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:** PRECCDFGF
2. **Software Version:** 3.01
3. **Document Version:** 3.01
4. **ERMS #:** 577631

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	8/10/22 Date
14.	Todd Zeitler **Technical Reviewer** (*print*)	*Signature on File* Signature	8/22/22 Date
15.	Shelly R. Nielsen **QA Reviewer** (*print*)	Shelly R. Nielsen Signature	8/29/22 Date
16.	Steve Wagner **Responsible Manager** (*print*)	*Signature on File* Signature	8/23/22 Date
17.	Jennifer Long **SCM Coordinator** (*print*)	*Signature on File* Signature	8/25/22 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:** PRECCDFGF
2. **Software Version:** 3.01
3. **Document Version:** 3.01
4. **ERMS #:** 577631

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	8/10/2022 Date
16.	Todd Zeitler **Technical Reviewer** (*print*)	*Signature on File* Signature	8/22/2022 Date
17.	Shelly R. Nielsen **QA Reviewer** (*print*)	Shelly R. Nielsen Signature	8-29-2022 Date
18.	Steve Wagner **Responsible Manager** (*print*)	*Signature on File* Signature	8/23/2022 Date
19.	Jennifer Long **SCM Coordinator** (*print*)	*Signature on File* Signature	8/25/2022 Date

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WIPP PA

Design Document and User's Manual

for

PRECCDFGF Version 3.01

Document Version 3.01

ERMS #577631

August 2022

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1.0 INTRODUCTION AND SCOPE

This Design Document and User's Manual for PRECCDFGF Version 3.01 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 Solaris cluster.

1.1 Software Identification

Code Name:	PRECCDFGF
Version:	3.01
CVS Repository:	/data/cvs/CVSLIB/WIPP_CODES/PA_CODES/PRECCDFGF
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

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.

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2.0 REQUIREMENTS

The requirements for PRECCDFGF are listed in the Requirements Document, Verification and Validation Plan, and Validation Document for PRECCDFGF Version 3.01 (Brunell, 2022b), and are repeated here.

2.1 Functional Requirements

The functional requirements for PRECCDFGF Version 3.01 are:

R.1 PRECCDFGF will consolidate all data inputs and create the release table (RELTAB) file required by CCDFGF.

R.2 PRECCDFGF will verify the header records in each release table written by SUMMARIZE and CUTTINGS_S. If the header information does not match the expected format, PRECCDFGF will produce an error and abort the run.

R.3 If PRECCDFGF requires a parameter value that is not located in the expected Computational Database (CDB) input file, PRECCDFGF will produce an error and abort the run.

2.2 External Interface Requirements

The external interface requirements for PRECCDFGF Version 3.01 are listed below:

R.4 PRECCDFGF must be able to accept command-line arguments at run time.

R.5 PRECCDFGF must read text output files produced by SUMMARIZE, EPAUNI, and CUTTINGS_S.

R.6 PRECCDGF will retrieve constant and sampled parameter values required by CCDFGF from CDB files produced by POSTLHS and MATSET.

2.3 Other Requirements

There are no other requirements for PRECCDFGF.

2.4 Functionality Not Tested

All code functionality is covered in the requirements and test cases.

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3.0 MAJOR SOFTWARE COMPONENTS

This section describes the organization of the PRECCDFGF source code, required object libraries, and the structure and content of the input and output files for PRECCDFGF.

PRECCDFGF is implemented in FORTRAN. All subroutines and functions are found in the file Preccdfgf.f. 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 the file preccdfgf.inc.

Additionally, PRECCDFGF utilizes the WIPP PA libraries CAMDAT_LIB, CAMCON_LIB, and CAMSUPES_LIB to access functions and subroutines that read CDB files and that write QA-related information to output files and screen output.

3.1 Object Libraries

PRECCDFGF uses the following object libraries:

- CAMDAT_LIB: reads and writes information to CAMDAT files. PRECCDFGF links to subroutines DBSETUP, DBIOPEN, DBICLOSE, DBISIZES, DBIELBLK, and DBIPROP.

