Appendix E

NUCLEAR WASTE MANAGEMENT PROCEDURE Sandia National Laboratories	**Design Document Criteria**	**Form Number: NP 19-1-4** **Page 1 of 1**

1. **Software Name:** CCDFGF
2. **Software Version:** 8.01
3. **Document Version:** 8.01
4. **ERMS #:** 577625

Prior to sign-off of the DD, all items shall be appropriately addressed by the code sponsor so that "**Yes**" may be checked. Include this form as part of the DD.

Are the following appropriately defined and documented in the DD?

5. Major Software Components ☒ Yes
6. Technical description of the software with respect to: theoretical basis, embodied mathematical model, major control flow, control logic, and data structures ☒ Yes
7. Functionalities and interfaces of object components, functions, and subroutines. ☒ Yes
8. Allowable or prescribed ranges for inputs and outputs ☒ Yes
9. Verifiability: Is the design verifiable through testing or other means? ☒ Yes
10. Consistency and Traceability: Is the design consistent with and traceable to the software's requirements? ☒ Yes
11. Technical Feasibility: Is the design technically feasible? ☒ Yes
12. Implementation: Is the design presented in sufficient detail to allow for implementation as computer software? ☒ Yes

13.	Sarah Brunell **Code Team/Sponsor** (*print*)	*Signature on File* Signature	8/11/22 Date
14.	Clifford Hansen **Technical Reviewer** (*print*)	*Signature on File* Signature	8/11/22 Date
15.	Shelly R. Nielsen **QA Reviewer** (*print*)	Shelly R. Nielsen Signature	8/22/22 Date
16.	Steve Wagner **Responsible Manager** (*print*)	*Signature on File* Signature	8/16/22 Date
17.	Jennifer Long **SCM Coordinator** (*print*)	*Signature on File* Signature	8/17/22 Date

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Appendix G

NUCLEAR WASTE MANAGEMENT PROCEDURE Sandia National Laboratories	**User's Manual Criteria**	**Form Number: NP 19-1-6** **Page 1 of 1**

Does the User's Manual contain as appropriate:

1. **Software Name:** CCDFGF
2. **Software Version:** 8.01
3. **Document Version:** 8.01
4. **ERMS #:** 577625

Prior to sign-off of the User's Manual, all items shall be appropriately addressed by the code sponsor so that "**Yes**" or "**N/A**" may be checked. Include this form as part of the User's Manual.

5.	A statement(s) of functional requirements (consistent with those in the RD)?	☒	Yes		
6.	An explanation of the mathematical model and numerical models, where applicable as based on code functionality?	☒	Yes	☐	N/A
7.	Physical and mathematical assumptions, where applicable as based on code functionality?	☒	Yes	☐	N/A
8.	The capabilities and limitations inherent in the software?	☒	Yes		
9.	Instructions that describe the user's interaction with the software?	☒	Yes		
10.	The identification of input parameters, formats, and valid ranges?	☒	Yes		
11.	Messages initiated as a result of improper input and how the user can respond?	☒	Yes		
12.	The identification and description of output specifications and formats?	☒	Yes		
13.	A description of any required training necessary to use the software?	☒	Yes		
14.	The identification of components of the code that were not tested?	☐	Yes	☒	N/A

15.	Sarah Brunell **Code Team/Sponsor** (*print*)	*Signature on File* Signature	8/11/2022 Date
16.	Clifford Hansen **Technical Reviewer** (*print*)	*Signature on File* Signature	8/11/2022 Date
17.	Shelly R. Nielsen **QA Reviewer** (*print*)	Shelly R. Nielsen Signature	8/22/2022 Date
18.	Steve Wagner **Responsible Manager** (*print*)	*Signature on File* Signature	8/16/2022 Date
19.	Jennifer Long **SCM Coordinator** (*print*)	*Signature on File* Signature	8/17/2022 Date

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WIPP PA

Design Document and User's Manual

for

CCDFGF Version 8.01

Document Version 8.01

ERMS #577625

August 2022

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1.0 INTRODUCTION AND SCOPE

This Design Document and User's Manual for CCDFGF Version 8.01 describes the following major features of software design: software components, theoretical basis, mathematical model, control flow and logic, data structures, and functionality and the interfaces of subroutines. It also describes in detail the allowed or prescribed ranges for input data and user interface, in accordance with the Nuclear Waste Management Procedure NP 19-1 Software Requirements (Long, 2020). This code is used by the Sandia National Laboratories' Performance Assessment (PA) Department in support of the performance assessment calculations for the Waste Isolation Pilot Plant (WIPP). It is controlled under the software configuration management system CVS (Concurrent Versions System) on the Linux platform.

1.1 Software Identification

Code Name:	CCDFGF
Version:	8.01
CVS Repository:	/data/cvs/CVSLIB/WIPP_CODES/PA_CODES/CCDFGF
Platform:	CentOS 7/Dell PowerEdge C6420
Host:	fwm.sandia.gov
Compiler:	Gfortran/GCC 8.2.0

1.2 Points of Contact

Code Sponsor:	Sarah Brunell	sbrunel@sandia.gov	(575) 234-0038

1.3 Code Overview

The code CCDFGF is part of the PA system. CCDFGF is the computer program that constructs complementary cumulative distribution functions (CCDFs) of releases from the WIPP repository using Monte Carlo procedures. This code synthesizes the releases calculated by other PA system components and compares the performance of WIPP to the limits established in the regulations.

CCDFGF Version 7.0 and above writes its output data to a database for post-processing. The user must provide the name of the database, the analysis name (e.g., CRA19), the analysis revision (usually 0), and the replicate number. The binned data and the statistics are stored for each vector.

CCDFGF calculates the following eight statistics for each variable and each vector: mean of the data across the set of futures, the median, the 95th percentile value, the standard deviation, the proportion of non-zero values, the maximum release value, the probability associated with the maximum release, and the minimum bin value for the results.

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2.0 REQUIREMENTS

CCDFGF is the computer code that constructs CCDFs of releases from the WIPP repository using Monte Carlo procedures. Requirements for the CCDFGF code fall into five categories: functional requirements, performance requirements, code attributes, external interfaces, and other requirements.

2.1 Functional Requirements

The functional requirements for CCDFGF are listed below.

R.1 CCDFGF must construct individual CCDFs that account for aleatory uncertainty about the future of the repository.

R.2 CCDFGF must construct a distribution of CCDFs that results from epistemic uncertainty.

R.3 CCDFGF must incorporate the potential for intrusions into brine pockets in the Castile Formation.

R.4 CCDFGF will account for the effects of intrusions into each separate waste panel. In addition, CCDFGF will group panels into 4 groups to be consistent with the current representation of the repository. The total number of panels, panel number, and probability of drilling into each panel will be specified in the control file. Panel groups (lower, middle, upper, or other) and adjacency relationships (same, connected, adjacent, or non-adjacent) will also be defined in the control file.

R.5 CCDFGF will incorporate a random number generating function that can generate repeatable streams of random numbers from an input seed.

R.6 CCDFGF will utilize tables of radionuclide concentrations across one or more panel brine volumes. The number of brine volume-concentration tables will be specified in the PRECCDFGF output (RELTAB) file.

R.7 CCDFGF must be able to simulate a variable number of panels. The maximum panel number will be specified in the control file.

R.8 CCDFGF must be able to simulate releases from the Culebra using a variable number of Culebra release points. The release point for each panel will be specified in the control file.

2.2 External Interface Requirements

The external interface requirements are listed below:

R.9 CCDFGF must take as input the results of the component models used in an assessment. These results are assembled into an input file by PRECCDFGF (Brunell, 2022b). CCDFGF produces the CCDF specified in 40 CFR 191 (EPA, 1985).

R.10 CCDFGF will write the binned data and the statistics to a database specified by the user at run time.

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2.3 Other Requirements

There are no other requirements for CCDFGF.

2.4 Functionality Not Tested

CCDFGF has the ability to treat borehole diameter as a stochastic variable for each intrusion by sampling a borehole diameter from a triangular distribution and then scaling the cuttings and cavings volumes by the square of the ratio of the sampled borehole diameter to the value used by CUTTINGS_S. Line 9 of the control input file is set to 'T' to select this option, however this code functionality is untested in CCDFGF Version 8.01. The only functionality fully qualified for use in CCDFGF Version 8.01 is to use a fixed borehole diameter, which is selected by specifying 'F' on Line 9 of the control input file. The value of the fixed borehole diameter (in meters) should be specified as the first value on Line 10 of this file. The remaining two values on Line 10 are ignored by CCDFGF when using a fixed borehole diameter, however the first value is duplicated by convention.

3.0 MAJOR SOFTWARE COMPONENTS

This section describes the organization of the CCDFGF source code, and the structure and content of the input and output files for CCDFGF.

CCDFGF is implemented in FORTRAN. All subroutines and functions are found in a single file. To avoid lengthy argument lists for subroutines and functions, and to provide variables with global scope, numerous variables are declared and grouped into COMMON blocks in 27 separate "include" files with file type "*.inc*". Additionally, CCDFGF makes use of the WIPP PA libraries CAMCON_LIB, CAMSUPES_LIB, and DB_LIB to standardize common user interface and I/O functions (Gilkey, 2006a and 2006b). These libraries are linked to the CCDFGF executable during the build process as documented in the CCDFGF Implementation Document (Brunell, 2022c).

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3.1 Object Libraries

CCDFGF uses the following object libraries:

- CAMCON_LIB: provides general-use functions, such as handling command line arguments, displaying standardized output, and parsing free-field input. CCDFGF links to subroutines FILDFNAM, FILRDNAMS, FILWRNAMS, QAABORT, QABANNER, QACPUS, and QASETUP.

- CAMSUPES_LIB: provides machine-dependent functions. CCDFGF does not directly link to any subroutines in the CAMSUPES_LIB; this library is instead used by the other object libraries.

- DB_LIB: retrieves information from the Performance Assessment Parameter Database or stores/retrieves information from the PA_Results database. CCDFGF links to subroutines RDBCLOSE, RDBDELETECCDF, RDBLOADCCDF, RDBOPEN, and RDBPREPCCDF.

3.2 Input Files

A number of input files are needed to execute CCDFGF. Input files fall into three categories: release and transport data, model parameters, and simulation control parameters. Input files are specified using command line arguments as described in Section 8.0.

3.2.1 Release Table (RELTAB) Input File

The RELTAB input file consolidates all the release information from the various models for input to the CCDFGF code. The RELTAB file is an ASCII file produced by the PRECCDFGF code and can be very large, but has a well-defined structure. The file has a relatively small section of information that is common to all vectors, followed by a lengthy data section for each vector.

The RELTAB file starts with a listing of constant parameter values obtained from the parameter database. Next, the RELTAB file contains maximum array dimensions for spallings, direct brine releases (DBR), and flows to the Culebra; these values are used in CCDFGF to dimension data structures. Following these array dimensions, the RELTAB file contains two title records, followed by a line reporting the number of vectors to follow in the file and a line reporting the number of Culebra release points for each vector in the file.

The remainder of the RELTAB file is a series of data groups, one group for each vector. Within each group are the following sections of data: sampled parameters; cuttings and cavings releases; spallings releases; direct brine releases; releases to the Culebra; and transport through the Culebra. Except for the first vector, the structure of each data section is the same for each vector. Some data, such as interpolation times, are written to the data section for the first vector only.

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3.2.1.1 Sampled Parameters Section

For each vector, the RELTAB file lists the values of sampled parameters. In CCDFGF, the only sampled parameter is the probability of a drilling intrusion encountering a brine pocket below the repository.

3.2.1.2 Cuttings and Cavings Releases Data Section

The cuttings and cavings release data section starts with three lines of data that are repeated for every vector. The first line that gives the vector number, an unused flag, and the text CUTTINGS RELEASE TABLE. The second line provides data for contact handled (CH) waste: the number of interpolation times; the number of CH waste streams; the area of a drilling intrusion into CH waste with cavings included; and the drill bit diameter. The third line provides data for remote handled (RH) waste: the number of interpolation times; the number of RH waste streams; and the area of a drilling intrusion into CH waste with cavings included. PRECCDFGF uses the drill diameter to calculate the area of a drilling intrusion into RH waste and assumes no increase in area due to cavings.

For the first vector only, the first three lines are followed by additional data, as follows:

- the probability of encountering each CH waste stream
- the probability of encountering each RH waste stream
- the interpolation times for CH waste stream activities
- the interpolation times for RH waste stream activities
- the activities of each CH waste stream at the interpolation times in EPA units per m^3, written from the first time to the last time for each CH waste stream, from the first CH waste stream to the last.
- the activities of each RH waste stream at the interpolation times in EPA units per m^3, written from the first time to the last time for each RH waste stream, from the first RH waste stream to the last.

3.2.1.3 Spallings Releases Data Section

The spallings release data section starts with one line that gives the vector number, an unused flag, and the text SPALLINGS RELEASE TABLES. The data section next contains the number of interpolation times for spallings releases, the interpolation times and the activity of the CH waste in EPA units per m^3 at these interpolation times. Next, the spallings release section contains three blocks of data, for E0, E1 and E2 intrusions.

The E0 intrusion block has four components for the lower, middle, upper and other panel groups. In each component is one data segment comprising a single time series. The time series is described by the number of interpolation times, a list of interpolation times, and the spallings releases at the interpolation times.

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The E1 and E2 intrusion block has four components for same, connected, adjacent, and non-adjacent panel groups. Each panel group component has a series of data segments, and starts with the number of data segments in the component. Each segment comprises a single time series. The time series is described by the number of interpolation times, a list of interpolation times, and the spallings releases at the interpolation times. The E2 intrusion block has the same structure as the E1 intrusion block.

3.2.1.4 Direct Brine Releases (DBR) Data Section

The DBR release data section starts with one line that gives the vector number, an unused flag, and the text DIRECT BRINE RELEASE TABLES. The data section next contains a data block with the concentrations of mobilized radionuclides for DBR releases. This data block lists the number of interpolation times and number of panel brine volumes, followed by the interpolation times, and the panel brine volumes (m^3). Next, the concentrations (EPA Units/m^3) for four radionuclides (Am241, Pu239, U234 and Th230) and total concentration in EPA units per m^3 at each interpolation time for the E0, E1, and E2 scenarios are listed, in that order. When multiple panel brine volumes are considered in the calculations, concentrations are listed in blocks from the first to last brine volume for the E0 scenario, followed by the same data ordering for the E1 then E2 scenarios.

Next, the DBR release section contains three blocks of data, for E0, E1 and E2 intrusions. The structure of each block is the same as the corresponding block in the spallings release section.

The E0 intrusion block has four components for the lower, middle, upper, and other panel groups. Each component lists the number of interpolation times, the interpolation times, DBRs at each interpolation time, and the DBR volumes at each interpolation time.

The E1 intrusion block has four components for the same, connected, adjacent, and non-adjacent panel groups; these panel groups correspond to the release input files for the lower, middle, upper, and other intrusions, respectively. Each panel group component has a series of data segments, and starts with the number of data segments in the component. Each segment consists of a number of interpolation times, a list of interpolation times, and the DBR releases at the interpolation times. The E2 intrusion block has the same structure as the E1 intrusion block.

3.2.1.5 Releases to Culebra Data Section

The releases to Culebra data section starts with one line that gives the vector number, an unused flag, and the text RELEASES TO CULEBRA RELEASE TABLES.

For the first vector only, immediately after the first line of the releases to Culebra data section, the RELTAB file presents the number of colloid species, the number of decay chains, the number of members in each decay chain, and names of the four radionuclides. Next, the interpolation times for releases to Culebra data section are listed for each of four scenarios: E0, E1, E2, and E1E2. The interpolation times for each scenario consist of one or more blocks of data. The RELTAB file lists the number of blocks, then for each block, the file lists the number of times and then the interpolation times.

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The remainder of the releases to Culebra data section is repeated for each vector. First, the colloid species fractions are listed; for each radionuclide in the order listed for vector one, the data specify the colloid species fraction for each colloid species.

Next, the releases to Culebra data section lists the flows to the Culebra for the E0, E1, E2, and E1E2 scenarios. For each scenario, the RELTAB file contains a number of blocks of data, corresponding to the number of blocks of interpolation times for that scenario. For each block the number of interpolation times are listed, followed by the flow to the Culebra in Curies for each radionuclide in the order listed for vector one. These data are followed by three additional segments of data, listing the releases out the marker beds, Dewey Lake, and to the surface for the E0 scenario. The marker bed, Dewey Lake, and surface releases are in EPA units thus are not listed by radionuclide.

3.2.1.6 Culebra Transport Data Section

The Culebra transport data section starts with one line that gives the vector number, an unused flag, and the text TRANSPORT FROM CULEBRA RELEASE TABLES.

For the first vector only, immediately after the first line of the Culebra transport data sections, the RELTAB file presents the total activity of TRU radionuclides in Curies in the repository. Next, the RELTAB file lists for each of four radionuclides: the decay rate (yr^{-1}); the number of moles in a kg of the radionuclide; the specific activity (unitless); and the release limit (Curies) per unit of waste. Next the RELTAB file lists the number of interpolation times for Culebra transport, followed by the interpolation times.

The remainder of the Culebra transport data section is repeated for each vector. The first line lists the Culebra release point referenced for the current block of data, followed by a sequence of data blocks. For each radionuclide there are two blocks: the first for partially-mined conditions, and the second for fully-mined conditions. Each block lists the amount (in kg) transported to the LWB from a 1 kg source placed in the Culebra at each interpolation time. For each vector, this data format is repeated once for each of the number of Culebra release points specified at the top of the RELTAB file.

3.2.2 Control File

The Control file is used to control the execution of CCDFGF. The first 26 lines of the file are always present whereas the remainder of the file varies depending on whether order statistics are to be output, whether minimum and maximum values are to be specified for the output histogram tables and on the number of panels to be represented in the repository. Table 3-1 lists the records in the control file; and example control file is shown in Figure 3-1.

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Table 3-1. Control File Data for Fixed Records

Record	Data Description	Data types
1	First title line	Character (130 characters at most)
2	Second title line	Character (130 characters at most)
3	Number of futures per observation	Integer
4	Number of observation for detailed print	Integer
5	Observation indices	Blank delimited list of integers
6	Number of futures for detailed print	Integer
7	Futures indices	Blank delimited list of integers
8	End time (yr)	Floating point
9	Simulate variable borehole diameters	Logical (Value of T is unqualified)
10	Borehole diameter range and mode above repository (m)	Three blank delimited floating point numbers (Minimum, Maximum and Mode)
11	Number of waste streams to average for CH wastes and RH wastes	Two blank delimited integers
12	Number of intrusions to deplete each brine pocket	Integer
13	Spallings reference (T=after E1) and no. of intrusions	Logical and integer
14	Blowout reference (T=after E1) and no. of intrusions	Logical and integer
15	Random number generator seed	Integer
16	Relative roundoff tolerance	Floating point
17	Generate only (0), read (1) or store (2) random numbers	Integer
18	Use repository-scale concentrations for spalling calculations	Logical
19	Use volume fraction as probability for release of cuttings	Logical
20	Write the binned distribution data to a file	Logical
21	Write tables of the sorted results	Logical
22	Write summary statistics	Logical
23	Export the mean and median across observations within frequency (Y)	Logical
24	Number of order statistics to be exported	Integer
25	The order statistics to be exported	Blank delimited list of integers
26	Number of variables (N) for which minimum and maximum values will be specified for controlling the X-axis of the histogram	Integer
27 to 27+N	Number of the variable, the minimum and maximum values	Blank-delimited list of integers followed by 2 floating point numbers
28+N	The Culebra release point designated for undisturbed releases.	Integer (I2 format)
29+N	The number of panels (P) to be represented, maximum of 50.	Integer (I2 format)
30+N to 31+N	Comment sections	Comments
32+N to 32+N+P	Panel specific data, formatted as panel number (I2, 1x), panel group (A1, 1x), Culebra release point associated with the panel (I2, 1x), and probability of intruding the panel (F11.9, 1x). This is then followed by P columns representing the adjacency relationship between the current panel and the panel represented by the column number listed in the first comment line at the bottom of the control file (A1, 1x).	Types as indicated by format.

