# Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant

**Appendix CCDFGF** 



## United States Department of Energy Waste Isolation Pilot Plant



Carlsbad Area Office Carlsbad, New Mexico

# Design Document for CCDFGF and GRIDFLO

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## **Design Document for CCDFGF and GRIDFLO**

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## Acknowledgment



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1.	Introduction	1
2.	Theoretical Overview	3
	2.1 EN1: Probabilistic Characterization of Different Futures	4
	2.2 EN7: Estimation of Releases	
	2.3 EN3. Probabilistic Characterization of Parameter Uncertainty	6
3.	Sampling of Futures	
	3.1 Probability Space ( $S_{st}$ , $S_{st}$ , $p_{st}$ ) for Stochastic Uncertainty	
	3.2 Generation of Individual Futures	
4.	Construction of Releases to Accessible Environment for Individual Futures	25
	4.1 Mechanistic Results for Specific Futures	
	4.2 Construction of Cuttings Releases	
	4.3 Construction of Blowout Releases	
	4.4 Construction of Spallings Releases	
	4.5 Radionuclide Transport Away from Repository by Flowing Brine	
	4.6 Radionuclide Transport Through Anhydrite Marker Beds	41
	4.7 Radionuclide Transport Through Dewey Lakes Red Beds	
	4.8 Radionuclide Transport Through Abandoned Borehole to Surface	
	4.9 Radionuclide Transport Through Culebra Dolomite	
	4.10 CCDF Construction	
	4.11 Data Assembly	51
5.	Fluid Flow and Radionuclide Transport for E1E2 Intrusions	
	5.1 Rationale for GRIDFLO	53
	5.2 Mathematical Structure of GRIDFLO	
	5.3 Implementation of GRIDFLO	
6.	Code Architecture	61
	6.1 Control Flow	61
	611 Initialization	61
	6.1.2 Calculation Structure	
	613 Borehole Intrusions	
$\frown$	6.1.4 Releases to Accessible Environment	
	6.1.5 Flow to the Culebra	
$(\mathbf{i}_{i})$	6.1.6 Repository Flow and Transport (GRIDFLO Option)	
$\bigcirc$	6.1.7 Result Distributions	
	6.2 Control Logic	
	6.3 Data Structures	65
	6.3.1 Run Control Parameters	
	6.3.2 Repository Nodalization Parameters	65
•	6.3.3 Inventory Parameters (GRIDFLO Option)	
	6.3.4 Accessible Environment Release Parameters	

### CONTENTS

6.3.5 Borehole Definition Parameters (Optional)	<b>6</b> 6
6.4 Allowable/Prescribed Ranges for Input/Output	67
6.5. Verifiability	
6.6 Consistency/Traceability	
6.7 Technical Feasibility	
6.8 Implementation	
6.8.1 Input Parameter Definitions	69
6.8.2 Repository Nodalization	
6.8.3 Leg Property Definitions	
6.8.4 Leg Property Modification.	
6.8.5 Borehole Intrusion Parameters	70
6.8.6 Node Pressure Heads	
6.8.7 Repository Flow Rate Calculations	
6.8.8 Repository Species Transport	
6.8.9 Releases to Accessible Environment	72
6.8.10 Result Distributions	72
7. Summary	75
8. References	77
Appendix A: Linearity of Equations in SECO-TRANSPORT	A-1
Appendix B: Memo from Rebecca L. Blaine Illustrating Linearity of SECO-TRANSPORT Calculations	<b>B</b> -1

.

## Figures

Figur	re de la companya de	Pa
2.1	Boundary line and associated CCDF specified in 40 CFR 191, Subpart B.	
2.2	Models used in 1996 WIPP PA.	6
2.3	Distribution of CCDFs resulting from possible values for $\mathbf{x}_{su} \in S_{su}$	8
2.4	Distribution of exceedance probabilities due to subjective uncertainty.	8
2.5	Example CCDF distribution from 1992 WIPP PA.	9
3.1	Example of discretized drilling locations	13
3.2	Sampling of time intervals between drilling intrusions from cumulative distribution function (CDF)	
	associated with drilling rate $\lambda = \lambda_d$	17
3.3	Hypothetical example of specification of node properties	23
4.1	Pairs of drilling intrusions used in the calculation of blowout releases.	34
5.1	Coordinate system for calculation of flow within the experimental, operations and waste disposal	
	regions of the WIPP	
5.2	Flow paths associated with a single node in the repository	56

### Tables

-

-

.

3.1	Probability of Different Numbers of Drilling Intrusions over 9900 yrs for Different Drilling Rates	16
3.2	Required Input and Associated Calculations to Generate Single Future x <sub>st</sub> of Form Shown in Eqs.	
	(2.2) and (3.1)	18
3.3	Anticipated Definition of $D_P$ for Use in 1996 WIPP PA. Under Option A in CCDFGF, the	
	implications of borehole permeability will be accounted for directly from the values assigned to p <sub>i</sub>	21
3.4	Algorithm to Sample Time of a Drilling Intrusion with	24
4.1	Results from Baseline Inventory (BIR) and Calculations with CUTTINGS Transferred to CCDFGF	
	for Use in Determination of Releases Due to Cuttings Removal	28
4.2	Calculation of Cuttings Release $f_C$ for an Arbitrary Future $\mathbf{x}_{st}$	29
4.3	Results from Calculations with BLOWOUT Transferred to CCDFGF for Use in Determination of	
	Releases Due to Blowout	31
4.4	Results from Calculations with PANEL Transferred to CCDFGF for Use in Determination of Releases	
	Due to Blowout and Spallings	35
4.5	Calculation of Blowout Release $f_{BL}$ for an Arbitrary Future $\mathbf{x}_{st}$	36
4.6	Extension of Limited Number of BLOWOUT Calculations to Obtain Results in Table 4.3.	37
4.7	Results from Calculations with NUTS and PANEL Related to Radionuclide Transport Away from the	
	Repository by Flowing Brine Transferred to CCDFGF	38
4.8	Construction of Radionuclide Releases into the Culebra Dolomite Without Use of GRIDFLO for an	
	Arbitrary Future x <sub>st</sub>	42
4.9	Calculation of Anhydrite Marker Bed Release $f_{MB}$ for an Arbitrary Future $\mathbf{x}_{st}$	44
4.10	Results from Calculations with SECO-TRANSPORT Transferred to CCDFGF for Use in	
	Determination of Releases Due to Groundwater Transport in the Culebra Dolomite	46
4.11	Calculation of Groundwater Transport Release $f_{ST}$ through the Culebra Dolomite for an Arbitrary	
	Future X <sub>st</sub>	48

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#### 1. Introduction

The Waste Isolation Pilot Plant (WIPP) is located in southeastern New Mexico and is being developed by the U.S. Department of Energy (DOE) as a disposal facility for transuranic (TRU) waste.<sup>1,2</sup> The WIPP must comply with various environmental regulations, including 40 CFR 191, Subpart B, *Environmental Radiation Protection Standards for the Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes*,<sup>3</sup> and 40 CFR 268.6, *Petitions to Allow Land Disposal of a Waste Prohibited Under Subpart C of Part* 268.<sup>4</sup> As part of the development process for the WIPP, a sequence of performance assessments (PAs) has been carried out by Sandia National Laboratories (SNL) to organize knowledge currently available about the WIPP and to provide guidance for future research and development efforts.<sup>5,6</sup> The next iteration of these PAs is currently underway at SNL and will form the basis for an application by the DOE to the U.S. Environmental Protection Agency (EPA) in late 1996 for the certification of the WIPP for the disposal of TRU waste.

An important part of the compliance certification application (CCA) for the WIPP is the complementary cumulative distribution function (CCDF) for comparison with the release limits specified in 40 CFR 191.13. In the 1991 and 1992 WIPP PAs, this CCDF was constructed with a procedure based on importance sampling.<sup>7</sup> To provide greater flexibility and improved use of available information, the CCA will use a Monte Carlo procedure for CCDF construction.<sup>8</sup> A similar procedure was also used in the systems prioritization methodology.<sup>9</sup>

This document describes the program CCDFGF that will be written to implement a Monte Carlo CCDF construction in the CCA. The purpose of CCDFGF will be to assemble results obtained from calculations performed with a number of different programs (e.g., BRAGFLO, PANEL, NUTS, SECO-FLOW, SECO-TRANSPORT, CUTTINGS, BLOWOUT) into the CCDF specified in 40 CFR 191.13.

The theoretical basis for CCDFGF is presented in Chapter 2. As described there, three basic entities underlie CCDFGF: (1) a probability space that characterizes the likelihood of different disruptions that could occur at the WIPP site over the next 10,000 yr, (2) a probability space that characterizes the uncertainty in the required inputs to the CCA, and (3) a function f that estimates consequences (e.g., the EPA normalized release) conditional on a specific set of disruptions and a specific set of input values.

The manner in which the probability space for different futures is defined and sampled from is described in Chapter 3. The manner in which the probability space for uncertain parameters is defined and sampled from is outside the scope of CCDFGF and not treated in this presentation, although Chapter 2 does give a high-level overview of how this sampling fits into the overall analysis.

The function f, in concept, is the outcome of the combined operation of the previously indicated programs. However, it is not possible to directly evaluate f with these programs for all possible sets of values that must be

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considered in CCDF construction. As a result, CCDFGF must use a relatively small number of mechanistic calculations to evaluate, i.e., approximate, f for the large number of different futures that must be considered in CCDF construction.

Two options are supplied within CCDFGF for evaluation of f. The first option, designated Option A for algebraic construction, involves algebra manipulation of mechanistic results to produce normalized releases to the accessible environment for specific, randomly selected futures. The construction of f under Option A is described in Chapter 4. The second option, designated Option GF as a mnemonic for GRIDFLO, differs from Option A in the use of a more sophisticated procedure (i.e., the GRIDFLO submodule of CCDFGF) to estimate releases from the repository to the Culebra Dolomite in the presence of two or more drilling intrusions of which at least one penetrates pressurized brine (i.e., a brine pocket) in the Castile Formation. Option GF is intended for use in situations that involve large, slowly depressurizing brine pockets in the Castile Formation. The determination of radionuclide releases from the repository to the Culebra under Option GF is described in Chapter 5.

The report then ends with a sequence of chapters that describe the structure of the program (i.e., CCDFGF) that will implement the computational procedures described in Chapters 2, 3, 4 and 5.

#### 2. Theoretical Overview

When viewed at a high-level, three basic entities underlie the PAs conducted by SNL for the WIPP,

- EN1: a probabilistic characterization of the likelihood of different futures occurring at the WIPP site over the next 10,000 yr,
- EN2: a procedure for estimating the radionuclide releases to the accessible environment associated with each of the possible futures that could occur at the WIPP site over the next 10,000 yr,
- EN3: a probabilistic characterization of the uncertainty in the parameters used in the definition of EN1 and EN2.

Together, EN1 and EN2 give rise to the CCDF specified in 40 CFR 191 (Fig. 2.1), and EN3 gives rise to an assessment of the confidence with which the location of this CCDF can be estimated.

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



Figure 2.1. Boundary line and associated CCDF specified in 40 CFR 191, Subpart B.

- Q1: What occurrences could take place at the WIPP site over the next 10,000 yr?
- Q2: How likely are the different occurrences that could take place at the WIPP site over the next 10,000 yr?
- Q3: What are the consequences of the different occurrences that could take place at the WIPP site over the next 10,000 yr?

and one question about the WIPP PA,

Q4: How much confidence should be placed in answers to the first three 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.

#### 2.1 EN1: Probabilistic Characterization of Different Futures

The entity EN1 is the outcome of the scenario development process for the WIPP and provides a probabilistic characterization of the likelihood of different futures that could occur at the WIPP site over the next 10,000 yr, with the period of 10,000 yr specified in 40 CFR 191. When viewed formally, EN1 is defined by a probability space ( $S_{st}$ ,  $\mathcal{L}_{st}$ ,  $p_{st}$ ), with the sample space  $S_{st}$  given by

$$S_{st} = {\mathbf{x}_{st}: \mathbf{x}_{st} \text{ is a possible 10,000 yr sequence of occurrences at the WIPP}.$$
 (2.1)

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

As a reminder, a probability space (S, A, p) consists of three components: a set S that contains everything that could occur for the particular "universe" under consideration, a suitably restricted set S of subsets of S and a function p defined for elements of S that actually defines probability. In the terminology of probability theory, S is the sample space, the elements of S are elementary events, and the subsets of S contained in S are events. In most applied problems, the function p defined on S is replaced by a probability density function (PDF) d (e.g.,  $d_{st}$  in Fig. 2.1).

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. In addition, 40 CFR 194 specifies that the occurrence of mining within the land withdrawal boundary must be included in the analysis. As a result, the elements  $\mathbf{x}_{st}$  of  $S_{st}$  are anticipated to be vectors of the form

$$\mathbf{x}_{st} = [\underbrace{t_1, p_1, l_1, a_1, d_1, k_1, b_1}_{1^{\text{st}} \text{ intrusion}}, \underbrace{t_2, p_2, l_2, a_2, d_2, k_2, b_2}_{2^{\text{nd}} \text{ intrusion}}, \ldots, \underbrace{t_n, p_n, l_n, a_n, d_n, k_n, b_n}_{n^{\text{th}} \text{ intrusion}}, t_{min}]$$
(2.2)

in the 1996 WIPP PA, where *n* is the number of drilling intrusions,  $t_i$ ,  $p_i$ ,  $l_i$ ,  $a_i$ ,  $d_i$ ,  $k_i$  and  $b_i$  correspond to the time (yr), plugging (i.e., sealing) pattern, location, activity level (Ci/m<sup>2</sup>), diameter (m), permeability (m<sup>2</sup>), and possible penetration of pressurized brine in the Castile Formation of the *t*<sup>th</sup> drilling intrusion, and  $t_{min}$  is the time at which potash mining occurs within the land withdrawal boundary. In the development of  $(S_{st}, A_{st}, p_{st})$ , the probabilistic characterization of *n*,  $t_i$  and  $l_i$  will derive from the assumption that drilling intrusions occur randomly in time and space (i.e., follow a Poisson process), the probabilistic characterization of  $p_i$ ,  $d_i$  and  $k_i$  will derive from current drilling practices in the sedimentary basin (i.e., the Delaware Basin) in which the WIPP is located, and the probabilistic characterization for  $t_{min}$  follows from the guidance in 40 CFR 194<sup>10</sup> that the occurrence of potash mining within the land withdrawal to occur randomly in time (i.e., follow a Poisson process with a rate constant of  $\lambda_m = 10^{-4} \text{ yr}^{-1}$ ).

With respect to the previously indicated questions,  $S_{st}$  provides an answer to Q1, while  $L_{st}$  and  $p_{st}$  provide an answer to Q2. In practice, Q2 will be answered by specifying distributions for n,  $t_i$ ,  $p_i$ ,  $l_i$ ,  $a_i$ ,  $d_i$ ,  $k_i$  and  $b_i$  which in turn lead to definitions for  $L_{st}$  and  $p_{st}$ . The CCDF in 40 CFR 191 will be obtained by evaluating an integral involving ( $S_{st}$ ,  $L_{st}$ ,  $p_{st}$ ) (Fig. 2.1).

#### 2.2 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  $S_{st}$ ) that could occur at the WIPP. Estimation of environmental releases corresponds to evaluation of the function f in Fig. 2.1. Release mechanisms associated with f include direct removal to the surface at the time of a drilling intrusion (i.e., cuttings, spallings, brine flow) and release subsequent to a drilling intrusion due to brine flow up a borehole with a degraded plug (i.e., groundwater transport).

The primary computational models intended for use in the 1996 WIPP PA are illustrated in Fig. 2.2. Most of these models involve the numerical solution of partial differential equations used to represent material deformation, fluid flow and radionuclide transport. It is the models indicated in Fig. 2.2 that actually define the function f in Fig. 2.1.

The models in Fig. 2.2 are too complex to permit a closed form evaluation of the integral in Fig. 2.1 that defines the CCDF specified in 40 CFR 191. Rather, a Monte Carlo procedure will be used. Specifically, elements  $\mathbf{x}_{st,i}$ , i = 1, 2, ..., nS, will be randomly sampled from  $S_{st}$  in consistency with the definition of  $(S_{st}, S_{st}, p_{st})$ . Then, the integral in Fig. 2.1, and hence the associated CCDF, will be approximated by





Figure 2.2. Models used in 1996 WIPP PA.

$$prob(Rel > R) = \int_{\mathcal{S}_{st}} \delta_R[f(\mathbf{x}_{st})] d_{st}(\mathbf{x}_{st}) dV_{st} \doteq \sum_{i=1}^{nS} \delta_R[f(\mathbf{x}_{st,i})] / nS.$$
(2.3)

The models in Fig. 2.2 are too computationally intensive to permit their evaluation for every element  $\mathbf{x}_{st,i}$  of  $S_{st}$  in Eq. (2.3). Due to this constraint, the models in Fig. 2.2 will be evaluated for representative elements of  $S_{st}$  and then the results of these evaluations will be used to construct values of f for the large number of  $\mathbf{x}_{st,i}$  (e.g.,  $1000 \le nS \le 10,000$ ) in Eq. (2.3).

With respect to the previously indicated questions, the models in Fig. 2.2 are providing an answer to Q3.

#### 2.3 EN3: Probabilistic Characterization of Parameter Uncertainty

The entity EN3 is the outcome of the data development effort for the WIPP and provides a probabilistic characterization of the uncertainty in the parameters that underlie the WIPP PA. When viewed formally, EN3 is defined by a probability space ( $S_{su}$ ,  $J_{su}$ ,  $p_{su}$ ), with the sample space  $S_{su}$  given by

$$S_{su} = \{\mathbf{x}_{su}: \mathbf{x}_{su} \text{ is possibly the correct vector of parameter values to use in the WIPP PA}\}.$$
 (2.4)

The subscript *su* refers to subjective (i.e., epistemic) uncertainty and is used because  $(S_{su}, S_{su}, p_{su})$  is providing a probabilistic characterization of where the appropriate inputs to use in the WIPP PA are believed to be located. In practice, some elements of  $\mathbf{x}_{su}$  affect the definition of  $(S_{st}, S_{st}, p_{st})$  (e.g., the rate constant  $\lambda$  used to define the



Poisson process for drilling intrusions or the mode of the distribution of borehole permeabilities) and other elements relate to the models in Fig. 2.2 that determine the function f in Fig. 2.1 and Eq. (2.3) (e.g., radionuclide solubilities in Castile brine or fracture spacing in the Culebra Dolomite).

If the value for  $\mathbf{x}_{su}$  was precisely known, then the CCDF in Fig. 2.1 could be determined with certainty and compared with the boundary line specified in 40 CFR 191. However, given the complexity of the WIPP site and the 10,000 yr time period under consideration,  $\mathbf{x}_{su}$  can never be known with certainty. Rather, uncertainty in  $\mathbf{x}_{su}$  as characterized by  $(S_{su}, S_{su}, p_{su})$  will lead to a distribution of CCDFs (Fig. 2.3). The proximity of this distribution to the boundary line in Fig. 2.1 provides an indication of the confidence with which 40 CFR 191 will be met.

