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

1. **Software Name:** PRECCDFGF
2. **Software Version:** 1.01
3. **Document Version:** 1.03
4. **ERMS #:** 539295

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. Allowable or Prescribed Ranges for Inputs and Outputs ☒ Yes
8. Verifiability: Is the design verifiable through testing or other means? ☒ Yes
9. Consistency and Traceability: Is the design consistent with and traceable to the software's requirements? ☒ Yes
10. Technical Feasibility: Is the design technically feasible? ☒ Yes
11. Implementation: Is the design presented in sufficient detail to allow for implementation as computer software? ☒ Yes

Eric Vugrin 12. **Code Team/Sponsor** (*print*)	Eric Vugrin Signature	7/11/05 Date
Sean Dunagan 13. **Technical Reviewer** (*print*)	Eric Vugrin for Sean Dunagan Signature	7/11/05 Date
David Kessel 14. **Responsible Manager** (*print*)	David Kessel Signature	7/11/05 Date
Jennifer Long 15. **SCM Coordinator** (*print*)	Jennifer Long Signature	7/12/05 Date

Key for check boxes above:

Check **Yes** for each item reviewed and found acceptable

WIPP PA

DESIGN DOCUMENT

for

PRECCDFGF (Version 1.01)

Document Version 1.03

ERMS# 539295

July 2005

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1.0 INTRODUCTION

This document serves as a Design Document for the PRECCDFGF program as used in the Waste Isolation Pilot Plant (WIPP) Performance Assessment (PA) calculation. As such, it provides an overview of PRECDDFGF and describes its code architecture.

Three significant modifications have been made to the requirements for PRECCDFGF version 1.01. The first is that when PRECCDFGF version 1.01 reads data for direct solids releases, it will read the text output file written directly by CUTTINGS_S version 6.00 or higher instead of a series of SUMMARIZE output files. Secondly, when reading the release tables written by SUMMARIZE and CUTTINGS_S, PRECCDFGF version 1.01 will read header records at the start of the files to ensure that the fields in the files correspond to the values expected by the READ statements in the code itself. The headers denote the order of the data in the input file, and failure of the header to match the expected text will cause PRECCDFGF to abort its execution with appropriate error messages being logged. Finally, whereas PRECCDFGF version 1.00D read a text output file from LHS to get data about the sampled parameter GLOBAL:PBRINE, version 1.01 will read a set of CAMDAT files generated by POSTLHS to obtain this data. Thus, PRECCDFGF will no longer be required to read output files from LHS.

These modifications require a revision of the discussion of the input files. Additionally, discussion of the header verification capability has been added to Section 6.3.

1.1 Software Identifier

Code Name:	PRECCDFGF
WIPP Prefix:	CCGF1
Version:	1.01

1.2 Points of Contact

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1.3 Code Overview

PRECCDFGF is a preprocessor for the code CCDFGF. PRECCDFGF collates the output from all other WIPP PA codes, retrieves parameter values, and formats this data into output files to be

used by CCDFGF. Requirements for PRECCDFGF fall into five categories: functional requirements, performance requirements, code attributes, external interfaces, and other requirements.

2.0 REQUIREMENTS

The requirements for PRECCDFGF are listed in the *WIPP PA Requirements Document for PRECCDFGF Version 1.01* (WIPP PA 2005a). The requirements are repeated here for the reader's convenience.

2.1 Functional Requirements

R.1 PRECCDFGF will read release tables written by SUMMARIZE.

R.2 PRECCDGF will retrieve constant and sampled parameter values required by CCDFGF from a Computational Database (CDB) file.

R.3 PRECCDFGF will read output from EPAUNI.

R.4 PRECCDFGF will consolidate all data inputs and create the release table (RELTAB) file required by CCDFGF.

R.5 PRECCDFGF will read the text output file from CUTTINGS_S versions 6.00 or higher.

R.6 PRECCDFGF will read the header records in the release tables written by SUMMARIZE and the text output file from CUTTINGS_S. Failure of the header to match the expected text will cause PRECCDFGF to abort its execution with appropriate error messages being logged.

2.2 Performance Requirements

PRECCDFGF should run on a COMPAQ Alpha ES40. Run-time should be less than one hour for one replicate of WIPP PA.