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```
TEST CASE FOR WIPP DRILLING INTRUSION SCENARIO
    (SECOND TITLE RECORD)
 2           NUMBER OF FUTURES PER OBS
 8           NUMBER OF OBSERVATION FOR DETAILED PRINT
 1 2 3 4 5 6 7 8        OBSERVATION INDICE
 2           NUMBER OF FUTURES FOR DETAILED PRINT
 1 2         FUTURES INDICES
 10000.      END TIME (YR)
 F           Simulate variable borehole diameters
 0.3111  0.3111  0.3111  BOREHOLE DIAMETER RANGE AND MODE ABOVE REPOSITORY (M)
 3  1        NUMBER OF WASTE STREAMS TO AVG FOR CH WASTES AND RH WASTES
 1000        NUMBER OF INTRUSIONS TO DEPLETE EACH BRINE POCKET
 F      1000 SPALLINGS REFERENCE (T=AFTER E1) AND NUMBER OF INTRUSIONS
 F      1000 BLOWOUT REFERENCE (T=AFTER E1) AND NUMBER OF INTRUSIONS
 1701        RANDOM NUMBER GENERATOR SEED
 1.0E-6      RELATIVE ROUNDOFF TOLERANCE
 1           Generate only(0), read(1) or store(2) random numbers
 T           Use repository-scale concentrations for spalling calculations
 F           Use volume fraction as probability for release of cuttings
 T           Write the binned distribution data to a file
 F           Write tables of the sorted results
 F           Write summary statistics
 F           Export the mean and median across observations within frequency (Y)
 0           Number of order statistics to be exported
 1 7 8       The order statistics to be exported
 0           Number of result-histogram minimum and maximum override values (X-axis)
 01          CULEBRA RELEASE POINT FOR UNDISTURBED RELEASES
 12          NUMBER OF PANELS (MUST BE 2-DIGIT INTEGER)
! PANEL NUMBER, PANEL GROUP, CULEBRA RELEASE POINT GROUP,
! PANEL INTRUSION PROBABILITY, ADJACENCY RELATIONSHIPS
 1 U 01 0.083000000 S A A A A A A A A N N N N N N N N
 2 U 01 0.083000000 A S A A A A A A A N N N N N N N N
 3 M 01 0.083000000 A A S C C C A A C A N N N N N N N N
 4 M 01 0.083000000 A A C S C C A A C A N N N N N N N N
 5 L 01 0.083000000 A A C C S C A A C A N N N N N N N N
 6 M 01 0.083000000 A A C C C S A A C A N N N N N N N N
 7 U 01 0.083000000 A A A A A A S A A A N N N N N N N N
 8 U 01 0.083000000 A A A A A A A S A A N N N N N N N N
 9 M 01 0.083000000 A A C C C C A A S A N N N N N N N N
10 U 01 0.083000000 A A A A A A A A A S N N N N N N N N
11 O 01 0.085000000 N N N N N N N N N S A A A A A A A A
12 O 01 0.085000000 N N N N N N N N N A S A A A A A A A
!    PANEL # COLUMN 1 2 3 4 5 6 7 8 910111213141516171819
! S = Same; C = Connected; A = Adjacent; N = NonAdjacent
!
!
```

Figure 3-1. Example Control File Data

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Optional descriptions can be used on each record following the data. A title for the analysis can be assigned to records 1 and 2. Record 3 lists the number of futures to be run for each observation (observations are also referred to as vectors). This value is generally 10000. Records 4 through 7 are used to control the printing of diagnostic data. Record 4 lists the number of results to be included in the diagnostic output, and record 5 lists the indices of the results to be printed. Record 6 lists the number of futures to be included in the diagnostic output and record 7 list the numbers of the futures to be printed. Record 8 lists the time for the end of the simulation, which is normally 10,000 years. The borehole diameter used in CCDFGF is normally read in from the RELTAB file but can be sampled from a triangular distribution as well; however, the capability to sample the borehole diameter from a triangular distribution is unqualified functionality in CCDFGF Version 8.01. Record 9 is used to signal whether the diameter of the boreholes should be sampled in CCDFGF as a stochastic value, and record 10 specifies the minimum, mode and maximum for the triangular distribution to be used.

Record 11 specifies the number of contact-handled (CH) and remote-handled (RH) waste streams to be averaged. The number of waste streams to be averaged reflects the number of waste streams likely to be encountered when a borehole encounters the waste. Assuming complete randomness in emplacement at the scale of barrels, one might expect three randomly-selected waste streams to be sampled since the barrels are stacked three high. If clustering of the barrels by waste stream is assumed then the number of CH waste streams to be averaged could be reduced to as little as 1. Since RH waste is assumed to be stored horizontally in the walls of the repository, only one RH waste container is currently expected to be sampled during each intrusion.

Record 12 lists the number of intrusions to deplete the brine pocket. By setting this number to a value that exceeds the number of intrusions expected over the period of the simulation, such as 1000 for a 10,000 year simulation, then the simulation proceeds as if the brine pocket can never be depleted. If a low value is set then the brine pocket is assumed to be depleted once it is penetrated that many times which then eliminates the possibility of having an E1 intrusion event.

Records 13 and 14 are used to limit the number of spallings releases and direct brine releases, respectively, following the first E1 event. Each record has a logical value (T or F for true or false) that controls whether the type of release should be limited. That logical is followed by an integer number for the maximum number of releases that are allowed if the logical parameter is set to true.

Record 15 sets the random number seed. This value should be a positive integer. Because the pseudo-random number generators used in computer simulations repeat the same sequence of numbers given the same starting value (seed), specifying the seed enables analysts to better inter-compare model results. Using different seeds is expected to generate a somewhat different set of results, although in the long run one would not expect much difference to be observed in the mean or median behavior of the model.

Record 16 is the relative round-off tolerance, which is used to set the level above which computed results are considered to be valid. Complex computations involving combinations of large and small values invariably contain rounding errors. The errors can be either positive or negative and, if treated as precise values, can lead to erroneous results. The relative tolerance value ensures that computed values less than the expected precision of a calculation are treated as zero.

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Record 17 expands the control of the random number generator by allowing one to save to a file the entire set of values generated by the random number generator during a run of the code, or to specify that the random numbers are to be read from a file instead of being generated at run-time. A value of 0 indicates that random numbers are to be generated but not saved, 1 that the values are to be read from a file, and 2 that the numbers are to be generated and saved to a file. This feature enables the analysts to ensure that the sequence of random values between runs of the model are identical, and also enables the analyst to construct a file for testing the model that contains a series of values that will cause the simulation to follow a known sequence of events.

Record 18 controls how CCDFGF treats waste emplacement. If set to true (T), CCDFGF treats the repository as a single unit when computing spallings releases and interpolates the release using spallings data from the RELTAB input file. If set to false (F) CCDFGF computes spallings releases based on the concentrations in the cuttings and cavings for the intruded panel.

Record 19 lists a logical value that controls whether the volume fraction is to be used in determining whether waste is encountered by a borehole when computing releases in cuttings and cavings. If a value of true (T) is listed then the probability of a borehole encountering waste is computed from the volume fraction. The process of encountering waste is then treated as a stochastic process using that probability. If a value of false (F) is assigned to record 19 then the volume fraction is simply treated as a weight factor in the release.

CCDFGF Version 7.00 and above saves results for constructing the CCDFs by counting the number of values that fall within a set of intervals, or bins. The limits on the bins are adjusted during the execution of the code to ensure that the data fall within a pre-determined number of bins; the number of bins (161 in CCDFGF Version 8.01) is specified in the include file *param1.inc*. This method for constructing the CCDFs is controlled by the logical value assigned to record 20. A value of true (T) specifies that CCDFs will be written to the output file designated at runtime.

An additional method for constructing CCDFs is also provided. This alternative method creates a pair of files of the values for each result. These files contain the data generated for each vector sorted in increasing order. One of the files is constructed as a Y-many-X format, where Y is the probability and X the value. The names of these files are "Result" with a 2-digit index for the result and ".txt" appended. The other file in the pair is constructed from interpolation as an X-many-Y format and is named "Result" with a 2-digit index for the result and "_XMY.txt" appended. The X-many-Y format is produced in order to allow the easy construction of confidence of tolerance intervals in the vertical direction. These data can also be used to generate the CCDFs. Record 21 contains a logical value to control the use of this alternative method, if set to true (T), the alternative files are generated.

Record 22 controls the generation of summary statistics for the output variables. The summary statistics include the mean, median, standard deviation, number of observations, minimum value, maximum value, minimum value greater than 0, geometric mean, geometric standard deviation, number of values greater than 0, and the nominal 10th and 90th percentiles. A value of true (T) will cause the summary statistics to be generated and printed to the file "SummaryStatistics.txt."

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In addition, this alternative method enables one to export the mean and median across the CCDFs (controlled by the logical value assigned to record 23) and order statistics that can be used to construct distribution-free tolerance intervals (controlled by records 24 and 25). Record 23 must contain true (T) to export the mean, median and order statistics or false (F) to suppress the exportation of the statistics. Record 24 lists the number of order statistics to be exported and record 25 has a blank-delimited list of the order statistics to be exported. The order statistics are indexed from 1 to *n,* where 1 is the index of smallest value and *n* is the index of the largest value of the *n* futures simulated. The number of records in the remaining portion of the control file is variable and depends on whether one wants to control the range of the X-axis of the CCDFs constructed using the binned data. By default the range of the bins, i.e. the range of the X-axis, for the binned data that can be used to generate CCDFs depends on the minimum and maximum of the data. The default scaling for the binned data can be changed for a result by specifying an alternative minimum and maximum value. Record 26 lists the number of results, *n*, which are to have their default scaling overridden. Records 27 through 27+*n* then list a triplet of numbers: the index of the result (an integer), the minimum and the maximum values as floating point numbers. Note that the minimum and maximum values listed in the control file are used to set the bin sizes instead of the actual minimum and maximum values observed in the data and are not necessarily the endpoints for the X-axis of the CCDF. The method used to assign data to a bin depends on using bins that increase in width by powers of two, so the actual range could exceed the range specified.

Record 28+*n* is used to designate which Culebra release point should be used by CCDFGF to evaluate releases from the Culebra for the undisturbed scenario.

The configuration of the panels is specified in the final block of records. Record 29+*n* lists the number of waste panels in the repository, *p*. This is followed by two comment lines (records 30+*n* and 31+*n*) describing the following block of data for convenient reference by the analyst. Each of the last *p* records, 32+*n*+*p*, lists the panel number, the panel group to which it belongs (L, M, U, or O for lower, middler, upper, or other, respectively), the Culebra release point assigned to the panel, the probability of intruding the panel, and a list of single characters representing the adjacency relationships between the panel and each of the other panels in the repository (S, C, A, or N for same, connected, adjacent, or non-adjacent panels, respectively). Panel numbers must be consecutive integer values starting with 1. The adjacency relationships listed for the panels must show symmetric relationships in the sense that if panel 5 is adjacent to panel 1, then panel 1 must be adjacent to panel 5.

3.2.3 Random Numbers File

The random numbers file is an optional file that contains a list of values generated by the RAN3 pseudo-random number generator. It can be used for both input and output, depending on the option selected in the control file. The file is an unformatted (binary) file consisting of a double precision floating point number followed by a four byte character value. The character string is a tag passed to RAN3 when it is referenced and can be used to identify where each value was used at the time the file is generated. On input a warning message is written to standard output if the tag from the file does not match the tag passed on the call to RAN3.

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3.3 Output Files

The number of output files created by CCDFGF depends on the options set in the control file, as described in Section 3.2.

3.3.1 Results as CCDFs from Binned Data

The CCDF results file is an ASCII (text) file containing data that can be used to construct the graphs of the CCDFs for the results. The file has a set of header records that define the data followed by the numeric data. The first record of the file is simply a title (Figure 3-2). The next record lists the following values: the maximum index of observations, the maximum index of futures, the maximum index of results, the maximum index of "other" results, the maximum index of base results, the number of species, and the number of bins. The numeric data are referenced using a 0-based indexing scheme so that the number of the various results is one more than the maximum index. Thus, in the example shown in Figure 3-2, there are a total of 36 output summary release data; descriptions of these variables follow record 2. The first 17 variables constitute the "base" results, which are fixed. The "other" results are the first 11 variables of the base results representing variables for release pathways other than Culebra transport. After the 17 base results, 5 variable descriptions are listed constituting releases for each species to the Culebra in a dissolved state, to the Culebra as colloids, the total releases to the Culebra, the releases from the Culebra per Culebra release point, and the total releases from the Culebra. In the example shown in Figure 3-2, there are 4 radionuclide species. With 5 output variables per species, including variables associated with the single Culebra release point, the result is 20 release variables. The remaining records in the file are the values for the output variables.

A set of CCDF data is composed of three records. The first record lists the observation (vector) number, the index of the result, the mean of the data across the set of futures, the median, the 95th percentile value, the standard deviation, the proportion of non-zero values, the value associated with the peak of the distribution, the probability associated with the peak, and the minimum bin value for the results. Note that the mean and standard deviation calculation treats negative results as zero. The second and third records list the bin values for each of the bins (161 in the example of Figure 3-2) and the associated probabilities, respectively. The triplets of records are ordered by observation and then by results within observation. The eight statistics written to the output file are also written to the database.

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```
  TEST CASE FOR WIPP DRILLING INTRUSION SCENARIO
       8       2       35       10       15       4      161
Buffer
Cuttings and Cavings
Spallings
Direct Brine
Cuttings and Cavings Volume
Spallings Volume
Direct Brine Volume
Marker Beds
Dewey Lake
Direct Surface
Cut+Spall+DirectBrine
Total To Culebra-D
Total To Culebra-C
Total To Culebra
Total From Culebra
Total
Am241 to Culebra-D
Pu239 to Culebra-D
U234 to Culebra-D
Th230 to Culebra-D
Am241 to Culebra-C
Pu239 to Culebra-C
U234 to Culebra-C
Th230 to Culebra-C
Total Am241 to Culebra
Total Pu239 to Culebra
Total U234 to Culebra
Total Th230 to Culebra
Total Am241 from Cul-CRP-01
Total Pu239 from Cul-CRP-01
Total U234 from Cul-CRP-01
Total Th230 from Cul-CRP-01
Total Am241 from Culebra
Total Pu239 from Culebra
Total U234 from Culebra
Total Th230 from Culebra
    1    0 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000E+00.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00
 0.000E+00
```

Figure 3-2. A Portion of the File Containing Binned Output Data

3.3.2 Diagnostic Output File

The diagnostic output file contains data that describe many of the execution paths that were followed and the data that were used in computing releases. The contents of the file include many descriptions to help interpret the data (Figure 3-3). The structure of the file is highly variable because it depends on the paths taken in the simulation and these paths are determined by the stochastic events that are simulated. The number and selection of the observations tracked in the diagnostic file is controlled by the data in records 4 and 5 of the control file (Figure 3-3).

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```
 NUMBER OF OBSERVATIONS                      =         8
 NUMBER OF FUTURES PER OBSERVATION                     2

 RELEASE TABLE REPOSITORY FLOWS

 DETAILED PRINTING FOR FOLLOWING OBSERVATIONS:
         1    2    3    4    5    6    7    8

 DETAILED PRINTING FOR FOLLOWING FUTURES:
         1    2

 End TIME (YR)                               = 1.000E+04

                                                          MINIMUM   MAXIMUM    MODE
 BOREHOLE DIAMETER DISTRIBUTION (M) ABOVE REPOSITORY     3.111E-01 3.111E-01 3.111E-01
 WASTE STREAMS TO AVG FOR CH WASTE CUTTINGS   =         3
 WASTE STREAMS TO AVG FOR RH WASTE CUTTINGS   =         1
 WASTE TYPE (NONE,CH,RH) PROB FOR REGION 1    = 0.000E+00 8.762E-01 1.238E-01
 INTRUSIONS TO DEPLETE THE BRINE POCKET       = 1000
 SPALLINGS RELEASES BEGIN WITH INITIAL INTRUSION AND END AFTER 1000 INTRUSIONS
 BLOWOUT RELEASES BEGIN WITH INITIAL INTRUSION AND END AFTER 1000 INTRUSIONS