The distribution of CCDFs in Fig. 2.3 can be summarized by distributions of exceedance probabilities conditional on individual release values (Fig. 2.4). This distribution is defined by a double integral over  $S_{su}$  and  $S_{st}$ . In practice, this integral is too complex to permit a closed-form evaluation. Instead, the WIPP PA uses Latin hypercube sampling<sup>7</sup> to evaluate the integral over  $S_{su}$  and, as indicated in Eq. (2.3), simple random sampling to evaluate the integral over  $S_{st}$ . Specifically, a Latin hypercube sample  $\mathbf{x}_{su,k}$ , k = 1, 2, ..., nLHS, is generated from  $S_{su}$ in consistency with the definition of  $(S_{su}, S_{su}, p_{su})$  and a random sample  $\mathbf{x}_{st,i}$ , i = 1, 2, ..., nS, is generated from  $S_{st}$ in consistency with the definition of  $(S_{su}, S_{su}, p_{su})$ . The probability  $prob(p \leq P|R)$  in Fig. 2.4 is then approximated by

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

$$(2.5)$$

The result of the preceding calculation is typically displayed by plotting percentile values (e.g.,  $P_{0.1}$ ,  $P_{0.5}$ ,  $P_{0.9}$  from Fig. 2.4) and also mean values for exceedance probabilities above the corresponding release values (i.e., R) and then connecting these points to form continuous curves (Fig. 2.5). The proximity of these curves to the indicated boundary line provides an indication of the confidence with which 40 CFR 191 will be met.

With respect to the previously indicated questions,  $(S_{su}, S_{su}, p_{su})$  and results derived from  $(S_{su}, S_{su}, p_{su})$  (e.g., the distributions in Figs. 2.3, 2.4 and 2.5) are providing an answer to Q4.



Figure 2.3. Distribution of CCDFs resulting from possible values for  $\mathbf{x}_{su} \in S_{su}$ .



Figure 2.4. Distribution of exceedance probabilities due to subjective uncertainty.



Figure 2.5. Example CCDF distribution from 1992 WIPP PA.

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#### 3. Sampling of Futures

#### 3.1 Probability Space $(S_{st}, J_{st}, p_{st})$ for Stochastic Uncertainty

The probability space  $(S_{st}, J_{st}, p_{st})$  provides a probabilistic characterization of the events that could occur at the WIPP over the next 10,000 yr. As indicated in Eq. (2.1), the sample space  $S_{st}$  consists of all possible 10,000 yr futures that could occur at the WIPP subsequent to decommissioning. The final definition of  $(S_{st}, J_{st}, p_{st})$  for the 1996 WIPP PA can only be made after the Features, Events, and Processes (FEPs) screening process is complete. Past reviews have concluded that exploratory drilling for natural resources constitutes the only type of future occurrence with sufficient likelihood and potential for initiating releases to the accessible environment to merit inclusion in the definition of  $(S_{st}, J_{st}, p_{st})$ . Further, 40 CFR 194 requires that the occurrence of potash mining within the land withdrawal boundary must be included in the analysis. Therefore, this discussion will proceed under the assumption that drilling intrusions and the occurrence of potash mining within the land withdrawal boundary are the only events that require incorporation into  $(S_{st}, J_{st}, p_{st})$ . However, the conceptual structure in use and its associated computational implementation should be sufficiently general to allow the incorporation of other types of events into  $(S_{st}, J_{st}, p_{st})$  should this be required (although possibly with some additional programming required).

The following assumptions will underlie the definition of  $(S_{st}, S_{st}, p_{st})$ :

(1) Drilling intrusions occur randomly in time and space (i.e., follow a Poisson process). This process will be defined by a rate term  $\lambda_d$  (units: yr<sup>-1</sup>), with  $\lambda_d$  defined by the drilling rate (e.g., 48 boreholes/km<sup>2</sup>/10<sup>4</sup> yr) and the area of the repository (or possibly some larger area if the depletion of pressurized brine pockets in the Castile Formation or the penetration of disturbed rock zones around the repository are deemed to be significant).

(2) Different sealing (i.e., plugging) patterns are used for different drilling intrusions. At present, three potential sealing patterns are anticipated for the 1996 WIPP PA: (a) full concrete plug through Salado Formation to Bell Canyon Formation with a permeability of  $5 \times 10^{-17}$  m<sup>2</sup>, (b) two plug configuration with plugs at Rustler/Salado and Castile/Bell Canyon interfaces, and (c) three plug configuration with plugs at Rustler/Salado, Salado/Castile and Castile/Bell Canyon interfaces. Specifically, the variation in plugging patterns will be defined by a distribution  $D_{PL}$ .

(3) There is a distribution of waste concentration (Ci/m<sup>2</sup>) within the repository. In past WIPP PAs, this distribution has been implemented by discretizing the waste into five activity levels with a probability  $pA_i$ , i = 1, 2, ..., 5, that a randomly placed borehole through the repository will pass through waste of activity level *i*. For the definition of  $(S_{st}, \mathcal{L}_{st}, p_{st})$ , activity level will be assumed to follow a distribution  $D_A$ , where  $D_A$  can be either continuous or discrete. For the 1996 WIPP PA, it is anticipated that  $D_A$  will be based on the distinction between penetrating contact handled (CH) and remote handled (RH) waste and the individual waste streams associated with each of these waste types.

(4) There is a distribution of drillbit diameters in use (i.e., different drilling intrusions will use different drillbit diameters). The 1991 and 1992 WIPP PAs assumed that all drilling intrusions would use the same drillbit diameter but that the correct value for this diameter was not known; in contrast, the SPM analyses assumed a distribution of drillbit diameters across different drilling intrusions. Specifically, the variation of drillbit diameters across different drilling intrusions will be assumed to follow a distribution  $D_{DB}$ , where  $D_{DB}$  can be either continuous or discrete.

(5) Different drilling intrusions can result in boreholes with different permeabilities. Past analyses for the WIPP have assumed that *all* boreholes rapidly evolve to the same permeability, although there was assumed to be large uncertainty in what this asymptotic (i.e., long term) permeability was. This does not seem to be reasonable as different boreholes will be plugged in different ways and thus can be reasonably anticipated to have different asymptotic permeabilities. This variability across drilling intrusions is specifically recognized by the EPA in the following statement (Ref. 10, p. 5776):

For the specific case of borehole seals, EPA is further proposing that boreholes shall be assumed to be sealed at the rate boreholes have been sealed over the past 50 years in the Delaware Basin and that natural processes will degrade or otherwise affect the permeability of boreholes over the regulatory time frame.

In consistency with the preceding guidance, the variation in permeability across different drilling intrusions will be assumed to follow a distribution  $D_P$ , where  $D_P$  can be either continuous or discrete. A further option will be to define time-dependent distributions for permeabilities above and below the repository, possibly with a specified correlation between these two permeabilities. The distinction between permeability above and below the repository is potentially important due to the role that such permeabilities might play in diverting brine flow from a pressurized brine pocket through the repository.

(6) For the purpose of initiating groundwater transport calculations, the repository (and possibly an adjacent area) will be discretized into a finite number of locations (i.e., nodes) at which drilling intrusions can occur (Fig. 3.1). A discrete probability distribution  $D_L$  will define the probability that a randomly placed intrusion into the repository (or possibly an adjacent area if such areas are included in the analysis) will occur at a given location. Specifically,  $D_L$  will consist of a sequence of probabilities  $pL_i$ , i = 1, 2, ..., nL, where  $pL_i$  is the probability that a randomly placed drilling intrusion will occur at location  $L_i$  and nL is the number of discretized locations in use. Due to the assumption that drilling intrusions occur randomly in space,  $pL_i$  will derive from the area associated with location  $L_i$ . Further, each location  $L_i$  can be identified as either being above or not above pressurized brine in the Castile Formation. Thus,  $L_i$  will play an important role in the definition of E1, E2 and E1E2 scenarios, where an E1 scenario designates a subset of  $S_{st}$  in which a single drilling intrusion passes through the repository and penetrates pressurized brine, an E1E2 scenario designates a subset of  $S_{st}$  in which a single drilling intrusion passes through the repository and penetrates pressurized brine, and E1E2 scenario designates a subset of  $S_{st}$  in which a single drilling intrusion passes through the repository and penetrates pressurized brine, and E1E2 scenario designates a subset of  $S_{st}$  in which two or more drilling intrusions pass through the repository, with at least one of these intrusions penetrating pressurized brine.



Figure 3.1. Example of discretized drilling locations. Such locations and their associated probabilities will be userspecified input.

(7) A given drilling intrusion may or may not penetrate pressurized brine in the Castile Formation. If the pressurized brine is present in large contiguous areas, then the location of the drilling intrusion (see (6) above) is sufficient to determine whether or not pressurized brine is penetrated. However, if variation in the location of pressurized brine occurs on a finer scale than the specification of the nodes in (6) above, then an additional determination must be made to specify whether or not a given drilling intrusion penetrates pressurized brine. Specifically, a discrete probability distribution  $D_B$  can be used to characterize the likelihood that a randomly placed drilling intrusion through the Castile Formation in the vicinity of the waste panels will encounter pressurized brine. Possibilities for  $D_B$  include a single probability for encountering pressurized brine anywhere in the vicinity of the WIPP and a different probability for intrusions in the vicinity of each of the nodes in (6) above.

(8) The occurrence of potash mining within the land withdrawal boundary occurs randomly in time (i.e., follows a Poisson process). This process will be defined by a rate term  $\lambda_m$  (units: yr<sup>-1</sup>). Guidance in 40 CFR 194 specifies  $\lambda_m = 1 \times 10^{-4}$  yr<sup>-1</sup>.

The probability space ( $S_{st}$ ,  $\mathcal{L}_{st}$ ,  $p_{st}$ ) will be defined by the rate terms  $\lambda_d$  and  $\lambda_m$ , which can be constant or time dependent, and the distributions  $D_{PL}$ ,  $D_A$ ,  $D_{DB}$ ,  $D_P$ ,  $D_L$  and  $D_B$ . Specifically, the elements of  $\mathbf{x}_{st}$  of  $S_{st}$  will be vectors of the form

$$\mathbf{x}_{st} = [t_1, p_1, l_1, a_1, d_1, k_1, b_1, t_2, p_2, l_2, a_2, d_2, k_2, b_2, \dots, t_n, p_n, l_n, a_n, d_n, k_n, b_n, t_{min}, 0, 0, 0, 0, 0, \dots], \quad (3.1)$$

where

- $t_i = \text{time (yr) of } i^{\text{th}} \text{ drilling intrusion,}$
- $p_i$  = plugging pattern used for *i*<sup>th</sup> drilling intrusion,
- $l_i = \text{location}$  (dimensionless) of *i*<sup>th</sup> drilling intrusion (i.e., node associated with *i*<sup>th</sup> drilling intrusion),
- $a_i$  = activity level of waste penetrated by *i*<sup>th</sup> drilling intrusion,
- $d_i$  = drillbit diameter (m) used in *i*<sup>th</sup> drilling intrusion,
- $k_i$  = permeability (m<sup>2</sup>) for *i*<sup>th</sup> drilling intrusion (Note: if permeabilities above and below the repository are assumed to be different, then two permeabilities will be required for each drilling intrusion; a time dependence for borehole permeability is also possible),
- $b_i$  = designator (dimensionless) for penetration of pressurized brine in the Castile Formation (i.e.,  $b_i$  = 0, 1 implies nonpenetration and penetration, respectively, of pressurized brine),
- n = number of drilling intrusions in the 10,000 yr future defined by  $\mathbf{x}_{st}$ ,

 $t_{min}$  = time of occurrence (yr) of potash mining within the land withdrawal boundary,

the  $t_i$  are assumed to be ordered so that  $t_i \le t_{i+1}$  for i = 1, 2, ..., n-1, and the trailing 0's in Eq. (3.1) are place holders to bring  $\mathbf{x}_{st}$  up to the dimensionality assumed for  $S_{st}$  (and in general will be omitted for notational simplicity).

In concept, *n* could be any positive integer, with the result that  $S_{st}$  is a subset of  $R^{\infty}$ . As a reminder,  $R^{\infty}$  denotes the set of all real-valued vectors of infinite length. In practice, the probability of a large number of drilling intrusions (e.g., > 15) will be small (e.g., < 10<sup>-4</sup>) (Table 3.1). Thus,  $S_{st}$  would effectively be a subset of  $R^{106}$  if the occurrence of more than 15 drilling intrusions over 10,000 yr was probabilistically insignificant given the definition of  $\lambda_d$  (i.e., 106 = 7 \* 15 + 1, where 7 is the number of real-valued quantities associated with each drilling intrusion in Eq. (3.1) and the number 1 derives from  $t_{min}$ ). For perspective, the probabilities of different numbers of drilling intrusions that result for different  $\lambda_d$ 's are shown in Table 3.1.

Given  $\lambda_d$ ,  $\lambda_m$  and the distributions  $D_{PL}$ ,  $D_A$ ,  $D_{DB}$ ,  $D_P$ ,  $D_L$  and  $D_B$ , the set  $\mathcal{L}_{st}$  and the function  $p_{st}$  can be formally developed.<sup>11</sup> However, this is not necessary for the computational implementation of the 1996 WIPP PA and therefore will not be done. Rather, random sampling defined by  $\lambda_d$ ,  $\lambda_m$ ,  $D_{PL}$ ,  $D_A$ ,  $D_{DB}$ ,  $D_P$ ,  $D_L$  and  $D_B$  will be used to select elements  $\mathbf{x}_{st}$  of  $S_{st}$  in the numerical approximation of the integral in Eq. (2.8) with the summation in Eq. (2.11).

#### 3.2 Generation of Individual Futures

The random sampling to generate an element  $\mathbf{x}_{st}$  of  $S_{st}$  will operate in the following manner. The drilling rate  $\lambda_d$  will be used to generate the times at which drilling intrusions occur. For a Poisson process with a constant  $\lambda_d$  (i.e., a stationary process), the cumulative distribution function (CDF) for the time  $\Delta t$  between the successive events is given by (Ref. 12, p. 113):

$$prob(t \le \Delta t) = 1 - e^{-\lambda} d^{\Delta t}.$$
(3.2)

A uniformly distributed random number can be selected from [0, 1]. Then, solution of

$$r_1 = 1 - e^{-\lambda_d t_1} \tag{3.3}$$

for  $t_1$  gives the time of the first drilling intrusion (Fig. 3.2). If 100 yr of administrative control is assumed, then 100 yr would be added to the  $t_1$  obtained in Eq. (3.3) to obtain the time of the first drilling intrusion. Selection of a second random number  $r_2$  and solution of

$$r_2 = 1 - e^{-\lambda} d^{\Delta t_1} \tag{3.4}$$

n: No. BHs <sup>a</sup>	$prob(n)^{b}$ : Probability of $n BH_s$			
	25 BHs/10 <sup>4</sup> yr km <sup>2</sup> $\lambda_d = 3.147E-04 \text{ yr}^{-1c}$	30 BHs/10 <sup>4</sup> yr km <sup>2</sup> $\lambda_d = 3.776E-04 \text{ yr}^{-1}$	48 BHs/10 <sup>4</sup> yr km <sup>2</sup> $\lambda_d = 6.050E-04 \text{ yr}^{-1}$	62.5 BHs/10 <sup>4</sup> yr km <sup>2</sup> $\lambda_d = 7.868E-04 \text{ yr}^{-1}$
0	4.435E-02	2.379E-02	2.505E-03	4.143E-04
I	1.382E-01	8.893E-02	1.500E-02	3.227E-03
2	2.153E-01	`1.662E01	4.493E-02	1.257E-02
3	2.236E-01	2.072E-01	8.970E-02	3.263E-02
4	1.741E-01	1.936E-01	1.343E-01	6.354E-02
5	1.085E-01	1.448E-01	1.609E01	9.898E-02
6	5.634E-02	9.021E-02	1.606E-01	1.285E-01
7	2.507E-02	4.818E-02	1.374E-01	1.430E-01
8	9.765E-03	2.252E-02	1.029E-01	1.392E-01
9	3.380E-03	9.354E-03	6.848E-02	1.205E-01
10	1.053E-03	3.497E-03	4.101E-02	9.382E-02
11	2.983E04	1.189E-03	2.233E-02	6.643E-02
12	7.744E-05	3.703E-04	1.115E-02	4.312E-02
13	1.856E-05	1.065E-04	5.136E-03	2.584E-02
14	4.130E-06	2.844E05	2.197E-03	1.437E-02
15	<u>8.579E-07</u>	<u>7.088E-06</u>	<u>8.773E-04</u>	7.463E-03
	1.000E+00	1.000E+00	9.995E-01	9.935E-01

Table 3.1. Probability of Different Numbers of Drilling Intrusions over 9900 yrs for Different Drilling Rates

a  $BHs \sim Boreholes$ 

b  $prob(n) = \left[ \left(9900 \lambda_d \right)^n / n! \right] \exp \left(-9900 \lambda_d \right)$ 

c  $\lambda_d = (25/10^4 \text{ yr km}^2) (0.1259 \text{ km}^2)$ , where 0.1259 km<sup>2</sup> is the waste disposal area used in the 1992 WIPP PA.

for  $\Delta t_1$  gives the time interval between the first and second drilling intrusions, with the outcome that  $t_2 = t_1 + \Delta t_1$ . This process can be continued until a time  $t_{n+1}$  is generated that exceeds 10,000 yr. The times  $t_1, t_2, ..., t_n$  then constitute the drilling times in  $\mathbf{x}_{st}$  in Eq. (3.1). The mining time  $t_{min}$  is sampled in a similar manner. An additional 6n uniformly distributed random numbers from [0, 1] can then be used to generate the elements  $p_i, l_i, a_i, d_i, k_i, b_i, i =$ 1, 2, ..., n, of  $\mathbf{x}_{st}$  from the distributions  $D_{PL}$ ,  $D_A$ ,  $D_{DB}$ ,  $D_P$ ,  $D_L$ ,  $D_B$ . A detailed description of the algorithm for generating individual futures is given in Table 3.2. Further, a hypothetical example of the specification of node properties is given in Fig. 3.3.

The discussion in this section has assumed that drilling intrusions and potash mining within the land withdrawal boundary are the only events involved in the definition of  $\mathbf{x}_{st}$  in Eq. (3.1) and hence in the sample space  $S_{st}$  for stochastic uncertainty. If the FEPs screening process identifies additional potential occurrences that should be included in the definition of  $(S_{st}, S_{st}, p_{st})$ , this should present no conceptual problem. Such occurrences will be incorporated into the definition of  $\mathbf{x}_{st}$  and their associated probabilities used in the sampling process described in the preceding paragraph. For example, if deemed sufficiently important to the calculation of normalized releases, climatic change could be incorporated into the definition of  $\mathbf{x}_{st}$  and hence  $(S_{st}, S_{st}, p_{st})$ .



#### **Time Between Drilling Intrusions**

Figure 3.2. Sampling of time intervals between drilling intrusions from cumulative distribution function (CDF) associated with drilling rate  $\lambda = \lambda_d$ .