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

- CAMSUPES_LIB: provides machine-dependent functions. PRECCDFGF links to subroutines MCINIT, MDINIT.

3.2 Input Files

A number of input files are needed to execute PRECCDFGF. Input files fall into four categories:

1. control files
2. release data
3. inventory data
4. parameter data.

The following sections describe each type of input file.

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3.2.1 Control Input Files

PRECCDFGF Verion 3.01 requires two input control files: a map file and an intrusion times file.

3.2.1.1 Map File

The map file is a text file containing a map of input data file names to logical variable names. The map file is specified by the command line keyword "-map". An example map file is shown in Figure 1. The logical variables expected in the map file are fixed as displayed in Figure 1, with the exceptions of the radionuclide concentration files (logical variables PNL_CON*n*_S1$INP and PNL_CON*n*_S2$INP, where *n* denotes the number of brine volumes, maximum 5), and the Culebra transport files (logical variables ST2D*c*_FM$INP and ST2D*c*_PM$INP, where *c* represents the associated Culebra release point). The map file must contain logical variable names for at least one brine volume and at least one Culebra release point. For each brine volume, a pair of logical variable names are expected for scenarios S1 and S2. For each Culebra release point, a pair of logical variable names are expected for the full mining and partial mining scenarios.

The logical variable names in the map file are all required. The logical variable names may be listed in any order, but all must be provided. The logical variable names include information such as scenario number (e.g., "S1") and intrusion time (e.g., "T100") that must be consistent with the data contained in the release data input files (Section 3.2.2).