2.3 Attribute Requirements

PRECCDFGF will be written in a transparent, structured manner to facilitate verification of the correct consolidation of release tables into the release data file for CCDFGF.

PRECCDFGF will include comments in the code to assist in code maintenance. Each subroutine or function will include a header describing its purpose and a list of variables that are passed to or from the subroutine or function. In addition, comments will identify the purpose of IF statements and DO loops.

PRECCDFGF will be written with standard FORTRAN 95, and will compile on OpenVMS and on Windows platforms.

PRECCDFGF will meet all applicable WIPP QA requirements.

2.4 External Interface Requirements

PRECCDFGF must read output from SUMMARIZE, POSTLHS, and EPAUNI and the text output file from CUTTINGS_S version 6.00 or higher to produce the release data input file for CCDFGF. PRECCDFGF must be able to read Computational Database (CDB) files. PRECCDFGF must be able to accept command-line arguments at run time.

2.5 Other Requirements

None.

3.0 DESIGN OVERVIEW

This section describes the structure and content of the input and output files from PRECCDFGF. Since PRECCDFGF primarily consolidates multiple files into a single release data file for CCDFGF, the structure of the input and output files determines the design of the PRECCDFGF code.

3.1 I/O Description

The files associated with running PRECCDFGF are described below.

3.1.1 Input files

A number of input files are needed to execute PRECCDFGF. Input files fall into three categories: release data; inventory data; and parameter data.

The vast majority of the input files for PRECCDFGF are created by SUMMARIZE. SUMMARIZE version 3.00 was created by modifying SUMMARIZE version 2.20 (WIPP PA 2005c). In addition to its previous functionality, SUMMARIZE version 3.00 has an additional driver, the PRECCDFGF driver, to format SUMMARIZE output files. This driver is used to create the SUMMARIZE input files for PRECCDFGF version 1.01, and the formats of these files differ from the formats of input files for previous versions of PRECCDFGF. The main difference is the addition of a three line header to these files. The first line contains three numbers, and these numbers indicate the number of vectors in the file, the number of different times for the data, and the number of fields of data excluding vector and time, respectively. The second line denotes the order that the fields appear in the following rows of data, and the third line indicates the type of CAMDAT variable for each field (except vector and time) listed in the

second line. This header is then followed by a blank line. The following sections contain examples of these headers for each type of input file.

Release data input files

Many input files contain release data calculated by other WIPP PA codes; all of these files except the ones containing direct solids release data are produced by running the code SUMMARIZE to process the output of the other WIPP PA codes. The files containing the direct solids release data are produced by the code CUTTINGS_S version 6.00 or higher.

There are four types of release data input files: direct brine releases; direct solids releases; Salado transport releases; and Culebra transport releases. The content of each type of release data input file is described below.

- Direct brine releases

  Direct brine release data files are generated by running SUMMARIZE on the output of the direct brine release calculation, done by the BRAGFLO code. For each replicate, PRECCDFGF expects a total of 78 direct brine release files assigned to the logical names listed in Table 1.

Table 1. Logical Names for Direct Brine Release Data Files

Logical name		
DBR_S1_*P*_T*ttttt*$INP	*P* = U, L, M	*ttttt* = 100, 350, 1000, 3000, 5000, 10000
DBR_S2_*P*_T*ttttt*$INP	*P* = U, L, M	*ttttt* = 550, 750, 2000, 4000, 10000
DBR_S3_*P*_T*ttttt*$INP	*P* = U, L, M	*ttttt* = 1200, 1400, 3000, 5000, 10000
DBR_S4_*P*_T*ttttt*$INP	*P* = U, L, M	*ttttt* = 550, 750, 2000, 4000, 10000
DBR_S5_*P*_T*ttttt*$INP	*P* = U, L, M	*ttttt* = 1200, 1400, 3000, 5000, 10000

Each direct brine release input file has three header rows that are used to identify the data that appears in each of the following columns of data, and the subroutine OPENSUMMARIZEFILE reads this header to verify that the data in the input file is in the order that is required by PRECCDFGF. Figure 1 contains an example of the header for a DBR input file.

