterated integrals (Helton 1993). Thus, p_{st} can be defined in concept but does not have a simple form that can be easily displayed.

The fundamental scenarios E0, E1, E2, and E1E2 have infinitely many elements because the drilling intrusions and mining events can occur throughout the regulatory period. However, scenarios involving drilling intrusions that occur at specific times will have a probability of zero. For example, the scenario

$$\mathcal{S} = \left\{ \mathbf{x}_{st} : \mathbf{x}_{st} = \left[t_1 = 350\,yr,\ e_1 = 1,\ l_1,\ b_1 = 1,\ p_1 = 2,\ \mathbf{a}_1,\ t_{min} \right] \right\}, \qquad (23)$$

where e_1, $\mathbf{a}_1$ and t_{min} are arbitrary, contains infinitely many futures (i.e., infinitely many $\mathbf{x}_{st}$ meet the criteria to belong to $\mathcal{S}$ due to the infinite number of values that l_1, $\mathbf{a}_1$, and t_{min} can assume) and also has a probability of zero (i.e., $p_{st}(\mathcal{S}) = 0$) because t_1 is restricted to a single value. Sets that contain single elements of X_{st} are also scenarios, but such scenarios will typically have a probability of zero; the only single element scenario that has a nonzero probability contains the future that has no drilling intrusions and no mining.

Releases from the repository are calculated (i.e. the function f in Figure PA-1 is evaluated) for a small number of elements belonging to each of the four fundamental scenarios (Sections PA-6.7 and PA-6.8). Releases for an arbitrary element $\mathbf{x}_{st}$ of X_{st} are estimated from the results of the fundamental scenarios (Section PA-6.8); these releases are used to construct CCDFs by Equation (4).

PA-3.10 Historical Review of CCDF Construction

The 1991 and 1992 WIPP PAs used an approach to the construction of the CCDF specified in 40 CFR § 191.13 based on the exhaustive division of X_{st} into a collection of mutually exclusive scenarios $S_{st,i}$, i = 1, 2, …, nS (Helton and Iuzzolino 1993). A probability $p_{st}(S_{st,i})$ and a normalized release R_i were then calculated for each scenario $S_{st,i}$ and used to construct the CCDF specified in 40 CFR § 191.13. Due to the complexity of the elements $\mathbf{x}_{st}$ of X_{st} (see Equation (3)), this approach was not used in the CCA PA. In particular, the decomposition of X_{st} into a suitable and defensible collection of scenarios $S_{st,i}$, i = 1, 2, …, nS, is quite difficult. Further, once these scenarios are defined, it is necessary to calculate their probabilities $p_{st}(S_{st,i})$, which is also not easy. Although the calculation of the probabilities $p_{st}(S_{st,i})$ is difficult, the development of an appropriate and acceptable decomposition of X_{st} into the scenarios $S_{st,i}$ posed a great challenge. Accordingly, the CCA PA used the Monte

Carlo approach to CCDF construction indicated in Equation (4), thus avoiding the difficulties associated with decomposing X_{st} into a collection of mutually exclusive scenarios and then calculating the probabilities of these scenarios. The CRA-2004 PA uses the same approach as used in the CCA PA.

PA-4.0 ESTIMATION OF RELEASES

This section describes how releases to the accessible environment are estimated for a particular future in the CRA-2004 PA.

PA-4.1 Results for Specific Futures

The function $f\left(\mathbf{x}_{st}\right)$ (Figure PA-1) estimates the radionuclide releases to the accessible environment associated with each of the possible futures $\mathbf{x}_{st}$ that could occur at the WIPP site over the next 10,000 years. In practice, f is quite complex and is constructed by the models implemented in computer programs used to simulate important processes and releases at the WIPP. In the context of these models, f has the form

$$\begin{aligned} f\left(\mathbf{x}_{st}\right) = & f_C\left(\mathbf{x}_{st}\right) + f_{SP}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right] + f_{DBR}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right] \\ & + f_{MB}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right] + f_{DL}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right] + f_S\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right], \\ & + f_{ST}\left[\mathbf{x}_{st,0}, f_{MF}\left(\mathbf{x}_{st}\right), f_{NP}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]\right] \end{aligned} \tag{24}$$

where

$\mathbf{x}_{st}$ ~ ***particular future under consideration,***

$\mathbf{x}_{st,0}$ ~ ***future involving no drilling intrusions but a mining event at the same time t_{min} as in $\mathbf{x}_{st}$,***

$f_C\left(\mathbf{x}_{st}\right)$ ~ ***cuttings and cavings release to accessible environment for $\mathbf{x}_{st}$ calculated with CUTTINGS_S,***