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```
! These are the input files for Test 2
 EPAUNI_CCH$INP          ./Input/epu_ccgf_test_ch.dat
 EPAUNI_CRH$INP          ./Input/epu_ccgf_test_rh.dat
 PNL_CON1_S1$INP         ./Input/sum_panel_con_t1_b1_s1.tbl
 PNL_CON1_S2$INP         ./Input/sum_panel_con_t1_b1_s2.tbl
 PNL_CON2_S1$INP         ./Input/sum_panel_con_t1_b2_s1.tbl
 PNL_CON2_S2$INP         ./Input/sum_panel_con_t1_b2_s2.tbl
 DBR_S1_L_T100$INP       ./Input/sum_bf4_ccgf_test_r1_s1_l_t100.tbl
 DBR_S1_L_T350$INP       ./Input/sum_bf4_ccgf_test_r1_s1_l_t350.tbl
 DBR_S1_L_T1000$INP      ./Input/sum_bf4_ccgf_test_r1_s1_l_t1000.tbl
 DBR_S1_L_T3000$INP      ./Input/sum_bf4_ccgf_test_r1_s1_l_t3000.tbl
 DBR_S1_L_T5000$INP      ./Input/sum_bf4_ccgf_test_r1_s1_l_t5000.tbl
 DBR_S1_L_T10000$INP     ./Input/sum_bf4_ccgf_test_r1_s1_l_t10000.tbl
 DBR_S1_M_T100$INP       ./Input/sum_bf4_ccgf_test_r1_s1_m_t100.tbl
 DBR_S1_M_T350$INP       ./Input/sum_bf4_ccgf_test_r1_s1_m_t350.tbl
 DBR_S1_M_T1000$INP      ./Input/sum_bf4_ccgf_test_r1_s1_m_t1000.tbl
 DBR_S1_M_T3000$INP      ./Input/sum_bf4_ccgf_test_r1_s1_m_t3000.tbl
 DBR_S1_M_T5000$INP      ./Input/sum_bf4_ccgf_test_r1_s1_m_t5000.tbl
 DBR_S1_M_T10000$INP     ./Input/sum_bf4_ccgf_test_r1_s1_m_t10000.tbl
 DBR_S1_U_T100$INP       ./Input/sum_bf4_ccgf_test_r1_s1_u_t100.tbl
 DBR_S1_U_T350$INP       ./Input/sum_bf4_ccgf_test_r1_s1_u_t350.tbl
 DBR_S1_U_T1000$INP      ./Input/sum_bf4_ccgf_test_r1_s1_u_t1000.tbl
 DBR_S1_U_T3000$INP      ./Input/sum_bf4_ccgf_test_r1_s1_u_t3000.tbl
 DBR_S1_U_T5000$INP      ./Input/sum_bf4_ccgf_test_r1_s1_u_t5000.tbl
 DBR_S1_U_T10000$INP     ./Input/sum_bf4_ccgf_test_r1_s1_u_t10000.tbl
 DBR_S1_O_T100$INP       ./Input/sum_bf4_ccgf_test_r1_s1_o_t100.tbl
 DBR_S1_O_T350$INP       ./Input/sum_bf4_ccgf_test_r1_s1_o_t350.tbl
 DBR_S1_O_T1000$INP      ./Input/sum_bf4_ccgf_test_r1_s1_o_t1000.tbl
 DBR_S1_O_T3000$INP      ./Input/sum_bf4_ccgf_test_r1_s1_o_t3000.tbl
 DBR_S1_O_T5000$INP      ./Input/sum_bf4_ccgf_test_r1_s1_o_t5000.tbl
 DBR_S1_O_T10000$INP     ./Input/sum_bf4_ccgf_test_r1_s1_o_t10000.tbl
 DBR_S2_L_T550$INP       ./Input/sum_bf4_ccgf_test_r1_s2_l_t550.tbl
 DBR_S2_L_T750$INP       ./Input/sum_bf4_ccgf_test_r1_s2_l_t750.tbl
 DBR_S2_L_T2000$INP      ./Input/sum_bf4_ccgf_test_r1_s2_l_t2000.tbl
 DBR_S2_L_T4000$INP      ./Input/sum_bf4_ccgf_test_r1_s2_l_t4000.tbl
 DBR_S2_L_T10000$INP     ./Input/sum_bf4_ccgf_test_r1_s2_l_t10000.tbl
 DBR_S2_M_T550$INP       ./Input/sum_bf4_ccgf_test_r1_s2_m_t550.tbl
 DBR_S2_M_T750$INP       ./Input/sum_bf4_ccgf_test_r1_s2_m_t750.tbl
 DBR_S2_M_T2000$INP      ./Input/sum_bf4_ccgf_test_r1_s2_m_t2000.tbl
 DBR_S2_M_T4000$INP      ./Input/sum_bf4_ccgf_test_r1_s2_m_t4000.tbl
 DBR_S2_M_T10000$INP     ./Input/sum_bf4_ccgf_test_r1_s2_m_t10000.tbl
 DBR_S2_U_T550$INP       ./Input/sum_bf4_ccgf_test_r1_s2_u_t550.tbl
 DBR_S2_U_T750$INP       ./Input/sum_bf4_ccgf_test_r1_s2_u_t750.tbl
 DBR_S2_U_T2000$INP      ./Input/sum_bf4_ccgf_test_r1_s2_u_t2000.tbl
 DBR_S2_U_T4000$INP      ./Input/sum_bf4_ccgf_test_r1_s2_u_t4000.tbl
 DBR_S2_U_T10000$INP     ./Input/sum_bf4_ccgf_test_r1_s2_u_t10000.tbl
 DBR_S2_O_T550$INP       ./Input/sum_bf4_ccgf_test_r1_s2_o_t550.tbl
 DBR_S2_O_T750$INP       ./Input/sum_bf4_ccgf_test_r1_s2_o_t750.tbl
 DBR_S2_O_T2000$INP      ./Input/sum_bf4_ccgf_test_r1_s2_o_t2000.tbl
 DBR_S2_O_T4000$INP      ./Input/sum_bf4_ccgf_test_r1_s2_o_t4000.tbl
 DBR_S2_O_T10000$INP     ./Input/sum_bf4_ccgf_test_r1_s2_o_t10000.tbl
 DBR_S3_L_T1200$INP      ./Input/sum_bf4_ccgf_test_r1_s3_l_t1200.tbl
 DBR_S3_L_T1400$INP      ./Input/sum_bf4_ccgf_test_r1_s3_l_t1400.tbl
 DBR_S3_L_T3000$INP      ./Input/sum_bf4_ccgf_test_r1_s3_l_t3000.tbl