The three header rows are followed by three columns of data, with one row of data for each vector. The first column contains the vector number, the second column contains the time, and the third column contains the volume of brine released in m^3. Only the third column is used by PRECCDFGF; these data are read by the subroutine PREBS.

```
         8         1         1

vector time          BRIN_REL

                     [H]
```

Figure 1 Header for DBR Summarize Files

- Direct Solids Releases

For each replicate PRECCDFGF version 1.01 requires one direct solids release data file that is created by running CUTTINGS_S version 6.00 or higher. This file is assigned to the logical SPALL$INP. The *User's Manual for CUTTINGS_S version 6.00* (WIPP PA 2005b) describes this file in the following manner:

> The first line of the output data file is a header record with the following columns:
> 1. the number of scenarios (5 for regulatory calculations)
> 2. the number of vectors (100 for regulatory calculations)
> 3. the number of cavities (3 for regulatory calculations)
>
> The second line lists the number of intrusion times for each scenario (6 in scenario 1 and 5 intrusions in scenarios 2-5 for regulatory calculations), in the order that the scenarios were defined on the master control file and are written on the output data file. The order required for regulatory calculations is 1,2,4,3,5.
>
> The third line is a comment that describes the data columns for the data lines.
>
> The data lines follow. The data lines are ordered by scenario, then cavity, then intrusion time, and finally vector. Thus, all the data for a particular scenario appears together, and the vector index increments each line. The scenario order is determined by the order they were defined on the master control file. Each data line has the following columns:
> 1. the scenario number,
> 2. the cavity abbreviation,
> 3. the intrusion time,
> 4. the vector number,
> 5. the drill diameter (m),
> 6. the footprint area of the material brought to the surface by cuttings and cavings (m^2), and
> 7. the volume of the material brought to the surface by spallings (m^3).

PRECCDFGF calls the subroutine OPENSPALLINGS to read the header, and the drill diameter and cuttings and cavings area are read in the subroutine PRECUT. Spallings volume is read in the subroutine PREBS. An excerpt from of the CUTTINGS_S data file can be found in Appendix A.

- Salado transport releases

PRECCDFGF uses two types of data files for Salado transport releases. One set of data files are generated by running SUMMARIZE on the output of the NUTS code for scenarios S1 though S5. The second set are generated by running SUMMARIZE on the output of the PANEL code for the S6 scenario only. Both types of data files are read by the subroutine PRENUT.

For each replicate, PRECCDFGF expects a total of 22 Salado transport release files assigned to the logical names listed in Table 2.

Table 2. Logical Names for Salado Transport Release Data Files

Logical name	
NUTS_S1$INP	
NUTS_S2_*ttt*$INP	*ttt* = 100, 350
NUTS_S3_*tttt*$INP	*tttt* = 1000, 3000, 5000, 7000, 9000
NUTS_S4_*ttt*$INP	*ttt* = 100, 350
NUTS_S5_*tttt*$INP	*tttt* = 1000, 3000, 5000, 7000, 9000
PNL_S6_tttt$INP	*tttt* = 100, 350, 1000, 2000, 4000, 6000, 9000

Figure 2 and Figure 3 contain headers for these files , and these headers are used to identify the data that appears in each of the following columns of data. The subroutine OPENSUMMARIZEFILE reads this header to verify that the data in the input file is in the order that is required by PRECCDFGF. Each file contains one block of data for each vector. In each block are seven columns of data in the files, with one row of data for each time interval of 50 years, beginning at the time of intrusion. The first column is the vector number and the second column contains the time; these two columns are not used by PRECCDFGF. The third through sixth columns contain the amount of radionuclide (in Curies) released to the Culebra (dissolved or sorbed to colloids) during each time interval for four radionuclides: Am241, Pu239, U234, and Th230.