 CULEBRA RELEASE POINT FOR UNDISTURBED RELEASES =         1

 RELATIVE ROUNDOFF TOLERANCE                 = 1.000E-06

 Obs    1, Future      1, Mining Time:  4999.99 years

 OBS    1, FUTURE      1, DRILL INTRUSION   1, TIME(YR)=1.200E+03,  PANEL  5 (LOWER )
      PLUG PATTERN 2, DRILL DIAM(M)=(3.111E-01)
      EXCAVATED   , NO BRINE POCKET HAS
           CUTTINGS RELEASE
      CH WASTE, A(M2)=1.000E-01, HT(M)=3.960E+00, VOL(M3)=3.960E-01, VOL FRAC=3.860E-01, FINAL
VOL(M3)=1.529E-01
      WASTE STREAM    1, INTERP TIMES(YR)=(1.000E+03,3.000E+03), RELEASES(EPA/M3)=(5.000E+00,5.000E+00),
RELEASE(EPA/M3)=5.000E+00
      WASTE STREAM    2, INTERP TIMES(YR)=(1.000E+03,3.000E+03), RELEASES(EPA/M3)=(7.273E+00,5.657E+00),
RELEASE(EPA/M3)=7.111E+00
      WASTE STREAM    3, INTERP TIMES(YR)=(1.000E+03,3.000E+03), RELEASES(EPA/M3)=(9.182E+00,7.364E+00),
RELEASE(EPA/M3)=9.000E+00
      WASTE STREAM(S) AVGD=  3, AVG CONC(EPA/M3)=2.716E+00, RELEASE(EPA)=1.076E+00
           SPALLINGS RELEASE
      INTERP TIMES(YR)=(1.000E+03,3.000E+03), VOLS(M3)=(0.000E+00,0.000E+00), VOL(M3)=0.000E+00
      INTERP TIMES(YR)=(1.000E+03,3.000E+03), CONCS(EPA/M3)=(1.715E+01,1.391E+01), CONC(EPA/M3)=6.495E+00,
SPALLINGS RELEASE(EPA)=0.000E+00
           DBR RELEASE      INTERP TIMES(YR)=(1.000E+03,3.000E+03), VOLS(M3)=(0.000E+00,0.000E+00),
VOL(M3)=0.000E+00
           PVOLS =(2.000E+03,2.000E+03), PVOLUME=2.000E+03
      INTERP TIMES(YR)=(1.000E+03,3.000E+03), CONCS(EPA/M3)=(0.000E+00,0.000E+00), CONC(EPA/M3)=0.000E+00,
DBR RELEASE(EPA)=0.000E+00
      Am241 CONCS(Ci/M3)=(0.000E+00,0.000E+00), CONC(Ci/M3)=0.000E+00, DBR RELEASE(Ci)=0.000E+00
      Pu239 CONCS(Ci/M3)=(0.000E+00,0.000E+00), CONC(Ci/M3)=0.000E+00, DBR RELEASE(Ci)=0.000E+00
      U234  CONCS(Ci/M3)=(0.000E+00,0.000E+00), CONC(Ci/M3)=0.000E+00, DBR RELEASE(Ci)=0.000E+00
      Th230 CONCS(Ci/M3)=(0.000E+00,0.000E+00), CONC(Ci/M3)=0.000E+00, DBR RELEASE(Ci)=0.000E+00
           CUMULATIVE RELEASES (EPA):  CUTTINGS=1.076E+00, SPALLINGS=0.000E+00, BLOWOUTS=0.000E+00,
TOTAL=1.076E+00
           CUMULATIVE VOLUME RELEASES (M3):  CUTTINGS=3.960E-01, SPALLINGS=0.000E+00, BLOWOUTS=0.000E+00
```

Figure 3-3. A Portion of the Diagnostic Output File

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3.3.3 Summary Statistics

Summary statistics by vector and results across futures are printed to the file *SummaryStatistics.txt*. The first record of the file is a header record listing the vector numbers (Figure 3-4). Statistics for each result are then listed. These statistics include the mean, median, standard deviation (SD), number of futures (N), minimum, maximum, minimum of values greater than 0, the geometric mean (GM), the geometric standard deviation (GSD), the number of positive, non-zero values (n>0), and the nominal 10^{th} and 90^{th} percentiles of the data. These data are provided primarily as a means for checking the results.

Variable	Vector 1	Vector 2	Vector 3	Vector 4	Vector 5	Vector 6	Vector 7
Cuttings and Cavings							
Mean:	0.2660D+02	0.5335D+02	0.1844D-03	0.1811D-03	0.1862D-03	0.1845D-03	0.1842D-03
Median:	0.2526D+02	0.5101D+02	0.1697D-03	0.1679D-03	0.1693D-03	0.1672D-03	0.1683D-03
SD:	0.1191D+02	0.2371D+02	0.2067D-03	0.2042D-03	0.2052D-03	0.2080D-03	0.2082D-03
N:	10000	10000	10000	10000	10000	10000	10000
Minimum:	0.3141D-03	0.2410D-03	0.0000D+00	0.0000D+00	0.0000D+00	0.0000D+00	0.0000D+00
Maximum:	0.8944D+02	0.1712D+03	0.1439D-02	0.1269D-02	0.1437D-02	0.1325D-02	0.1408D-02
Min > 0:	0.3141D-03	0.2410D-03	0.1535D-03	0.1535D-03	0.1535D-03	0.1535D-03	0.1536D-03
GM:	0.2361D+02	0.4729D+02	0.2886D-03	0.2862D-03	0.2876D-03	0.2881D-03	0.2885D-03
GSD:	0.1767D+01	0.1817D+01	0.1601D+01	0.1598D+01	0.1603D+01	0.1617D+01	0.1613D+01
n>0:	10000	10000	5676	5630	5755	5666	5653
Nominal 10%:	0.1241D+02	0.2506D+02	0.0000D+00	0.0000D+00	0.0000D+00	0.0000D+00	0.0000D+00
Nominal 90%:	0.4204D+02	0.8470D+02	0.4736D-03	0.4637D-03	0.4739D-03	0.4819D-03	0.4803D-03

Figure 3-4. A Portion of the *SummaryStatistics.txt* File

3.3.4 Unbinned Results

A pair of files can be generated for each results which contain the data needed to construct CCDFs without resorting to binning of the data. One of the pair is constructed as a Y-many-X format, where Y is the probability and X the value. The name of this file is "Result" with a 2-digit index for the result and ".txt" appended (e.g., for the example shown in Figure 3-2, Result02.txt would contain unbinned Cuttings and Cavings results). The data in the file are organized in comma-delimited columns, with one column for each vector and one row for each future. The first row in the file consists of a description for each column. The first column contains the cumulative probability value for each future and a description of the variable (e.g., Prob_Cuttings and Cavings in our example). The next columns contain the value of the result at each probability for each vector. The per-vector columns can be followed by the mean, median, and a set of order statistics, depending on the options specified in the control file.

The other file in the pair is constructed from interpolation as an X-many-Y format and is named "Result" with a 2-digit index for the result and "_XMY.txt" appended (e.g., Result02_XMY.txt). The X-many-Y format is produced in order to allow for the easy construction of confidence of tolerance intervals in the vertical direction. The file is formatted similar to the "Results00.txt" file, using comma-delimited columns, except that the first column contains an interpolated result value followed by interpolated complementary probabilities for each vector and the optional statistics. The number of rows in the file is arbitrary but is currently set to 200 using a data statement in the subroutine called "SortFile".

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3.3.5 Binary Output

The results for each future and observation are saved to the file Results.bin. This file is an unformatted (binary) file. Each record in the file has the observation number as an integer followed by the values of the results as double precision floating point numbers. The Results.bin file is a temporary file and is used to store the data until the end of the run. At that time the data are read and used to create the various output files of for the CCDFs of the data. The number and types of output files depends on the selections made in the control file, but include the "CCGF_PRT_OUT" file and the paired "Results00.txt" and "Results00_XMY.txt" files (where the "00" in the file name is replaced by the index of the output variable).

4.0 MODELS AND METHODS

There are three primary questions about the WIPP:

Q1: What occurrences could take place at the WIPP site over the next 10,000 years?

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

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

and one question about the WIPP PA:

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

These questions give rise to a methodology, embodied in CCDFGF, for quantifying both the distribution of possible releases over the next 10,000 years and for characterizing the uncertainty in that distribution due to imperfect knowledge about the parameters contained in the models used to predict releases.

CCDFGF is used to assemble results obtained from calculations performed with a number of different models (e.g., BRAGFLO, PANEL, NUTS, SECOTP2D, and CUTTINGS_S) to produce CCDFs specified in 40 CFR 191 (EPA, 1985) and as shown in Figure 4-1. To produce the CCDFs, CCDFGF simulates the drilling of boreholes at the surface of the repository. Drilling location, depth (which determines whether the brine pocket is penetrated), and the type of plugging pattern are treated as stochastic parameters, necessitating the simulation of many possible realizations, or futures, in order to characterize the aleatory uncertainty of the results.

If the model results were free from uncertainty then the CCDF of the potential releases from the repository produced by this method would characterize the uncertainty in the releases due to the uncertainty of intrusion of the repository in the future (i.e., to the CCDF specified in 40 CFR 191) (EPA, 1985). However, there is also uncertainty associated with the model results due to the lack of precise knowledge about the values of the parameters used in the models, i.e., the epistemic uncertainty. Therefore, CCDFGF also incorporates this epistemic uncertainty into its estimate of the total uncertainty in the results by repeating the computation of results for a set of futures for each of a series of observations, or vectors, of the input data obtained from the various models. Each vector of input data is the result of a simulation in which the parameters of the model were sampled from distributions representing the epistemic uncertainty in their values. Thus for each

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vector of input data CCDFGF generates one CCDF for each output variable describing the probability of the output variable taking on various values. It is the set of CCDFs for the releases that characterizes the confidence with which the location of the CCDF of releases can be estimated.

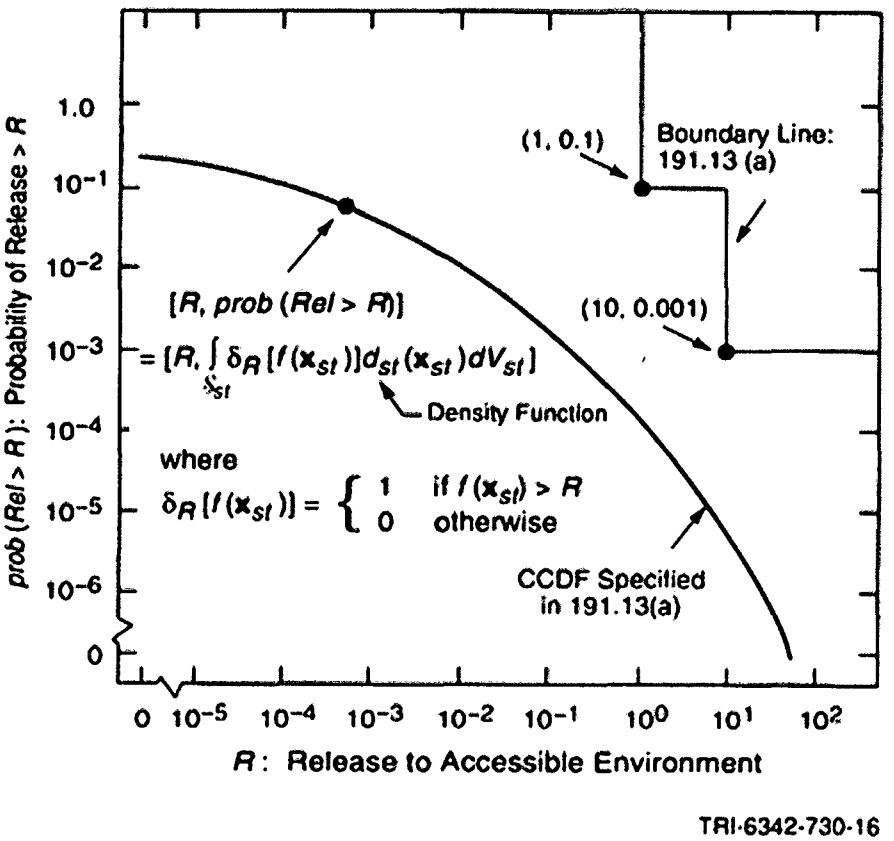


Figure 4-1. Boundary Line and Associated CCDF Specified in 40 CFR 191, Subpart B

4.1 Probabilistic Characterization of Different Futures

The outcome of the scenario development process for the WIPP provides a probabilistic characterization of the likelihood of different futures that could occur at the WIPP site over the next 10,000 years, where the period of 10,000 years is specified in 40 CFR 191 (EPA, 1985). When viewed formally, the set of possible futures is defined by a probability space (S_{st}, $\mathbf{S}_{st}$, p_{st}), with the sample space S_{st} given by

$$S_{st} = \{\mathbf{x}_{st}: \mathbf{x}_{st} \text{ is a possible 10,000-year sequence of occurrences at the WIPP}\}. \quad \text{Eq. (1)}$$

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

As a reminder, a probability space (S, $\mathbf{S}$, p) consists of three components: a set S that contains everything that could occur for the particular "universe" under consideration, a suitably restricted set $\mathbf{S}$ of subsets of S and a function p defined for elements of $\mathbf{S}$ that actually defines probability.

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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 $\mathcal{S}$ are events. In most applied problems, the function p defined on $\mathcal{S}$ is replaced by a probability density function (PDF) d (e.g., d_{st} in Figure 4-1).

With respect to the previously indicated questions, S_{st} provides an answer to Q1, while $\mathcal{S}_{st}$ and p_{st} provide an answer to Q2. In practice, Q2 will be answered by specifying distributions for the individual aleatory quantities (see discussion of n, t_i, p_i, l_i, a_i, d_i, p_i and b_i in Section 4.4.1) which in turn lead to definitions for $\mathcal{S}_{st}$ and p_{st}. The CCDF in 40 CFR 191 (EPA, 1985) will be obtained by evaluating an integral involving (S_{st}, $\mathcal{S}_{st}$, p_{st}) (Figure 4-1).

4.2 Estimation of Releases

Estimation of environmental releases corresponds to evaluation of the function f in Figure 4-1. Release mechanisms associated with f include direct removal to the surface at the time of a drilling intrusion (i.e., cuttings and cavings, spallings, brine flow) and releases subsequent to a drilling intrusion due to brine flow up a borehole with a degraded plug (i.e., groundwater transport). These processes are simulated using the set of models (Figure 4-2). 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 Figure 4-2 that actually define the function f in Figure 4-1.

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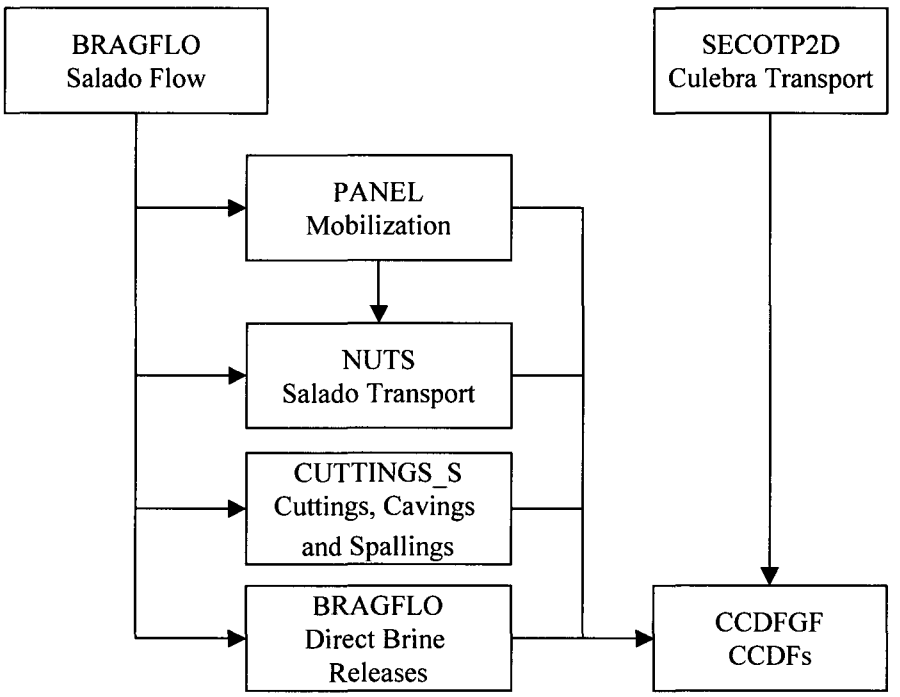


Figure 4-2. Models Used in WIPP PA

The models in Figure 4-2 are too computationally intensive to permit their evaluation for every element $\mathbf{x}_{st,i}$ of S_{st} in Eq. (2). Due to this constraint, the models in Figure 4-2 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., $1{,}000 \leq nS \leq 10{,}000$) in Eq. (2).

$$prob(Rel > R) = \int_{S_{st}} \delta_R[f(\mathbf{x}_{st})]\, d_{st}(\mathbf{x}_{st}) dV_{st} \doteq \sum_{i=1}^{nS} \delta_R[f(\mathbf{x}_{st,i})]/nS \qquad \text{Eq. (2)}$$

With respect to the previously indicated questions, the models in Figure 4-2 are providing an answer to Q3.

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4.3 Probabilistic Characterization of Parameter Uncertainty

The total uncertainty on the probability of releases includes not only the aleatory uncertainty described in Section 4.2, but also epistemic uncertainty due to uncertainty about the values of the parameters that underlie the WIPP PA. When viewed formally, parameter uncertainty is defined by a probability space $(S_{su}, \mathbf{S}_{su}, p_{su})$, with the sample space S_{su} given by

$$S_{su} = \{\mathbf{x}_{su}: \mathbf{x}_{su} \text{ is possibly the correct vector of parameter values to use in the WIPP PA}\}. \quad \text{Eq. (3)}$$

the subscript *su* refers to subjectively-specified epistemic uncertainty and is used because $(S_{su}, \mathbf{S}_{su}, p_{su})$ 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 $(S_{st}, \mathbf{S}_{st}, p_{st})$ (e.g., the rate constant λ 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 Figure 4-2 that determine the function f in Figure 4-1 and Eq. (2) (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 Figure 4-1 could be determined with certainty and compared with the boundary line specified in 40 CFR 191 (EPA, 1985). However, given the complexity of the WIPP site and the 10,000-year time period under consideration, $\mathbf{x}_{su}$ can never be known with certainty. Rather, uncertainty in $\mathbf{x}_{su}$ as characterized by $(S_{su}, \mathbf{S}_{su}, p_{su})$ will lead to a distribution of CCDFs (Figure 4-3). The proximity of this distribution to the boundary line in Figure 4-1 provides an indication of the confidence with which 40 CFR 191 (EPA, 1985) will be met.

The distribution of CCDFs can be summarized by distributions of exceedance probabilities conditional on individual release values (Figure 4-4). 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 to evaluate the integral over S_{su} and, as indicated in Eq. (4), simple random sampling to evaluate the integral over S_{st}. Specifically, a Latin hypercube sample $\mathbf{x}_{su,k}$, $k = 1, 2, \ldots, nLHS$, is generated from S_{su} in consistency with the definition of $(S_{su}, \mathbf{S}_{su}, p_{su})$ and a random sample $\mathbf{x}_{st,i}$, $i = 1, 2, \ldots, nS$, is generated from S_{st} in consistency with the definition of $(S_{st}, \mathbf{S}_{st}, p_{st})$.