 DBR_S3_L_T5000$INP      ./Input/sum_bf4_ccgf_test_r1_s3_l_t5000.tbl
```

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```
DBR_S3_L_T10000$INP    ./Input/sum_bf4_ccgf_test_r1_s3_l_t10000.tbl
DBR_S3_M_T1200$INP     ./Input/sum_bf4_ccgf_test_r1_s3_m_t1200.tbl
DBR_S3_M_T1400$INP     ./Input/sum_bf4_ccgf_test_r1_s3_m_t1400.tbl
DBR_S3_M_T3000$INP     ./Input/sum_bf4_ccgf_test_r1_s3_m_t3000.tbl
DBR_S3_M_T5000$INP     ./Input/sum_bf4_ccgf_test_r1_s3_m_t5000.tbl
DBR_S3_M_T10000$INP    ./Input/sum_bf4_ccgf_test_r1_s3_m_t10000.tbl
DBR_S3_U_T1200$INP     ./Input/sum_bf4_ccgf_test_r1_s3_u_t1200.tbl
DBR_S3_U_T1400$INP     ./Input/sum_bf4_ccgf_test_r1_s3_u_t1400.tbl
DBR_S3_U_T3000$INP     ./Input/sum_bf4_ccgf_test_r1_s3_u_t3000.tbl
DBR_S3_U_T5000$INP     ./Input/sum_bf4_ccgf_test_r1_s3_u_t5000.tbl
DBR_S3_U_T10000$INP    ./Input/sum_bf4_ccgf_test_r1_s3_u_t10000.tbl
DBR_S3_O_T1200$INP     ./Input/sum_bf4_ccgf_test_r1_s3_o_t1200.tbl
DBR_S3_O_T1400$INP     ./Input/sum_bf4_ccgf_test_r1_s3_o_t1400.tbl
DBR_S3_O_T3000$INP     ./Input/sum_bf4_ccgf_test_r1_s3_o_t3000.tbl
DBR_S3_O_T5000$INP     ./Input/sum_bf4_ccgf_test_r1_s3_o_t5000.tbl
DBR_S3_O_T10000$INP    ./Input/sum_bf4_ccgf_test_r1_s3_o_t10000.tbl
DBR_S4_L_T550$INP      ./Input/sum_bf4_ccgf_test_r1_s4_l_t550.tbl
DBR_S4_L_T750$INP      ./Input/sum_bf4_ccgf_test_r1_s4_l_t750.tbl
DBR_S4_L_T2000$INP     ./Input/sum_bf4_ccgf_test_r1_s4_l_t2000.tbl
DBR_S4_L_T4000$INP     ./Input/sum_bf4_ccgf_test_r1_s4_l_t4000.tbl
DBR_S4_L_T10000$INP    ./Input/sum_bf4_ccgf_test_r1_s4_l_t10000.tbl
DBR_S4_M_T550$INP      ./Input/sum_bf4_ccgf_test_r1_s4_m_t550.tbl
DBR_S4_M_T750$INP      ./Input/sum_bf4_ccgf_test_r1_s4_m_t750.tbl
DBR_S4_M_T2000$INP     ./Input/sum_bf4_ccgf_test_r1_s4_m_t2000.tbl
DBR_S4_M_T4000$INP     ./Input/sum_bf4_ccgf_test_r1_s4_m_t4000.tbl
DBR_S4_M_T10000$INP    ./Input/sum_bf4_ccgf_test_r1_s4_m_t10000.tbl
DBR_S4_U_T550$INP      ./Input/sum_bf4_ccgf_test_r1_s4_u_t550.tbl
DBR_S4_U_T750$INP      ./Input/sum_bf4_ccgf_test_r1_s4_u_t750.tbl
DBR_S4_U_T2000$INP     ./Input/sum_bf4_ccgf_test_r1_s4_u_t2000.tbl
DBR_S4_U_T4000$INP     ./Input/sum_bf4_ccgf_test_r1_s4_u_t4000.tbl
DBR_S4_U_T10000$INP    ./Input/sum_bf4_ccgf_test_r1_s4_u_t10000.tbl
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DBR_S4_O_T2000$INP     ./Input/sum_bf4_ccgf_test_r1_s4_o_t2000.tbl
DBR_S4_O_T4000$INP     ./Input/sum_bf4_ccgf_test_r1_s4_o_t4000.tbl
DBR_S4_O_T10000$INP    ./Input/sum_bf4_ccgf_test_r1_s4_o_t10000.tbl
DBR_S5_L_T1200$INP     ./Input/sum_bf4_ccgf_test_r1_s5_l_t1200.tbl
DBR_S5_L_T1400$INP     ./Input/sum_bf4_ccgf_test_r1_s5_l_t1400.tbl
DBR_S5_L_T3000$INP     ./Input/sum_bf4_ccgf_test_r1_s5_l_t3000.tbl
DBR_S5_L_T5000$INP     ./Input/sum_bf4_ccgf_test_r1_s5_l_t5000.tbl
DBR_S5_L_T10000$INP    ./Input/sum_bf4_ccgf_test_r1_s5_l_t10000.tbl
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DBR_S5_M_T1400$INP     ./Input/sum_bf4_ccgf_test_r1_s5_m_t1400.tbl
DBR_S5_M_T3000$INP     ./Input/sum_bf4_ccgf_test_r1_s5_m_t3000.tbl
DBR_S5_M_T5000$INP     ./Input/sum_bf4_ccgf_test_r1_s5_m_t5000.tbl
DBR_S5_M_T10000$INP    ./Input/sum_bf4_ccgf_test_r1_s5_m_t10000.tbl
DBR_S5_U_T1200$INP     ./Input/sum_bf4_ccgf_test_r1_s5_u_t1200.tbl
DBR_S5_U_T1400$INP     ./Input/sum_bf4_ccgf_test_r1_s5_u_t1400.tbl
DBR_S5_U_T3000$INP     ./Input/sum_bf4_ccgf_test_r1_s5_u_t3000.tbl
DBR_S5_U_T5000$INP     ./Input/sum_bf4_ccgf_test_r1_s5_u_t5000.tbl
DBR_S5_U_T10000$INP    ./Input/sum_bf4_ccgf_test_r1_s5_u_t10000.tbl
DBR_S5_O_T1200$INP     ./Input/sum_bf4_ccgf_test_r1_s5_o_t1200.tbl
DBR_S5_O_T1400$INP     ./Input/sum_bf4_ccgf_test_r1_s5_o_t1400.tbl
DBR_S5_O_T3000$INP     ./Input/sum_bf4_ccgf_test_r1_s5_o_t3000.tbl
DBR_S5_O_T5000$INP     ./Input/sum_bf4_ccgf_test_r1_s5_o_t5000.tbl
```