In the files obtained from NUTS, the seventh column contains the concentration of EPA units released to the Culebra during each time interval. In the files obtained from PANEL, the seventh column is not used by PRECCDFGF. However, the seventh column is required to contain data to allow the same code in PRECCDFGF to read both types of Salado flow release data files.

```
          8       199         5

   vector time    A00AM241    A00PU239       A00U234        A00TH230       EPALWMBT

                                [G]          [G]            [G]            [G]            [G]
```

Figure 2 Header for NUTS Summarize Files

```
        8       199         5

vector time    LDCAM241       LDCPU239       LDCU234        LDCTH230       SDCPB210

                             [H]            [H]            [H]            [H]            [H]
```

Figure 3 Header for Scenario 6 PANEL SUMMARIZE File

- Culebra transport releases

Culebra transport release data files are generated by running SUMMARIZE on the output of the Culebra transport calculation, done by the SECOTP2D code. For each replicate, PRECCDFGF expects a two Culebra transport release files assigned to the logical names ST2D_PM$INP and ST2D_FM$INP for the partial mining and full mining cases, respectively.

These input files are similar in structure to the Salado transport releases. Figure 4 contains the header for these files, and the headers are used to identify the data that appears in each of the following columns of data. The subroutine OPENSUMMARIZEFILE reads this header to verify that the data in the input file is in the order that is required by PRECCDFGF. Each file contains one block of data for each vector. In each block are seven columns of data in the files, with one row of data for each time interval of 50 years, beginning at the time of intrusion. The first column is the vector number and the second column contains the time; these two columns are not used by PRECCDFGF. The third through sixth columns contain the fractional amount (in kg) of each of four dissolved radionuclides (Am241, Pu239, U234, and Th230) that are transported through the Culebra to the Land Withdrawal Boundary (LWB) from a 1 kg source of each radionuclide placed in the Culebra during the time interval. The seventh column contains the amount (in kg) of Th230 that is transported through the Culebra to the Land Withdrawal Boundary (LWB) as a daughter product from a 1 kg source of U234 placed in the Culebra during the time interval.

```
         8       200         5

vector time          MT2AM241    MT2PU239    MT2U234     MT2TH230    MT2TH23A

                     [H]         [H]         [H]         [H]         [H]
```

Figure 4 Header for SECOTP2D SUMMARIZE Files

Inventory data input files

PRECCDFGF reads four input files containing inventory data: one file for solid CH waste, one file for solid RH waste, and two files for mobilized radionuclides, either dissolved or sorbed to colloids in the Castile and Salado brines.

- Contact-handled waste stream

The inventory of CH waste streams are provided to PRECCDFGF in a single input file assigned to the logical EPAUNI_CCH$INP. The inventory is tabulated and decayed over time by the code EPAUNI. As currently configured, PRECCDFGF reads the CH output file from EPAUNI. This file should contain three blocks of data: indexes; intrusion times; and waste stream data.

PRECCDFGF first skips four header lines, then reads the number of CH waste streams and the number of decay times from the fifth and sixth lines. PRECCDFGF reads these numbers starting in column 13 of the EPAUNI output file.

PRECCDFGF skips six more header lines and then reads the intrusion times. Each intrusion time is read from a single line starting in the eighth column.

PRECCDFGF skips another five header lines, then reads one row of data for each CH waste stream. For each CH waste stream, the row of data contains the waste stream number, the probability of an intrusion hitting the waste stream, then a sequence of activity densities in the waste stream, one activity density for each intrusion time. Activity densities are given in EPA units per m^3.

PRECCDFGF calculates the activity density on a repository scale for use in CCDFGF by summing the products of the probability of encountering each waste stream multiplied by the activity density of the waste stream.

- Remote-handled waste stream

The inventory of RH waste streams are provided to PRECCDFGF in a single input file assigned to the logical EPAUNI_CRH$INP. The inventory is tabulated and decayed over

time by the code EPAUNI. PRECCDFGF reads the RH output file from EPAUNI, which has the same structure as the CH waste stream data file. WIPP PA assumes that all RH waste is lumped into a single RH waste stream.

- Mobilized radionuclides

Mobilized radionuclides are either dissolved or sorbed to colloids. The concentration of mobilized radionuclides is used to calculated radionuclides in direct brine releases. Mobilized radionuclide files are generated by running SUMMARIZE on the output of the PANEL code. For each replicate, PRECCDFGF expects two files containing the amounts of mobilized radionuclides, one for Salado brines and one for Castile brines, assigned to the logicals PNL_CON_S1$INP and PNL_CON_S2$INP, respectively. Since Scenario S1 uses Salado brine and Scenario S2 uses Castile brine, these two scenarios cover the range of possible brines, and thus mobilized radionuclide concentrations are not calculated for the other scenarios. Rather, for Scenarios S4 and S5 (E2 intrusions) mobilized radionuclide concentrations are equal to those for Scenario S1 (E0 conditions); for Scenario S3 and S6 (E1 intrusion and E1E2 intrusion, respectively) mobilized radionuclide concentrations are equal to those for Scenario S2 (E1 intrusion.)