Table 3.2. Required Input and Associated Calculations to Generate Single Future  $\mathbf{x}_{st}$  of Form Shown in Eqs. (2.2) and (3.1)

		Required Input
λ <sub>d</sub>	£	drilling rate $(yr^{-1})$ , which is a function of a drilling rate per unit area (e.g., 48 drilling intrusions/km <sup>2</sup> 10 <sup>4</sup> yr) and the area encompassed by the nodalization in Fig. 3.1
λ <sub>m</sub>	=	mining rate (yr <sup>-1</sup> ), which is specified to be $1 \times 10^{-4}$ yr <sup>-1</sup> in 40 CFR 194
nPL	Ŧ	number of plugging patterns in use in vicinity of the WIPP (e.g., 3)
pPL(j)	=	probability that a drilling intrusion will be sealed with plugging pattern $j$ , $j = 1, 2,, nPL$ (e.g., 1 ~ full concrete plug through Salado Formation to Bell Canyon Formation with a permeability of $5 \times 10^{-17}$ m <sup>2</sup> , 2~ two plug configuration with concrete plugs at Rustler/Salado interface and Castile/Bell Canyon interfaces, 3~ three plug configuration with concrete plugs at Rustler/Salado, Salado/Castile and Castile/Bell Canyon interfaces). The effects of these three plugging patterns on release modes from the repository will be written into the code for use with Option A (see Table 3.2).
nR	=	number of regions in repository (e.g., $nR = 3$ if the experimental area, operations area and waste disposal area are identified as separate regions)
pR(j)	=	probability that a random drilling intrusion into the <i>nR</i> regions will occur in region $j, j = 1, 2,, nR$ (i.e., $pR(j)$ is the ratio of the area of region $j$ to the total area of all regions)
pW(j, k)		probability that a random drilling intrusion into the excavated area of region j will encounter waste of type k, $k = 1, 2, 3$ , where 1~ no waste, 2~ CH waste, 3~ RH waste
nN(j)	=	number of nodes used in nodalization of region j
pN(j, k)	=	probability that a random drilling intrusion into region j will occur at node k, $k = 1, 2,, nNE(j)$
pE(j,k)	=	probability that a random drilling intrusion into region $j$ at node $k$ will encounter an excavated area of the repository (i.e., $1 - pE(j)$ is the probability that a random drilling intrusion into region $j$ at node $k$ will not encounter an excavated area)
pB(j, k)	Ŧ	probability that a drilling intrusion assigned to node $k$ of region $j$ will encounter pressurized brine in the Castile Formation
nBP	=	number of brine pockets
nD(p)	=	number of drilling intrusions required to deplete brine pocket $p, p = 1, 2,, nBP$
iB(j, k)	-	integer identifier indicating brine pocket associated with node k of region j (i.e., $iB(j, k)$ is an integer between 0 and $nBP$ )
-	Ŧ	number of waste panels (e.g., 10)

- iP(j, k) = integer identifier indicating waste panel associated with node k of region j (i.e., iP(j, k) is an integer between 0 and nP with iP(j, k) = 0 implying node not contained in a waste panel and iP(j, k) = p implying that node contained in waste panel p). Allows identification of  $l_i$  with specific waste panels.
  - iL(j) = integer identifier that indicates whether panel j is to be considered a lower panel (i.e., iL(j) = 1) or an upper panel (i.e., iL(j) = 2) for purpose of implementing blowout and spallings releases, j = 1, 2, ..., nP (e.g., iL(j) = 1 for Panels 4, 5 and Southern Equivalent Panel in Fig. 3.1 and iL(j) = 2 for Panels 1, 2, 3, 6, 7, 8 and Northern Equivalent Panel in Fig. 3.1)
    - tA = time period (e.g., 100 yr) over which active institutional controls are effective
- tPICD = length of time (yr) subsequent to end of active institutional controls over which passive institutional controls (PICs) are effective in reducing the rate of inadvertent human intrusion due to exploratory drilling (e.g., 700 yr)
- fPICD = reduction fraction for rate of inadvertent human intrusion due to exploratory drilling in the presence of PICs (i.e., the drilling rate is  $fPICD \lambda_d$  in the presence of PICs)
- *tPICM* = length of time (yr) subsequent to end of active institutional controls over which passive institutional controls (PICs) are effective in reducing the rate of inadvertent human intrusion due to potash mining (e.g., 700 yr)
- fPICM = reduction fraction for rate of inadvertent human intrusion due to potash mining in the presence of PICs (i.e., the mining rate is  $fPICM \lambda_m$  in the presence of PICs)
  - tM = length of time period (yr) over which the  $t_i$  and  $t_{min}$  are defined (i.e., 10,000 yr in analyses to show compliance with 40 CFR 191.13)
  - $D_{DB}$  = distribution of drillbit diameters. Supplied by user-defined subroutine; initially define as a triangular distribution with user-specified minimum, mode and maximum above and below repository; may be degenerate in 1996 WIPP PA (i.e., only one drillbit diameter in use)
  - $D_P$  = distribution of borehole permeability. Supplied by user-defined subroutine; initially define as a log triangular distribution with user specified minimum, mode and maximum above and below repository; may be degenerate (i.e., only one borehole permeability in use). In concept,  $k_i$  could be a time-dependent function with different values above and below the repository. See Table 3.3.

Generation of  $\mathbf{x}_{st} = [t_1, p_1, l_1, a_1, d_1, k_1, b_1, t_2, p_2, l_2, a_2, d_2, k_2, b_2, \dots, t_n, p_n, l_n, a_n, d_n, k_n, b_n, t_{min}]$ 

1. Sample  $t_1$  with a time dependent  $\lambda_d$  given by

$$\lambda_d(t) = 0 \qquad \text{if } 0 \le t \le tA$$
$$= fPICD \lambda_d \qquad \text{if } tA < t \le tA + tPICD$$
$$= \lambda_d \qquad \text{if } t > tA + tPICD$$

The actual generation of  $t_1$  and subsequent intrusion times is based on sampling the elapsed time between intrusions as indicated in conjunction with Fig. 3.2 (see Table 3.4).

- 2. Sample  $p_1$  with pPL(j)
- 3. Sample  $l_1$  and  $b_1$ 
  - 3.1 Use pR(j) to determine region in which intrusion occurs
  - 3.2 Use pN(j,k) to determine node at which intrusion occurs
  - 3.3 Use pB(j,k) to determine if intrusion penetrates pressurized brine
  - 3.4 Increment counter nH(iB(j, k)) if pressurized brine is penetrated and  $p_1 = 2$  to provide count of number of penetrations into each brine pocket (counter not incremented for  $p_1 = 1$ , 3, because of limited potential for brine depletion with these plugging patterns)
  - 3.5 Use pE(j,k) to determine if intrusion penetrates excavated area
    - 3.5.1 Case 1: Intrusion does not penetrate excavated area. Return to Step 1, generate new  $t_1$  by using  $\lambda_d$ (t) to sample elapsed time from initial  $t_1$  to new  $t_1$  and repeat Step 2 (i.e., the initial  $t_1$  is dropped from consideration because it did not penetrate an excavated area in the repository)
    - 3.5.2 Case 2: Intrusion penetrates excavated area
      - 3.5.2.1 Assign  $l_1$  integer identifier for node penetrated by drilling intrusion
      - 3.5.2.2 Assign  $b_1$  as follows:
        - $b_1 = 0$  if  $p_1 = 1$  (i.e., an intrusion that involves no long term brine flow from the repository to the Culebra due to low borehole permeability)
          - = 1 if  $p_1 = 2$ , drilling intrusion penetrates brine pocket p, and  $nH(p) \le nD(p)$  (i.e., an E1 intrusion into brine pocket p that can result in brine flow to the repository)
          - = 2 if (1)  $p_1 = 2$ , drilling intrusion penetrates brine pocket p, and nH(p) > nD(p), (2)  $p_1 = 2$  and drilling intrusion does not penetrate brine pocket, or (3)  $p_1 = 3$  (i.e., an E2 intrusion)

5

- 4. Sample  $a_1$  with use of pW(j, k)
- 5. Sample  $d_1$  with use of  $D_{DB}$
- 6. Sample  $k_1$  with use of  $D_P$

- 7. Repeat Steps 1 6 to determine properties (i.e.,  $t_2$ ,  $p_2$ ,  $l_2$ ,  $a_2$ ,  $d_2$ ,  $k_2$ ,  $b_2$ ) of 2<sup>nd</sup> drilling intrusion
- 8. Continue until  $t_{n+1} > tM$  (i.e., 10,000 yr in analyses to show compliance with 40 CFR 191.13); the 1<sup>st</sup> n intrusions define the drilling intrusions associated with  $\mathbf{x}_{st}$
- 9. Sample  $t_{min}$  (see Table 3.4) with a time dependent  $\lambda_m$  given by

$\lambda_m(t)$	= 0	$\text{if } 0 \le t \le tA$
	$= fPICM \lambda_m$	$if tA < t \le tA + tPICM$
	$= \lambda_m$	if tA + tPICM < t

- 1. Include an option where  $t_{min}$  is set to the largest integer multiple of 100 yr that is less than or equal to the sampled value of  $t_{min}$ . That is,  $t_{min} = 100 * AINT(t_{min} / 100)$  as a FORTRAN assignment, where AINT is the greatest integer function.
- 2. Check to see how hard it is to develop the input so that  $k_i$  is always specified as a vector  $\mathbf{k}_i$  of time-dependent values above and below the repository as indicated in the discussion for  $D_P$  above.
- 3. The distribution  $D_{PL}$  indicated in the text is defined by pPL(j);  $D_L$  is defined by pR(j), pE(j), pNE(j, k), pNN(j, k);  $D_A$  is defined by pW(j, k);  $D_B$  is defined by pBE(j, k).

Table 3.3. Anticipated Definition of  $D_P$  for Use in 1996 WIPP PA. Under Option A in CCDFGF, the implications of borehole permeability will be accounted for directly from the values assigned to  $p_i$  (i.e.,  $k_i$  will not be used). However, the permeability assignments indicated in this table will influence the details of the BRAGFLO calculations performed to support the use of CCDFGF.

- $DPL_{R-S}$  = distribution of plug life expectancy at the Rustler/Salado interface (e.g., degenerate with a single value of 200 yr)
- $DPL_{S-C}$  = distribution of plug life expectancy at the Salado/Castile interface (e.g., log triangular from 500 to 50000 yr with a mode at 5000 yr)
  - BHP = permeability (m<sup>2</sup>) of a sand-filled borehole

Algorithm to define  $D_P$ :

1. Use pPL(j) to define plugging pattern  $p_i$  used with *i*<sup>th</sup> drilling intrusion (see Table 3.2 for definition of pPL(j))



2. Assignment for  $p_i = 1$ 

$k_i = 1 \times 10^{-9} \mathrm{m}^2$	above Rustler/Salado interface for $t_i \le t \le t_i + \Delta t_{R-S}$ , where $\Delta t_{R-S}$ is randomly sampled	
	according to DPL <sub>R-S</sub>	

- = BHP above Rustler/Salado interface for  $t_i + \Delta t_{R-S} < t$
- =  $5 \times 10^{-17} \text{ m}^2$  below Rustler/Salado interface for  $t_i \le t$
- 3. Assignment for  $p_i = 2$ 
  - $k_i = 1 \times 10^{-9} \text{ m}^2$  above and below seal at Rustler/Salado interface for  $t_i \le t \le t_i + \Delta t_{R-S}$ , where  $\Delta t_{R-S}$  is randomly sampled according to DPL<sub>R-S</sub>
    - =  $5 \times 10^{-17} \text{ m}^2$  in seal at Rustler/Salado interface for  $t_i \le t \le t_i + \Delta t_{R-S}$
    - = BHP in entire borehole for  $t_i + \Delta t_{R-S} < t \le t_i + \Delta t_{R-S} + 1000 \text{ yr}$
    - = BHP above bottom of waste panel for  $t_i + \Delta t_{R-S} + 1000$  yr < t
    - = BHP/10 below bottom of waste panel for  $t_i + \Delta t_{R-S} + 1000$  yr < t
- 4. Assignment for  $p_i = 3$ . Same as in Step 3 but seal at Salado/Castile interface is assigned a value of  $5 \times 10^{-17} \text{ m}^2$ and assumed to last for a time period  $\Delta t_{S-C}$ , which is randomly sampled according to  $DPL_{S-C}$  (with the restriction that  $\Delta t_{R-S} \leq \Delta t_{S-C}$ )

Determination of Releases:

- 1.  $p_1 = 1$ : Cuttings, blowout and spallings releases calculated. Permeability in borehole is assumed to be sufficiently low to prevent releases to the Culebra due to brine flow and also to affect the releases associated with any subsequent intrusions (i.e., is same as no intrusion except for cuttings, blowout and spallings releases).
- 2.  $p_i = 2$ : Standard case for which BRAGFLO calculations will be performed. All release modes considered.
- 3.  $p_i = 3$ : Define to be same as E2 intrusion at time  $t_i$ . Rationale is that the dominant character of an E1 intrusion is the open borehole between the brine pocket and the waste panel for  $t_i \le t \le t_i + \Delta t_{R-S}$ ; this condition will not occur for  $p_i = 3$  because  $\Delta t_{R-S} \le \Delta t_{S-C}$ .

ſſ



$$nR = 3; pR(1) = pR(2) = 0.1, pR(3) = 0.8; nN(1) = nN(2) = 9, nN(3) = 72$$
$$pN(j, k) = 1/nN(j), k = 1, ..., nN(j), j = 1, 2, 3$$
$$\begin{bmatrix} 1 & k = 1 \\ 0 & k = 1 \end{bmatrix}$$

$$pW(1, k) = pW(2, k) = \begin{cases} 1 & k = 1 \\ 0 & k = 2 \\ 0 & k = 3 \end{cases} pW(3, k) = \begin{cases} 0 & k = 1 \\ 0.9 & k = 2 \\ 0.1 & k = 3 \end{cases}$$

 $nB = 2, \ pB(j, k) = \begin{cases} 0.1 & \text{if node } k \text{ underlain by pressurized brine} \\ 0 & \text{if node } k \text{ not underlain by pressurized brine} \end{cases}$ 

 $iB(j, k) = \begin{cases} i & \text{if node } k \text{ underlain by brine pocket } i \\ 0 & \text{if node } k \text{ not underlain by pressurized brine} \end{cases}$ 

 $A(j, k) = \text{total area (units}^2)$  associated with node k

$$E(j, k) = \text{excavated area (units}^2)$$
 associated with node k  
 $pE(j, k) = E(j, k)/A(j, k)$ 

$$pE(j, k) = E(j, k)/A(j, k)$$

$$iP(1,k)=iP(2,k)=0$$

 $iP(3, k) = 1, k = 7, 8, 9, 16, 17, 18, \dots, iP(3, k) = 8, k = 1, 2, 3, 10, 11, 12, \dots$ 

$$iL(j) = \begin{cases} 1 & j = 1, 2, 3, 6, 7, 8, 9 \\ 2 & j = 4, 5, 10 \end{cases}$$





Table 3.4. Algorithm to Sample Time of a Drilling Intrusion with

$$\lambda(t) = \begin{cases} \mu = fPIC \ \lambda & \text{for } tA \le t \le tA + tPIC \\ \lambda & \text{for } tA + tPIC < t \end{cases}$$

1. Sample random number r from uniform distribution on [0, 1]. Then,

$$r = 1 - \exp(-\mu\Delta t_1) \Rightarrow \Delta t_1 = \left[-\ln(1-r)\right]/\mu.$$

Two cases:

- 1.1 If  $tA + \Delta t_1 \le tA + tPIC$ , then  $t_1 = tA + \Delta t_1$ .
- 1.2 If  $tA + \Delta t_1 > tA + tPIC$ , then sample new random r and determine new  $\Delta t_1$ :

$$r = 1 - \exp(-\lambda \Delta t_1) \Rightarrow \Delta t_1 = \left[-\ln(1-r)\right]/\lambda.$$

Then,  $t_1 = tA + tPIC + \Delta t_1$ .

- 2. Repeat process to obtain  $t_2$ . Two cases:
  - 2.1 If  $t_1 < tA + tPIC$ , then identical Step 1 except that tA is replaced by  $t_1$ , and the two cases are based on the inequalities

 $t_1 + \Delta t_2 \le t_1 + tPIC$  and  $t_1 + \Delta t_2 > t_1 + tPIC$ .

- 2.2 If  $t_1 > tA + tPIC$ , then identical to Step 1.2 except that tA + tPIC is replaced by  $t_1$
- 3. Repeat Step 2 to obtain  $t_3, t_4, ..., t_{n+1}$ , where  $t_{n+1}$  is the first time to exceed tM (=10000 yr). Then,  $t_1, t_2, ..., t_n$  are the desired times.

#### 4. Construction of Releases to Accessible Environment for Individual Futures

#### 4.1 Mechanistic Results for Specific Futures

Each sampled future of the form indicated in Eqs. (2.2) and (3.1) will require the determination of a normalized release to the accessible environment. Determination of this release corresponds to evaluation of the function f in Eq. (2.3), which in turn requires evaluation of the programs in Fig. 2.2. Specifically, f is given by

$$f(\mathbf{x}_{st}) = f_{C}(\mathbf{x}_{st}) + f_{BL}[\mathbf{x}_{st}, f_{B}(\mathbf{x}_{st})] + f_{SP}[\mathbf{x}_{st}, f_{B}(\mathbf{x}_{st})] + f_{MB}[\mathbf{x}_{st}, f_{B}(\mathbf{x}_{st})] + f_{DL}[\mathbf{x}_{st}, f_{B}(\mathbf{x}_{st})] + f_{S}[\mathbf{x}_{st}, f_{B}(\mathbf{x}_{st})] + f_{S-T}\{\mathbf{x}_{st,0}, f_{S-F}(\mathbf{x}_{st,0}), f_{N-P-G}[\mathbf{x}_{st}, f_{B}(\mathbf{x}_{st})]\},$$
(4.1)

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  $\mathbf{x}_{st}$ ,
- $f_C(\mathbf{x}_{st}) \sim$  cuttings release to accessible environment for  $\mathbf{x}_{st}$  calculated with CUTTINGS,
- $f_B(\mathbf{x}_{st})$  ~ results calculated for  $\mathbf{x}_{st}$  with BRAGFLO; in practice,  $f_B(\mathbf{x}_{st})$  would be a vector containing a large amount of information,
- $f_{BL}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$  ~ blowout release to accessible environment for  $\mathbf{x}_{st}$  calculated with a modified version of BRAGFLO designated BLOWOUT; this calculation requires BRAGFLO results (i.e.,  $f_B(\mathbf{x}_{st})$ ) as input,
- $f_{SP}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})] \sim$  spallings release to accessible environment for  $\mathbf{x}_{st}$  calculated with the spallings model contained in CUTTINGS; this calculation requires BRAGFLO results (i.e.,  $f_B(\mathbf{x}_{st})$ ) as input,
- $f_{MB}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})] \sim$  release through anhydrite marker beds to accessible environment for  $\mathbf{x}_{st}$  calculated with NUTS; this calculation requires BRAGFLO results (i.e.,  $f_B(\mathbf{x}_{st})$ ) as input,
- $f_{DL}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})] \sim$  release through Dewey Lakes Red Beds to accessible environment for  $\mathbf{x}_{st}$  calculated with NUTS; this calculation requires BRAGFLO results (i.e.,  $f_B(\mathbf{x}_{st})$ ) as input,
- $f_S[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})] \sim$  release to land surface due to brine flow up a plugged borehole for  $\mathbf{x}_{st}$  calculated with NUTS or PANEL; this calculation requires BRAGFLO results (i.e.,  $f_B(\mathbf{x}_{st})$ ) as input,

 $f_{S-F}(\mathbf{x}_{st,0})$  ~ flow field calculated for  $\mathbf{x}_{st,0}$  with SECO-FLOW,

 $f_{N-P-G}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$  ~ release to Culebra for  $\mathbf{x}_{st}$  calculated with NUTS, PANEL and/or GRIDFLO as appropriate; this calculation requires BRAGFLO results (i.e.,  $f_B(\mathbf{x}_{st})$ ) as input,

 $f_{S-T} \{ \mathbf{x}_{st,0}, f_{S-F}(\mathbf{x}_{st,0}), f_{N-P-G}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})] \}$  ~ groundwater transport release through Culebra to accessible environment calculated with SECO-TRANSPORT; this calculation requires SECO-FLOW results (i.e.,  $f_{S-F}(\mathbf{x}_{st,0})$ ) and NUTS, PANEL and/or GRIDFLO results (i.e.,  $f_{N-P-G}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ) as input;  $\mathbf{x}_{st,0}$  is used as an argument to  $f_{S-T}$  because drilling intrusions are assumed to cause no perturbations to the flow field in the Culebra.