$f_B\left(\mathbf{x}_{st}\right)$ ~ ***two-phase flow in and around the repository calculated for $\mathbf{x}_{st}$ with BRAGFLO; in practice, $f_B\left(\mathbf{x}_{st}\right)$ is a vector containing a large amount of information, including pressure and brine saturation in various geologic members,***

$f_{SP}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]$ ~ ***spallings release to accessible environment for $\mathbf{x}_{st}$ calculated with the spallings model contained in CUTTINGS_S; this calculation requires repository conditions calculated by $f_B\left(\mathbf{x}_{st}\right)$ as input,***

$f_{DBR}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]$ ~ ***direct brine release to accessible environment for $\mathbf{x}_{st}$ also calculated with BRAGFLO; this calculation requires repository conditions calculated by $f_B\left(\mathbf{x}_{st}\right)$ as input,***

$f_{MB}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]$ ~ release through anhydrite marker beds to accessible environment for $\mathbf{x}_{st}$ calculated with NUTS; this calculation requires flows in and around the repository calculated by $f_B\left(\mathbf{x}_{st}\right)$ as input,

$f_{DL}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]$ ~ release through Dewey Lake Red Beds to accessible environment for $\mathbf{x}_{st}$ calculated with NUTS; this calculation requires flows in and around the repository calculated by $f_B\left(\mathbf{x}_{st}\right)$ as input,

$f_{S}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]$ ~ release to land surface due to brine flow up a plugged borehole for $\mathbf{x}_{st}$ calculated with NUTS or PANEL; this calculation requires flows in and around the repository calculated by $f_B\left(\mathbf{x}_{st}\right)$ as input,

$f_{MF}\left(\mathbf{x}_{st,0}\right)$ ~ flow field in the Culebra calculated for $\mathbf{x}_{st,0}$ with MODFLOW,

$f_{NP}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]$ ~ release to Culebra for $\mathbf{x}_{st}$ calculated with NUTS or PANEL as appropriate; this calculation requires flows in and around the repository calculated by $f_B\left(\mathbf{x}_{st}\right)$ as input, and

$f_{ST}\left[\mathbf{x}_{st,0}, f_{MF}\left(\mathbf{x}_{st,0}\right), f_{NP}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]\right]$ ~ groundwater transport release through Culebra to accessible environment calculated with SECOTP2D.This calculation requires MODFLOW results (i.e., $f_{MF}\left(\mathbf{x}_{st,0}\right)$) and NUTS or PANEL results (i.e., $f_{NP}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]$ as input; $\mathbf{x}_{st,0}$ is used as an argument to f_{ST} because drilling intrusions are assumed to cause no perturbations to the flow field in the Culebra.

The remainder of this section describes the mathematical structure of the mechanistic models that underlie the component functions of f in Equation (24).

The Monte Carlo CCDF construction procedure, implemented in the code CCDFGF (WIPP PA 2003a), uses a sample of size nS = 10,000 in the CRA-2004 PA. The individual programs that estimate releases do not run fast enough to allow this number of evaluations of f. As a result, a two-step procedure is being used to evaluate f in the calculation of the integral in Equation (4). First, f and its component functions are evaluated with the procedures (i.e., models) described in this section for a group of preselected futures. Second, values of $f\left(\mathbf{x}_{st,i}\right)$ for the randomly selected futures $\mathbf{x}_{st,i}$ used in the numerical evaluation of the integral in Equation (4) are then constructed from results obtained in the first step. These constructions are described in Sections PA-6.7 and PA-6.8, and produce the evaluations of f that are actually used in Equation (4).

For notational simplicity, the functions on the right hand side of Equation (24) will typically be written with only $\mathbf{x}_{st}$ as an argument (e.g., $f_{SP}\left(\mathbf{x}_{st}\right)$ will be used instead of $f_{SP}\left[\mathbf{x}_{st}, f_B\left(\mathbf{x}_{st}\right)\right]$). However, the underlying dependency on the other arguments will still be present.