Figure 5 contains the header for these files, and the headers are used to identify the data that appears in each of the following columns of data. The subroutine OPENSUMMARIZEFILE reads this header to verify that the data in the input file is in the order that is required by PRECCDFGF. Each file contains one block of data for each vector. Within each block are nine rows of data, one row for each of the following times: 100, 125, 175, 350, 1000, 3000, 5000, 7500, and 10000 years. Each block of data contains seven columns. The first column is the vector number and the second column is the time in years. The third through sixth columns contain the concentration in Curies/m^3 of mobilized radionuclide for Am241, Pu239, U234, and Th230, in that order. The seventh column contains the concentration in EPA units/m^3 of all mobilized radionuclides.

```
      8         9         5

vector time        CLEAM241    CLEPU239    CLEU234     CLETH230    CNETOTAL

                   [H]         [H]         [H]         [H]         [H]
```

Figure 5 Header for PANEL_CON SUMMARIZE Files

Parameter data input files

- Sampled parameter values

PRECCDFGF version 1.01 requires one sampled parameter, GLOBAL:PBRINE, the probability that a drilling intrusion encounters a brine pocket below the repository. This sampled parameter value is provided to PRECCDFGF by a set CAMDAT files that are

generated by the code POSTLHS. PRECCDFGF version 1.01 requires that a template for the names of these files be entered in a command line argument.

- Constant parameter values

PRECCDFGF requires parameter values from the WIPP PA Parameter Database (PAPDB). PRECCDFGF reads these parameters from an input file in the CDB format. Table 3 lists the parameters used by PRECCDFGF; the code uses a variable name, while the parameter database uses both a material name and a property name for each parameter.

Table 3. Constant Parameters Used in PRECCDFGF

Variable name	Material	Property
ContactHandledWasteArea	REFCON	AREA_CH
RemoteHandledWasteArea	REFCON	AREA_RH
EXVOL	REFCON	VREPOS
ACTI	GLOBAL	TA
VolumeFractionContactWaste	REFCON	FVW
VolumeFractionRemoteHandledWaste	REFCON	FVRW
FinalDrillingRate	GLOBAL	LAMDAD
PluggingPatternProb(1)	GLOBAL	ONEPLG
PluggingPatternProb(2)	GLOBAL	TWOPLG
PluggingPatternProb(3)	GLOBAL	THREEPLG
FinalMiningRate	GLOBAL	MINERT
MiningTransitionTime	GLOBAL	TPICM
DrillingTransitionTime	GLOBAL	TPICD
InitialMiningReduction	GLOBAL	FPICM
InitialDrillingReduction	GLOBAL	FPICD
HeightContactHandledWaste	BLOWOUT	HREPOS
HeightRemoteHandledWaste	REFCON	HRH
BermArea	REFCON	ABERM
WUF	BOREHOLE	WUF

- Colloidal mobilization fractions

Releases to the Culebra are provided to PRECCDFGF in the Salado transport data files. These releases are reported as the total amount (in Curies) of mobilized radionuclides, both dissolved and sorbed to colloids. WIPP PA treats four colloid species: humic, actinide intrinsic, microbial and mineral fragment. WIPP PA assumes that humic colloids transport as do dissolved radionuclides, and that other colloid species are not transported through the Culebra. Hence the fraction of mobilized actinide present in each colloid species is needed to calculate the release through the Culebra.

Colloidal mobilization fractions are calculated in the code PANEL and are extracted by running the SUMMARIZE code on the PANEL output. PRECCDFGF expects two colloidal mobilization fraction data files assigned to the logicals COLLOID_S1$INP and COLLOID_S2$INP.