At present, releases to the accessible environment due to flow through the Dewey Lakes Red Beds (i.e.,  $f_{DL}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ) and also long-term flow up an abandoned borehole (i.e.,  $f_S[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ) are anticipated to be zero in the 1996 WIPP PA (i.e., there is no upward flow in a plugged and abandoned borehole above the Culebra).

Based on experience from the SPM analyses, the Monte Carlo CCDF construction procedure indicated in Eq. (2.3) and to be implemented by CCDFGF will require a sample size between 1000 and 10,000 (i.e.,  $1000 \le nS \le$  10,000 in Eq. (2.3)). The individual programs in Fig. 2.2 do not run fast enough to allow this number of evaluations of *f*. As a result, it will be necessary to evaluate the programs in Fig. 2.2 for a limited number of futures and then to use this limited number of evaluations to construct the releases for the large number of futures that must be considered in Eq. (2.3).

Until the final assumptions for the 1996 WIPP PA are decided upon and preliminary calculations with these assumptions are performed and analyzed, it is difficult to select an appropriate set of futures for evaluation with the models in Fig. 2.2 and also to decide on appropriate ways to use these results to estimate the releases for additional futures. However, to build and test the structure of CCDFGF, some assumptions have to be made about the calculations that will be performed with the models in Fig. 2.2. Therefore, this chapter will assume that certain calculated results with the models in Fig. 2.2 are available and then describe a way to use these results in the evaluation of the function f in Eqs. (2.3) and (4.1). Unfortunately, the possibility cannot be avoided that last minute recoding of the manipulations described in this chapter may be required to make the most appropriate use of the necessarily limited number of mechanistic calculations that will be performed.

For notational simplicity at later points in this presentation, the functions on the right hand side of Eq. (4.1) will typically be written with only  $\mathbf{x}_{st}$  an argument (e.g.,  $f_{BL}(\mathbf{x}_{st})$  will be used instead of  $f_{BL}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ). However, the underlying dependency on the other arguments will still be present.

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#### 4.2 Construction of Cuttings Releases

Cuttings releases will be constructed with results from the CUTTINGS program. Specifically, CUTTINGS will provide the cross-sectional areas of drilling intrusions through CH- and RH-waste. These areas will then be combined with the effective height of the waste and the concentration in individual waste streams to obtain cuttings releases.

The information being supplied to CCDFGF for use in the calculation of cuttings releases is given in Table 4.1. Further, the computational formulas used to determine the cuttings release (i.e.,  $f_C(\mathbf{x}_{st})$ ) are given in Table 4.2.

#### 4.3 Construction of Blowout Releases

Blowout releases will be constructed from brine releases (m<sup>3</sup>) to the surface obtained from a specialized formulation of BRAGFLO, designated by the name BLOWOUT, and radionuclide concentrations (EPA units/m<sup>3</sup>) in brine calculated by PANEL. The results transferred to CCDFGF from BLOWOUT and PANEL are summarized in Tables 4.3 and 4.4. Further, the computational formulas used to determine the blowout release (i.e.,  $f_{BL}(\mathbf{x}_{st})$ ) are given in Table 4.5.

In practice, it may not be possible to perform BLOWOUT calculations for all the cases indicated in Table 4.3. In this case, the calculations that are performed will have to be extended to give results for the cases for which calculations are not performed. The manner in which this can be done is described in Table 4.6 and Fig. 4.1.

#### 4.4 Construction of Spallings Releases

The construction of the spallings release  $f_{SP}(\mathbf{x}_{st})$  is identical to that described in Sect. 4.3 for the calculation of blowout releases except that volumes of solid material released will be used rather than volumes of brine. These solid releases will be calculated with the spallings submodel of the CUTTINGS program.

The table of input values for spallings releases will be identical in structure to that shown in Table 4.3 for blowout releases (i.e., to obtain the table of input values for the spallings calculation, simply modify Table 4.3 by replacing the letters "*BL*" in the variable names with the letters "*SP*," replacing the word "blowout" with the word "spallings"), and changing the release units from "m<sup>3</sup> brine" to "m<sup>3</sup> solids." Further, similar modifications hold for the computational formulas in Table 4.5 with the additional requirement that the dissolved concentrations (i.e., CAVGE0D( $t_i$ ), CAVGE2D( $t_i$ ), CAVGE1D( $t_i$ )) be replaced by a concentration per unit volume of solid waste (i.e., CAVG( $t_i$ ) • DWS, where CAVG( $t_i$ ) is concentration in waste at time  $t_i$ , EPA units/kg, and DWS is the density of the solid components of the waste, kg/m<sup>3</sup>; see Table 4.4).



 

 Table 4.1
 Results from Baseline Inventory (BIR) and Calculations with CUTTINGS Transferred to CCDFGF for Use in Determination of Releases Due to Cuttings Removal. The information in this table will repeat for each element in a sample.

#### Results Transferred to CCDFGF

DBDIAM: Drillbit diameter (m) used in calculation of cuttings releases (e.g., 0.311 m ~ 12.25 in.)

NCH: Number of waste streams for CH waste (e.g., 569)

ACH: Cross-sectional area (m<sup>2</sup>) of waste removed by drilling intrusion through CH waste (calculated by CUTTINGS)

HCH: Emplaced height (m) of CH waste (i.e., ACH • HCH equals volume of original (uncompacted) waste removed by a drilling intrusion) (e.g., 3.96 m)

FCH: Fraction of volume removed by drilling intrusion through portion of repository containing CH waste that is actually CH waste (e.g., 0.4; see Sect. 3.1.1, SAND92-0700/3)

PCH (ICH): Probability that a randomly sampled unit (i.e., drum) of CH waste will come from waste stream ICH, ICH = 1, 2, ..., NCH (Note:  $\Sigma_i$  PCH(i) = 1)

NTMCH: Number of times at which radionuclide concentrations are calculated for CH waste (e.g., 9)

TMCH (ITMCH): Times (yr) at which radionuclide concentrations are calculated for CH waste, ITMCH = 1, 2, ..., NTMCH (e.g., 100, 125, 175, 350, 1000, 3000, 5000, 7500, 10000 yr)

CCH (ICH, ITMCH): Radionuclide concentration (EPA units/m<sup>3</sup>, where EPA unit refers to the normalized radionuclide unit defined in 40 CFR 194<sup>3</sup>) in CH waste stream ICH at time TMCH (ITMCH), ICH = 1, 2, ..., NCH and ITMCH = 1, 2, ..., NTMCH

NSMPCH: Number of waste streams intersected by a single drilling intrusion through CH waste (e.g., 3)

NRH, ARH, HRH, FRH, PRH (IRH), NTMRH, TMRH (ITMRH), CRH (IRH, ITMRH, NSMPRH): Same as NCH, ACH, HCH, PCH (ICH), NTMCH, TMCH (ITMCH), CCH (ICH, ITMCH), NSMPCH but for RH waste

Conceptual Structure of Transfer File for One Sample Element

DBDIAM	(e.g.,	0.311	m)

NCH (e.g., 569)

ACH

HCH (e.g., 3.96 m)

FCH (e.g., 0.4)

PCH (ICH): ICH = 1, ..., NCH

NTMCH (e.g., 9)


```
TMCH (ITMCH): ITMCH = 1, ..., NTMCH (e.g., 100, 125, 175, 350, 1000, 3000, 5000, 7500, 10000)

CCH (ICH, ITMCH): (ITMCH = 1, ..., NTMCH), ICH = 1, ..., NCH

NRH (e.g., 1)

ARH (e.g., DBDIAM)

HRH (e.g., )

FRH (e.g., 1)

PRH (IRH): IRH = 1, ..., NRH

NTMRH (e.g., 9)

TMRH (ITMRH): ITMRH = 1, ..., NTMRH (e.g., 100, 125, 175, 350, 1000, 3000, 5000, 7500, 10000)

CRH (IRH, ITMRH): (ITMRH = 1, ..., NTMRH), IRH = 1, ..., NRH
```

Table 4.2. Calculation of Cuttings Release  $f_C$  for an Arbitrary Future  $\mathbf{x}_{st}$ 

#### Arbitrary future:

 $\mathbf{x}_{st} = [t_1, p_1, l_1, a_1, d_1, k_1, b_1, t_2, p_2, l_2, a_2, d_2, k_2, b_2, \dots, t_n, p_n, l_n, a_n, d_n, k_n, b_n, t_{min}]$ 

Notation: $cW_{ij}$  = concentration (EPA units/m<sup>3</sup>) in waste stream j at time  $t_i$ 

$$= \begin{cases} \text{CCH}(j, t_i)^2 & \text{if } a_i \sim \text{CH waste} \\ \text{CRH}(j, t_i) & \text{if } a_i \sim \text{RH waste} \end{cases}$$

 $v_i$  = volume (m<sup>3</sup>) of waste removed by *i*<sup>th</sup> drilling intrusion

$$= \begin{cases} ACH HCH & \text{if } a_i \sim CH \text{ waste} \\ ARH HRH & \text{if } a_i \sim RH \text{ waste} \end{cases}$$

 $fW_i$  = fraction of removed volume that is waste

$$=\begin{cases} FCH & \text{if } a_i \sim CH \text{ waste} \\ FRH & \text{if } a_i \sim RH \text{ waste} \end{cases}$$

 $\delta$  = drillbit diameter (m)

= DBDIAM

-

m(i) = number of waste streams intersected by i<sup>th</sup> drilling intrusion

 $\begin{cases} NSMPCH & \text{if } a_i \sim CH \text{ waste} \\ NSMPRH & \text{if } a_i \sim RH \text{ waste} \end{cases}$ 



n(i) = number of waste streams associated with waste class (i.e., CH or RH) intersected by  $i^{\text{th}}$  drilling intrusion

$$= \begin{cases} \text{NCH} & \text{if } a_i \sim \text{CH waste} \\ \text{NRH} & \text{if } a_i \sim \text{RH waste} \end{cases}$$

 $\pi_{ij}$  = probability of waste stream j for waste class (i.e., CH or RH) intersected by i<sup>th</sup> drilling intrusion

$$=\begin{cases} PCH(j) & \text{if } a_i \sim CH \text{ waste} \\ PRH(j) & \text{if } a_i \sim RH \text{ waste} \end{cases}$$

j(i, r) = integer randomly selected from 1, 2, ..., n(i) according to probabilities  $\pi_{ij}$ ,  $j = 1, 2, ..., n_{(i)}$ , for r = 1, 2, ..., m(i)

Evaluation of  $f_C(\mathbf{x}_{st})$ :

$$\overline{cW_i}^b = 0 \qquad \text{if } a_i \sim \text{no waste}$$

$$= \left(\sum_{r=1}^{m(i)} \overline{cW_{i, j(i, r)}}\right) / m(i) \qquad \text{if } a_i \sim \text{CH or RH waste}$$

$$f_C(\mathbf{x}_{st}) = \sum_{i=1}^n (d_i / \delta)^2 fW_i v_i \overline{cW_i}$$

<sup>a</sup> Interpolation is implied when a real value appears in an array rather than an integer. Thus,

$$CCH(j, t_i) = CCH(j, l) + \left[\frac{t_i - TMCH(l)}{TMCH(l+1) - TMCH(l)}\right] [CCH(j, l+1) - CCH(j, l)],$$

where l is the largest integer such that  $TMCH(l) \le t_i$ . This notational convention will be used repeatedly to simplify the description of computational procedures that require interpolation.

<sup>b</sup> Technically, j(i, r) is the outcome of stochastic uncertainty (i.e., variation in the cuttings release due to random variation in where the *i*<sup>th</sup> drilling intrusion occurs). Thus, j(i, r) is actually part of the definition of  $a_i$  discussed in Chapt. 3. When viewed in this manner,  $a_i$  becomes a vector of the form  $\mathbf{a}_i = [a_i, j(i, r), r = 1, 2, ..., m(i)]$ .



# Table 4.3. Results from Calculations with BLOWOUT Transferred to CCDFGF for Use in Determination of Releases Due to Blowout. The information in this table will repeat for each sample element.

#### Results Transferred to CCDFGF

NTMBLEOL: Number of times at which blowout releases are calculated with BLOWOUT for an E0 (i.e., initial) intrusion into the lower waste panel (e.g., 12)

TMBLEOL (ITM): Times (yr) at which blowout releases are calculated for an E0 intrusion into the lower waste panel, ITM = 1, 2, ..., NTMBLEOL (e.g., 100, 350, 1000, 2000, 3000, ..., 10000 yr)

RBLEOL (ITM): Blowout release (m<sup>3</sup> brine) for an E0 intrusion into the lower waste panel at time TMBLEOL (ITM), ITM = 1, 2, ..., NTMBLEOL

NTMBLEOU, TMBLEOU, RBLEOU (ITM): Same as NTMBLEOL, TMBLEOL, RBLEOL (ITM) but for intrusion into the upper waste panels

NTMBLE1S: Number of times at which initial E1 intrusions (i.e., into pressurized brine in the Castile Formation) occur for use in calculation of blowout releases for second and subsequent intrusions into the same waste panel (e.g., 7). See Fig. 4.1 for temporal structure of calculations for second intrusions into the repository.

TMBLE1S (ITM1): Times (yr) at which initial E1 intrusions occur for use in calculation of blowout releases for second and subsequent intrusions into same waste panel, ITM1 = 1, 2, ..., NTMBLE1S (e.g., 100, 350, 1000, 3000, 5000, 7500, 10000 yr)

NTBLE1S2 (ITM1): Number of times at which a second intrusion into a waste panel occurs following an initial E1 intrusion into that panel at time TMBLE1S (ITM1), ITM1 = 1, 2, ..., NTMBLE1S (e.g., 13, 13, 12, 9, 7, 5, 1)

TMBLE1S2 (ITM1, ITM2): Times (yr) at which a second intrusion into a waste panel occurs following an initial E1 intrusion into that panel at time TMBLE1S (ITM1), ITM2 = 1, 2, ..., NTBLE1S2 (ITM1) and ITM1 = 1, 2, ..., NTMBLE1S (e.g., TMBLE1S(1) = 100 yr: 100, 300, 500, 1000, 2000, ..., 10000 yr; TMBLE1S(2) = 350 yr: 350, 550, 750, 1000, 3000, ..., 10000 yr; TMBLE1S(3) = 1000 yr: 1000, 1200, 1400, 2000, 3000, ..., 10000 yr; TMBLE1S(4) = 3000 yr: 3000, 3200, 3400, 4000, 5000, ..., 10000 yr; TMBLE1S(5) = 7500 yr: 7500, 7700, 7900, 9000, 10000 yr; TMBLE1S(6) = 10000 yr: 10000 yr)

RBLE1S2 (ITM1 ITM2): Blowout release (m<sup>3</sup> brine) for a second intrusion into a waste panel at time TMBLE1S2 (ITM2, ITM1) that previously experienced an initial E1 intrusion at time TMBLE1S (ITM1), ITM2 = 1, 2, ..., NTBLE1S2 (ITM1) and ITM1 = 1, 2, ..., NTMBLE1S

NTMBLE1D, TMBLE1D (ITM1), NTBLE1D2 (ITM1), TMBLE1D2 (ITM1, ITM2), RBLE1D2 (ITM1, ITM2): Same as NTMBLE1S, TMBLE1S, NTBLE1S2 (ITM1), TMBLE1S2 (ITM1, ITM2), RBLE1S2 (ITM1, ITM2) except that the second intrusion is into a different waste panel than the first intrusion

NTMBLE2S, TMBLE2S (ITM1), NTBLE2S2 (ITM1), TMBLE2S2 (ITM1, ITM2), RBLE2S2 (ITM1, ITM2), NTMBLE2D, TMBLE2D (ITM1), NTBLE2D2 (ITM1), TMBLE2D2 (ITM1, ITM2), RBLE2D2 (ITM1, ITM2): Same as NTMBLE1S, TMBLE1S (ITM1), NTBLE1S2 (ITM1), TMBLE1S2 (ITM1, ITM2), RBLE1S2 (ITM1, ITM2), NTMBLE1D, TMBLE1D (ITM1), NTBLE1D (ITM1), TMBLE1D2 (ITM1, ITM2), RBLE1D2 (ITM1, ITM2) except for an initial E2 intrusion (i.e., an intrusion that does not penetrate pressurized brine in the Castile Formation) rather than an initial E1 intrusion

Conceptual Structure of Transfer File for One Sample Element

NTMBLE0L (e.g., 12)

TMBLE0L (ITM): ITM = 1, ..., NTMBLE0L (e.g., 100, 350, 1000, 2000, 3000, ..., 10000 yr)

RBLEOL (ITM): ITM = 1, ..., NTMBLEOL

NTMBLE0U (e.g., 12)

TMBLE0U (ITM): ITM = 1, ..., NTMBLE0U (e.g., 100, 350, 1000, 2000, 3000, ..., 10000 yr)

RBLEOU (ITM): ITM = 1, ..., NTMBLEOU

NTMBLE1S (e.g., 7)

TMBLE1S (ITM1): ITM1 = 1, ..., NTMBLE1S (e.g., 100, 350, 1000, 3000, 5000, 7500, 10000 yr)

NTBLE1S2 (ITM1): ITM1 = 1, ..., NTMBLE1S (e.g., 13, 13, 12, 9, 7, 5, 1)

TMBLE1S2 (ITM1, ITME2): (ITM2 = 1, ..., NTBLE1S2 (ITM1), ITM1 = 1, ..., NTMBLE1S (e.g., 100, 300, 500, 1000, 2000, ..., 10000; 350, 550, 750, 1000, 2000, ..., 10000; 1000, 1200, 1400, 2000, 3000, ..., 10000; 3000, 3200, 3400, 4000, 5000, ..., 10000; 5000, 5200, 5400, 6000, 7000, ..., 10000; 7500, 7700, 7900, 9000, 10000; 10000)

RBLE1S2 (ITM1, ITM2): (ITM2 = 1, ..., NTBLE1S2 (ITM1)), ITM1 = 1, ..., NTMBLE1S

NTMBLE1D (e.g., 7)

TMBLE1D (ITM1): ITM1 = 1, ..., NTMBLE1D (e.g., 100, 350, 1000, 3000, 5000, 7500, 10000 yr)

NTBLE1D2 (ITM1): ITM1 = 1, ..., NTMBLE1D (e.g., 13, 13, 12, 9, 7, 5, 1)

TMBLE1D2 (ITM1, ITM2): (ITM2 = 1, ..., NTBLE1D2 (ITM1), ITM1 = 1, ..., NTMBLE1D (e.g., 100, 300, 500, 1000, 2000, ..., 10000; 350, 550, 750, 1000, 2000, ..., 10000; 1000, 1200, 1400, 2000, 3000, ..., 10000; 3000, 3200, 3400, 4000, 5000, ..., 10000; 5000, 5200, 5400, 6000, 7000, ..., 10000; 7500, 7700, 7900, 9000, 10000; 10000)

RBLE1D2 (ITM1, ITM2): (ITM2 = 1, ..., NTBLE1D2 (ITM1)), ITM1 = 1, ..., NTMBLE1D

NTMBLE2S (e.g., 7)

TMBLE2S (ITM1): ITM1 = 1, ..., NTMBLE2S (e.g., 100, 350, 1000, 3000, 5000, 7500, 10000 yr)

NTBLE2S2 (ITM1): ITM1 = 1, ..., NTMBLE2S (e.g., 13, 13, 12, 9, 7, 5, 1)

TMBLE2S2 (ITM1, ITM2): (ITM2 = 1, ..., NTBLE2S2 (ITM1), ITM1 = 1, ..., NTMBLE2S (e.g., 100, 300, 500, 1000, 2000, ..., 10000; 350, 550, 750, 1000, 2000, ..., 10000; 1000, 1200, 1400, 2000, 3000, ..., 10000; 3000, 3200, 3400, 4000, 5000, ..., 10000; 5000, 5200, 5400, 6000, 7000, ..., 10000; 7500, 7700, 7900, 9000, 10000; 10000)

RBLE2S2 (ITM1, ITM2): (ITM2 = 1, ..., NTBLE2S2 (ITM1)), ITM1 = 1, ..., NTMBLE2S

NTMBLE2D (e.g., 7)

TMBLE2D (ITM1): ITM1 = 1, ..., NTMBLE2D (e.g., 100, 350, 1000, 3000, 5000, 7500, 10000 yr)

NTBLE2D2 (ITM1): ITM1 = 1, ..., NTMBLE2D (e.g., 13, 13, 12, 9, 7, 5, 1)

TMBLE2D2 (ITM1, ITM2): (ITM2 = 1, ..., NTBLE2D2 (ITM1), ITM1 = 1, ..., NTMBLE2D (e.g., 100, 300, 500, 1000, 2000, ..., 10000; 350, 550, 750, 1000, 2000, ..., 10000; 1000, 1200, 1400, 2000, 3000, ..., 10000; 3000, 3200, 3400, 4000, 5000, ..., 10000; 5000, 5200, 5400, 6000, 7000, ..., 10000; 7500, 7700, 7900, 9000, 10000; 10000)

RBLE2D2 (ITM1, ITM2): (ITM2 = 1, ..., NTBLE2D2 (ITM1)), ITM1 = 1, ..., NTMBLE2D



TRI-6342-4696-0

Fig. 4.1. Pairs of drilling intrusions used in the calculation of blowout releases. Solid points (•) represent calculations performed with BLOWOUT; open points (O) represent results constructed from BLOWOUT calculations. Points in table correspond to pairs of times at which RBLE1S (ITM1, ITM2), RBLE1D (ITM1, ITM2), RBLE2S (ITM1, ITM2) and RBLE2D (ITM1, ITM2) will be generated for use in CCDF constructions.