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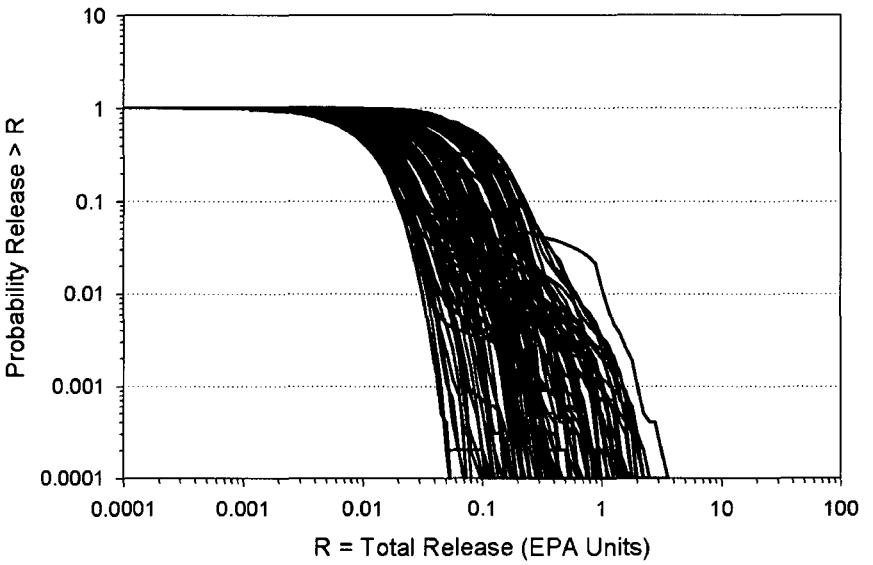


Figure 4-3. Example CCDF Distribution from 2009 PABC

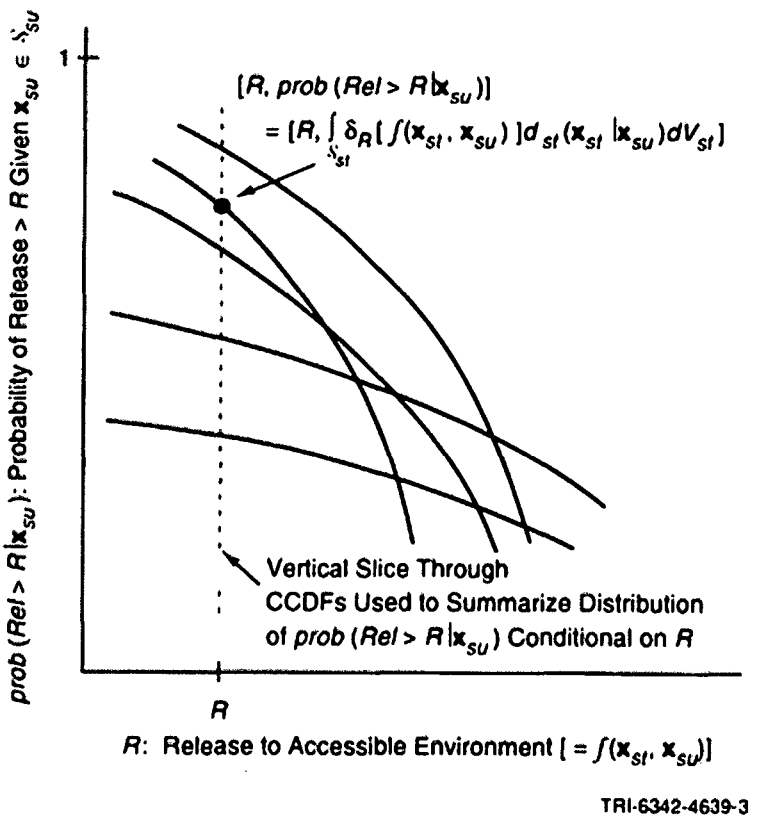


Figure 4-4. Summarizing Distribution of CCDFs

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The probability $prob(p \leq P|R)$ in Figure 4-4 is then approximated by

$$prob(p \leq P|R) \doteq 1 - \sum_{k=1}^{nLHS} \delta_P \left[\sum_{i=1}^{nS} \delta_R \left[f\left(\mathbf{x}_{st,i}, \mathbf{x}_{su,k}\right) \right] / nS \right] / nLHS \qquad \text{Eq. (4)}$$

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 Figure 4-5) and also mean values for exceedance probabilities above the corresponding release values (i.e., R) and then connecting these points to form continuous curves (Figure 4-5). 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}, $\boldsymbol{S}_{su}$, p_{su}) and results derived from (S_{su}, $\boldsymbol{S}_{su}$, p_{su}) (e.g., the distributions in Figure 4-3, Figure 4-4, and Figure 4-5) are providing an answer to Q4.

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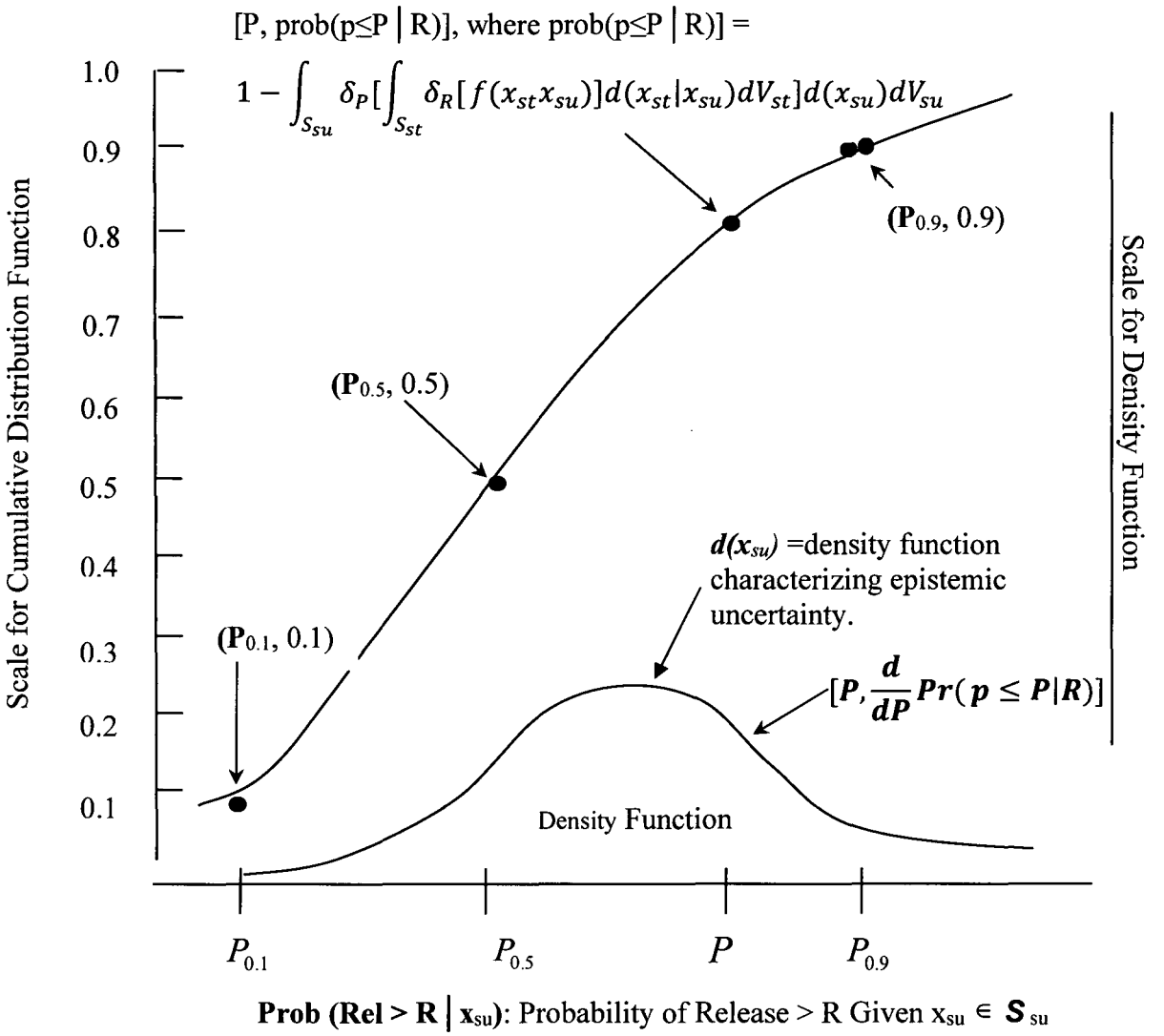


Figure 4-5. Distribution of Exceedance Probabilities Due to Epistemic Uncertainty

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4.4 Sampling of Futures

4.4.1 Probability Space (S_{st}, $\mathbb{S}_{st}$, p_{st}) for Stochastic Uncertainty

The probability space (S_{st}, $\mathbb{S}_{st}$, 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. (1), the sample space S_{st} consists of all possible 10,000 yr futures that could occur at the WIPP subsequent to decommissioning. 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}, $\mathbb{S}_{st}$, p_{st}). Further, 40 CFR 194 (EPA, 1995) requires that the occurrence of potash mining within the land withdrawal boundary must be included in the analysis. Therefore, drilling intrusions and the occurrence of potash mining within the land withdrawal boundary are the only events that require incorporation into (S_{st}, $\mathbb{S}_{st}$, p_{st}).

The following assumptions will underlie the definition of (S_{st}, $\mathbb{S}_{st}$, 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 λ_d (units: yr^{-1}), with λ_d defined by the drilling rate per unit area (e.g., 5.98×10^{-3} yr^{-1} km^{-1}) and the area of the repository.

(2) Different sealing (i.e., plugging) patterns are used for different drilling intrusions. At present, three potential sealing patterns are considered: (a) full concrete plug through Salado Formation to Bell Canyon Formation, (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^2) within the repository. For the definition of (S_{st}, $\mathbb{S}_{st}$, p_{st}), activity level will be assumed to follow a distribution D_A, where D_A can be either continuous or discrete. In WIPP PA, D_A is 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 drill bit diameters in use (i.e., different drilling intrusions will use different drill bit diameters). Two methods will be provided for the sampling of drill bit diameters. In the first method it is assumed that all drilling intrusions would use the same drill bit diameter but that the correct value for this diameter was not known, i.e., that the uncertainty in drill bit diameter is epistemic. In the second method it is assumed that drill bit diameters vary randomly across different drilling intrusions. Specifically, the aleatory variation of drill bit diameters across different drilling intrusions will be assumed to follow a triangular distribution D_{DB}. As discussed in Section 2.4, the second method is an untested capability of CCDFGF Version 8.01. The selection of the method to be used is specified in the control file.

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(5) 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. One node will be assigned to each waste panel. 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, $i = 1, 2, \ldots nL$, where pL_i is the probability that a randomly placed drilling intrusion will occur at panel location L_i and nL is the number of waste panels in use. Due to the assumption that drilling intrusions occur randomly in space, pL_i will derive from the area associated with panel location L_i.

(6) A given drilling intrusion may or may not penetrate pressurized brine in the Castile Formation. Specifically, a single probability D_B can be used to characterize the likelihood that a randomly placed drilling intrusion through the Castile Formation will encounter pressurized brine.

(7) 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 λ_m (units: yr^{-1}). Guidance in 40 CFR 194 (EPA, 1995) specifies $\lambda_m = 1\times10^{-4}$ yr^{-1}.

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

$$\mathbf{x}_{st} = [t_1, w_1, p_1, l_1, a_1, d_1, b_1, t_2, w_2, p_2, l_2, a_2, d_2, b_2, \ldots, t_n, w_n, p_n, l_n, a_n, d_n, b_n, t_{min}, 0, 0, 0, 0, 0, \ldots] \quad \text{Eq. (5)}$$

where

t_i=time (yr) of i^{th} drilling intrusion,

w_i = designator (dimensionless) for penetration of an excavated area of the repository (i.e., $w_i = 0, 1$ implies nonpenetration and penetration, respectively, of an excavated area),

p_i=plugging pattern used for i^{th} drilling intrusion,

l_i=location (dimensionless) of i^{th} drilling intrusion (i.e., node associated with i^{th} drilling intrusion),

a_i=activity level (waste stream) of waste penetrated by i^{th} drilling intrusion,

d_i=borehole diameter (m) used in i^{th} drilling intrusion,

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-year future defined by $\mathbf{x}_{st}$, and

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

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The t_i are assumed to be ordered so that $t_i \leq t_{i+1}$ for $i = 1, 2, \ldots, n-1$, and the trailing 0's in Eq. (5) 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). Random sampling defined by λ_d, λ_m, D_{PL}, D_A, D_{DB}, 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) with the summation in Eq. (4).

4.4.2 Generation of Individual Futures

There are four stochastic processes simulated in CCDFGF that control the generation of individual futures. These processes are 1) drilling and mining intrusions, 2) the penetration of CH or RH waste, 3) plugging of boreholes and 4) penetration of the brine pocket. The first two processes require the use of two or more stochastic variables.

4.4.3 Drilling Intrusions

The random sampling to generate an element $\mathbf{x}_{st}$ of S_{st} will operate in the following manner. The drilling rate λ_d will be used to generate the times at which drilling intrusions occur. For a Poisson process with a constant λ_d (i.e., a stationary process), the cumulative distribution function (CDF) for the time Δt between the successive events is (Mood, 1974):

$$prob(t \leq \Delta t) = 1 - e^{-\lambda_d \Delta t} \qquad \text{Eq. (6)}$$

A uniformly distributed random number, r_1, can be selected from [0, 1]. Then, solution of

$$t_1 = -log(1 - r_1)/\lambda_d \qquad \text{Eq. (7)}$$

for t_1 gives the time of the first drilling intrusion. If 100 years of administrative control is assumed, then 100 years would be added to the t_1 obtained in Eq. (7) to obtain the time of the first drilling intrusion. Selection of a second random number r_2 and solution of

$$\Delta t = -log(1 - r_2)/\lambda_d \qquad \text{Eq. (8)}$$

for Δt gives the time interval between the first and second drilling intrusions, with the outcome that $t_2 = t_1 + \Delta t$. This process can be continued until a time t_{n+1} is generated that exceeds 10,000 years. The times $t_1, t_2, \ldots, t_n$ then constitute the drilling times in $\mathbf{x}_{st}$ in Eq. (5). The mining time t_{min} is sampled in a similar manner. The status of the repository with regard to having had a mining intrusion determines the mining scenario used when selecting data for computing the release of dissolved radionuclides through the Culebra. The drilling and mining rates are read from the parameter section of the RELTAB file.

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4.4.3.1 Locations of Intrusions

The waste panels of the repository each have a single drilling node. The intruded panels are determined by randomly selecting one of the drilling nodes based on the probabilities of intruding the various panels. The number of panels is specified in the control file. Also specified for each panel are its panel group (lower, middle, upper, or other), the probability of intrusion, and the panel's adjacency relationship (same, connected, adjacent, non-adjacent) with all waste panels, including itself.

4.4.3.2 Borehole Diameter

A borehole diameter for each input vector is normally read from the cuttings and cavings release section of the RELTAB file. The diameter in the RELTAB file is the value used by CUTTINGS_S to calculate the volume of cuttings and cavings. CCDFGF can treat borehole diameter as a stochastic variable for each intrusion by sampling a drill bit diameter from a triangular distribution and then scaling the cuttings and cavings volumes by the square of the ratio of the sampled drill bit diameter to the value used by CUTTINGS_S. This code functionality is untested in CCDFGF Version 8.01. The default diameter is the first of the three values specified in line 10 of the control file. The default diameter can also be interpreted as the minimum of a triangular distribution of diameters that can be sampled as an optional stochastic variable in CCDFGF. The remaining two values on line 10 represent the mode and maximum for the distribution. The selection of the option to sample the borehole diameter is specified in line 9 of the control file.

4.4.4 Penetration of Waste

There are three stochastic processes involved with the penetration of waste. The first process determines whether or not an excavated area is penetrated. The probability of penetration of an excavated area is equal to the sum of the areas occupied by CH and RH waste divided by the berm area. These three parameters are read from the parameter section of the RELTAB file.

The second process determines whether CH waste or RH waste is encountered. These probabilities are equal to the area of contact handled waste and area of remote handled waste, respectively, divided by the sum of these two areas. Each CH and RH waste stream is assigned a probability of being encountered. These probabilities are read from the cuttings and cavings release section of the RELTAB file. The third stochastic process determines which of the waste streams were encountered for each of the waste streams to be averaged. The number of CH and RH waste streams to be averaged is specified in the control file. Because the waste barrels are stacked three high, it is possible to encounter as many as three different waste streams in a penetration. Setting the number of CH waste streams to 3 simulates the assumption that waste is randomly emplaced at the scale of barrels. Setting the number of CH waste streams to 1 or 2 simulates clustering of the barrels by waste stream. Since RH waste is assumed to be stored horizontally in the walls of the repository, only one RH waste container is currently expected to be sampled during each intrusion.

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4.4.5 Plugging Pattern

Three potential borehole plugging patterns are simulated in CCDFGF: (1) full concrete plug through Salado Formation to Bell Canyon Formation ; (2) two plug configuration with plugs at Rustler/Salado and Castile/Bell Canyon interfaces; (3) three plug configuration with plugs at Rustler/Salado, Salado/Castile and Castile/Bell Canyon interfaces. The probability for each plugging pattern is read from the parameters section of the RELTAB file. A plugging pattern is randomly selected, based on the probabilities, for each borehole that is simulated. Plugging pattern is one condition that is used to set the type of intrusion scenario.

4.4.6 Penetration of Brine

The probability of penetrating the brine pocket is read from the RELTAB file and can be different for each vector. If an intrusion penetrates the brine pocket, an excavated area is penetrated and the brine pocket has not been depleted due to an excess of intrusion events then the intrusion scenario is either E1 or an E2. E1 intrusions occur only for plugging pattern 2, whereas E2 intrusions occur only for plugging pattern 3 and if there have been no previous E1-type intrusions. If the brine pocket is not penetrated and the plugging pattern is 2 or 3 then the intrusion scenario is E2. An intrusion for which plugging pattern 1, the solid plug, is selected is treated as if the waste were not penetrated by the intrusion.

4.5 Mechanistic Results for Specific Futures

Each sampled future of the form indicated in Eq. (6) will require the determination of a normalized release to the accessible environment. Determination of this release corresponds to evaluation of the function $f(x_{st,l},\ x_{su,i})$ in Eq. (4), which in turn requires evaluation of the models in Figure 4-2. Specifically, f is given by

$$\begin{aligned} f(\mathbf{x}_{st}) &= f_C(\mathbf{x}_{st}) + f_{DBR}[\mathbf{x}_{st},\ f_B(\mathbf{x}_{st})] + f_{SP}[\mathbf{x}_{st},\ f_B(\mathbf{x}_{st})] \\ &\quad + f_{MB}[\mathbf{x}_{st},\ f_B(\mathbf{x}_{st})] + f_{DL}[\mathbf{x}_{st},\ f_B(\mathbf{x}_{st})] + f_S[\mathbf{x}_{st},\ f_B(\mathbf{x}_{st})] \\ &\quad + f_{S-T}\{\mathbf{x}_{st,0},\ f_{S-F}(\mathbf{x}_{st,0}), f_{N-P-G}[\mathbf{x}_{st},\ f_B(\mathbf{x}_{st})]\} \end{aligned} \qquad \text{Eq. (9)}$$

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 $\mathbf{x}_{st}$,

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

$f_B(\mathbf{x}_{st})$ ~ 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,

$f_{DBR}[\mathbf{x}_{st},\ f_B(\mathbf{x}_{st})]$ ~ direct brine release to accessible environment for $\mathbf{x}_{st}$ calculated with BRAGFLO,

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$f_{SP}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ 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,

$f_{MB}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ 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,

$f_{DL}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ 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,

$f_S[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ 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 SECOTP2D,

$f_{N-P-G}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$ ~ release to Culebra for $\mathbf{x}_{st}$ calculated with NUTS and PANEL; 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 SECOTP2D; this calculation requires NUTS and PANEL 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.