Colloidal mobilization fractions vary by vector and by the type of brine assumed to predominate in the waste-filled area. Since Scenario S1 uses Salado brine and Scenario S2 uses Castile brine, these two scenarios cover the range of possible brines, and thus colloidal mobilization fractions are not calculated for the other scenarios. Rather, for Scenarios S4 and S5 (E2 intrusions) colloidal mobilization fractions are equal to those for Scenario S1 (E0 conditions); for Scenario S3 and S6 (E1 intrusion and E1E2 intrusion, respectively) colloidal mobilization fractions are equal to those for Scenario S2 (E1 intrusion.)

These input files have three header rows followed by fourteen columns of data, with one row for each vector. Figure 6 contains the header for these files, and the headers are used to identify the data that appears in each of the following columns of data. The subroutine OPENSUMMARIZEFILE reads this header to verify that the data in the input file is in the order that is required by PRECCDFGF. The first column is the vector and the second column is the time; neither column is used by PRECCDFGF. The remaining twelve columns contain three colloidal mobilization fractions for each of four radionuclides: Am241, Pu239, U234, and Th230. Columns three, four and five contain the colloidal mobilization fractions for microbial, actinide intrinsic, and mineral fragment colloids for Am241. Columns six through fourteen contain the colloidal mobilization fractions Pu239, U234 and Th230 in the same order. WIPP PA assumes that humic colloids transport exactly the same as do dissolved radionuclides; consequently, no colloidal mobilization fraction is used for humic colloids.

```
       8        1       12

vector time FRCMIC FRCINT  FRCMIN  FRCMIC  FRCINT  FRCMIN  FRCMIC  FRCINT  FRCMIN
FRCMIC         FRCINT         FRCMIN

       [P:32]   [P:32]   [P:32] [P:40]   [P:40]   [P:40]    [P:44]    [P:44]     [P:44]

  [P:43]         [P:43]         [P:43]
```

Figure 6 Header for Colliod Mobilization SUMMARIZE FILES.
Note that the first, second, and third lines in this figure are contained on one line in the file itself. The same is true for the fourth and fifth lines of figure.

3.1.2 Output Files

PRECCDFGF generates an ASCII file containing the parameter values and the consolidated release information from the various input files.

Release Table (RELTAB) output file

The RELTAB output file consolidates all the release information from the various input data files for input to the CCDFGF code. The RELTAB file 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 for use by the code CCDFGF. Next, the RELTAB file contains maximum array dimensions for spallings, DBR, and flows to the Culebra; these values are used in CCDFGF to dimension data structures that will contain release data. 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.

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 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.

- Sampled parameters section

  The RELTAB file lists the values of sampled parameters for each vector. In version 1.01, the only sampled parameter is the probability of a drilling intrusion encountering a brine pocket below the repository.

- Cuttings releases data section

  The cuttings 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 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 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.

- 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 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 three components for the lower, middle and upper panel groups. In each component are the number of interpolation times, the interpolation times, and the spallings volumes at each interpolation time.

The E1 intrusion block has three components for the same, different-by-one, and different-by-two panel groups; these panel groups correspond to the release input files for the lower, middle, and upper 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 spallings releases at the interpolation times. The E2 intrusion block has the same structure as the E1 intrusion block.

- 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; the data block first lists the number of interpolation times, interpolation times, then the concentrations at each interpolation time for the E0, E1, and E2 scenarios, in that order.

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 three components for the lower, middle and upper panel groups. In each component are the number of interpolation times, the interpolation times, and the DBR volumes at each interpolation time.

The E1 intrusion block has three components for the same, different-by-one, and different-by-two panel groups; these panel groups correspond to the release input files for the lower, middle, and upper 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.

- 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 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.

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.

- 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. For each of four radionuclides, the RELTAB file lists: the decay rate (yr^{-1}); the number of moles in a kg of the radionuclide; the specific activity (); 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 Culebra transport data section comprises 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.

3.2 Design Constraints

PRECCDFGF must be able to read data from computational database (CDB) formatted files, using the utilities in WIPP PA libraries CAMDAT_LIB, CAMCON_LIB and SDBREAD_LIB, as necessary.

3.3 Other Design Considerations

There are no other design considerations for PRECCDFGF.

4.0 THEORETICAL OVERVIEW

PRECCDFGF does not model any physical processes or perform any complex mathematics. The only calculations in PRECCDFGF are unit conversions (from Curies to kg, for example.) Thus, there is no significant theoretical basis for any portion of PRECCDFGF.