 Table 4.4.
 Results from Calculations with PANEL Transferred to CCDFGF for Use in Determination of Releases

 Due to Blowout and Spallings.
 The information in this table will repeat for each sample element.

**Results Transferred to CCDFGF** 

NTMAVG: Number of times at which average radionuclide concentrations over the entire repository are calculated (e.g., 9)

TMAVG (ITMA): Times (yr) at which average radionuclide concentrations are calculated, ITMA = 1, 2, ..., NTMAVG (e.g., 100, 125, 175, 350, 1000, 3000, 5000, 7500, 10000 yr)

CAVG (ITMA): Radionuclide concentration (EPA units/kg) in repository averaged over all waste streams at time TMAVG (ITMA), ITMA = 1, 2, ..., NTMAVG

DWS: Density (kg/m<sup>3</sup>) of the solid components of the waste. Product of CAVG (ITMA) and DWS gives radionuclide concentration (EPA units/m<sup>3</sup>) in solid material removed in a spallings release at time TMAVG (ITMA)

CAVGE0D (ITMA): Dissolved radionuclide concentration (EPA units/m<sup>3</sup>) in repository averaged over all waste streams under E0 (i.e., undisturbed) conditions at time TMAVG (ITMA), ITMA = 1, 2, ..., NTMAVG

CAVGE1D (ITMA): Dissolved radionuclide concentration (EPA units/ $m^3$ ) in repository averaged over all waste streams at time TMAVG (ITMA) subsequent to an E1 intrusion, ITMA = 1, 2, ..., NTMAVG

CAVGE2D (ITMA): Same as CAVGE1D but for an E2 intrusion

Conceptual Structure of Transfer File for One Sample Element

NTMAVG (e.g., 9)

TMAVG (ITMA): ITMA = 1, ..., NTMAVG (e.g., 100, 125, 175, 350, 1000, 3000, 5000, 7500, 10000)

CAVG (ITMA): ITMA = 1, ..., NTMAVG

CAVGEOD (ITMA): ITMA = 1, ..., NTMAVG

CAVGE1D (ITMA): ITMA = 1, ..., NTMAVG

CAVGE2D (ITMA): ITMA = 1, ..., NTMAVG

Arbitrary future:

$$\mathbf{x}_{st} = [t_1, p_1, l_1, a_1, d_1, k_1, b_1, t_2, p_2, l_2, a_2, d_2, k_2, b_2, \dots, t_n, p_n, l_n, a_n, d_n, k_n, b_n, t_{min}]$$

Release  $rBL_i$  for intrusion into a pressurized repository (i.e., i = 1 or  $b_i = 0$  for j = 1, 2, ..., i - 1):

$$rBL_{i} = 0$$
 if  $l_{i}$  not in waste panel or  $a_{i} \sim no$   
= VBLE0U $(t_{i})^{a}$  CAVGE0D $(t_{i})$  if  $l_{i}$  in upper waste panels  
= VBLE0L $(t_{i})$  CAVGE0D $(t_{i})$  if  $l_{i}$  in lower waste panels

Release  $rBL_i$  for  $i^{th}$  intrusion into a depressurized repository with no E1 intrusion in first i-1 intrusions (i.e.,  $b_k = 0$  for  $k = 1, 2, ..., j-1, b_j = 2, b_k \neq 1$  for k = j + 1, j + 2, ..., i-1):

or RH waste

 $rBL_{i} = 0$   $= VBLE2S2(t_{j}, t_{i})^{b}$   $CAVGE2D(t_{i})$   $if l_{j}, l_{i} \text{ in same waste panel}$   $= VBLE2D2(t_{j}, t_{i})^{c}$   $CAVGE2D(t_{i})$   $if l_{j}, l_{i} \text{ in different waste panels}$ 

Release  $rBL_i$  for *i*<sup>th</sup> intrusion into a depressurized repository with first E1 intrusion at time  $t_j < t_i$  (i.e.,  $b_k \neq 1$  for  $k = 1, 2, ..., j - 1, b_j = 1$ ):

 $rBL_{i} = 0$   $= VBLE1S2(t_{j}, t_{i}) CAVGE1D(t_{i})$   $= VBLE1D2(t_{j}, t_{i}) CAVGE1D(t_{i})$   $= VBLE1D2(t_{j}, t_{i}) CAVGE1D(t_{i})$   $= t_{i}$   $= t_{i}$ 

Set criterion for terminating blowout release:

nMX	=	n	No termination criterion, use blowout releases from all intrusions
	=	$\min \{nBL, n\}$	Terminate after first nBL intrusions
	Ξ	$\min \{nE1 + nBL, n\}$	Terminate after first <i>nBL</i> intrusions following initial E1 intrusion at time $t_{nE1}$
	Ξ	$\min \{nP, n\}$	Terminate after first intrusion time $t_{nP}$ at which the borehole permeability $k_{nP}$ exceeds a specified value

Evaluation of  $f_{BL}(\mathbf{x}_{st})$ :

$$f_{BL}(\mathbf{x}_{st}) = \sum_{i=1}^{nMX} rBL_i$$

<sup>&</sup>lt;sup>a</sup> Here and elsewhere, appearance of a real quantity as an array subscript implies interpolation (see Table 4.2).

<sup>&</sup>lt;sup>b</sup> Here and elsewhere, appearance of two real quantities as array subscripts implies two dimensional interpolation.

Table 4.6. Extension of Limited Number of BLOWOUT Calculations to Obtain Results in Table 4.3.

#### Anticipated Blowout Calculations for 1996 WIPP PA

Initial (i.e., E0) intrusion into lower waste panel at 100, 350, 1000, 2000, 3000, ..., 10000 yr. Defines RBLE0L (ITM), ITM = 1, 2, ..., 12

Initial (i.e., E0) intrusion into upper waste panel at 100, 350, 1000, 2000, 3000, ..., 10000 yr. Defines RBLE0U (ITM), ITM = 1, 2, ..., 12

Initial E1 intrusion at 350 yr followed by intrusion into same waste panel at 550, 750, 1000, 2000, 3000, ..., 10000 yr. Defines RBLE1S (2, ITM2), ITM2 = 2, 3, ..., 13

Initial E1 intrusion at 350 yr followed by intrusions into different waste panel at 550, 750, 1000, 2000, 3000, ..., 10000 yr. Defines RBLE2D (2, ITM2), ITM2 = 2, 3, ..., 13

Initial E1 intrusion at 1000 yr followed by intrusion into same waste panel at 1200, 1400, 2000, 3000, ..., 10000 yr. Defines RBLE1S (3, ITM2), ITM2 = 2, 3, ..., 12

Initial E1 intrusion at 1000 yr followed by intrusion into different waste panel at 1200, 1400, 2000, 3000, ..., 10000 yr. Defines RBLE1D (3, ITM2), ITM2 = 2, 3, ..., 12

Same results calculated for intrusions subsequent to an E2 intrusion (i.e., RBLE2S (2, ITM2), RBLE2D (2, ITM2), RBLE2D (3, ITM2))

Extension of Calculated Results (See Fig. 4.1)

- 1. For initial intrusions at 350 and 1000 yr, assign same value for second intrusion at  $\Delta t = 0$  yr as for second intrusion at  $\Delta t = 200$  yr.
- 2. For initial intrusion at 100 yr, assign value for second intrusion by interpolating on  $\Delta t$  for initial intrusion at 350 yr; value for  $\Delta t = 9900$  yr requires extrapolation.
- 3. For initial intrusion at 3000, 5000, 7500 and 10000 yr, assign value for second intrusion by interpolating on  $\Delta t$  for initial intrusion at 1000 yr.

As for blowout calculations, the number of cases for which calculations can be performed will be less than the number of cases indicated in Table 4.3. Thus, it will be necessary to use the extension procedures described in Table 4.6 and Fig. 4.1.

## 4.5 Radionuclide Transport Away from Repository by Flowing Brine

The information from calculations with NUTS and PANEL that will be transferred to CCDFGF for use in the estimation of radionuclide transport away from the repository by flowing brine is listed in Table 4.7.

 Table 4.7.
 Results from Calculations with NUTS and PANEL Related to Radionuclide Transport Away from the Repository by Flowing Brine Transferred to CCDFGF. The information in this table will repeat for each sample element

#### **Results Transferred to CCDFGF**

NDCHAIN: Number of decay chains (e.g., 3)

NMBR (ICH): Number of elements in decay chain ICH, ICH = 1, 2, ..., NDCHAIN (e.g., 1, 1, 2)

RDECAY (ICH, IMBR): Decay constant  $(yr^{-1})$  for element IMBR of decay chain ICH, IMBR = 1, 2, ..., NMBR (ICH) and ICH = 1, 2, ..., NDCHAIN (e.g., \_\_, \_\_, \_\_)

CNVRTCM (ICH, IMBR): Conversion factor from curies to moles (mole/Ci) for element IMBR of decay chain ICH, IMBR = 1, 2, ..., NMBR (ICH) and ICH = 1, 2, ..., NDCHAIN (e.g., \_\_, \_\_, \_\_)

CNVRTKM (ICH, IMBR): Conversion factor from kilograms to moles (mole/kg) for element IMBR of decay chain ICH, IMBR = 1, 2, ..., NMBR (ICH) and ICH  $\approx$  1, 2, ..., NDCHAIN (e.g., \_\_, \_\_, \_\_)

NMDCMBR (ICH, IMBR): Name of member IMBR of decay chain ICH, IMBR = 1, 2, ..., NMBR (ICH) and ICH = 1, 2, ..., NDCHAIN (e.g., Pu-239, Am-241, U-234, Th-230)

RLIMIT (ICH, IMBR): EPA release limit (Ci) for element IMBR of decay chain ICH, IMBR = 1, 2, ..., NMBR (ICH) and ICH = 1, 2, ..., NDCHAIN (e.g., 100, 100, 100, 10 Ci)

TOTINV: Total inventory (Ci) of  $\alpha$ -emitting radionuclides placed in repository with halflives greater than 20 yr (e.g.,  $4.07 \times 10^6$  Ci)

NCOLSP: Number of colloid species (e.g., 4)

FRDCLE0 (ICOL, ICH, IMBR): Fraction of element IMBR of decay chain ICH attached to colloid specie ICOL for undisturbed (i.e., E0) conditions, IMBR = 1, 2, ..., NMBR (ICH), ICH = 1, 2, ..., NDCHAIN and ICOL = 1, 2, ..., NCOLSP

FRDCLE1 (ICOL, ICH, IMBR), FRDCLE2 (ICOL, ICH, IMBR): Same as FRDCLE0 (ICOL, ICH, IMBR) except for E1 and E2 intrusions, respectively

NTMRELE0: Number of times used to define intervals over which releases from the repository under undisturbed (i.e., E0) conditions due to brine flow are recorded (e.g., 198)

TMGWRPE0 (ITM): Times (yr) used to define intervals over which releases from the repository under undisturbed (i.e., E0) conditions due to brine flow are recorded, ITM = 1, 2, ..., NTMRELE0 (e.g., 100, 150, 200, ..., 9950, 10000)

RCGWRPE0 (ICH, IMBR, ITM): Cumulative release (kg) of element IMBR of decay chain ICH from the repository to the Culebra under undisturbed (i.e., E0) conditions through time TMGWRPE0 (ITM) due to brine flow, ITM = 1, 2, ..., NTMRELE0, IMBR = 1, 2, ..., NMBR (ICH) and ICH = 1, 2, ..., NDCHAIN

RAGWRPE0 (ITM): Cumulative release (EPA units) of all radioactive species from the repository to the accessible environment under undisturbed (i.e., E0) conditions through time TMGWRPE0 (ITM) due to brine flow in the anhydrite marker beds, ITM = 1, 2, ..., NTMRELE0

Table 4.7. Continued

NTME1: Number of times at which calculations for E1 intrusions are performed (e.g., 7)

TME1 (ITME1): Times (yr) at which calculations for E1 intrusions are performed, ITME1 = 1, 2, ..., NTME1 (e.g., 100, 350, 1000, 3000, 5000, 7000, 9000 yr)

NTMRELE1 (ITME1): Number of times used to define intervals over which releases from the repository are recorded for an E1 intrusion at time TME1 (ITME1), ITME1 = 1, 2, ..., NTME1 (e.g., 198, 193, 180, 140, 100, 60, 20)

TMGWRPE1 (ITME1, ITM): Times (yr) used to define intervals over which releases from the repository due to brine transport are recorded for an E1 intrusion at time TME1 (ITME1), ITME1 = 1, 2, ..., NTME1 and ITM = 1, 2, ..., NTMRELE1 (ITME1)

RGWRPE1 (ITME1, ICH, IMBR, ITM): Cumulative release (kg) of element IMBR of decay chain ICH from the repository to the Culebra through time TMGWRPE1 (ITME1, ITM) due to brine flow for an E1 intrusion at time TME1 (ITME1), ITM = 1, 2, ..., NTMRELE1 (ITME1), IMBR = 1, 2, ..., NMBR (ICH), ICH = 1, 2, ..., NDCHAIN, and ITME1 = 1, 2, ..., NTME1

RAGWRPE1 (ITME1, ITM): Cumulative release (EPA units) from the repository to the accessible environment through time TMGWRPE1 (ITME1, ITM) due to brine flow in the anhydrite marker beds for an E1 intrusion at time TME1 (ITME1), ITME1 = 1, 2, ..., NTME1 and ITM = 1, 2, ..., NTMRELE1 (ITME1)

NTME2, TME2 (ITME2), NTMRELE2 (ITME2), TMGWRPE2 (ITME2, ITM), RCGWRPE2 (ITME2, ICH, IMBR, ITM), RAGWRPE2 (ITME2, ITM): Same as NTME1, TME1 (ITME1), NTMRELE1 (ITME1), TMGWRPE1 (ITME1, ITM), RCGWRPE1 (ITME1, ICH, IMBR, ITM), RAGWRPE1 (ITME1, ITM) but for an E2 intrusion in place at time TME2 (ITME2)

NTME12, TME12 (ITME12), NTMRELE12 (ITME12), TMGWRPE12 (ITME12, ITM), RCGWRPE12 (ITME12, ICH, IMBR, ITM), RAGWRPE12 (ITME12, ITM): Same as NTME1, TME1 (ITME1), NTMRELE1 (ITME1), TMGWRPE1 (ITME1, ITM), RCGWRPE1 (ITME1, ICH, IMBR, ITM), RAGWRPE1 (ITME1, ITM) but for an E1E2 intrusion in place at time TME12 (ITME12)

Conceptual Structure of Transfer File for One Sample Element

NDCHAIN (e.g., 3)

NMBR (ICH): ICH = 1, ..., NDCHAIN (e.g., 1, 1, 2)

NMDCMBR (ICH, IMBR): (IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN (e.g., Pu-239, Am-241, U-234, Th-230)

RDECAY (ICH, IMBR): (IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN (e.g., \_\_\_, \_\_\_, \_\_\_)

CNVRTCM (ICH, IMBR): (IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN (e.g., \_\_\_, \_\_\_, \_\_\_, \_\_\_)

RLIMIT (ICH, IMBR): (IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN (e.g., 100, 100, 100, 100 Ci)

TOTINV (e.g.,  $4.07 \times 10^6$  Ci)

NCOLSP (e.g., 4)

FRDCLE0 (ICOL, ICH, IMBR): ((IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN), ICOL = 1, ..., NCOLSP

FRDCLE1 (ICOL, ICH, IMBR): ((IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN), ICOL = 1, ..., NCOLSP

FRDCLE2 (ICOL, ICH, IMBR): ((IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN), ICOL = 1, ..., NCOLSP

NTMRELE0 (e.g., 198)

TMGWRPE0 (ITM): ITM = 1, ..., NTMRELE0 (e.g., 100, 150, 200, ..., 9950, 10000)

RCGWRP (ICH, IMBR, ITM): ((ITM = 1, ..., NTMRELE0), IMBR = 1, ..., NMBR (ICH), ICH = 1, ..., NDCHAIN

RAGWRPE0 (ITM): ITM = 1, ..., NTMRELE0

NTME1 (e.g., 7)

TME1 (ITME1): ITME1 = 1, ..., NTME1 (e.g., 100, 350, 1000, 3000, 5000, 7000, 9000)

NTMRELE1 (ITME1): ITME1 = 1, ..., NTME1 (e.g., 198, 193, 180, 140, 100, 60, 20)

TMGWRPE1 (ITME1, ITM): (ITM = 1, ..., NTMRELE1 (ITME1), ITME1 = 1, ..., NTME1 (e.g., TTME1 =  $1 \sim 100 \text{ yr}$ : 100, 150, 200, ..., 9950, 10000; ITME1 =  $2 \sim 350 \text{ yr}$ : 350, 400, 450, ..., 9950, 10000, ...; ITME1 =  $7 \sim 9000 \text{ yr}$ : 9000, 9050, 9100, ..., 10000)

RCGWRPE1 (ITME1, ICH, IMBR, ITM): (((ITM = 1, ..., NTMRELE1 (ITME1)), IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN), ITME1 = 1, ..., NTME1

RAGWRPE1 (ITME1, ITM): (ITM = 1, ..., NTMRELE1 (ITME1)), ITME1 = 1, ..., NTME1

NTME2 (e.g., 7)

TME2 (ITME2): ITME2 = 1, ..., NTME2 (e.g., 100, 350, 1000, 3000, 5000, 7000, 9000)

NTMRELE2 (ITME2): ITME2 = 1, ..., NTME2 (e.g., 198, 193, 180, 140, 100, 60, 20)

TMGWRPE2 (ITME2, ITM): (ITM = 1, ..., NTMRELE2 (ITME2)), ITME2 = 1, ..., NTME2 (e.g., see TMGWRPE1)

RCGWRPE2 (ITME2, ICH, IMBR, ITM): (((ITM = 1, ..., NTMRELE2 (ITME2)), IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN), ITME2 = 1, ..., NTME2 RAGWRPE2 (ITME2, ITM): (ITM = 1, ..., NTMRELE2 (ITME2)), ITME2 = 1, ..., NTME2 NTME12 (e.g., 7) TME12 (ITME12): ITME2 = 1, ..., NTME12 (e.g., 100, 350, 1000, 3000, 5000, 7000, 9000) NTMRELE12 (ITME12): ITME2 = 1, ..., NTME12 (e.g., 198, 193, 180, 140, 100, 60, 20) TMGWRPE12 (ITME2, ITM): (ITM = 1, ..., NTMRELE12 (ITME2)), ITME12 = 1, ..., NTME12 (e.g., see TMGWRPE1) RCGWRPE12 (ITME12, ICH, IMBR, ITM): (((ITM = 1, ..., NTMRELE12 (ITME12)), IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN), ITME12 = 1, ..., NTMRELE12 (ITME12)), ITME12 = 1, ..., NTME12

Two options will be available for the construction of releases from the repository to the Culebra by flowing brine. The first option, Option A, is based on algebraic manipulation of results from NUTS and/or PANEL for all patterns of drilling intrusions, including E1E2 intrusions. This construction procedure is described in Table 4.8.