Based on previous experience, the Monte Carlo CCDF construction procedure indicated in Eq. (2) will require a sample size between 1,000 and 10,000 (i.e., $1{,}000 \leq nS \leq 10{,}000$ in Eq. (2)) to be implemented by CCDFGF. The individual codes in Figure 4-2 do not run fast enough to allow this number of evaluations of f. As a result, it will be necessary to evaluate the models in Figure 4-2 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).

Henceforth, for notational simplicity, the functions on the right hand side of Eq. (9) will typically be written with only $\mathbf{x}_{st}$ as an argument (e.g., $f_{DBR}(\mathbf{x}_{st})$ will be used instead of $f_{DBR}[\mathbf{x}_{st}, f_B(\mathbf{x}_{st})]$). However, the underlying dependency on the other arguments will still be present.

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4.6 Construction of Cuttings and Cavings Releases

The computation for a release of cuttings and cavings is depicted in Figure 4-6. The repository volume removed by cuttings and cavings is calculated as

$$V_w = A_w \times H_w \times \left(\frac{D_b}{D_d}\right)^2 \qquad \text{Eq. (10)}$$

where V_w is the volume of the repository removed by cuttings and cavings, A_w is the cross sectional area of the borehole for the borehole diameter D_d used in the cuttings and cavings release table, H_w is the height of the repository, D_b is the drill diameter used in the CCDFGF calculations and w is the type of waste. The CCDFGF drill diameter is either a constant obtained from the control file or a stochastic value sampled from a triangular distribution defined using parameters in the control file. As discussed in Section 2.4, the capability to use a triangular distribution to define the borehole diameter is untested in CCDFGF Version 8.01. The selection of the option to use a constant drill diameter or to sample it is specified in the control file. The repository volume is multiplied by the volume-fraction adjusted concentration to determine the cuttings and cavings release.

1. **Get the waste type**

The waste type is determined by selecting either CH or RH based on the probability of encountering the waste. These probabilities are computed as

$$p_{CH} = \frac{A_{CH}}{A_{CH}+A_{RH}} \qquad \text{Eq. (11)}$$

and

$$p_{RH} = \frac{A_{RH}}{A_{CH}+A_{RH}} = 1 - p_{CH} \qquad \text{Eq. (12)}$$

where p_{CH} and p_{RH} are the probabilities of encountering CH and RH waste, respectively, A_{CH} is the area of contact handled waste, and A_{RH} is the area of remote handled waste. The selection is made by generating a random number in the range [0,1] and comparing it to p_{CH}. If the generated value is less that p_{CH} then CH waste is selected, otherwise RH waste is selected.

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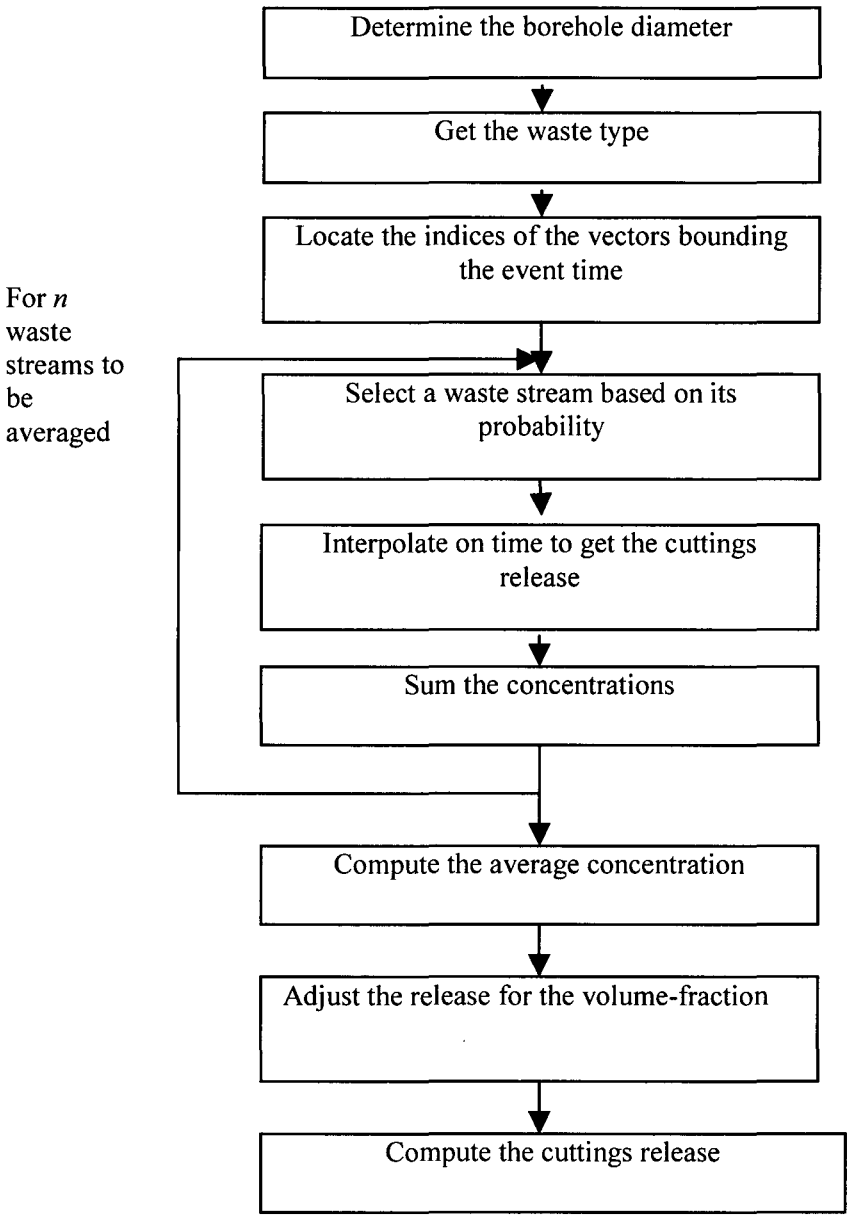


Figure 4-6. Calculation of cuttings and cavings releases

2. Locate the indices of the vectors bounding the event time

Cuttings and cavings release tables are provided for only a subset of all possible intrusion time. The release for the simulated event is obtained by interpolating the release from the cuttings and cavings table. The data to be interpolated are selected by finding the table entries whose times, $t_{c,i}$ and $t_{c,j}$, bracket the simulated intrusion time, i.e.,

$$t_{c,i} \leq t \leq t_{c,j} \qquad \text{Eq. (13)}$$

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3. **Loop across the number of waste streams to be averaged**

The numbers of CH and RH waste streams to be averaged, n_{CH} and n_{RH}, are specified in the control file.

4. **Select a waste stream based on its probability**

The waste stream is selected by generating a random number on the range [0,1] and then comparing it to a table of discrete, cumulative probabilities that are read from the cuttings and cavings release section of the RELTAB file. The activity index, A, is the index of the first table entry that exceeds the random number.

5. **Interpolate on time to get the cuttings and cavings release concentration**

The cuttings and cavings release concentration is interpolated from the cuttings and cavings release table for the given time of the intrusion (t), waste type (T), activity index (A), and the bounding time indices (i,j).

$$C_{T,A,t} = R_{T,A,i} + \frac{t - t_{c,i}}{t_{c,j} - t_{c,i}} \times \left(R_{T,A,j} - R_{T,A,i}\right) \qquad \text{Eq. (14)}$$

6. **Sum the concentrations**

Sum the concentrations across all waste streams to be averaged.

7. **Compute the average concentration**

Divide the sum of the concentrations by the number of waste streams to be averaged, n_T.

$$C_c = \frac{\sum_1^{n_T} C_{T,A,t}}{n_T} \qquad \text{Eq. (15)}$$

8. **Adjust average concentration for the volume-fraction**

A parameter set in the control file determines whether the volume fraction is to be used as a weighting factor or as a probability to determining how much waste is encountered by a borehole. If treated as a weighting factor then the average release is simply multiplied by the volume fraction. If treated as a probability then the average release is multiplied by 1 if a random number in the range [0,1] is less than the volume fraction, or 0 otherwise. Thus, C_r, the adjusted release concentration, is computed as:

$$C_r = \begin{cases} C_c \times V_f & if\ constant \\ C_c \times x & if\ probability, where\ x = 0\ or\ 1 \end{cases} \qquad \text{Eq. (16)}$$

9. **Compute the cuttings and cavings release**

The cuttings and cavings release is computed as the product of the volume-fraction adjusted average concentration, and the volume of waste, V_w, i.e.,

$$f_C(x_{st}) = V_w \times C_r \qquad \text{Eq. (17)}$$

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4.7 Determining Conditions for Direct Brine Releases, Spallings and Transport

Direct brine release and spallings are calculated conditional on the location of previous intrusions and on the conditions in the intruded panel and the repository at the time of the intrusion. Intrusions into the repository can change the conditions in and around the repository and hence affect releases from subsequent intrusions. The other WIPP PA models calculate releases for the initial intrusion into an undisturbed repository and for the second intrusion into the repository, based on the location and type of the first intrusion. CCDFGF calculates releases from the third and subsequent intrusions from the data for releases for the second intrusion.

4.7.1 Determining Repository and Panel Conditions

Direct brine releases and spallings, and releases by radionuclide transport require a determination of the conditions in the intruded panel and in the repository at the time of the intrusion. CCDFGF assigns one of four conditions to each panel:

- E0 – the panel has not been intruded by drilling
- E1 – the panel has one previous E1 intrusions (intersects a brine reservoir in the Castile)
- E2 – the panel has one or more previous E2 intrusions (none intersect brine reservoirs)
- E1E2 – the panel has at least two previous intrusions, at least one of which is an E1 intrusion

CCDFGF assigns one of three conditions to the repository:

- E0 – the repository is undisturbed by drilling
- E1 – the repository has at least one E1 intrusion
- E2 – the repository has one or more E2 intrusions but no E1 intrusions

Panel conditions are used to determine releases by transport through the Culebra. Repository conditions are used to determine direct releases for each intrusion by direct brine releases and spallings.

When an intrusion occurs, the conditions for the intruded panel and the repository are updated according to the rules above. Figure 4-7 shows the algorithm for determining the type of intrusion.

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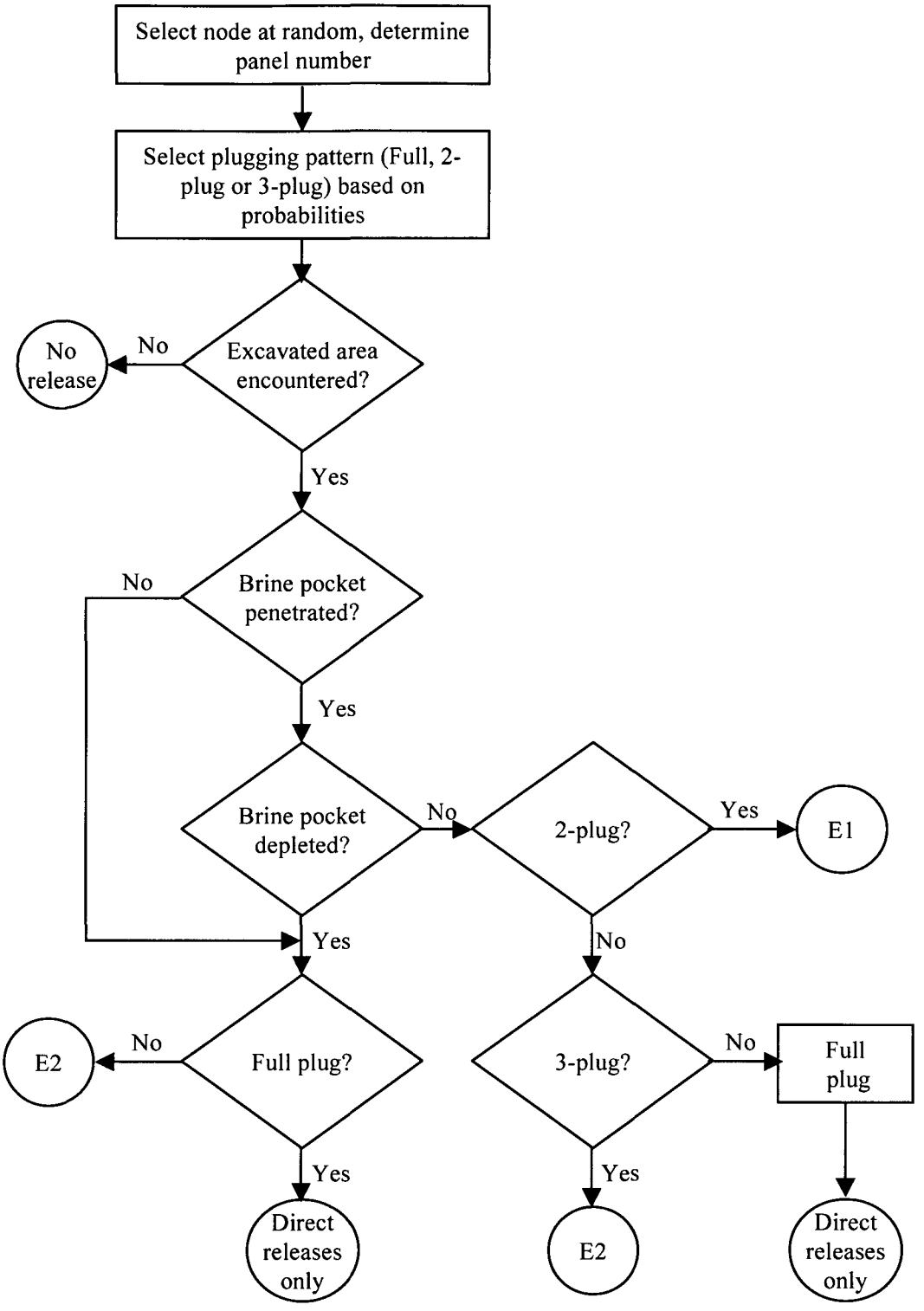


Figure 4-7. The determination of the type of intrusion

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4.7.2 Determining Distance from Previous Intrusions

Direct brine release and spallings require a determination of the distance between the panel hit by the current intrusion and the panels hit by previous intrusions. The number of panels and the panel group to which each panel is assigned is read from the control file. CCDFGF groups the panels into four groups: lower, middle, upper, and other.

Direct brine releases for subsequent intrusions are modeled in BRAGFLO by one of four intrusions: lower, middle, upper, and other corresponding to the four panel groups (also termed panel cavities). In modeling a second intrusion it is assumed that the initial intrusion was made into the lower panel. First intrusions into the lower panel are believed to maximize releases of second intrusions. Thus, a subsequent intrusion into a lower panel represents an intrusion into a previously intruded ("same") panel. The "middle" intrusion represents an intrusion into an undisturbed panel that is connected to a previously disturbed panel. Connected panels do not have any panel closures between them. The "upper" intrusion represents an intrusion into an undisturbed panel that is adjacent to a previously disturbed panel. Adjacent panels have at least one panel closure between them and are in the same section of the repository. The "other" intrusion represents an intrusion into an undisturbed panel that is non-adjacent to any previously disturbed panels. Non-adjacent panels are in different sections of the respository (south vs. west).

CCDFGF uses the release tables from BRAGFLO for these four cases (same, connected, adjacent, and non-adjacent) when modeling second and subsequent intrusions no matter where the first intrusion actually occurred. In addition, in CCDFGF, the selection of the time and location category (same, connected, adjacent, and non-adjacent) of the "previous" intrusion depends on the repository condition. The repository condition is determined by the intrusion of greatest consequence across all panels prior to the current intrusion. E1 intrusions are assumed to be of greater consequence than E2 intrusions. Likewise, the condition of each panel is equal to the intrusion of greatest consequence into the panel prior to the current intrusion. The previous intrusion is selected by finding the closest panel (same, connected, adjacent, or non-adjacent) whose intrusion condition, excluding the current intrusion, is equal to the repository condition. The time of the previous intrusion is the time of the most recent intrusion having the greatest consequence and closest distance.

4.8 Construction of Direct Brine Releases

Direct brine releases (also termed blowout releases) are calculated for all intrusions that encounter CH waste. Direct brine releases are constructed from brine releases (m^3) to the surface obtained from BRAGFLO and radionuclide concentrations in brine ($C_{DBR,RS,t}$ having units of EPA units/m^3) calculated by PANEL. These data are read from the RELTAB file. The radionuclide concentrations depend on the type of brine, which is reflected by the state of the repository, on time (t) of the release and on the volume of brine in the panel. Both the volume of brine in the panel and the volume of brine released depend on the time of the initial intrusion and, if previously intruded, the time since the initial intrusion.

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The calculations of the volume of brine released from the repository by an intrusion event and the volume of brine in the intruded panel of the repository at the time of the event both involve a two-dimensional interpolation based on the time of the original intrusion and, if the repository was intruded previously, the time to the subsequent intrusion. The release volume data tables and the panel volumes tables distinguish between the first intrusion and subsequent intrusions. The release volume and panel volume data for the initial (E0) intrusion are further distinguished by the panel group (lower, middle, upper, or other). The data for the release and panel volumes for the initial intrusion consists of release and panel volumes, respectively, at each of a series of intrusion times. The initial release volume and initial panel volume at any arbitrary time are computed by linear interpolation on their respective data. The data to be interpolated are selected by finding the table entries whose times, $t_{DBR,i}$ and $t_{DBR,j}$, bracket the simulated intrusion time; i.e.,

$$t_{DBR,i} \leq t \leq t_{DBR,j} \qquad \text{Eq. (18)}$$

and then the release and panel volumes are interpolated from the corresponding release volumes for the appropriate panel location (L):

$$V_{DBR} = V_{DBR,L,i} + \frac{t - t_{DBR,i}}{t_{DBR,j} - t_{DBR,i}} \times (V_{DBR,L,j} - V_{DBR,L,i}) \qquad \text{Eq. (19)}$$

$$V_{Panel} = V_{Panel,L,i} + \frac{t - t_{DBR,i}}{t_{DBR,j} - t_{DBR,i}} \times (V_{Panel,L,j} - V_{Panel,L,i}) \qquad \text{Eq. (20)}$$

Here $V_{x,L,i}$ and $V_{x,L,j}$are values interpolated using the simulated intrusion time from tables of release (x=*DBR*) or panel (x=*Panel*) volumes at selected times following specific initial intrusion times (those bracketing the simulated initial intrusion time)(Figure 4-8).

The data for the release volumes and panel volumes for subsequent intrusions are distinguished by the current state of the repository (E1 or E2) and the relative distance between the intruded panel and the panel of the initial intrusion (same, connected, adjacent, or non-adjacent). The algorithms for determining repository conditions and distance between intrusions are described in Section 4.7.

For each of the eight combinations of repository state and relative distance, release volumes and panel volumes for subsequent intrusions are computed for a set of pairs of times (t_i, t_j), where t_i is an initial intrusion time and t_j is a subsequent intrusion time. For each of a set of values of t_i, release and panel volumes are computed for a series of subsequent intrusion times t_j, represented by the vertical columns of solid circles in Figure 4-8. Each set of release data or panel volumes can be viewed as a grid of discrete values on a continuous surface. In Figure 4-8, BH1 and BH2 are the first and second intrusions (bore holes) at times 160 and 340, respectively and Δt is the length of time following the first intrusion that the second intrusion occurs, i.e., 180. Before values of releases or panel volumes are calculated, the algorithm identifies the two series of data in which the initial times bracket the time of the initial intrusion, termed here the left and right series. In this example, the left series starts at t_i=100 and the right series starts at t_i=350. The value at BH1 is found by interpolating between the first values in the left and right series (i.e., between releases at (100, 100) and (350, 350)), using E0 repository conditions. Getting the value at BH2 involves three interpolations. The first interpolation yields I1 at (100, 280) by interpolation within the left series of values; the second interpolation yields I2 at (350, 530) by interpolation within the right series of values. V_{DBR} or V_{Panel} at BH2 is computed at (160, 340) by interpolation between I1 at (100, 280) and I2 at (350, 530),