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```
DBR_S5_O_T10000$INP    ./Input/sum_bf4_ccgf_test_r1_s5_o_t10000.tbl
SPALL$INP              ./Input/cusp_ccgf_test.tbl
COLLOID_S1$INP         ./Input/sum_panel_st_ccgf_t1_s1.tbl
COLLOID_S2$INP         ./Input/sum_panel_st_ccgf_t1_s2.tbl
NUTS_S1$INP            ./Input/sum_nut_ccgf_t1_s1.tbl
NUTS_S2_100$INP        ./Input/sum_nut_ccgf_t1_s2_t100.tbl
NUTS_S2_350$INP        ./Input/sum_nut_ccgf_t1_s2_t350.tbl
NUTS_S3_1000$INP       ./Input/sum_nut_ccgf_t1_s3_t1000.tbl
NUTS_S3_3000$INP       ./Input/sum_nut_ccgf_t1_s3_t3000.tbl
NUTS_S3_5000$INP       ./Input/sum_nut_ccgf_t1_s3_t5000.tbl
NUTS_S3_7000$INP       ./Input/sum_nut_ccgf_t1_s3_t7000.tbl
NUTS_S3_9000$INP       ./Input/sum_nut_ccgf_t1_s3_t9000.tbl
NUTS_S4_100$INP        ./Input/sum_nut_ccgf_t1_s4_t100.tbl
NUTS_S4_350$INP        ./Input/sum_nut_ccgf_t1_s4_t350.tbl
NUTS_S5_1000$INP       ./Input/sum_nut_ccgf_t1_s5_t1000.tbl
NUTS_S5_3000$INP       ./Input/sum_nut_ccgf_t1_s5_t3000.tbl
NUTS_S5_5000$INP       ./Input/sum_nut_ccgf_t1_s5_t5000.tbl
NUTS_S5_7000$INP       ./Input/sum_nut_ccgf_t1_s5_t7000.tbl
NUTS_S5_9000$INP       ./Input/sum_nut_ccgf_t1_s5_t9000.tbl
PNL_S6_100$INP         ./Input/sum_panel_int_ccgf_t1_s6_t00100.tbl
PNL_S6_350$INP         ./Input/sum_panel_int_ccgf_t1_s6_t00350.tbl
PNL_S6_1000$INP        ./Input/sum_panel_int_ccgf_t1_s6_t01000.tbl
PNL_S6_2000$INP        ./Input/sum_panel_int_ccgf_t1_s6_t02000.tbl
PNL_S6_4000$INP        ./Input/sum_panel_int_ccgf_t1_s6_t04000.tbl
PNL_S6_6000$INP        ./Input/sum_panel_int_ccgf_t1_s6_t06000.tbl
PNL_S6_9000$INP        ./Input/sum_panel_int_ccgf_t1_s6_t09000.tbl
ST2D1_FM$INP           ./Input/sum_st2d_ccgf_t1_c1_mf.tbl
ST2D1_PM$INP           ./Input/sum_st2d_ccgf_t1_c1_mp.tbl
ST2D2_FM$INP           ./Input/sum_st2d_ccgf_t1_c2_mf.tbl
ST2D2_PM$INP           ./Input/sum_st2d_ccgf_t1_c2_mp.tbl
```

Figure 1. Example Map File

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3.2.1.2 Intrusion Times File

The intrusion times file is a text file containing an ordered list of times used to construct interpolated time series of direct brine releases (DBRs) and spallings for scenarios S2 through S5 (interpolation times for scenario S1 are hardwired, and the S6 scenario uses times for the S3 scenario). The intrusion times file is specified by the command line keyword "-times". The file INTRUSIONTIMES.IN should contain the data shown in Figure 2. The file contains seven groups of times, and times increase within each group to 10,000 years.