The major topics considered in this chapter are two-phase flow in the vicinity of the repository as modeled by BRAGFLO (i.e., f_B) (Section PA-4.2), radionuclide transport in the vicinity of the repository as modeled by NUTS (i.e., f_{MB}, f_{DL}, f_S, f_{NP}) (Section PA-4.3), radionuclide transport in the vicinity of the repository as modeled by PANEL (i.e., f_S, f_{NP}) (Section PA-4.4), cuttings and cavings releases to the surface as modeled by CUTTINGS_S (i.e., f_C) (Section PA-4.5), spallings releases to the surface as modeled by DRSPALL and CUTTINGS_S (i.e., f_{SP}) (Section PA-4.6), direct brine releases to the surface as modeled by BRAGFLO (i.e., f_{DBR}) (Section PA-4.7), brine flow in the Culebra as modeled by MODFLOW (i.e., f_{MF}) (Section PA-4.8), and radionuclide transport in the Culebra as modeled by SECOTP2D (i.e., f_{ST}) (Section PA-4.9).

PA-4.2 Two-Phase Flow: BRAGFLO

Quantification of the effects of gas and brine flow on radionuclide transport from the repository requires use of a two-phase (brine and gas) flow code. For the CRA-2004 PA, the DOE uses the two-phase flow code BRAGFLO to simulate gas and brine flow in and around the repository (WIPP PA 2003b). Additionally, the BRAGFLO code incorporates the effects of disposal room consolidation and closure, gas generation, and rock fracturing in response to gas pressure. This section describes the mathematical models on which BRAGFLO is based, the representation of the repository in the model, and the numerical techniques employed in the solution.

PA-4.2.1 Mathematical Description

Two-phase flow in the vicinity of the repository is represented by the following system of two conservation equations, two constraint equations, and three equations of state:

Gas Conservation

$$\nabla \bullet \left[\frac{\alpha \rho_g \mathbf{K}_g k_{rg}}{\mu_g} \left(\nabla p_g + \rho_g g \nabla h \right) \right] + \alpha q_{wg} + \alpha q_{rg} = \alpha \frac{\partial \left(\phi \rho_g S_g \right)}{\partial t}, \tag{25a}$$

Brine Conservation

$$\nabla \bullet \left[\frac{\alpha \rho_b \mathbf{K}_b k_{rb}}{\mu_b} \left(\nabla p_b + \rho_b g \nabla h \right) \right] + \alpha q_{wb} + \alpha q_{rb} = \alpha \frac{\partial \left(\phi \rho_b S_b \right)}{\partial t}, \tag{25b}$$

Saturation Constraint

$$S_g + S_b = 1, \qquad (25c)$$

Capillary Pressure Constraint

$$p_C = p_g - p_b = f\left(S_b\right), \qquad (25d)$$

Gas Density

ρ_g ***(determined by Redlich-Kwong-Soave equation of state; see Equation (46)),*** ***(25e)***

Brine Density

$$\rho_b = \rho_0 \exp\left[\beta_b\left(\rho_b - \rho_{b0}\right)\right], \text{ and} \qquad (25f)$$

Formation Porosity

$$\phi_b = \phi_0 \exp\left[\beta_f\left(\rho_b - \rho_{b0}\right)\right], \qquad (25g)$$

where

g = ***acceleration due to gravity (m/s^2)***

h = ***vertical distance from a reference location (m)***

K_l = ***permeability tensor (m^2) for fluid l (l = g ~ gas, l = b ~ brine)***

k_{rl} = ***relative permeability (dimensionless) to fluid l***

p_C = ***capillary pressure (Pa)***

p_l = ***pressure of fluid l (Pa)***

q_{rl} = ***rate of production (or consumption, if negative) of fluid l due to chemical reaction (kg/m^3 s)***

q_{wl} = ***rate of injection (or removal, if negative) of fluid l (kg/m^3 s)***

S_l = ***saturation of fluid l (dimensionless)***

t = ***time (s)***

α = ***geometry factor (m)***

ρ_l = ***density of fluid l (kg/m^3)***

μ_l = viscosity of fluid l (Pa s)

ϕ = porosity (dimensionless)

ϕ_0 = reference (i.e., initial) porosity (dimensionless)

p_{b0} = reference (i.e., initial) brine pressure (Pa), constant in Equation (25f) and spatially variable in Equation (25g)

ρ_0 = reference (i.e., initial) brine density (kg/m^3)

β_f = pore compressibility (Pa^{-1})

β_b = brine compressibility (Pa^{-1}).

The conservation equations are valid in one (i.e., $\nabla = [\partial/\partial x]$), two (i.e., $\nabla = [\partial/\partial x, \partial/\partial y]$) and three (i.e., $\nabla = [\partial/\partial x, \partial/\partial y, \partial/\partial z]$) dimensions. In the CRA-2004 PA, the preceding system of equations is used to model two-phase fluid flow within the two-dimensional region shown in Figure PA-8. The details of this system are now discussed.