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$$V_{DBR} = \mathrm{I1} + \frac{160-100}{350-100} \times (\mathrm{I2} - \mathrm{I1}) \qquad \text{Eq. (21)}$$

The calculation of panel volume, V_{Panel}, at the time of the second intrusion uses the same methodology.

$$V_{Panel} = \mathrm{I1} + \frac{160-100}{350-100} \times (\mathrm{I2} - \mathrm{I1}) \qquad \text{Eq. (22)}$$

The calculation of the concentration of radionuclides in the brine at the time of release depends upon the volume of brine in the panel. Tables of brine concentrations are read from the RELTAB file for a set of panel brine volumes at specific times and for the various states of the repository. Given V_{Panel}, the time of the intrusion and the state of the repository the concentration is calculated using the interpolation

$$C_{DBR} = C_{DBR,RS,V_{Panel},i} + \frac{t-t_{BC,i}}{t_{BC,j}-t_{BC,i}} \times (C_{DBR,RS,V_{Panel},j} - C_{DBR,RS,V_{Panel},i}) \qquad \text{Eq. (23)}$$

as shown in Figure 4-9. Here $C_{DBR,RS,V_{Panel},j}$ and $C_{DBR,RS,V_{Panel},i}$ are values interpolated from tables of concentrations at selected volumes using the current simulated volume.

The computation of direct brine releases is outlined in Figure 4-10. If the maximum number of boreholes yielding direct brine flow is exceeded then it is assumed that no release occurs. Otherwise, the direct brine release is computed as the product of the release concentration and the volume, V_{DBR}, i.e.,

$$f_{DBR}(x_{st}) = V_{DBR} \times C_{DBR} \qquad \text{Eq. (24)}$$

The maximum number of boreholes yielding direct brine flow is specified in the control file.

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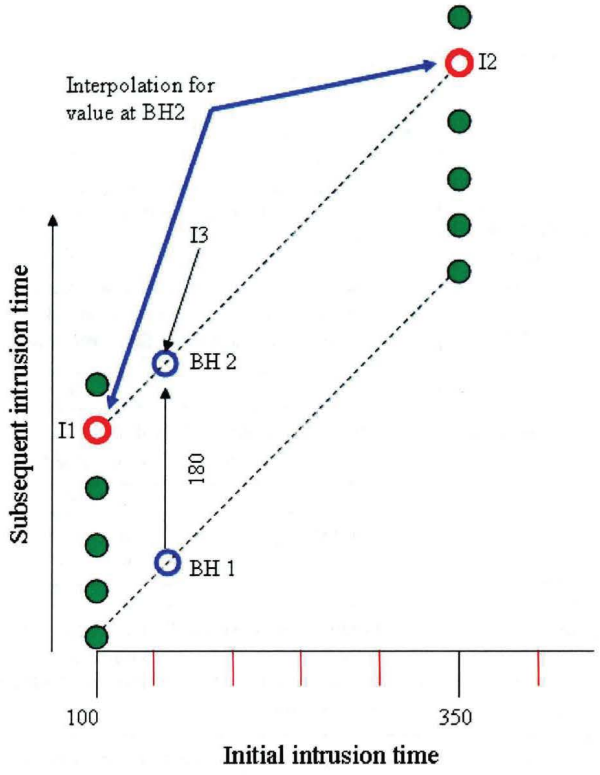


Figure 4-8. Interpolations for direct brine releases

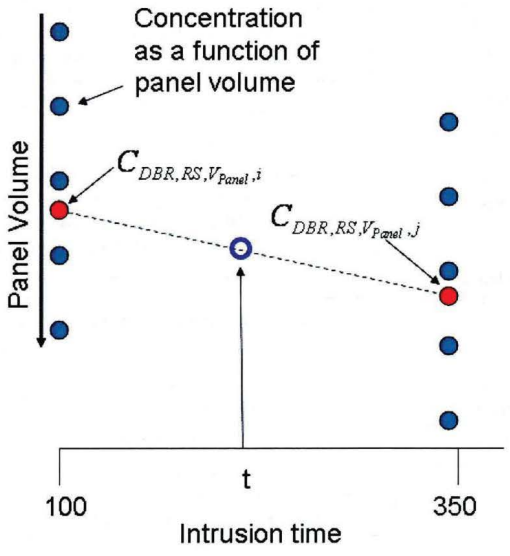


Figure 4-9. Concentration is a function of intrusion time and panel volume

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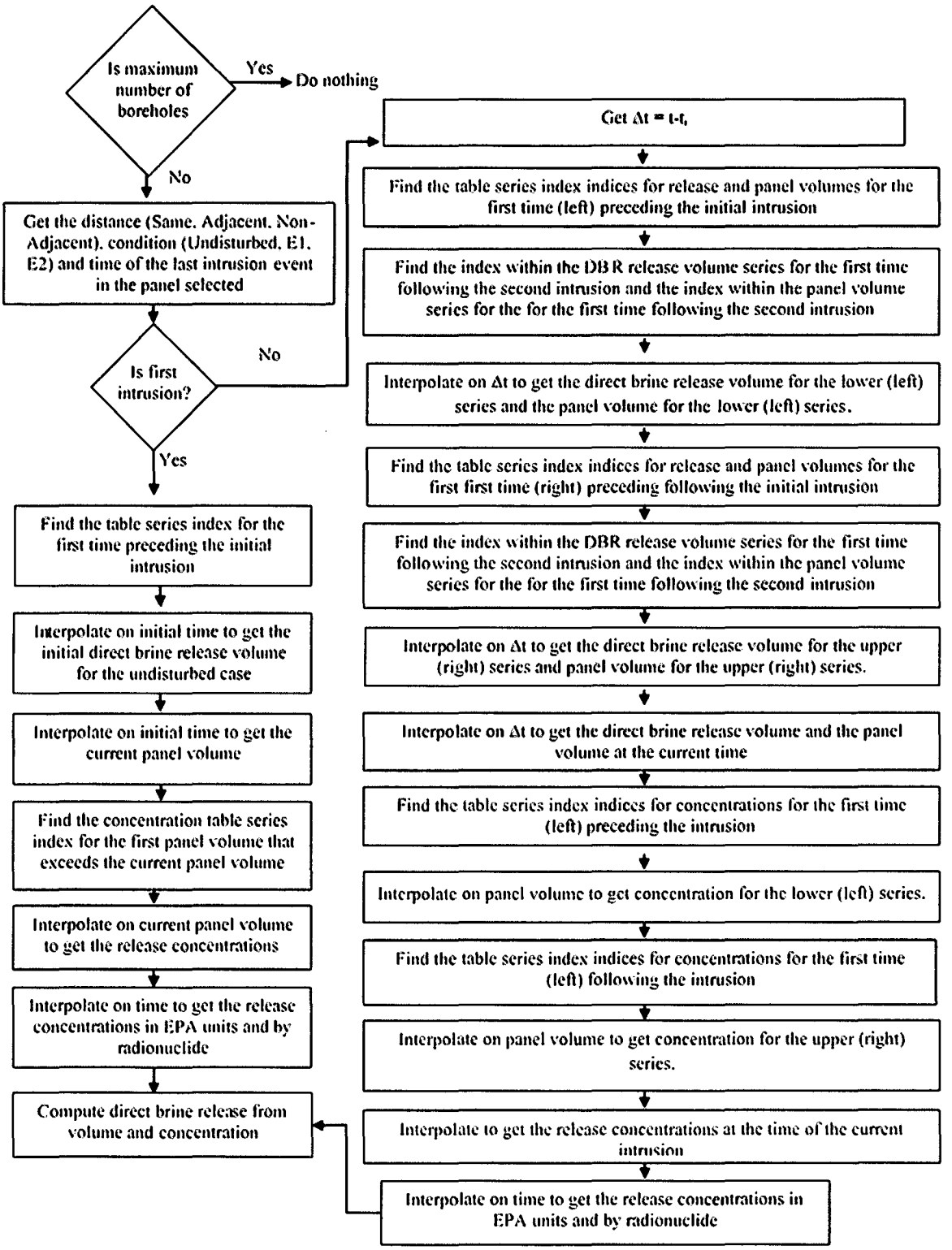


Figure 4-10. Computation of Direct Brine Releases

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4.9 Construction of Spallings Releases

Spallings releases are calculated for all intrusions that encounter CH waste. The construction of the spallings release $f_{SP}(x_{st})$ is nearly identical to that described in Section 4.8 for the calculation of direct brine releases, except that volumes of solid material released will be used rather than volumes of brine (Figure 4-11). These solid releases are calculated with the spallings submodel of the CUTTINGS_S code. For the initial intrusion, the data for the volume of spallings depends only on the time of release and the panel group (lower, middle, upper, or other). For subsequent releases, the data depends on the current state of the repository (E1 or E2) and the relative distance between the intruded panel and the panel of the initial intrusion (same, connected, adjacent, or non-adjacent). For each of the eight combinations of these factors, releases are computed for the discrete set of times described in Section 4.8. Interpolation of the spallings release volumes uses the same scheme depicted in Figure 4-8 and described in Section 4.8.

The concentration of radionuclides in the spallings can be computed using one of two methods, either repository scale or local scale, with the selection of the method determined by the control file. The repository scale method computes the concentration by interpolation on the data read from the spallings section of the RELTAB file, which depend only on the release time. The local scale method uses the concentration computed for the cuttings and cavings release as the concentration for the spallings as well.

4.10 Radionuclide Transport

CCDFGF implements the PA assumptions that the primary path for radionuclide transport from the repository is up through boreholes to the Culebra, then through the Culebra to the land withdrawal boundary (LWB). Data from the NUTS and PANEL codes are used in CCDFGF to estimate radionuclide transport through boreholes to the Culebra; these results are combined with data from the code SECOTP2D to compute transport through the Culebra to the LWB. For future development, CCDFGF includes logic to compute releases by other pathways: through the anhydrite marker beds; to the Dewey Lake red beds; and to the surface. Data for these release pathways are not currently provided by PRECCDFGF. These pathways will not be discussed further in this design document.

NUTS and PANEL compute the release to the Culebra over time from panels with three types of condition: E1, E2 and E1E2. An E1E2 condition results from the combination of two or more intrusions into the same panel, at least one of which is an E1 intrusion. Each borehole may create a pathway for releases to the Culebra. The first E1 or E2 intrusion in each panel creates a release path, with the radionuclide releases taken from the appropriate NUTS data. Subsequent E2 intrusions into a panel with only E2 intrusions do not cause additional releases; WIPP PA assumes that a subsequent E2 intrusion into a panel having only earlier E2 intrusions does not provide a significant source of additional brine, and thus does not release additional radionuclides to the Culebra. A subsequent E1 intrusion changes the panel's condition to E1E2, as does a E2 intrusion into a panel that has an earlier E1 intrusion. Once E1E2 conditions exist in a panel, they persist throughout the regulatory period. However, releases from a panel with E1E2 conditions are restarted for each subsequent E1 intrusion into that panel, since additional E1 intrusions may introduce new volumes of brine to the panel.

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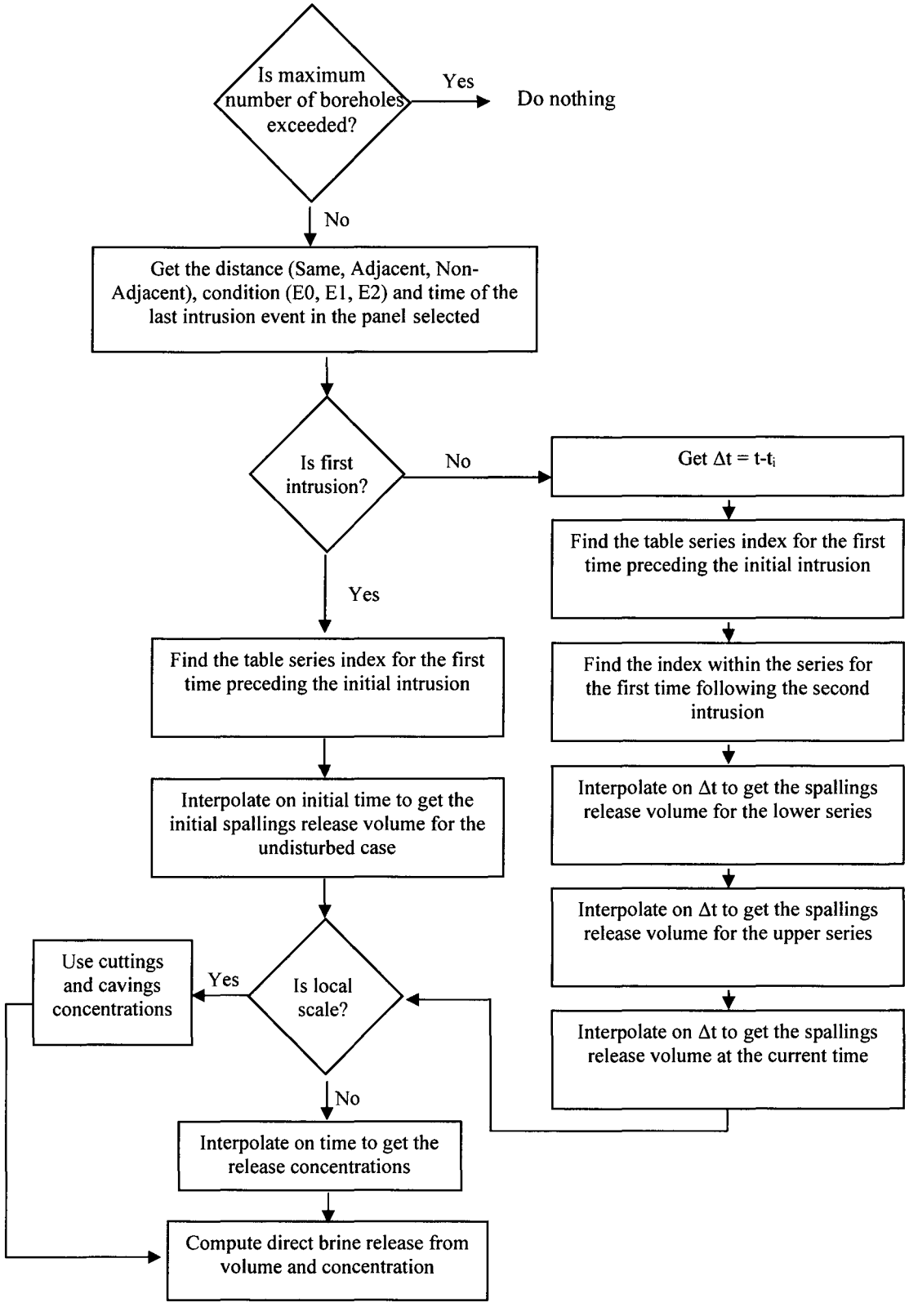


Figure 4-11. Computation of Spallings Releases

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Releases to the Culebra are summed for each radionuclide species at each point in time across all release pathways to the Culebra. Figure 4-12 shows the algorithm for computing total releases to the Culebra for all release pathways. The data give the cumulative amount of each radionuclide released to the Culebra at 50 year intervals. The computation of release to the Culebra for each intrusion is similar to the computations for spallings and direct brine releases; however, the releases to the Culebra are input as cumulative amounts. The activity release for an interval of time is the difference between the cumulative release at the end of the interval and the cumulative release at the start of the interval.

The total release through the Culebra is calculated for each radionuclide by

$$R = \sum_{t_i \le t_m} r(t_i) f_{PM}(t_i) + \sum_{t_i > t_m} r(t_i) f_{FM}(t_i) \qquad \text{Eq. (25)}$$

where $r(t_i)$ is the release to the Culebra in kg at time t_i and $f_{PM}(t_i)$ and $f_{FM}(t_i)$ are the fractions of a unit source placed in the Culebra in the interval (t_{i-1}, t_i) that reaches the LWB by the end of the 10,000 year regulatory period, for partial mined and fully mined conditions within the LWB, respectively. The function $f(t)$ changes when mining occurs within the LWB; hence the sum in the equation above is evaluated in two parts, where t_m is the time that mining occurs. The fractional amounts are computed by the code SECOTP2D, as a set of fractions at the boundary for various times following a unit release occurring between 0 and 50 years. To facilitate use of this data in CCDFGF, PRECCDFGF reverses the time-ordering of the data such that the fraction associated with year 200, for example, represents the release at the boundary at year 10,000 for a releases occurring between 150 and 200 years.

4.10.1 Release to Culebra for a Single Intrusion

For each intrusion, the code first constructs a series of values for the cumulative activity releases to the Culebra (intermediate interpolation in Figure 4-13). The activity release data used in the interpolation depend on the panel condition prior to the intrusion (E0, E1, E2, or E1E2), radionuclide species (^{239}Pu, ^{241}Am, etc.) and the time for the start of the release. The two neighboring series with times that bracket the intrusion time are located. These series are used to construct, using linear interpolation, the curve for the release (in kg) to the Culebra at the intrusion time. A second interpolation on this constructed curve is next performed in order to align the release times with the times for releases through the Culebra, which are provided at 50-year intervals. Cumulative activity releases through the Culebra for a single intrusion are tabulated from the time of the intrusion until the next E1 or E1E2 intrusion into the same panel, or until the end of the regulatory period if there are no more boreholes into the currently intruded panel. After the cumulative releases are tabulated and aligned with the times for the releases through the Culebra, the activity release for each interval of time is computed as the difference between the cumulative release at the end of the interval and the cumulative release at the start of the interval.

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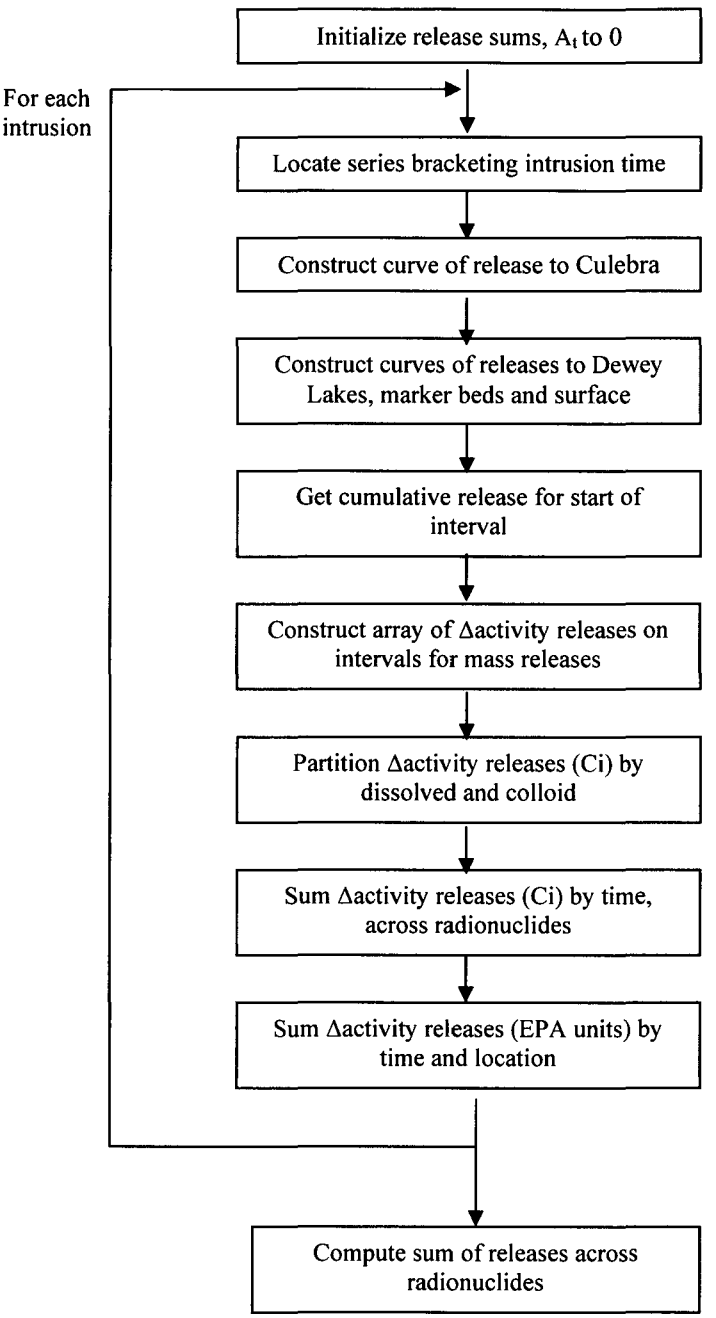


Figure 4-12. Computations of Releases by Transport

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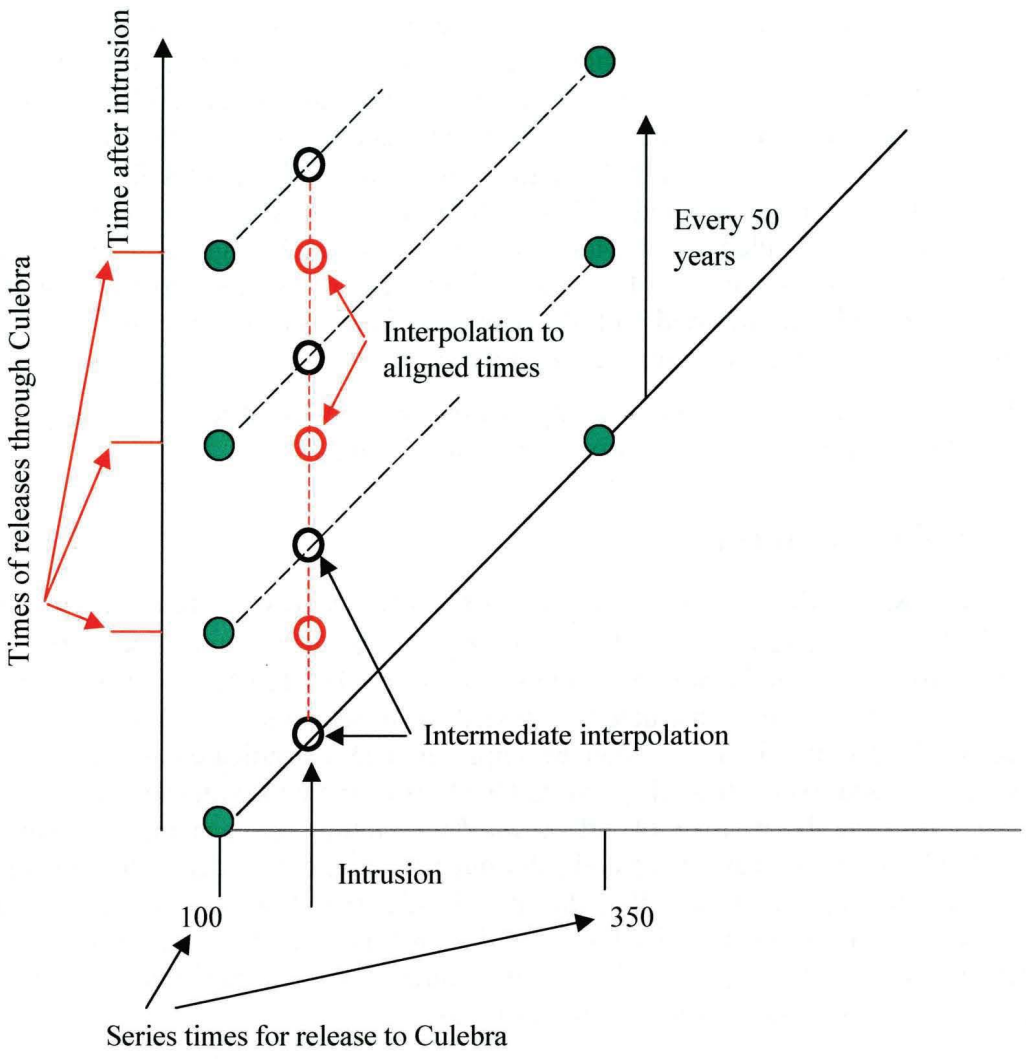


Figure 4-13. Interpolation for Release to the Culebra for a Single Intrusion

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4.10.2 Releases Through the Culebra

The above process for releases to the Culebra is repeated for each intrusion event in a future, accumulating a total release to the Culebra for each time interval and each radionuclide. The total releases to the Culebra includes both dissolved radionuclides and radionuclides sorbed to colloids. Before transport through the Culebra, the incremental activity release data are partitioned into dissolved and colloid releases by multiplying them by radionuclide-specific factors for the fraction dissolved and the fraction on colloids. This partition implements the assumptions about which colloids transport in the Culebra and which do not. Transport through the Culebra is computed assuming dissolved radionuclides only; hence, if colloids are assumed to transport through the Culebra, these colloids are included with the dissolved fraction of the release to the Culebra and are transported as if the radionuclides were dissolved.

The total release through the Culebra is computed by Eq. (25). Total releases through the Culebra are converted to EPA units before construction of the CCDFs.

4.11 CCDF Construction

For each vector $\mathbf{x}_{su,k}$ in the space of epistemic uncertainty, CCDFGF samples a sequence $\mathbf{x}_{st,i}$, i = 1, 2, …, nS of futures. A sample size of nS = 10000 has been shown to be adequate to construct a CCDF for comparison with the boundary line specified in 40 CFR 191.13 (EPA, 1985). A release $f(\mathbf{x}_{st,i})$ for each future is then constructed as described in Sections 4.1 – 4.9. Once the $f(\mathbf{x}_{st,i})$ are evaluated, the CCDF in Figure 4-1 can be approximated as indicated in Eq. (2). 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). In addition, all values for $f(\mathbf{x}_{st,i})$ are saved and subsequently ordered in order to provide an alternative method for constructing the CCDFs. In addition to the CCDF in Figure 4-1 over all release modes, it will be possible to obtain CCDFs for individual release modes (e.g., cuttings and cavings, spallings, direct brine releases, to Culebra, through marker beds, from Culebra). The logic for the production of the CCDFs is diagrammed in Figure 5-1.

The CCDF construction indicated in this section is for a single sample element $\mathbf{x}_{su,k}$ of the form indicated in Eq. (1). Repeated generation of CCDFs for individual sample elements $\mathbf{x}_{su,k}$, (i.e., for the vectors representing epistemic uncertainty in the model results) will lead to the distribution of CCDFs of Figure 4-5.

4.12 Random Number Generation

The RAN3 pseudorandom number generator (Press et al., 1992) implements an algorithm described by Knuth (1981) based on the subtractive method. The algorithm was chosen because it is portable across platforms and because it has a long cycle period, which is the number of values that can be generated before repeating the same sequence of values. The cycle period is 2^{55}-1 (Knuth, 1981; Vattulainen et al., 1995). The method employs a shuffling of values stored in an array. This shuffling strategy helps to extend the cycle period and to overcome potential problems such as sequential correlation.

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5.0 CONTROL FLOW AND LOGIC

The main program calls subroutines that record information for quality assurance purposes, reads input files, initializes variables, then executes two nested loops, the outer loop over vectors (realizations) and the inner loop over futures. Within each iteration of the inner loop a number of boreholes are simulated and releases from each intrusion are tabulated. The results over a future are assembled into a single point on the CCDF for each result (e.g., total releases, spallings releases). Points over all futures comprise the CCDFs for a realization. After generating the CCDFs the main program writes output files and terminates.

The following input data are required to run CCDFGF:

1. Run control parameters (see Section 3.2.2)
2. Release data tables (see Section 3.2.1):
   a) Cuttings and cavings
   b) Spallings
   c) Direct brine releases
   d) Releases to the Culebra
   e) Releases from the Culebra

CCDFGF runs without any other user interaction. Figure 5-1 shows the order in which input files are processed, and the order of events leading to the creation of CCDFs.

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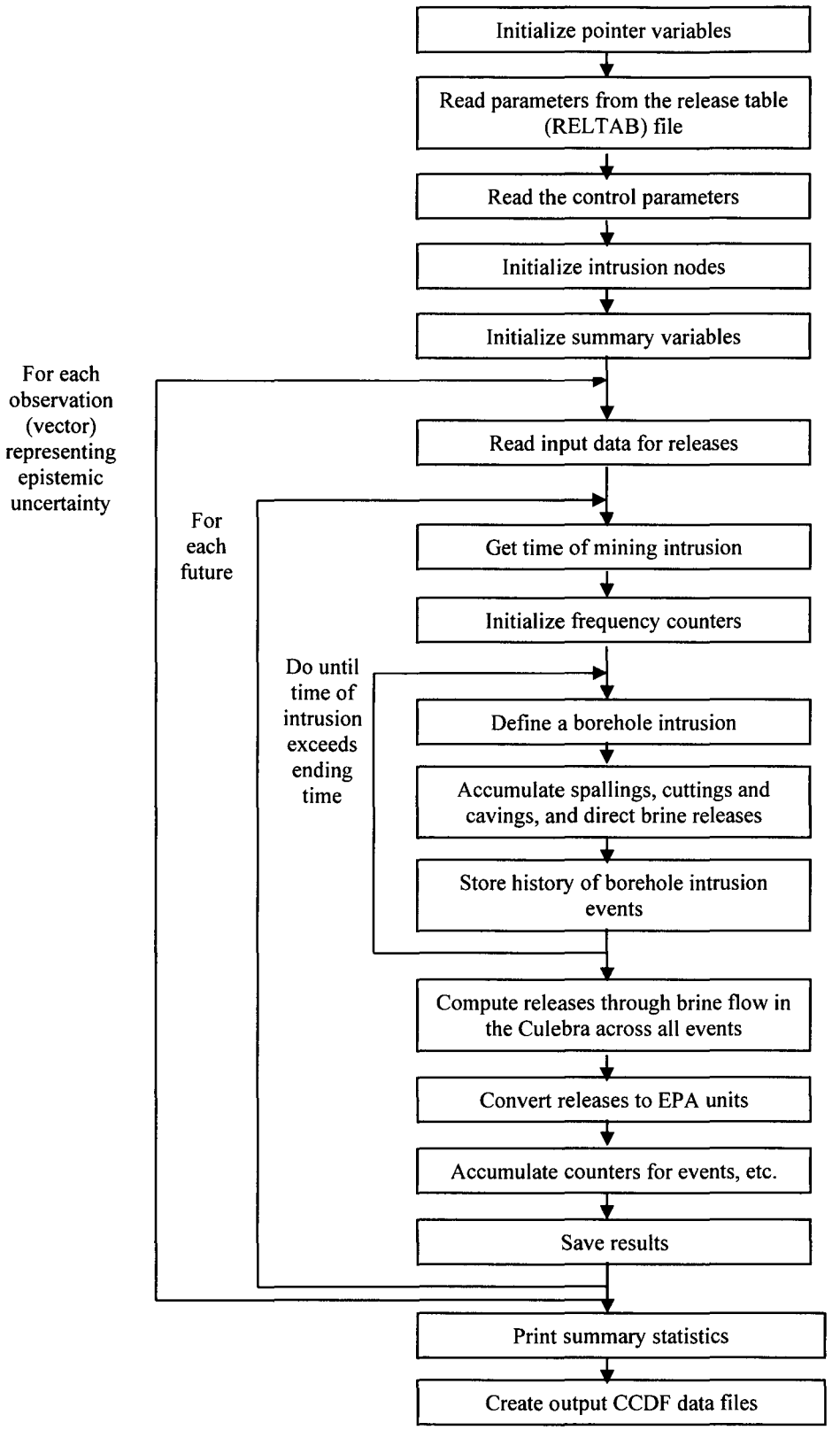


Figure 5-1. Flow of Processing of Input Data to Produce CCDFs

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5.1 Data Structures

The following is a list of all the routines and functions of CCDFGF, with a brief description, including the main program and entry routines (Table 5-1). For details of these subroutines and functions, please refer to the source code.