```
100.
300.
500.
1000.
2000.
3000.
4000.
10000.
350.
550.
750.
2000.
4000.
10000.
1000.
1200.
1400.
3000.
5000.
10000.
3000.
3200.
3400.
5000.
7000.
10000.
5000.
5200.
5400.
7000.
9000.
10000.
7500.
7700.
7900.
9000.
10000.
10000.
```

Figure 2. Example Intrusion Times File

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3.2.2 Release Data Input Files

There are four types of release data input files:

1. direct solids releases, created by the code CUTTINGS_S.
2. direct brine releases, created by the code SUMMARIZE.
3. Salado transport releases, created by the code SUMMARIZE.
4. Culebra transport releases, created by the code SUMMARIZE.

The content of each type of release data input file is described in the following sections.

Release data files created by SUMMARIZE contain a common three-line header. The first line contains three numbers:

- the number of vectors in the file
- the number of different times for the data
- the number of columns of data excluding vector and time.

The second line contains text labels for each column of data, and the third line indicates the CAMDAT variable type (H for History, G for Global, P for Property) for each column listed in the second line. The three line header is followed by a blank line. The subroutine OPENSUMMARIZEFILE reads this header.

For PRECCDFGF Version 2.00 or later, the formats of release data files differ from the formats of files for earlier versions of PRECCDFGF. SUMMARIZE Version 3.01 and later has a driver, the PRECCDFGF driver, to format SUMMARIZE output files for PRECCDFGF Version 2.00 or later.

3.2.2.1 Direct Solids Releases

For each replicate, PRECCDFGF Version 3.01 requires one direct solids release data file assigned to the logical name SPALL$INP. The file contains three header lines, followed by a block of data.

The first header line contains three integer values:

1. the number of scenarios (5 for regulatory calculations)
2. the number of vectors (100 for regulatory calculations)
3. the number of cavities; i.e., regions in the BRAGFLO grid containing waste.

PRECCDFGF Version 3.01 requires 4 cavities. If a different number of cavities is indicated in the CUTTINGS_S input file, PRECCDFGF will produce an error message and abort the run.

The second header line contains five integer values that are the number of intrusion times for scenarios S1 through S5, in order.

The third header line contains seven text values that describe the seven columns in the data block.

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The data block contains seven columns:

1. Scenario number (integer)
2. Cavity identifier (character; e.g., L, M, U, O)
3. Intrusion time (float) in years
4. Vector number (integer)
5. Borehole diameter (float) in meters
6. Cuttings and cavings area (float) in square meters
7. Spallings volume (float) in cubic meters.

Lines in the data block are enumerated by vector, intrusion time, cavity then scenario. An example of the first 10 lines of the data block is shown in Figure 3.