The second option, Option GF, will involve the use of the GRIDFLO model to calculate brine flow and radionuclide transport in the repository and to the Culebra in the presence of E1E2 intrusions. The GRIDFLO option is intended for use when the repository is brine saturated and a constant or slowly changing potential is present that controls brine flow. Such conditions could exist subsequent to the penetration of a large, slowly depressurizing brine pocket or possibly in the presence of conditions that involve U-tube flow from the Culebra, to the repository, and then back to the Culebra. When the GRIDFLO option is selected,  $rE12(tE12_{pm}, j, k, t)$  in Table 4.8, which estimates radionuclide release in the presence of an E1E2 intrusion, is replaced by a calculated release obtained from use of GRIDFLO. Otherwise, the overall computational structure in Table 4.8 remains unchanged. The details of GRIDFLO are described in Chapt. 5.

#### 4.6 Radionuclide Transport Through Anhydrite Marker Beds

Release through the anhydrite marker beds is based on calculations performed with NUTS. The relevant transport results calculated by NUTS are listed in Table 4.7. Then, the actual release for an arbitrary future  $\mathbf{x}_{st}$  is constructed with the procedure described in Table 4.9.

# Table 4.8. Construction of Radionuclide Releases into the Culebra Dolomite Without Use of GRIDFLO for an Arbitrary Future $x_{st}$

Arbitrary future:

$$\mathbf{x}_{st} = [t_1, p_1, l_1, a_1, d_1, k_1, b_1, t_2, p_2, l_2, a_2, d_2, k_2, b_2, \dots, t_n, p_n, l_n, a_n, d_n, k_n, b_n, t_{min}]$$

Notation:

nP = number of waste panels

nl(p) = number of drilling intrusions into waste panel p, p = 1, 2, ..., nP

 $t_{pi}$  = time (yr) of *i*<sup>th</sup> drilling intrusion into waste panel p, i = 1, 2, ..., nl(p), p = 1, 2, ..., nP

- nEl(p) = number of E1 intrusions into waste panel p (i.e., intrusions for which  $b_i = 1$ )
- nE2(p) = number of E2 intrusions into waste panel p (i.e., intrusions for which  $b_i = 2$ )

$$nE12(p) = \text{number_of } E1E2 \text{ intrusions into waste panel } p$$
, (see  $tE12_{pj}$  below)

 $tE1_{pj}$  = time (yr) of  $j^{\text{th}}$  E1 intrusion into waste panel p, j = 1, 2, ..., nE1(p)

 $tE2_{pj}$  = time (yr) of j<sup>th</sup> E2 intrusion into waste panel p, j = 1, 2, ..., nE2(p)

- $tE12_{pi}$  = time (yr) of 1<sup>st</sup> E1E2 intrusion into waste panel p (i.e., time when two or more drilling intrusions have penetrated waste panel p, of which at least one encounters pressurized brine in the Castile Formation; the relevant intrusions must have  $b_i = 1$  or 2; intrusions for which  $b_i = 0$  are not considered for determining long term releases from the repository to the Culebra)
- $tE12_{pj}$  = time (yr) of each E1 intrusion (i.e.,  $b_i = 1$ ) into waste panel p subsequent to  $tE12_{p1}$ , j = 2, 3, ..., nE12(p) (i.e.,  $tE1_{pj}$ , j = 2, 3, ..., nE1(p) if  $tE12_{p1} < tE1_{p2}$  and  $tE1_{pj}$ , j = 3, 4, ..., nE1(p) if  $tE12_{p1} = tE1_{p2}$ )
- rEO(j, k, l) = cumulative release (kg) of element k of decay chain j from the repository to the Culebra under undisturbed (i.e., E0) conditions through time l due to brine flow (= RCGWRPE0 (j, k, l))
- rE1(i, j, k, l) = cumulative release (kg) of element k of decay chain j from the repository to the Culebra from time i to time l due to brine flow with an El intrusion occurring at time i (=RGWRPE1 (i, j, k, l))
- rE2(i, j, k, l) = cumulative release (kg) of element k of decay chain j from the repository to the Culebra from time i to time l due to brine flow with an E2 intrusion occurring at time i (=RGWRPE2 (i, j, k, l))
- rE12(i, j, k, l) = cumulative release (kg) of element k of decay chain j from the repository to the Culebra from time i to time l due to brine flow with an E1E2 intrusion occurring at time i (=RGWRPE12 (i, j, k, l))

nC = number of colloid species (= NCOLSP)

- fCEO(s, j, k) = fraction of element k of decay chain j attached to colloid specie s under undisturbed (i.e., E0) conditions
- fCE1(s, j, k), fCE2(s, j, k): same as fCE0(s, j, k) but for conditions subsequent to E1 and E2 intrusions, respectively Cumulative release to Culebra:
  - $cRD_p(j, k, t)$  = cumulative dissolved release (kg) to Culebra through time t of element k of decay chain j from waste panel p

$$= 0 \text{ if } t \le t_{p1}$$

$$= \left[1 - \sum_{s=1}^{nC} fCE1(s, j, k)\right] rE1(t_{p1}, j, k, t) \quad \text{if } tE1_{p1} = t_{p1} < t \le t_{p2}$$

$$= \left[1 - \sum_{s=1}^{nC} fCE2(s, j, k)\right] rE2(t_{p1}, j, k, t) \quad \text{if } tE2_{p1} = t_{p1} < t \le tE1_{p1}$$

$$= \left[1 - \sum_{s=1}^{nC} fCE1(s, j, k)\right] rE12(tE12_{pm}, j, k, t) \quad \text{if } tE12_{pm} < t \le tE12_{p,m+1}, m = 1, 2, ..., nE12(p)$$

cRD(j, k, t) = cumulative dissolved release (Ci) from repository to Culebra through time t of element k of decay chain j

$$= \left[1 - \sum_{s=1}^{nC} fCE0(s, j, k)\right] rE0(j, k, t) \quad \text{if } t \le t_1$$
$$= \sum_{p=1}^{nP} cRD_p(j, k, t) \quad \text{if } t > t_1$$

 $cRC_p(s, j, k, t)$  = cumulative release (kg) from waste panel p to Culebra through time t of element k of decay chain j sorbed to colloid specie s

= 0 if 
$$t \le t_{p1}$$
  
=  $fCE1(s, j, k) rE1(t_{p1}, j, k, t)$  if  $tE1_{p1} = t_{p1} < t \le t_{p2}$ 



$$= fCE2(s, j, k) rE2(t_{p1}, j, k, t)$$
 if  $tE2_{p1} = t_{p1} < t \le tE1_{p1}$   

$$= fCE1(s, j, k) rE12(tE12_{pm}, j, k, t)$$
 if  $tE12_{pm} < t \le tE12_{p, m+1}, m = 1, 2, ..., nE12(p)$   

$$cRC(s, j, k, t) =$$
 cumulative release (kg) from repository to Culebra through time t of element k of decay chain  
j sorbed to colloid specie s  

$$= fCE0(s, j, k) rE0(j, k, t)$$
 if  $t \le t_1$   

$$= \sum_{j=1}^{n^p} cRC_p(s, j, k, t)$$
 if  $t > t_1$ 

Table 4.9. Calculation of Anhydrite Marker Bed Release  $f_{MB}$  for an Arbitrary Future  $\mathbf{x}_{st}$ 

Arbitrary future:

p=l

.

.

$$\mathbf{x}_{st} = [t_1, p_1, l_1, a_1, d_1, k_1, b_1, t_2, p_2, l_2, a_2, d_2, k_2, b_2, \dots, t_n, p_n, l_n, a_n, d_n, k_n, b_n, t_{min}]$$

Notation:

tE1 = time (yr) of first E1 intrusion (i.e., first intrusion for which  $b_i = 1$ )

tE2 = time (yr) of first E2 intrusion (i.e., first intrusion for which  $b_i = 2$ )

- rAE0(l) = cumulative release (EPA units) of all radioactive species from the repository to the accessible environment under undisturbed (i.e., E0) conditions through time l due to brine flow in the anhydrite marker beds (= RAGWRPE0(l))
- rAE1(i, l) = cumulative release (EPA units) of all radioactive species from the repository to the accessible environment between time *i* and time *l* with an E1 intrusion at time *i* due to brine flow in the anhydrite marker beds (= RAGWRPE1(*i*, *l*))

$$rAE2(i, l)$$
: same as  $rAE1(i, l)$  but for an E2 intrusion (= RAGWRPE2(i, l))

Evaluation of  $f_{MB}(\mathbf{x}_{st})$ :

 $f_{MB}(\mathbf{x}_{st}) = rAE0(t_l)$ 

 $+ rAE2(tE2, \min \{tE1, tM\}) \qquad \text{if } tE2 < tE1$  $+ rAE1(tE1, tM) \qquad \text{if } tE1 < tM$ 



#### 4.7 Radionuclide Transport Through Dewey Lakes Red Beds

At present, it is anticipated that there will be no significant transport through the Dewey Lakes Red Beds to the accessible environment. If such transport is observed to occur, it can be estimated as described in Sect. 4.6 or 4.9 depending on the level of resolution at which the modeling is done (i.e., with NUTS or SECO-TRANSPORT).

### 4.8 Radionuclide Transport Through Abandoned Borehole to Surface

At present, it is anticipated that there will be no radionuclide transport through abandoned boreholes to the surface. The transport referred to here is due to long-term brine flow through an abandoned (typically plugged) borehole, and is distinct from the blowout release considered in Sect. 4.3, which occurs through an open borehole at the time of drilling. If transport through abandoned boreholes is observed to occur, it can be estimated as described in Sect. 4.6 with results obtained from NUTS.

### 4.9 Radionuclide Transport Through Culebra Dolomite

Release through the Culebra Dolomite is based on calculations performed with the SECO-TRANSPORT model. Due to the linearity of the system of partial differential equations that underlies SECO-TRANSPORT (see Apps. A and B), it is possible to evaluate transport results for unit releases into the Culebra and then use these results to construct transport releases for arbitrary time-dependent releases into the Culebra.

The information transferred to CCDFGF for use in the construction of Culebra transport results is listed in Table 4.10. Further, the actual construction procedures are given in Table 4.11.

# 4.10 CCDF Construction

A sequence  $\mathbf{x}_{st,i}$ , i = 1, 2, ..., nS of futures will be sampled as indicated in Table 3.2. At present, it is anticipated that a sample size between nS = 1000 and nS = 10000 will be adequate to construct a CCDF for comparison with the boundary line specified in 40 CFR 191.13. A normalized release  $f(\mathbf{x}_{st,i})$  for each future will then be constructed as described in Sects. 4.1 - 4.9. Once the  $f(\mathbf{x}_{st,i})$  are evaluated, the CCDF in Fig. 2.1 can be approximated as indicated in Eq. (2.3). In practice, a binning technique can be used to construct the desired CCDF (i.e., the consequence axis is divided into a sequence of bins and the number of values for  $f(\mathbf{x}_{st,i})$  falling in each bin is accumulated); this avoids having to save and subsequently order all values for  $f(\mathbf{x}_{st,i})$ .

In addition to the CCDF in Fig. 2.1 over all release modes (see Eq. (4.1)), it will be possible to obtain CCDFs for individual release modes (e.g., cuttings, spallings, blowout, to Culebra, through marker beds, through Culebra).

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Table 4.10. Results from Calculations with SECO-TRANSPORT Transferred to CCDFGF for Use in Determination of Releases Due to Groundwater Transport in the Culebra Dolomite. The information in this table will repeat for each sample element

#### **Results Transferred to CCDFGF**

NDCHAIN: Number of decay chains (e.g., 3)

NMBR (ICH): Number of elements in decay chain ICH, ICH = 1, 2, ..., NDCHAIN (e.g., 1, 1, 2)

RDECAY (ICH, IMBR): Decay constant  $(yr^{-1})$  for element IMBR of decay chain ICH, IMBR = 1, 2, ..., NMBR (ICH) and ICH = 1, 2, ..., NDCHAIN (e.g., \_\_\_, \_\_\_, \_\_\_)

CNVRTKM (ICH, IMBR): Conversion factor from kg to moles (mole/kg) for element IMBR of decay chain ICH, IMBR = 1, 2, ..., NMBR (ICH) and ICH = 1, 2, ..., NDCHAIN (e.g., \_\_, \_\_, \_\_)

CNVRTKC (ICH, IMBR): Conversion factor from kg to Ci (Ci/kg) for element IMBR of decay chain ICH, IMBR = 1, 2, ..., NMBR (ICH) and ICH = 1, 2, ..., NDCHAIN (e.g., \_\_, \_\_, \_\_)

NMDCMBR (ICH, IMBR): Name of member IMBR of decay chain ICH, IMBR = 1, 2, ..., NMBR (ICH) and ICH = 1, 2, ..., NDCHAIN (e.g., Pu-239, Am-241, U-234, Th-230)

RLIMIT (ICH, IMBR): EPA release limit (Ci) for element IMBR of decay chain ICH, IMBR = 1, 2, ..., NMBR (ICH) (e.g., 100, 100, 100, 100 Ci)

TOTINV: Total inventory (Ci) of  $\alpha$ -emitting radionuclides placed in repository with halflives greater than 20 yr (e.g.,  $4.07 \times 10^6$  Ci)

NCOLSP: Number of colloid species (e.g., 4)

NTMGWTP: Number of times used to define intervals over which result of unit radionuclide release to the Culebra Dolomite is calculated (e.g., 198)

TMGWTR (ITM): Times that define intervals over which result of unit radionuclide release to the Culebra Dolomite is calculated (e.g., 100, 150, 200, ..., 9950, 10000 yr)

RRADAEU (ICH, IMBR, IDCND, ITM): Release (kg) to accessible environment for element IDCND of decay chain ICH due to a 1 kg dissolved release of element IMBR of decay chain ICH into the Culebra at the repository during time interval ITM (i.e., from TMGWTR (ITM) to TMGWTR (ITM + 1)) and subsequent transport under undisturbed (i.e., unmined) conditions, ITM = 1, 2, ..., NTMGWTP, IDCND = IMBR, IMBR + 1, ..., NMBR (ICH), IMBR = 1, 2, ..., NMBR (ICH), and ICH = 1, 2, ..., NDCHAIN (Note: IDCND counts over element IMBR of decay chain ICH and all of its daughters, i.e., to the end of decay chain ICH)

RRADAEM (ICH, IMBR, IDCND, ITM): Same as RRADAEU (ICH, IMBR, IDCND, ITM) but for radionuclide transport in the Culebra under disturbed (i.e., mined) conditions rather than undisturbed conditions

RCOLAEU (ICOL, ITM): Cumulative release (kg) to accessible environment through time TMGWTR (ITM) of colloid specie ICOL due to a 1 kg release of colloid specie ICOL into the Culebra at time TMGWTR (1) and subsequent transport under undisturbed conditions, ITM = 1, 2, ..., NTMGWTR and ICOL = 1, 2, ..., NCOLSP

RCOLAEM (ICOL, ITM): Same as RCOLAEU (ICOL, ITM) but for colloid transport in the Culebra under disturbed (i.e., mined ) conditions rather than undisturbed conditions

Conceptual Structure of Transfer File for One Sample Element

NDCHAIN (e.g., 3)

NMBR (ICH): ICH = 1, ..., NDCHAIN (e.g., 1, 1, 2)

NMDCMBR (ICH, IMBR): (IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN (e.g., Pu-239, Am-241, U-234, Th-230)

RDECAY (ICH, IMBR): (IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN (e.g., \_\_\_, \_\_\_, \_\_\_, \_\_\_, \_\_\_)

CNVRTKM (ICH, IMBR): (IMBR = 1, ..., NMBR (ICH), ICH = 1, ..., NDCHAIN (e.g., \_\_\_, \_\_\_, \_\_\_)

CNVRTKC (ICH, IMBR): (IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN (e.g., \_\_, \_\_, \_\_, \_\_)

RLIMIT (ICH, IMBR): (IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN (e.g., 100, 100, 100, 100 Ci)

TOTINV (e.g.,  $4.06 \times 10^6$  Ci)

NCOLSP (e.g., 4)

NTMGWTP (e.g., 198)

TMGWTR (ITM): ITM = 1, ..., NTMGWTP (e.g., 100, 150, 200, ..., 9950, 10000 yr)

RRADAEU (ICH, IMBR, IDCND, ITM): (((ITM = 1, ..., NTMGWTP), IDCND = IMBR, ..., NMBR (ICH)), IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN

RRADAEM (ICH, IMBR, IDCND, ITM): (((ITM = 1, ..., NTMGWTP), IDCND = IMBR, ..., NMBR (ICH)), IMBR = 1, ..., NMBR (ICH)), ICH = 1, ..., NDCHAIN

RCOLAEU (ICOL, ITM): (ITM = 1, ..., NTMGWTP), ICOL = 1, ..., NCOLSP

RCOLAEM (ICOL, ITM): (ITM = 1, ..., NTMGWTP), ICOL = 1, ..., NCOLSP



Table 4.11. Calculation of Groundwater Transport Release  $f_{ST}$  through the Culebra Dolomite for an Arbitrary Future  $\mathbf{x}_{st}$ 

Arbitrary future:

$$\mathbf{x}_{st} = \begin{bmatrix} t_1, p_1, l_1, a_1, d_1, k_1, b_1, t_2, p_2, l_2, a_2, d_2, k_2, b_2, \dots, t_n, p_n, l_n, a_n, d_n, k_n, b_n, t_{min} \end{bmatrix}$$

Notation:

- $\tau_m$  = times (yr) used to record results of unit release calculations with SECO-TRANSPORT for the Culebra [ = TMGWTR (m)], m = 1, 2, ..., nTI<sup>+</sup>+1 (=NTMGWTP-1)
- nTI = number of time intervals  $[\tau_m, \tau_{m+1}]$ , m = 1, 2, ..., nTI, defined by  $\tau_m, m = 1, 2, ..., nTI + 1$ (= NTMGWTP - 1)
- $cKM(j, k) = \text{conversion factor from kg to moles (mole/kg) for element k of decay chain j [= CNVRTCM (j, k)]$
- cMK(j, k) = conversion factor from moles to kg (kg/mole) for element k of decay chain j [=1/cKM(j, k)]
- $cKC(j, k) = \text{conversion factor from kg to Ci (Ci/kg) for element k of decay chain j [= CNVRTKC(j, k)]$ 
  - $\lambda(j, k) = \text{decay constant } (yr^{-1}) \text{ for element } k \text{ of decay chain } j [= \text{RDECAY } (j, k)]$ 
    - nDC = number of decay chains [= NDCHAIN]
  - nM(j) = number of members in decay chain j = NMBR(j)
  - rL(j, k) = EPA release limit (Ci) for element k of decay chain j = RLIMIT(j, k)
    - $tI = total inventory (Ci) of \alpha$ -emitting radionuclides placed in repository with halflives that exceed 20 yr [= TOTINV]
    - nC = number of colloid species [= NCOLSP]

Dissolved release rD(j, k) of element k of decay chain j:

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uR(j, k, l, m) = release (kg) to accessible environment of element l of decay chain j resulting from a 1 kg dissolved release of element k of decay chain j to the Culebra over time interval  $[\tau_m, \tau_{m+1}]$ 

$$\begin{cases} \text{RRADAEU}(j, k, l, m) & \text{if } \tau_{m+1} < t_{min} \\ \text{RRADAEM}(j, k, l, m) & \text{if } \tau_{m+1} \ge t_{min} \end{cases}$$

 $dRD(j, k, \tau_m, \tau_{m+1})$  = dissolved release (kg) to Culebra of element k of decay chain j over time interval  $[\tau_m, \tau_{m+1}]$ 

$$= cRD(j, k, \tau_{m+1}) - cRD(j, k, \tau_m)$$

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rD(j, k) = release (kg) to accessible environment of element k of decay chain j resulting from dissolved releases into the Culebra

$$= \sum_{m=1}^{nTI} \sum_{p=1}^{k} dRD(j, p, \tau_m, \tau_{m+1}) uR(j, p, k, m)$$

Colloidal release rC(j, k) of element k of decay chain j:

uC(s, l, m) = release (kg) to accessible environment of colloid specie s over time interval  $[\tau_m, \tau_{m+1}]$ resulting from a 1 kg release of colloid specie s to the Culebra over time interval  $[\tau_l, \tau_{l+1}]$ 

$$=\begin{cases} \text{RCOLAEU}(s, m+1-l) - \text{RCOLAEU}(s, m-l) & \text{if } \tau_{m+1} < t_{min} \\ \text{RCOLAEM}(s, m+1-l) - \text{RCOLAEM}(s, m-l) & \text{if } \tau_{m+1} \ge t_{min} \end{cases}$$

dRC(s, j, k, l) = amount (kg) of element k of decay chain j attached to colloid specie s released to Culebra over time interval  $[\tau_l, \tau_{l+1}]$ 

$$= cRC(s, j, k, \tau_{l+1}) - cRC(s, j, k, \tau_l)$$

 $aC(s, j, k, l, m) = \text{amount (kg) of element } k \text{ of decay chain } j \text{ attached to colloid specie } s \text{ over time interval } [\tau_m, \tau_{m+1}] \text{ due to releases over time interval } [\tau_l, \tau_{l+1}]$ 

$$= \left\{ \sum_{p=1}^{k} \left( \sum_{\substack{j=p \\ j \neq p}}^{k} \left[ \frac{\left[ \prod_{\substack{r=p \\ k}}^{k} \lambda(j,r) \right] / \lambda(j,k)}{\prod_{\substack{s=p \\ s \neq q}}^{k} \left[ \lambda(j,s) - \lambda(j,q) \right]} \right] \cdot \exp \left[ -\lambda(j,q) \left( \frac{\tau_m + \tau_{m+1}}{2} - \frac{\tau_l + \tau_{l+1}}{2} \right) \right] \right) \right\}$$
$$\cdot dRC(s, j, p, l) cKM(j, p) \left\{ cMK(j, k) \right\}$$

rCI(s, j, k, m) = amount (kg) of element k of decay chain j attached to colloid specie s released to accessible environment over time interval  $[\tau_m, \tau_{m+1}]$ 

$$= \sum_{l=1}^{m} aC(s, j, k, l, m) uC(s, l, m)$$

rC(j, k) = release (kg) to accessible environment of element k of decay chain j resulting from colloidal releases into the Culebra

$$= \sum_{s=1}^{nC} \sum_{m=1}^{nTI} rCI(s, j, k, m)$$

Evaluation of  $f_{ST}(\mathbf{x}_{st})$ :

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$$f_{ST}(\mathbf{x}_{st}) = \sum_{j=1}^{nDC} \sum_{k=1}^{nM(j)} \left\{ \frac{\left[ rD(j,k) + rC(j,k) \right] cKC(j,k)}{rL(j,k)} \right\} \left\{ \frac{10^6 \text{ Ci}}{tI} \right\}$$



The CCDF construction indicated in this section is for a single sample element  $\mathbf{x}_{su,k}$  of the form indicated in conjunction with Eq. (2.5). Repeated generation of CCDFs for individual sample elements  $\mathbf{x}_{su,k}$  will lead to distributions of CCDFs of the form illustrated in Figs. 2.3 - 2.5.

## 4.11 Data Assembly

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The initial component of CCDFGF will be a sequence of subroutines that collects and assembles the information indicated in Tables 4.1, 4.3 (and the equivalent table for spallings releases), 4.4, 4.6, 4.7 and 4.10. In general, this information will repeat for each sample element  $\mathbf{x}_{su,k}$  indicated in conjunction with Eq. (2.5).



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## 5. Fluid Flow and Radionuclide Transport for E1E2 Intrusions

#### 5.1 Rationale for GRIDFLO

In past PAs for the WIPP, groundwater releases to the Culebra have been dominated by E1E2 intrusions in which the repository is penetrated by two or more drilling intrusions, of which at least one penetrates pressurized brine and at least one does not penetrate pressurized brine. The potential for large releases results from the diversion of brine flow from the drilling intrusion that penetrated pressurized brine through the repository to the drilling intrusion that did not penetrate pressurized brine. In the context of the representation for  $\mathbf{x}_{st}$  in Eq. (2.2), an E1E2 intrusion occurs when  $n \ge 2$  and at least one of the locations  $l_i$  is above pressurized brine.

The modeling of this important intrusion event has been conservative in past PAs. In particular, all flow from the drilling intrusion that penetrates pressurized brine has been assumed to divert to the drilling intrusion that did not penetrate pressurized brine. This is a very conservative assumption because it is equivalent to assuming a perfect plug above the drilling intrusion that penetrates pressurized brine and no plug above the intrusion that does not penetrate pressurized brine. In reality, the amount of diverted brine should depend on the permeability of the two boreholes, the elevation of the two boreholes within the repository (as a reminder, the repository is built on a dip), the permeability of the material within the repository, and the length of the flow path between the two boreholes.

In addition, conservative assumptions have been made about the extent of the waste inventory that would be contacted by the brine diverting between the two boreholes. The 1991 and 1992 WIPP PAs assumed perfect panel seals and that an E1E2 type intrusion will produce a brine flow that contacted the entire inventory of a waste panel. The SPM analysis assumed no panel seals, with the result that an equivalent assumption would have implied that an E1E2 intrusion could contact the entire inventory of the repository. This did not seem reasonable and an *ad hoc* procedure based on the flow paths between the boreholes associated with an E1E2 intrusion was used to reduce the amount of contacted inventory.

In past analyses, BRAGFLO calculations have not been performed for E1E2 intrusions. Rather, BRAGFLO calculations have been performed for E1 intrusions (i.e., a single intrusion that penetrates both the repository and pressurized brine) and then the assumptions indicated in the two preceding paragraphs have been used in conjunction with PANEL to estimate E1E2 releases from E1 flow results.

Given both the potential importance of E1E2 intrusions and the many different occurrence patterns by which two or more drilling intrusions could give rise to an E1E2 intrusion, a modeling approach with more resolution was desirable. Desirable capabilities for such an approach include (1) representation of the geometry of the repository (Fig. 3.1), (2) treatment of multiple drilling intrusions (i.e.,  $\geq 2$ ), (3) incorporation of location of each drilling intrusion, (4) specification of different properties (i.e., diameter, permeability) for different boreholes,

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(5) specification of local properties within the repository (e.g., permeabilities), (6) specification of solubilities or distribution coefficients within the repository, (7) flexibility in the assignment of brine pocket locations and properties, and (8) numerical stability and rapid computation.

In general, it would be hard to meet the preceding desiderata. However, the E1E2 intrusions that are to be modeled are very special situations. In such intrusions, the repository fills with brine. Once the repository is filled with brine, the flow through the repository then depends on the pressure in the brine pocket(s), the permeabilities in the boreholes and the flow paths between boreholes in the repository, and the pressure in the Culebra. Past analyses have indicated that the pressures in brine pockets and in the Culebra tend to remain fixed. Because of this, Darcy's law can be used to describe the resultant constant flow system. Once this flow system is determined, the implementation of a radionuclide transport model within the repository and to the Culebra is relatively simple. The approach is now described in more detail. For convenience, the model being described will be referred to as the GRIDFLO model.

### 5.2 Mathematical Structure of GRIDFLO

The basic idea in GRIDFLO is to have a system of nodes in the repository defined on a rectilinear grid, with flow between these nodes taking place in the grid (Fig. 3.1). In addition, each node in the repository will have corresponding nodes in the Castile and Culebra that are directly below and above the repository node.

In setting up the problem, grid elements are assumed to run south (-) to north (+), east (-) to west (+) and down (-) to up (+). See Fig. 5.1. Further, the possible flow paths and data associated with a single node are shown in Fig. 5.2. For many nodes, all of the flow paths (i.e., legs) in Fig. 5.2 will not be used.

In setting up the mass balance equation at a node in the repository, flows

- (1) from the node to the north, west or up are assumed to remove brine and thus are negative; similarly, flows to the node from the north, west or up are assumed to add brine and thus are positive,
- (2) to the node from the south, east or down are assumed to add brine and thus are positive; similarly, flows from the node to the south, east or down are assumed to remove brine and thus are negative;

or, stated in an equivalent form with respect to Fig. 5.2,

(1) Flow in a positive direction in legs 1, 3 or 5 removes brine and flow in a negative direction in legs 1, 3 or 5 adds brine,



TRI-6334-206-21

Figure 5.1. Coordinate system for calculation of flow within the experimental, operations and waste disposal regions of the WIPP.



 $P \sim \text{pressure}$   $L \sim \text{length}$ 

A ~ cross -sectional area

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Figure 5.2. Flow paths associated with a single node in the repository.

(2) Flow in a positive direction in legs 2, 4 or 6 adds brine and flow in a negative direction in legs 2, 4 or 6 removes brine.

From the preceding conventions and Darcy's Law, net brine flow at a given node in the repository must be 0 and results in the following equation (see Fig. 5.2 for notation):

$$0 = \sum_{i=1}^{6} (\text{flow in leg } i)$$

 $0 \le \Rightarrow$  flow towards node (i.e., to south)  $0 \ge \Rightarrow$  flow away from node (i.e., to north)

$$=\delta_1\left(\frac{k_1A_1}{L_1}\right)\left(\overline{Z_1+P_1-Z_0-P_0}\right)$$

 $0 \le \Rightarrow$  flow towards node (i.e., to north)  $0 \ge \Rightarrow$  flow away from node (i.e., to south)

$$+\delta_2\left(\frac{k_2A_2}{L_2}\right)\left(\overline{Z_2+P_2-Z_0-P_0}\right)$$

 $0 \le$  flow towards node (i.e., to east)  $0 \ge$  flow away from node (i.e., to west)

$$+\delta_3\left(\frac{k_3A_3}{L_3}\right)\left(\overline{Z_3+P_3-Z_0-P_0}\right)$$

 $0 \le \Rightarrow$  flow towards node (i.e., to west)  $0 \ge \Rightarrow$  flow away from node (i.e., to east)

$$+\delta_4\left(\frac{k_4A_4}{L_4}\right)\left(\overline{Z_4+P_4-Z_0-P_0}\right)$$

 $0 \le$  flow towards node (i.e., down)  $0 \ge$  flow away from node (i.e., up)

$$+\delta_5\left(\frac{k_5A_5}{L_5}\right)\left(\overline{Z_5+P_5-Z_0-P_0}\right)$$

 $0 \le \Rightarrow$  flow towards node (i.e., up)  $0 \ge \Rightarrow$  flow away from node (i.e., down)

$$+\delta_6\left(\frac{k_6A_6}{L_6}\right)\left(\overline{Z_6+P_6-Z_0-P_0}\right)$$

where

$$\delta_i = \frac{\text{.f leg } i \text{ is defined}}{0 \text{ if leg } i \text{ is undefined}}$$

Thus,

(5.2)

(5.1)

$$= \left[\sum_{i=1}^{t} \varrho^{i} \left(\frac{\Gamma^{i}}{V_{i}V_{i}}\right) Z^{i} + \sum_{i=1}^{t} \varrho^{i} \left(\frac{\Gamma^{i}}{V_{i}V_{i}}\right) D^{i}_{i} - Z^{0} \sum_{i=1}^{t} \varrho^{i} \left(\frac{\Gamma^{i}}{V_{i}V_{i}}\right)\right] + \sum_{i=1}^{t} \varrho^{i} \left(\frac{\Gamma^{i}}{V_{i}V_{i}}\right) D^{i}_{i} + \left[-\frac{\Gamma^{i}}{\varrho}\right] Q^{i} \left(\frac{\Gamma^{i}}{V_{i}V_{i}}\right)\right] D^{0}_{i} \left(2^{2}3\right)$$

$$= \sum_{i=1}^{t} \varrho^{i} \left(\frac{\Gamma^{i}}{V_{i}V_{i}}\right) Z^{i} + \sum_{i=1}^{t} \varrho^{i} \left(\frac{\Gamma^{i}}{V_{i}V_{i}}\right) D^{i}_{i} - Z^{0} \sum_{i=1}^{t} \varrho^{i} \left(\frac{\Gamma^{i}}{V_{i}V_{i}}\right) - D^{0}_{i} \sum_{i=1}^{t} \varrho^{i} \left(\frac{\Gamma^{i}}{V_{i}V_{i}}\right) D^{0}_{i} \left(\frac{\Gamma^{i}}{V_{i}V_{i}}\right) D^{0}_{i} \left(2^{2}\right)$$

$$= \sum_{i=1}^{t} \varrho^{i} \left(\frac{\Gamma^{i}}{V_{i}V_{i}}\right) (Z^{i}_{i} + D^{i}_{i} - Z^{0} - D^{0}_{i})$$

$$= \sum_{i=1}^{t} \varrho^{i} \left(\frac{\Gamma^{i}}{V_{i}V_{i}}\right) (Z^{i}_{i} + D^{i}_{i} - Z^{0} - D^{0}_{i})$$

There will be one equation of the above form for each node in the repository, with  $P_0$ ,  $P_1$ ,  $P_2$ ,  $P_3$ ,  $P_4$  being the unknown variables. The pressures in the Castile (i.e.,  $P_6$ ) and the Culebra (i.e.,  $P_5$ ) are assumed to be known.

$$=\sum_{q=1}^{q} \delta_{i} \left( \frac{L_{q}}{L_{q}} \right) \left( Z_{0} - Z_{i} \right) - \sum_{q=2}^{q} \delta_{i} \left( \frac{L_{q}}{L_{q}} \right) P_{i} + Z_{0} \sum_{i=1}^{q} \delta_{i} \left( \frac{L_{q}}{L_{q}} \right) P_{i}$$

which can be viewed as one equation associated with the matrix representation

The preceding equation can also be written in the form

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$$\mathbf{A} = \begin{bmatrix} b_n \\ \vdots \\ b_n \end{bmatrix} \text{ is the vector of nonhomogeneous terms}$$
$$\mathbf{A} = \begin{bmatrix} b_n \\ \vdots \\ \vdots \\ b_n \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ b_n \end{bmatrix} \text{ is the vector of nonhomogeneous terms}$$

n = number of nodes in repository.

The coefficients (i.e.,  $a_{ij}$ ) in **A** will be defined by the coefficients on  $P_0$ ,  $P_1$ ,  $P_2$ ,  $P_3$ ,  $P_4$  in Eq. (4.4). The elements of **b** (i.e.,  $b_i$ ) will be defined by the right-hand side of Eq. (5.4). Solution of equations of the form shown in Eq. (5.5) is a standard problem in numerical linear algebra.<sup>13</sup>

The unknowns in Eq. (5.5) are the pressures at the nodes in the repository. Once these pressures are obtained by solving Eq. (5.5), Darcy's law can be used to define brine flow rates between the individual nodes. Once the brine flow rates are known, radionuclide transport calculations can be performed.

The transport calculation can be performed by treating each leg between two nodes (Fig. 3.1) as a "bucket" that contains a certain amount of brine, with this amount deriving from the porosity, cross-sectional area and length of the leg and the assumption that the leg is brine saturated. The brine concentration of each radionuclide within the leg is then set on the basis of an assumed solubility or  $K_d$  value. The amount of radionuclide exiting a leg in a given period of time and the legs to which this radionuclide is transported depends on the flows predicted by Darcy's law. In essence, Darcy's law tells how much brine is to be poured out of the leg (i.e., bucket) for a given interval of time. Dynamic control of time-step size can be used to select appropriate time steps. Further, the numerical implementation must account for radioactive decay and inventory limits.

### 5.3 Implementation of GRIDFLO

The GRIDFLO model provides an alternative to the use of BRAGFLO/NUTS/PANEL results to define the expression  $rE12(tE12_{pm\nu} j, k, t)$  in Table 4.8. Other than this substitution, the CCDF construction procedures in CCDFGF remain the same whether GRIDFLO or interpolation procedures as described in Table 4.8 are used to estimate releases from the repository to the Culebra for E1E2 intrusions.

The operation of GRIDFLO should be set up with two options. In Option 1, GRIDFLO operates on a single waste panel basis as described in Table 4.8 (i.e., E1E2 intrusions are considered only when the relevant drilling intrusions occur within the same waste panel). In Option 2, GRIDFLO operates over the entire repository (i.e., E1E2 intrusions can involve drilling intrusions anywhere in the repository).

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## 6. Code Architecture

# 6.1 Control Flow

# 6.1.1 Initialization

The following input parameters define analysis initialization:

- 1. Run control parameters
- 2. Repository inventory parameters
- 3. Repository grid nodalization parameters
- 4. Repository region and panel parameters
- 5. Release parameter tables for:
  - a. cuttings
  - b. spallings
  - c. blowouts
  - d. Marker Beds
  - e. Dewey Lakes
  - f. surface
  - g. flows to the Culebra
  - h. transport through the Culebra
- 6. Pre-defined individual borehole intrusion parameters (optional)

Grid leg (internode) properties are defined based on the grid nodalization properties. The intersections of the nodal specification lines correspond to the nodes. All node definitions are processed first. All area definitions are processed after all node definitions have been processed. The final specification for a given area takes precedence over all previous specifications for the same area.

# 6.1.2 Calculation Structure

Three run execution options are available:

- 1. Normal execution
- 2. Preprocessing execution
- 3. Intermediate execution

Option 1 is the normal execution option but must be preceded by an Option 2 execution. Option 2 must be executed prior to Options 1 or 3 to create release summary tables from previously calculated results from other analysis codes.

Option 3 is used for creating intermediate release results for analysis of release summary tables and is not required for normal execution.

A three-level looping structure is used as the basic calculation structure. The outer calculation loop corresponds to an observation loop, such as in Latin hypercube sampling. The next calculation loop corresponds to a time future loop. The inner calculation loop corresponds to individual timesteps for a single time future. The number of observations and the number of time futures per observation are specified in the run control parameters. The time futures correspond to the total length of time over which releases to the accessible environment are calculated. One or more time futures can be specified per observation.