Table 5-1. Description of Subroutines and Functions

Routine/Function Name	Description
CCDFGF	The main program of CCDFGF.
AccCulebraRelease	Accumulate releases for reporting
AccumulateIntrusionCounters	Accumulate intrusion counters for current time future (diagnostic)
CI	Function for confidence interval (standard error) on the mean probability.
DefineBorehole	Define current borehole properties.
DirectBrineReleases	Calculate direct brine release for current intrusion.
DrillingIntrusionDiameter	Determine drilling intrusion diameter.
DrillingLocation	Determine drilling intrusion panels and the plugging pattern. Get a drilling diameter and return the panel index.
DrillTime	Determine drilling intrusion times.
EPA_Releases	Convert species mass releases to EPA normalized releases and accumulate total releases to Culebra, from Culebra, and over all pathways.
ExceedsValue	Look up the first time that exceeds the current time.
ExceedsTime	Look up the first time that exceeds the current time.
ExponentialVariate	Return an exponential variate.
FindSeries	Find the series which has its initial time just prior or equal to the borehole time.
Heapsort	Do heapsort on an array. Based on method from W. H. Press et al. (1992)
Histogram	Assign the results to bins for later creation of plots.
InitialIntrusionVolume	Interpolate spalling release volumes.
InitializePanelMaps	Read region and panel parameters file.
InitializePanelsAndCounters	Initialize parameters and results for current future.

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Routine/Function Name	Description
InitializePointers	Initialize all pointer variables.
InitializeResultLabels	Initialize result distribution labels and open the output files.
InitializeResultDistributions	Initialize result distributions.
InitializeSummaryVariables	Initialize values for probabilistic intrusion summary and population doses.
INPUT	Open diagnostic output file and then read in the input parameter data and control variables.
InterpolateReleasesToCulebra	Interpolates and sums releases to Culebra, Marker Beds, Dewey Lake, and Surface for time interval TS to TE.
IntrusionProbabilities	Get the intrusion probabilities.
IntrusionVolume	Compute the interpolation for spalling release for the current intrusion.
LININT	Computes a linear interpolation.
MiningIntrusionTime	Determine mining intrusion time.
NuclineIndex	Return index number for nuclide name passed as NucID.
PanelDistance	Return the distance and condition for the release scenario.
PrintStatistics	Calculate and write summary statistics information for a completed run.
ProbabilityOfNIntrusions	Poisson function for probabilities for time futures with different numbers of drilling intrusions.
ProbabilityOneIntrusion	Output the probabilities for different numbers of intrusions.
RAN3	Returns a uniform random deviate between 0.0 and 1.0. Based on the method in W. H. Press et al. (1992).
RanInit	Initialize the random number generator.
ReadControlParameters	Read control parameters file.
ReadCuttingsRelease	Read cuttings and cavings release tables.
ReadDirectBrineRelease	Read direct brine release tables.
ReadReleaseTableHeader	Read summary release tables file headers.
ReadReleaseTables	Read release tables for current observation.
ReadReleaseThroughCulebra	Read summary tables for releases from the Culebra.
ReadReleaseToCulebra	Read summary tables for releases to the Cuelbra, Marker Beds, Dewey Lake, and the Surface.

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Routine/Function Name	Description
ReadSpallingsRelease	Read spallings release tables.
ReleaseByCuttings	Calculate cuttings and cavings release for current intrusion.
ReleaseBySpallings	Calculate spallings release for current intrusion.
ReleasesThroughCulebra	Accumulate releases to the Marker Beds, Dewey Lake, the Surface, and to and from the Culebra.
ResponseCurve	Return Y value by finding interval in Xarray containing X and then performing linear interpolation.
ResponseCurve0	Return Y value by finding interval in Xarray containing X and then performing linear interpolation. This routine is used to produce one X many Y CCDF curves.
RSP_LININT	Compute the interpolation on disturbed spalling releases.
SaveResults	Save results for analysis and creation of CCDF curves.
SetBoreholeCounters	Keep counter for all 18 combinations of TimesToTransition (before, after, either), waste penetration (PenetrateWaste = not penetrated, penetrated, total), and penetration of brine pocket. PenetrateBrine is 2 if brine penetrated, otherwise it is 1.
SortFile	Reload the results data, sort it into ascending order by result and vector, and create a text file for each result. Also compute the descriptive statistics. This routine can be used in a "stand alone" mode, with the exception that the result names will be generated as Result01, etc.
WriteDistributions	Write CCDF and summary for each result to file.

5.2 Allowable/Prescribed Ranges for Input and Output

CCDFGF does not check the validity of the data provided in the various input files. CCDFGF imposes no restrictions on the range of values in the input files.

6.0 REQUIRED USER TRAINING AND/OR BACKGROUND

CCDFGF Version 8.01 is implemented on the Linux platform. To exercise CCDFGF, users should have basic knowledge of Linux and access to the WIPP cluster computers or their functional equivalents.

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7.0 CAPABILITIES AND LIMITATIONS

CCDFGF is used to assemble results obtained from calculations performed with a number of different models (e.g., BRAGFLO, PANEL, NUTS, SECOTP2D, and CUTTINGS_S) to produce complementary cumulative distribution functions (CCDFs). The CCDFGF code is an essential part of the probabilistic modeling necessary for performance assessment of the WIPP site.

8.0 USER INTERACTIONS WITH THE SOFTWARE

CCDFGF Version 8.01 executes on a Linux platform. To execute CCDFGF, the executable name (ccdfgf) must be in the user's current PATH or referenced by its path name.

CCDFGF expects a number of command line arguments. The program arguments may either be positional (provided in order) or flagged (preceded by the appropriate flag). Flags always start with "–" and may be abbreviated. All positional arguments must be listed before any flagged arguments. The only difference between using positional and flagged arguments is that optional arguments may be omitted for flagged arguments.

Interactive users may request that the program prompt for any missing command line arguments by appending "?" to the command line.

CCDFGF expects the following command line arguments. Full information about the files is given in Section 3.0.

1. –input — The release table RELTAB input file, which consolidates all the release information from the various models for input to the CCDFGF code.
2. –user — The input control file.
3. –output — The output CCDF results file.
4. –debug — The output diagnostics file.
5. –analysis — The analysis name for the database.
6. –revision — The analysis revision for the database. It defaults to 0.
7. –replicate — The replicate number for the database.
8. –database — The database name. Official runs use the official database PA_Results which can only be edited by the run_mast user. Informal runs should use the user's personal database. The name of this database generally has the format PA_Results_xxx, where xxx is some combination of the user's login name. "NONE" requests no database output. Note that there will be no database output if record 20 in the input control file is False, indicating that no binned data should be written.

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9. –prefix — The prefix for the miscellaneous output debug files, as follows:
   - The binary data file, an internal scratch file which is always generated, but rarely examined. This file is named "*prefix*Data.bin". A unique name should be provided if multiple CCDFGF executions are being performed, for example, runs consisting of multiple replicates.
   - The pair of database text files, which CCDFGF uses to load data into the database. These files are named "*prefix*DBbind.temp" and "*prefix*DBstat.temp", but they should not need to be examined.
   - The optional set of paired unbinned results files, controlled by record 21 in the input control file. These files are named "*prefix*Result*nn*.txt" and "*prefix*Result*nn*_XMY.txt", where *nn* is the two-digit result number (01...37).
   - The optional summary statistics file, controlled by record 22 in the input control file. This file is named "*prefix*SumStats.txt".

10. –random — The random number file. This file is optional and may be input or output (as controlled by the input control file). The name of this file was previously hardcoded.

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9.0 ERROR MESSAGES

Error messages are printed to both the console (Table 9-1) and to the diagnostic output file (Table 9-2).

Table 9-1. Error Messages Written to the Console

Subroutine	Statement	Explanation
FindSeries	"Borehole time ",TStart," is less than the earliest time in the input table of transport to the Culebra"	A time for a borehole intrusion is less than the earliest series time in the Culebra data read in from PRECCDFGF's RELTAB file.
	"TStart exceeds tabular values in FindSeries"	A time for a borehole intrusion is greater than the last time in the Culebra data read in from PRECCDFGF's RELTAB file.
Histogram	"Out of data in input file"	Fatal error: The end of the file of unformatted result data used to construct CCDFs was encountered prematurely.
InitializePanelMap	"Error: MaxPanelNumber could not be read from the control file."	Fatal error: The number of panels could not be read from the control file.
	"ERROR: End of file reading panel information from the control file."	Fatal error: There were too few records of panel-specific information given the number of panels specified in the control file.
	"Error: Panel data could not be read from the control file."	Fatal error: An error occurred when reading the panel-specific records from the control file.
	"Error: Unknown adjacency:"	Fatal error: The symbol for adjacency relationships must be S, C, A, or N (or their lower case equivalents) and the character read from the control file did not match one of these.
	"ERROR:Distance matrix is unsymmetrical at …"	Fatal error: The specification of panel neighbors in the control file was asymmetric, e.g., Panel 1 was shown to be adjacent to Panel 5 but Panel 5 was not shown to be adjacent to Panel 1.
	"Error: Unknown group:"	Fatal error: The symbol for the group must be L, M, U, or O (or their lower case equivalents) and the symbol read from the control file did not match these.

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Subroutine	Statement	Explanation
InitializePanelMap (Continued)	ERROR:The panel probabilities sum to … . Aborted."	Fatal error: The probabilities assigned to the panels in the control file did not sum to 1.
InitializeResult Distributions	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 5'	Fatal error: Invalid value specified for MinNumberBinsPerOrderOfMag relative to MaxNumBins. A power of 2 is required.
INPUT	'>>>>>ERROR(S) ENCOUNTERED IN INPUT, EXECUTION TERMINATED 6'	Fatal error: Indicates that an input error occurred in reading data from the header section of the release tables (RELTAB) file, the control file or the dose parameters file.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 7'	Fatal error: An error was encountered when initializing the panel maps.
InterpolateReleasesTo Culebra	"Error in finding pointers into array of times of flow from Culebra"	Fatal error: The start time for the flow was greater than all of the times of releases from the Culebra in the release tables.
LININT	"Error in LININT. Denominator = 0"	Fatal error: The denominator for a linear interpolation was 0.
	X," less than minimum value ",X1," in LININT"	Fatal error: The independent value, X, for a linear interpolation was less than the minimum value of the interval to be interpolated.
	X," greater than maximum value ",X2," in LININT"	Fatal error: The independent value, X, for a linear interpolation was greater than the maximum value of the interval to be interpolated.
NuclideIndex	"Nuclide ",NucID," not found in NuclideIndex"	Fatal error: The nuclide name passed to the function is not in its list of known radionuclides (Am241, Pu239, U234, Th230)
RAN3	"Random number read does not match tag."	Fatal error: The tag field for the random number read from the input file does not match the tag passed to RAN3
	"Out of input data in RAN3. Terminating"	Fatal error: A random number was requested but the input file has no more data.
ReadControlParameters	"Random number file will be read"	Warning that random numbers will be read from the random number input file

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Subroutine	Statement	Explanation
ReadControlParameters (Continued)	"Random number file will be saved"	Warning that random numbers will be generated and written to the random number input file
	"Random numbers will only be generated"	Warning that random numbers will be generated but not written to the random number input file
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 70'	This error is raised if an error was encountered while reading from the control file, if the minimum diameter was 0 or exceeded the mode or the maximum, if the value of NumberOfCulebraReleasePts is out of range, or if the specified Culebra release point for undisturbed releases is out of range.
ReadCuttingsRelease	'>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 59',VectorNumber, IOBS	Fatal error: The observation (vector) number does not match the value specified in the release table file for cuttings and cavings releases.
	'>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 62'	Fatal error: The CH cuttings and cavings release data do not span the range of times possible for the simulation.
	'>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 63'	Fatal error: The RH cuttings and cavings release data do not span the range of times possible for the simulation.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 64'	Fatal error: An unknown type of error was encountered when reading the cuttings and cavings release table data.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 65'	Fatal error: An end-of-file was encountered when reading the cuttings and cavings release table data.
ReadDirectBrineRelease	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 28'	Fatal error: The observation (vector) number does not match the value specified in the release table file for direct brine releases.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 47'	Fatal error: An unknown type of error was encountered when reading the direct brine release table data.