```
     5      8      4
     6      5      5      5      5
SCN CAV     TIME         VEC     DRILDIAM       AREA_C         VOL_S
  1 L     1.00000E+02     1   3.111500E-01   1.000000E-01   0.000000E+00
  1 L     1.00000E+02     2   3.111500E-01   2.000000E-01   0.000000E+00
  1 L     1.00000E+02     3   3.111500E-01   0.000000E+00   1.000000E-02
  1 L     1.00000E+02     4   3.111500E-01   0.000000E+00   0.000000E+00
  1 L     1.00000E+02     5   3.111500E-01   0.000000E+00   0.000000E+00
  1 L     1.00000E+02     6   3.111500E-01   0.000000E+00   0.000000E+00
  1 L     1.00000E+02     7   3.111500E-01   0.000000E+00   0.000000E+00
```

Figure 3. Example of a Direct Solid Release File

3.2.2.2 Direct Brine Releases

Release data files for direct brine releases (DBRs) are created by the code SUMMARIZE. For each replicate, PRECCDFGF Version 3.01 requires a total of 104 direct brine release files assigned to the logical names listed in Table 3-1. Running PRECCDFGF with fewer input files will result in an error message and a failed code execution.

Table 3-1. Logical Names for Direct Brine Release Data Files

Logical Name	Cavity	Intrusion time
DBR_S1_*P*_T*tttt*$INP	*P* = L, M, U, O	*tttt* = 100, 350, 1000, 3000, 5000, 10000
DBR_S2_*P*_T*tttt*$INP	*P* = L, M, U, O	*tttt* = 550, 750, 2000, 4000, 10000
DBR_S3_*P*_T*tttt*$INP	*P* = L, M, U, O	*tttt* = 1200, 1400, 3000, 5000, 10000
DBR_S4_*P*_T*tttt*$INP	*P* = L, M, U, O	*tttt* = 550, 750, 2000, 4000, 10000
DBR_S5_*P*_T*tttt*$INP	*P* = L, M, U, O	*tttt* = 1200, 1400, 3000, 5000, 10000

PRECCDFGF allows for single or multiple panel brine volumes to be considered in the calculation of direct brine releases. The number of panel brine volumes is specified on the command line using the command line keyword '-nbrine'.

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Each DBR input file has a header as described in Section 3.2.2. Figure 4 contains an example of the header for a DBR input file.

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