5.0 MATHEMATICAL MODEL

PRECCDFGF does not model any physical processes. The only calculations done with PRECCDFGF are unit conversions and do not require and sophisticated equations.

6.0 CODE ARCHITECTURE

6.1 Control Flow and Logic

PRECCDFGF requires four command line arguments at run-time. The user must provide the name of the CDB file containing parameter values; the number of vectors to be analyzed (normally 100); the end time of the simulation (normally 10,000 years); and a template for the names of the POSTLHS CDB files. PRECCDFGF runs without any other user interaction.

6.2 Data Structures

The structures of input and output files are described in section 3.0 of this document. Internal data structures are standard variables, arrays, and pointers, which do not require further description.

6.3 Allowable / Prescribed Ranges for Input / Output

PRECCDFGF requires that the headers of the input files precisely match the formats described in Section 3.1.1. and, thus, ensures that the data in the input files is in the order required by PRECCDFGF. Failure of the headers to match will result in a terminal error and abortion of the calculations.

PRECCDFGF does not check the validity of the data provided in the various input files. PRECCDFGF imposes no restrictions on the range of values in the input files, and (with the exception of unit conversions) echoes these inputs to the output files.

6.4 Verifiability

PRECCDFGF will be verified by manual inspection of the output files resulting from a known set of input files. Parameter values will be provided in a CDB file; validation will use the GROPECDB utility to verify that PRECCDFGF correctly reads data from the CDB file. In addition, validation will demonstrate that the output RELTAB file can be read by CCDFGF.

7.0 REFERENCES

WIPP PA (Performance Assessment) 2005a. *Requirements Document for PRECCDFGF Version 1.01*. Sandia National Laboratories. Carlsbad, NM. ERMS# 539480.

WIPP PA (Performance Assessment) 2005b. *User's Manual for CUTTINGS_S Version 6.00*. Sandia National Laboratories. Carlsbad, NM. ERMS# 537039.

WIPP PA (Performance Assessment) 2005c. *Change Control Form for SUMMARIZE Version 2.20*. Sandia National Laboratories. Carlsbad, NM. ERMS# 540117.

APPENDIX A: DIRECT SOLIDS RELEASE DATA FILE

A sample direct solids release data file is shown below. This file is output by the code CUTTINGS_S.

Line 1 of the file specifies that there are five scenarios, four vectors, and three cavities. Line 2 specifies that there are six intrusion times for Scenario 1, five times for Scenarios 2 and 4, and four times for Scenario 3 and 5. Note that the scenarios do not have the same intrusion times and the scenarios are not in numerical order. The intrusion times and the ordering of the scenarios are specified in the master control file. Line 3 of the file is a comment describing the contents of the data lines that follow. The file contains 288 data lines (4 vectors * 3 cavities * (6+5+5+4+4) intrusion times per scenario). Many of the data lines have been removed for brevity and replaced with "…" and a comment (in italics) explaining what data lines have been removed.

```
     5     4     3
     6     5     5     4     4
SCN CAV     TIME          VEC     DRILDIAM       AREA_C         VOL_S
  1 L    1.00000E+02      1   3.111500E-01   2.128595E-01   0.000000E+00
  1 L    1.00000E+02      2   3.111500E-01   1.131132E-01   0.000000E+00
  1 L    1.00000E+02      3   3.111500E-01   7.603780E-02   0.000000E+00
  1 L    1.00000E+02      4   3.111500E-01   1.309525E-01   0.000000E+00
  1 L    3.50000E+02      1   3.111500E-01   2.128595E-01   0.000000E+00
  1 L    3.50000E+02      2   3.111500E-01   1.131132E-01   0.000000E+00
  1 L    3.50000E+02      3   3.111500E-01   7.603780E-02   0.000000E+00
  1 L    3.50000E+02      4   3.111500E-01   1.309525E-01   2.410427E-02
  1 L    1.00000E+03      1   3.111500E-01   2.128595E-01   0.000000E+00
  1 L    1.00000E+03      2   3.111500E-01   1.131132E-01   4.980908E-01
  1 L    1.00000E+03      3   3.111500E-01   7.603780E-02   0.000000E+00
  1 L    1.00000E+03      4   3.111500E-01   1.309525E-01   3.760077E-01
  1 L    3.00000E+03      1   3.111500E-01   2.128595E-01   0.000000E+00
  1 L    3.00000E+03      2   3.111500E-01   1.131132E-01   5.401633E-01
  1 L    3.00000E+03      3   3.111500E-01   7.603780E-02   0.000000E+00
  1 L    3.00000E+03      4   3.111500E-01   1.309525E-01   2.590723E-01
  1 L    5.00000E+03      1   3.111500E-01   2.128595E-01   0.000000E+00
  1 L    5.00000E+03      2   3.111500E-01   1.131132E-01   5.332199E-01
  1 L    5.00000E+03      3   3.111500E-01   7.603780E-02   0.000000E+00
  1 L    5.00000E+03      4   3.111500E-01   1.309525E-01   2.110886E-01
  1 L    1.00000E+04      1   3.111500E-01   2.128595E-01   0.000000E+00
  1 L    1.00000E+04      2   3.111500E-01   1.131132E-01   4.988766E-01
  1 L    1.00000E+04      3   3.111500E-01   7.603780E-02   0.000000E+00
  1 L    1.00000E+04      4   3.111500E-01   1.309525E-01   1.872676E-01
```

```
  1 M     1.00000E+02     1  3.111500E-01  2.128595E-01  0.000000E+00
  1 M     1.00000E+02     2  3.111500E-01  1.131132E-01  0.000000E+00
```