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Subroutine	Statement	Explanation
ReadDirectBrineRelease (Continued)	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 48'	Fatal error: An end-of-file was encountered when reading the direct brine release table data.
ReadReleaseTableHeader	'>>>>>TOTAL OF PLUGGING PATTERN PROBABILITIES ON RUN CONTROL PARAMETERS FILE NOT EQUAL TO 1.0 TPP=",TPP	Fatal error: The total of the probabilities for plugging patterns did not equal 1. A flag is set which terminates the program from the subroutine Input.
ReadReleaseTables	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 12':IOBS=",IOBS, "IOBST=",IOBST	Fatal error: The observation (vector) number does not match the value specified in the release table file.
ReadReleaseThrough Culebra	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 49'	Fatal error: The observation (vector) number does not match the value specified in the release table file for releases through the Culebra.
	"Nuclide order not consistent in ReadReleaseThroughCulebra,", &NuclideName(ISPC),"<>",Nuclide(ISPC).Name	Fatal error: An inconsistent ordering of nuclide data was detected.
	'>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 50'	Fatal error: The number of species in the release-tables file exceeds the maximum number of species allowed.
	'>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 51'	Fatal error: The maximum number of release times in the release tables file exceeds the maximum number of times allowed.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 52'	Fatal error: An unknown type of error was encountered when reading the release table data.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 53'	Fatal error: An end-of-file was encountered when reading the release table data.

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Subroutine	Statement	Explanation
ReadReleaseToCulebra	'>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 54'	Fatal error: The observation (vector) number does not match the value specified in the release table file for releases to the Culebra.
	'>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 55'	Fatal error: The number of species in the release tables file exceeds the maximum number of species allowed.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 57'	Fatal error: An unknown type of error was encountered when reading the release table data.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 58'	Fatal error: An end-of-file was encountered when reading the release table data.
ReadSpallingsRelease	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 71'	Fatal error: The observation (vector) number does not match the value specified in the release-tables file for spallings releases.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 72'	Fatal error: The spallings release tables do not span the range of potential intrusion times.
	'>>>>>SPALLINGS RELEASE TABLE DOES NOT SPAN POTENTIAL INTRUSION TIMES' '>>>>>(', AdminControlTime, ' TO ', TEnd, ' YR)'	
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 73'	Fatal error: The spallings release tables for the same, connected, adjacent, and non-adjacent tables do not span the range of potential intrusion times.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 75'	Fatal error: The times in the spallings release tables for undisturbed conditions are not in increasing order.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 76'	Fatal error: The times in the spallings release tables for disturbed conditions are not in increasing order.

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Subroutine	Statement	Explanation
ReadSpallingsRelease (Continued)	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 77'	Fatal error: The times in the spallings release tables for disturbed conditions are not in increasing order.
	'>>>>I/O ERROR ENCOUNTERED, EXECUTION TERMINATED IN ReadSpallingsRelease'	Fatal error: An unknown type of error was encountered when reading the spallings release table data.
	'>>REMATURE EOF ENCOUNTERED, EXECUTION TERMINATED IN ReadSpallingsRelease'	Fatal error: An end-of-file was encountered when reading the spallings release table data.
ResponseCurve	"Failure in ResponseCurve. ",x," not in interval ",Xarray(1)," - ",Xarray(n)	Fatal error: The piecewise linear interpolation function failed because the independent value, X, was not within the range of data passed in the input array.
RSP_LININT	"ERROR IN RSP_LININT. I=",I	Fatal error: The index passed must be 2 or greater because the value of the previous array element is the lower bound of the interpolation. A value of 1 or less was passed in.
	"ERROR IN RSP_LININT. DENOM = 0"	Fatal error: The denominator of the linear interpolation function was 0.
SortFile	"Out of data in input file"	Fatal error: The expected number of records in the sort file was not found.
IntrusionProbabilities	"Error: Unexpected case in IntrusionProbabilities"	Fatal error: An unexpected case was passed to the IntrusionProbabilities function.

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Table 9-2. Error Messages Written to the Diagnostic Output File

Subroutine	Statement	Explanation
DirectBrineReleases	'>>>>>NEGATIVE DBR RELEASE VOLUME'	Warning: The DBR release or volume was negative.
ReadControlParameters	'>>>>>DRILLING INTRUSION DIAMETER PARAMETERS ABOVE REPOSITORY MUST BE GREATER THAN 0.0'	Fatal error: There is an error in the drilling intrusion diameter parameters (minimum diameter was 0 or less).
	'>>>>>MIN DRILLING INTRUSION DIAMETER ABOVE REPOSITORY EXCEEDS MAX DRILLING INTRUSION DIAMETER'	Fatal error: There is an error in the drilling intrusion diameter parameters (minimum diameter exceeded the maximum).
	'>>>>>DRILLING INTRUSION DIAMETER MODE ABOVE REPOSITORY MUST BE IncludeD IN MIN/MAX DIAMETER RANGE'	Fatal error: There is an error in the drilling intrusion diameter parameters (minimum diameter exceeded the mode).
	'>>>>>VALUE OF NumberOfCulebraReleasePts MUST BE IN RANGE OF 1 TO MaxPanelNumber'	Fatal error: The value of NumberOfCulebraReleasePts is out of range.
	'>>>>>CULEBRA RELEASE POINT FOR UNDISTURBED RELEASES MUST BE IN RANGE OF 1 TO VALUE OF NumberOfCulebraReleasePts FROM RELTAB FILE'	Fatal error: Undisturbed Culebra releases are assigned to an invalid value in the control file.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 70'	Fatal error: This error is raised if an error was encountered while reading from the control file, if the minimum diameter was 0 or exceeded the mode or the maximum, if the value of NumberOfCulebraReleasePts is out of range, or if the specified Culebra release point for undisturbed releases is out of range.
	'>>>>>ERROR OPENING RUN CONTROL PARAMETERS FILE'	Fatal error: The run control parameter file could not be opened.
	'>>>>>I/O ERROR READING RUN CONTROL PARAMETERS FILE'	Fatal error: An unknown type of error was encountered when reading the control parameter file.
	'>>>>>PREMATURE EOF READING RUN CONTROL PARAMETERS FILE'	Fatal error: An end-of-file was encountered when reading the control parameter file.
ReadCuttingsRelease	'>>>>>INVALID OBSERVATION INDEX VALUE FOR CUTTINGS RELEASE TABLES', VectorNumber, IOBS	Fatal error: The observation (vector) number does not match the value specified in the release table file for cuttings and cavings releases.
	'>>>>>CUTTINGS CH RELEASE TABLE DOES NOT SPAN POTENTIAL INTRUSION'	Fatal error: The CH cuttings and cavings release data do not span the range of times possible for the simulation.
	'>>>>>TIMES (',AdminControlTime,' TO ',TEnd,' YR)'	

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Subroutine	Statement	Explanation
ReadCuttingsRelease (Continued)	'>>>CUTTINGS RH RELEASE TABLE DOES NOT SPAN POTENTIAL INTRUSION	Fatal error: The RH cuttings and cavings release data do not span the range of times possible for the simulation.
	'>>>TIMES (', AdminControlTime,' TO ',TEnd,' YR)'	
	'>>>>>I/O ERROR WHILE READING CUTTINGS RELEASE TABLES'	Fatal error: An unknown type of error was encountered when reading the cuttings and cavings release table data.
	'>>>>>PREMATURE EOF ENCOUNTERED READING CUTTINGS RELEASE TABLES'	Fatal error: An end-of-file was encountered when reading the cuttings and cavings release table data.
ReadDirectBrineRelease	'>>>>>INVALID OBSERVATION INDEX VALUE FOR BLOWOUT RELEASE TABLES'	Fatal error: The observation (vector) number does not match the value specified in the release table file for direct brine releases.
	'>>>>>I/O ERROR READING BLOWOUT RELEASE TABLES'	Fatal error: An unknown type of error was encountered when reading the direct brine release table data.
	'>>>>>PREMATURE EOF ENCOUNTERED READING BLOWOUT RELEASE TABLES'	Fatal error: An end-of-file was encountered when reading the direct brine release table data.
ReadLHS_SampleData	'>>>>>ERROR OPENING LHS FILE'	Fatal error: The LHS sample data file could not be opened.
	'>>>>>I/O ERROR READING LHS FILE'	Fatal error: An unknown type of error was encountered when reading the dose parameter data.
ReadReleaseTableHeader	'>>>>>TOTAL WASTE TYPE PROBABILITY NOT EQUAL 'TO 1.0 FOR REGION ', 1	Fatal error: The total of the probabilities for waste types did not equal 1. A flag is set which terminates the program from the subroutine Input.
	'>>>>>TOTAL OF PLUGGING PATTERN PROBABILITIES ON RUN CONTROL PARAMETERS FILE NOT EQUAL TO 1.0 TPP=",TPP	Fatal error: The total of the probabilities for plugging patterns did not equal 1. A flag is set which terminates the program from the subroutine Input.
	'>>>>>ERROR OPENING RELEASE SUMMARY TABLES FILE'	Fatal error: The release-tables file could not be opened.
	'>>>>>I/O ERROR READING HEADER RECORDS FROM RELEASE SUMMARY TABLES FILE'	Fatal error: An unknown type of error was encountered when reading the release table data.
	'>>>>>PREMATURE EOF ENCOUNTERED READING RELEASE SUMMARY TABLES FILE'	Fatal error: An end-of-file was encountered when reading the release table data.
ReadReleaseTables	'>>>>>INVALID OBSERVATION INDEX VALUE FOR LHS FILE'	Fatal error: The observation (vector) number does not match the value specified in the release table file.
ReadReleaseThrough Culebra	'>>>>>INVALID OBSERVATION INDEX VALUE FOR CULEBRA TRANSPORT TABLES'	Fatal error: The observation (vector) number does not match the value specified in the release table file for releases through the Culebra.

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Subroutine	Statement	Explanation
ReadReleaseThrough Culebra (Continued)	'>>>INCREASE VALUE OF PARAMETER MaxNumSpecies TO AT LEAST ', ISPC	Fatal error: The number of species in the release-tables file exceeds the maximum number of species allowed.
	'>>>INCREASE VALUE OF PARAMETER MAXTC TO AT LEAST ', nCulebraReleaseTimes	Fatal error: The maximum number of release times in the release tables file exceeds the maximum number of times allowed.
	'>>>UNEXPECTED VALUE FOR CULEBRA RELEASE POINT IN RELTAB FILE. EXPECTED ', iCRP, ' READ IN ',rCRP	Fatal error: The Culebra release point number does not match the value specified in the release table file for releases from the Culebra.
	'>>>>>I/O ERROR READING CULEBRA TRANSPORT RELEASE TABLES'	Fatal error: An unknown type of error was encountered when reading the release table data.
	'>>>>>PREMATURE EOF ENCOUNTERED READING CULEBRA TRANSPORT RELEASE TABLES'	Fatal error: An end-of-file was encountered when reading the release table data.
ReadReleaseToCulebra	'>>>INVALID OBSERVATION INDEX VALUE FOR CULEBRA RELEASE TABLES'	Fatal error: The observation (vector) number does not match the value specified in the release table file for releases to the Culebra.
	'>INCREASE VALUE OF PARAMETER MaxNumSpecies TO AT LEAST ', nSpecies	Fatal error: The number of species in the release tables file exceeds the maximum number of species allowed.
	'>>>>>I/O ERROR READING CULEBRA RELEASE TABLES'	Fatal error: An unknown type of error was encountered when reading the release table data.
	'>>>>>PREMATURE EOF ENCOUNTERED READING CULEBRA RELEASE TABLES'	Fatal error: An end-of-file was encountered when reading the release table data.
ReadSpallingsRelease	'>>>>>INVALID OBSERVATION INDEX VALUE FOR SPALLINGS RELEASE TABLES'	Fatal error: The observation (vector) number does not match the value specified in the release-tables file for spallings releases.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 72'	Fatal error: The spallings release tables do not span the range of potential intrusion times. This error is raised if the first spallings time occurs later than the end of the administrative control time.
	'>>>>>SPALLINGS RELEASE TABLE DOES NOT SPAN POTENTIAL INTRUSION TIMES	
	'>>>>>(', AdminControlTime, ' TO ', TEnd, ' YR)'	
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 73'	Fatal error: The spallings release tables do not span the range of potential intrusion times. This error is raised if the last spallings time occurs before the end of the simulation.
	'>>>>>SPALLINGS RELEASE TABLE DOES NOT SPAN POTENTIAL INTRUSION TIMES	
	>>>>>(',AdminControlTime,' TO ',TEnd,' YR)'	

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Subroutine	Statement	Explanation
ReadSpallingsRelease (Continued)	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 75'	Fatal error: The times in the spallings release tables for undisturbed conditions are not in increasing order.
	'>>>>>SPALLINGS RELEASE TIMES FOR UNDISTURBED CONDITIONS NOT IN INCREASING ORDER'	
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 76'	Fatal error: The times in the spallings release tables for disturbed conditions are not in increasing order.
	'>>>>>SPALLINGS RELEASE TIMES FOR ',E(Scenario),' INTRUSIONS NOT IN INCREASING ORDER'	This error is raised during validation of spallings times for the first intrusion.
	'>>>>>ERROR(S) ENCOUNTERED, EXECUTION TERMINATED 77'	Fatal error: The times in the spallings release tables for disturbed conditions are not in increasing order.
	'>>>>SPALLINGS RELEASE TIMES FOR ',E(Scenario),'E1 INTRUSIONS NOT IN INCREASING ORDER'	This error is raised during validation of spallings times for the second intrusion.
	'>>>>>I/O ERROR WHILE READING SPALLINGS RELEASE TABLES'	Fatal error: An unknown type of error was encountered when reading the spallings release table data.
	'>>>>>PREMATURE EOF ENCOUNTERED READING SPALLINGS RELEASE TABLES'	Fatal error: An end-of-file was encountered when reading the spallings release table data.
ReleaseByCuttings	'>>>>>NEGATIVE CUTTINGS RELEASE OR CUTTINGS VOLUME'	Warning: The cuttings and cavings release or volume was negative.
ReleaseBySpallings	'>>>>>NEGATIVE SPALLING RELEASE OR SPALLING VOLUME'	Warning: The spallings release or volume was negative.

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