#### 6.1.3 Borehole Intrusions

Borehole intrusions occur at randomly selected future times based on a Poisson distribution. The pressure head at the repository node corresponding to a borehole intrusion is altered depending on the formations the borehole penetrates outside of the repository, and this in turn affects the pressure heads for all other nodes in the repository.

## 6.1.4 Releases to Accessible Environment

Cuttings, spallings, and blowout releases for each borehole intrusion are interpolated from release tables versus drilling intrusion time. Releases to the Marker Beds, to the Dewey Lakes, and to the surface are interpolated from release tables versus time. Releases to the Culebra are determined either by interpolation from release tables versus time or by calculation of flow and transport depending on the locations and types of borehole intrusions that have occurred. Culebra transport releases are calculated based on previous unit release calculations to the Culebra.

#### 6.1.5 Flow to the Culebra

Flow to the Culebra is modeled using four different scenarios depending on the number and type of borehole intrusions that have occurred. Before any borehole intrusions occur, releases to the Culebra are interpolated from release tables for undisturbed conditions. After the first borehole intrusion has occurred, releases are interpolated from release tables for individual E1 intrusion scenarios and individual E2 intrusion scenarios. An E1 scenario is an intrusion that penetrates both the repository and a pressurized brine pocket below the repository. An E2 scenario is an intrusion that only penetrates the repository. After the first drilling intrusion that results in an E1E2 scenario, releases are calculated based on one of two methods: (1) interpolation of release tables for E1E2 scenarios or (2) modeling brine flow and associated species transport through the repository (GRIDFLO option). An E1E2 scenario is two or more borehole intrusions, at least one of which must be an E1 intrusion.

## 6.1.6 Repository Flow and Transport (GRIDFLO Option)

Grid leg (internode) flow rates can then be calculated based on the nodal pressure heads. A difference in the pressure heads between adjacent nodes translates into a flow from the high pressure node to the low pressure node. An Euler-type solution of a system of differential equations is used to model species transport based either on species solubility limits or on species  $K_d$  values. This solution is based on the assumption that species transport is essentially constant for each timestep. The species mass in the original waste, the brine solution, and the precipitated waste are reduced due to radioactive decay during each timestep.

## 6.1.7 Result Distributions

Result distributions for releases from the repository directly to the accessible environment and to the accessible environment through the Culebra formation are accumulated for each species being transported. Each result is based on the total species mass transported from the repository during a single time future. A series of time futures results in a distribution of releases corresponding to an observation. Result distributions are accumulated over all time futures for each observation for the following releases to the accessible environment:

- 1. Borehole cuttings
- 2. Borehole spallings
- 3. Borehole blowouts
- 4. Marker Beds transport
- 5. Dewey Lakes transport
- 6. Transport to the surface
- 7. Flows to the Culebra
- 8. Transport through the Culebra

In addition, flows to the Culebra and transport through the Culebra are quantified according to individual species and whether species are dissolved or are attached to colloids.

# 6.2 Control Logic


# 6.3 Data Structures

# 6.3.1 Run Control Parameters

The following parameters are defined on the run control parameter file:

- 1. Number of observations
- 2. Number of time futures per observation
- 3. Run execution option
- 4. Spatial solubility flag indicating spatially constant or variable solubility or Kd
- 5. Solubility limit flag indicating maximum solubility limit or K<sub>d</sub>
- 6. Initial and subsequent administrative control times
- 7. Flow and transport time parameters
- 8. Brine parameters
- 9. Total solids mass in repository
- 10. Elevations above mean sea level for Culebra and Castile formations
- 11. Pressure heads for Culebra and Castile formations
- 12. Drilling intrusion rates and parameters
- 13. Mining intrusion rates
- 14. Borehole diameter distribution parameters
- 15. Borehole permeability distribution parameters
- 16. Random number generator seed

# 6.3.2 Repository Nodalization Parameters

The following parameters are defined on the nodalization file. All x-distances and y-distances are referenced to a single point which can be either inside or outside the repository. All parameters refer to either nodal or area specifications:

- 1. Minimum x-distance
- 2. Maximum x-distance
- 3. Minimum y-distance
- 4. Maximum y-distance
- 5. Drift height
- 6. Driff width
- 7. Hydraulic conductivity
- 8. Porosity (pore fraction)



- 9. Waste fractions (0.0=shaft seal, 1.0=waste drift)
- 10. Elevation above mean sea level
- 11. Pressure head

# 6.3.3 Inventory Parameters (GRIDFLO Option)

The following parameters for the repository are read from the inventory file:

- 1. Species name
- 2. Species descendent name
- 3. Total species mass in repository
- 4. Minimum species solubility limit (kg/m<sup>3</sup>) or K<sub>d</sub> limit
- 5. Maximum species solubility limit (kg/m<sup>3</sup>) or Kd limit
- 6. Species radioactive half-life (if colloid, half-life=0.0)
- 7. Species molecular weight

# 6.3.4 Accessible Environment Release Parameters

Cuttings, spallings, and blowout releases for each borehole intrusion are interpolated from release tables versus drilling intrusion time. Releases to the Marker Beds, to the Dewey Lakes, and to the surface are interpolated from release tables versus time. Releases to the Culebra are dependent on the number and types of borehole intrusions that have occurred and are determined either by interpolation from release tables versus time or by calculation of flow and transport. Culebra transport releases are calculated based on unit releases to the Culebra.

## 6.3.5 Borehole Definition Parameters (Optional)

The following parameters are specified from the borehole parameter file. This file specification is optional. If this file is specified, boreholes are pre-defined. Each borehole intrusion is associated with a single repository node specified by x-node and y-node index specifications.

- 1. x-node index
- 2. y-node index
- 3. Diameter
- 4. Hydraulic conductivity

5. Elevation above mean sea level for penetrated formation (Culebra formation for upper borehole segment or Castile formation for lower borehole segment)

6. Pressure head of penetrated formation (Culebra formation for upper borehole segment or Castile formation for lower borehole segment)

7. Intrusion time

# 6.4. Allowable/Prescribed Ranges for Input/Output

Allowable ranges for input values are not restrictive except for validation of positive values and that parameters are valid relative to other input parameter specifications.

# 6.5 Verifiability

Most of the models involve simple algebraic manipulations. The following rates can be verified by simple algebraic manipulations for single intrusions and by probabilistic calculations for thousands of intrusions:

- 1. Drilling intrusion rate
- 2. Mining intrusion rate

Interpolation of summary tables for the following releases can be verified by simple algebraic manipulations:

- 1. Cuttings
  - a. Contact-handled (CH) waste
  - b. Remote-handled (RH) waste
- 2. Spallings
  - a. Undisturbed conditions
    - I. Upper waste panels (1,2,3,6,7,8,9)
    - II. Lower waste panels (4,5,10)
  - b. Previous E2 intrusion (no E1 intrusions)
    - I. Same waste panel
    - II. Different waste panel
  - c. Previous El intrusion
    - I. Same waste panel
    - II. Different waste panel

### 3. Blowouts

- a. Undisturbed conditions
  - I. Upper waste panels (1,2,3,6,7,8,9)
  - II. Lower waste panels (4,5,10)
- b. Previous E2 intrusion (no E1 intrusions)
  - I. Same waste panel
  - II. Different waste panel

- c. Previous E1 intrusion
  - I. Same waste panel
  - II. Different waste panel
- 4. Marker Beds
- 5. Dewey Lakes
- 6. Surface
- 7. Flows to the Culebra
  - a. Undisturbed conditions
  - b. Single E2 intrusions (no E1 intrusions)
  - c. Single E1 intrusions
  - d. E1E2 intrusion scenario
- 8. Transport through the Culebra
  - a. No mining intrusions
    - I. Dissolved species
    - II. Colloid species
  - b. Mining intrusions
    - I. Dissolved species
    - II. Colloid species

The GRIDFLO models requiring verification include:

- 1. Nodal pressure head calculations
- 2. Transport based on flows due to pressure/elevation head differences

Both of the above models can be verified by comparison to a two-node analytical solution to simulate onedimensional flow. A four-node analytical solution can then be used to verify two-dimensional flow between two nodes having two intermediate (alternate path) nodes.

## 6.6 Consistency/Traceability

All software will be constructed using modular coding techniques to facilitate the consistency of coded algorithms and the traceability of program flow in accordance with the Requirements Document for CCDFGF.

# 6.7 Technical Feasibility

The feasibility for implementing a banded matrix solver for the determination of node pressure heads has already been demonstrated. The implementation of the transport model has been demonstrated using the Euler-type solution for single species transport. All other models involve linear interpolation of release tables and verification of intrusion rates.

### 6.8 Implementation

# 6.8.1 Input Parameter Definitions

Run control parameters and associated input data are read first. The repository inventory parameters are read from the inventory file. Repository node parameter definitions are read from the nodalization file. Repository region and panel parameter definitions are read from the regions and panels file. If borehole intrusions are to be predefined, borehole intrusion parameters are read from the borehole parameter file. The following release tables are read from the summary release file for each observation:

- 1. Cuttings (to accessible environment)
- 2. Spallings (to accessible environment)
- 3. Blowouts (to accessible environment)
- 4. Marker Beds (to accessible environment)
- 5. Dewey Lakes (to accessible environment)
- 6. Surface (to accessible environment)
- 7. Flows to the Culebra
- 8. Transport through the Culebra (to accessible environment)

## 6.8.2 Repository Nodalization

Grid leg (internode) properties are defined based on the grid nodalization properties. The intersections of the nodal specification lines correspond to the nodes. All node definitions are processed first. All area definitions are processed after all node definitions have been processed. The last specification for a given area takes precedence over previous specifications for the same area.

## 6.8.3 Leg Property Definitions

All nodes are connected to up to six other nodes by internode legs, excepting those nodes lying on the outer border of the two-dimensional horizontal grid formed by all the nodes. Up to four of these six nodes lie in the horizontal grid representing the repository. The other two nodes are defined when a borehole intrusion occurs: a single node in the Culebra formation above the repository and a single node in the Castile formation below the repository. The following properties are initialized for each internode leg:

- 1. Height
- 2. Width
- 3. Hydraulic conductivity

- 4. Porosity
- 5. Flow rate
- 6. Total solids mass
- 7. Total pore volume available for brine
- 8. Waste fraction (0.0=shaft seal, 1.0=waste drift)

## 6.8.4 Leg Property Modification

Internode leg properties can be redefined or modified by specifying the x-distance and y-distance ranges with new property values corresponding to an area that is to be redefined. The properties for all legs overlapped by the specified the x-distance and y-distance ranges are redefined. Succeeding leg property specifications take precedence over any preceding specifications. A modified area can contain one or more nodes within its boundary but are not required to contain any nodes to redefine leg properties.

# 6.8.5 Borehole Intrusion Parameters

Borehole intrusion parameters can be defined either as direct input or as randomly defined parameters based on input ranges specified with the run control parameters. If the borehole intrusion parameters are defined as direct input, the coefficient matrix and nonhomogeneous vector corresponding to the nodal pressure heads is initialized based on no intrusions. The coefficient matrix and nonhomogeneous vector are then modified according to the borehole intrusion parameters. The resulting coefficient matrix and nonhomogeneous vector are then modified according to the borehole intrusion parameters. The resulting coefficient matrix and nonhomogeneous vector are solved using a banded matrix solver to determine the resulting nodal pressure heads. Grid leg (internode) flow rates can then be calculated based on the nodal pressure heads. A difference in the pressure heads between adjacent nodes translates into a flow from the high pressure node to the low pressure node.

A single set of parameters is required for the definition of each borehole intrusion which penetrates the Culebra and the repository. Two sets of parameters are required for a borehole intrusion which penetrates the Culebra formation, the repository, and the Castile formation. One set corresponds to the penetration from the Culebra formation to the repository (upper borehole). The second set corresponds to the penetrations from the repository to the Castile formation (lower borehole). The elevation and pressure head specifications correspond to either the Culebra formation or the Castile formation.

Borehole parameters can be specified for a borehole that penetrates the repository and the Castile formation but may not have a second specification corresponding to the borehole that penetrates the Culebra and the repository. The lower segment of a borehole specification is not required to have a corresponding upper segment borehole specification. When borehole parameters are not pre-defined, borehole parameters are randomly selected for defined ranges and distributions. An upper segment borehole is always associated with a lower segment borehole, but a lower segment borehole is not always associated with an upper segment borehole.

#### 6.8.6 Node Pressure Heads

The banded matrix solver parameters are defined based on the grid nodalization dimensions. The banded matrix solver uses a two-dimensional banded matrix and an associated one-dimensional nonhomogeneous vector to relate nodal pressure heads. The coefficient matrix and associated nonhomogeneous vector are then modified according to the borehole intrusion parameters at each borehole intrusion time. The resulting coefficient matrix and nonhomogeneous vector are solved using a back substitution banded matrix solver to determine the resulting nodal pressure heads.

#### 6.8.7 Repository Flow Rate Calculations

Grid leg (internode) flow rates can be calculated based on the nodal pressure heads. A difference in the pressure heads between adjacent nodes translates into a flow from the high pressure node to the low pressure node. Leg flow rates are calculated based on the following properties for the leg:

- 1. Length
- 2. Cross-sectional area
- 3. Hydraulic conductivity (calculated from permeability)
- 4. Pore volume
- 5. Elevations at each end of leg
- 6. Pressure heads at each end of leg

A positive flow rate indicates flow in the positive x-direction or positive y-direction. A negative flow rate indicates flow in the negative x-direction or negative y-direction. The magnitude of the flow rate determines the maximum timestep allowed for the transport calculations. The minimum ratio of each leg pore volume to the leg flow rate determines this maximum timestep for the transport calculations.

## 6.8.8 Repository Species Transport

Two basic transport models are used for the transport of species based on brine flow: (1) species solubility limits or (2) species  $K_d$  values determined as the ratio of concentration of the species in solid form to the concentration of the species in the brine. For the case of species solubility limits, the species is present in three physical forms: (1) original waste, (2) brine solution, and (3) precipitated waste. For the case of species  $K_d$  values, the species is present in two forms: (1) original waste and (2) brine solution. A range of either solubility limits or  $K_d$ values is specified for the entire repository grid and these solubility limits or  $K_d$  values can be applied as either spatially constant or spatially variable. A value chosen at random from this range based on a loguniform distribution may be used to specify either the solubility limit or  $K_d$  value for the entire grid or for a single leg within the grid. If the value is used for the entire grid, each leg is assigned the same value, resulting in a spatially constant solubility limit or  $K_d$  value. For a spatially variable solubility limit or  $K_d$  value, different values are randomly selected for each leg in the grid.

An Euler-type solution of a system of differential equations is used to model species transport based on either species solubility limits or species  $K_d$  values. This is based on the assumption that species transport is essentially constant for each timestep. The timestep must therefore be small enough to minimize inaccuracies due to this assumption. The maximum timestep allowed is based on the fact that the entire brine volume within a single leg cannot flow completely into adjacent legs during a single timestep. Total brine solution inflow and outflow for each leg are calculated based on the brine solution concentration of each leg at the beginning of the timestep. The species mass in the original waste, the brine solution, and the precipitated waste are reduced due to radioactive decay occurring during each timestep. The species mass in the brine solution is then compared to the solubility limit for the leg. If the brine species mass is greater than the solubility limit for the leg, the species mass in solution is reduced to the solubility limit, species mass from the precipitated waste in the grid cell. If the brine species mass to achieve the solubility limit, species mass from the precipitated waste. If the species mass in the brine species mass to achieve the solubility limit and the difference is removed from the precipitated waste.

### 6.8.9 Releases to Accessible Environment

Cuttings, spallings, and blowout releases for each borehole intrusion are interpolated from release tables versus drilling intrusion time. Releases to the Marker Beds, Dewey Lakes, and the surface for each timestep are interpolated from release tables versus time. Releases to the Culebra are determined either by interpolation from release tables versus time or by calculation of flow and transport depending on the locations and types of borehole intrusions that have occurred. Culebra transport releases are calculated based on previous unit release calculations to the Culebra.

## 6.8.10 Result Distributions

Result distributions are accumulated for each observation based on an auto-scaling algorithm which stores the distributions in the form of a histogram. These distributions can then be accumulated to determine a CCDF.

The following types of results are accumulated for total releases of one or more species to the accessible environment, summed over all intrusions:

- 1. Cuttings
- 2. Spallings
- 3. Blowouts
- 4. Marker Beds
- 5. Dewey Lakes
- 6. Surface
- 7. Flows to the Culebra
- 8. Transport through the Culebra

Flows to the Culebra and transport through the Culebra are accumulated separately for each species. Flows to the Culebra are modeled using four different scenarios depending on the locations and type of borehole intrusions that have occurred. Before any borehole intrusions occur, releases to the Culebra are interpolated from release tables for undisturbed conditions. After the first borehole intrusion has occurred, releases are interpolated from release tables for individual E1 and E2 intrusion scenarios. An E1 scenario is an intrusion that penetrates the repository and a pressurized brine pocket below the repository. An E2 scenario is an intrusion that penetrates only the repository. After the first drilling intrusion that results in an E1E2 scenario, releases are calculated by modeling brine flow and associated species transport through the repository. An E1E2 scenario is two or more borehole intrusions, one of which must be an E1 intrusion. All releases to the Culebra and all transport through the Culebra are accumulated for individual species and for the total release including all species.



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### 7. Summary

The Requirements Document for CCDFGF specifies the following conditions to be satisfied:

(1) assemble results calculated with BRAGFLO, NUTS, PANEL, CUTTINGS, BRINEFLO, SECO-TRANSPORT and possibly other WIPP PA codes to produce the CCDF specified in 40 CFR 191 (Fig. 2.1),

(2) allow brine pocket location in the Castile Formation to be specified as an input,

(3) construct the distribution of CCDFs that results from subjective uncertainty as indicated in Eq. (2.5) and Figs. 2.3, 2.4 and 2.5,

(4) be quick running (~ 5-10 min CPU time per individual CCDF construction on a VAS Alpha,

(5) have transparent, easily modified coding to facilitate the incorporation of changed assumptions into CCDF construction, and

(6) meet all applicable WIPP QA requirements.

In addition, CCDFGF shall contain a subroutine, to be called GRIDFLO (Fig. 2.2), that calculates releases based on Darcy flow for E1E2-type intrusions (i.e., futures of the form indicated in Eq. (2) that involve two or more drilling intrusions of which at least one penetrates pressurized brine in the Castile Formation). This subroutine must

(1) determine flow patterns through the repository that result from multiple drilling intrusions of which at least one penetrates pressurized brine in the Castile Formation,

(2) be based on Darcy's Law for single phase flow and incorporate (a) the location, diameter and permeability of individual boreholes above and below the repository, (b) the geometric structure of the repository including the waste handling and experimental regions, (c) the presence or absence of seals within the repository, (d) boundary pressures in the Castile Formation and the Culebra Dolomite, (e) radionuclide transport within the repository and to the Culebra Dolomite by flowing brine, including the effects of decay, sorption and solubility, and (f) the penetration or nonpenetration of pressurized brine in the Castile Formation by individual drilling intrusions,

(3) be fast running as several thousand calls to GRIDFLO will likely be required in each CCDF construction with CCDFGF (fast-running can be achieved by considering steady-state solutions to the equations that underlie Darcy's Law, with each solution requiring the evaluation of a single system of linear algebraic equations).

(4) have a stand-alone run capability for the analysis of specific patterns of drilling intrusions,

(5) meet all applicable WIPP QA requirements.



The code described in this document will satisfy the above requirements.

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