... *The 24 (6*4) data lines for Scenario 1, Cavity M, 6 intrusion times (100, 350, 1000, 3000, 5000, 10000), Vectors 1-4 follow the same pattern as for Cavity L above.*

```
  1 M     1.00000E+04     3  3.111500E-01  7.603780E-02  0.000000E+00
  1 M     1.00000E+04     4  3.111500E-01  1.309525E-01  1.864856E-01
  1 U     1.00000E+02     1  3.111500E-01  2.128595E-01  0.000000E+00
  1 U     1.00000E+02     2  3.111500E-01  1.131132E-01  0.000000E+00
```

... *The 24 data lines for Scenario 1, Cavity M, 6 intrusion times, Vectors 1-4.*

```
  1 U     1.00000E+04     4  3.111500E-01  1.309525E-01  1.846775E-01
  2 L     5.50000E+02     1  3.111500E-01  2.128595E-01  3.135009E-02
  2 L     5.50000E+02     2  3.111500E-01  1.131132E-01  2.227808E-01
```

... *The 60 (3*5*4) data lines for Scenario 2, 3 cavities (L,U,M), 5 intrusion times, Vectors 1-4 follows the same pattern as for Scenario 1 above.*

```
  2 U     1.00000E+04     4  3.111500E-01  1.309525E-01  0.000000E+00
  4 L     5.50000E+02     1  3.111500E-01  2.128595E-01  0.000000E+00
  4 L     5.50000E+02     2  3.111500E-01  1.131132E-01  2.248455E-01
```

... *The 60 data lines for Scenario 4, 3 cavities (L,U,M), 5 intrusion times, Vectors 1-4.*

```
  4 U     1.00000E+04     4  3.111500E-01  1.309525E-01  0.000000E+00
  3 L     1.20000E+03     1  3.111500E-01  2.128595E-01  3.691427E-02
  3 L     1.20000E+03     2  3.111500E-01  1.131132E-01  3.954772E-01
```

... *The 48 (3*4*4) data lines for Scenario 3, 3 cavities (L,U,M), 4 intrusion times, Vectors 1-4.*

```
  3 U     1.00000E+04     4  3.111500E-01  1.309525E-01  0.000000E+00
  5 L     1.20000E+03     1  3.111500E-01  2.128595E-01  0.000000E+00
  5 L     1.20000E+03     2  3.111500E-01  1.131132E-01  5.141423E-01
```

... *The 48 data lines for Scenario 5, 3 cavities (L,U,M), 4 intrusion times, Vectors 1-4.*

```
  5 U     1.00000E+04     4  3.111500E-01  1.309525E-01  0.000000E+00
```