The α term in Equation (25a) and Equation (25b) is a dimension-dependent geometry factor and is specified by

α = area normal to flow direction in one-dimensional flow (i.e., $\Delta y \Delta z$; units = m^2),

= thickness normal to flow plane in two-dimensional flow (i.e., Δz; units = m),

= 1 in three-dimensional flow (dimensionless). (26)

The CRA-2004 PA uses a two-dimensional geometry for computation of two-phase flow in the vicinity of the repository, and as a result, α is the thickness of the modeled region (i.e., Δz) normal to the flow plane (Figure PA-8). Due to the use of the two-dimensional grid in Figure PA-8, α is spatially dependent, with the values used for α defined in the column labeled "Δz." Specifically, α increases with distance away from the repository edge in both directions to incorporate the increasing pore volume through which fluid flow occurs. The method used in the CRA-2004 PA, called rectangular flaring, is illustrated in Figure PA-9 and ensures that the total volume surrounding the repository is conserved in the numerical grid. The equations and method used to determine α for the grid shown in Figure PA-8 are described in detail by Stein (2002a).

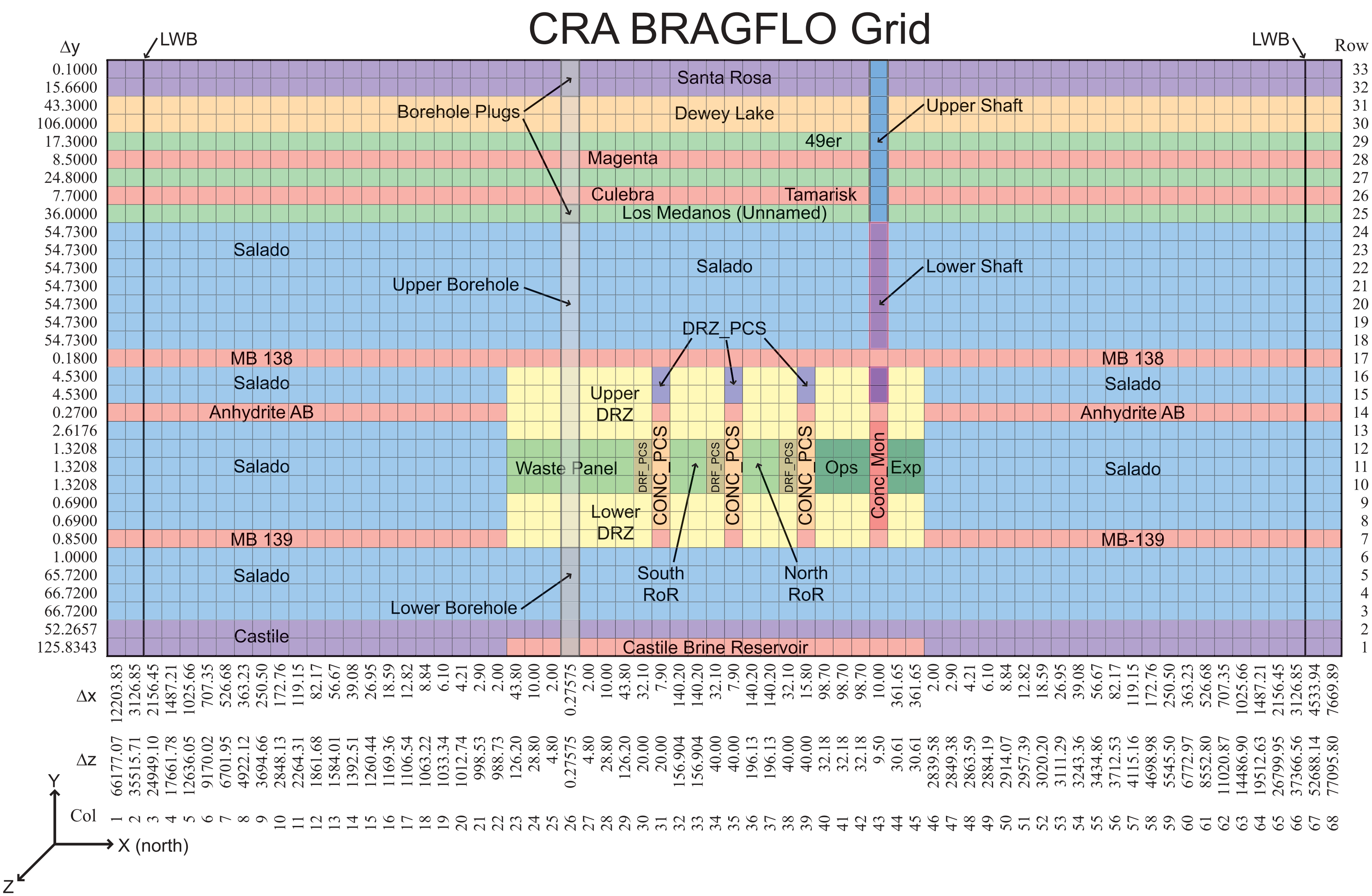
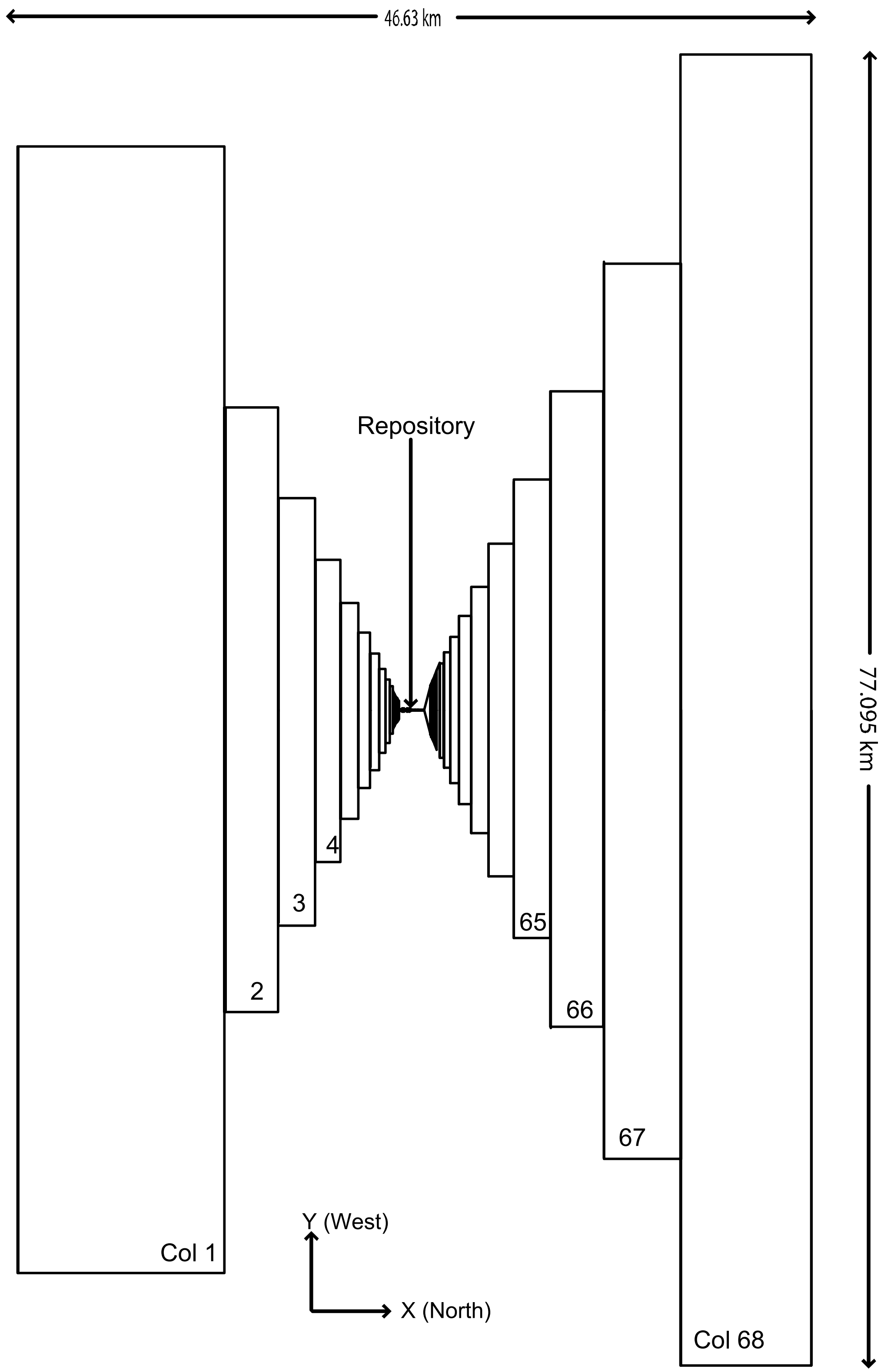


Figure PA-8. Computational Grid Used in BRAGFLO in the CRA-2004 PA.

1



2

3 *Figure PA-9. Definition of Element Depth in BRAGFLO Grid in the CRA-2004 PA.*