```
       8         1         2
vector time          BRIN_REL       PNLBRVOL
                     [H]            [H]

 1.000000E+00  1.369905E-01  0.000000E+00  2.000000E+03
 2.000000E+00  1.369905E-01  0.000000E+00  2.000000E+03
 3.000000E+00  1.369905E-01  0.000000E+00  2.000000E+03
 4.000000E+00  1.369905E-01  1.000000E-02  1.000000E+02
 5.000000E+00  1.369905E-01  0.000000E+00  2.000000E+03
 6.000000E+00  1.369905E-01  0.000000E+00  2.000000E+03
 7.000000E+00  1.369905E-01  0.000000E+00  2.000000E+03
 8.000000E+00  1.369905E-01  1.000000E-02  1.000000E+02
```

Figure 4. Example of a DBR file

3.2.2.3 Salado Transport Releases

PRECCDFGF uses two sets of data files for Salado transport releases. One set of data files is generated by running SUMMARIZE on the output of the NUTS code for scenarios S1 though S5. The second set is 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 3-2. Each file contains a three line header, followed by one blank line, as described in Section 3.2.2. Figure 5 and Figure 6 contain examples of the header of a file in each set.

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Table 3-2. File Names for Salado Transport Release Data Files

Logical Name	Intrusion time
NUTS_S1$INP	N/A
NUTS_S2_*ttt*$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

Each file contains one block of data for each vector; blocks are separated by one text line. In each block are seven columns, 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 after the intrusion. The third through sixth columns contain the mass of radionuclide (in Curies) transported through the Salado to the Culebra (dissolved or sorbed to colloids) during each time interval for four radionuclides: Am241, Pu239, U234, and Th230. In the files containing NUTS results, the seventh column contains the concentration of EPA units transported through the Salado to the Culebra during each time interval. In the files containing PANEL results, 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 transport release data files.

Figure 5. Example of a Header for a Salado Transport File from NUTS

```
       8      199        5
vector time         A00AM241      A00PU239      A00U234       A00TH230      EPALWMBT
                    [G]           [G]           [G]           [G]           [G]
```

Figure 6. Example of a Header for a Salado Transport File from PANEL

```
       8      199        5
vector time         LDCAM241      LDCPU239      LDCU234       LDCTH230      SDCPB210
                    [H]           [H]           [H]           [H]           [H]
```

3.2.2.4 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. PRECCDFGF allows for single or multiple Culebra release points to be considered in the calculation of Culebra releases. The number of Culebra release points is specified on the command line using the command line keyword '-crp'. If no value is provided at run time, PRECCDFGF assumes a default value of one.

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For each Culebra release point, PRECCDFGF expects two Culebra transport release files assigned to the logical names ST2D*c*_PM$INP and ST2D*c*_FM$INP, where *c* represents the release point number, for the partial mining and full mining cases, respectively.

The Culebra transport release input files contain a header as described in Section 3.2.2. Figure 7 shows an example of the header for these files.

Each file contains one block of data for each vector; blocks are separated by one text line. 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 after the intrusion. The third, fourth, fifth, and seventh columns contain the amount (as a fraction of 1 kg) of each of four dissolved radionuclides (Am241, Pu239, U234 and Th230, in that order) 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 between 0 and 50 years. The sixth column, labeled MT2TH230, 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 between 0 and 50 years.

Figure 7. Example of a Header for a Culebra Transport Release File

```
       8      200        5
vector time        MT2AM241      MT2PU239      MT2U234       MT2TH230      MT2TH23A
                   [H]           [H]           [H]           [H]           [H]
```

3.2.3 Inventory Data Files

PRECCDFGF reads four files containing inventory data: one file for contact-handled (CH) waste, one file for remote-handled (RH) waste, and two files for mobilized radionuclides, either dissolved or sorbed to colloids, in Castile and Salado brines, respectively.

3.2.3.1 Contact-Handled Waste Streams

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 lines, then reads the number of CH waste streams and the number of decay times from the fifth and sixth lines, starting in column 13 of the EPAUNI output file.

PRECCDFGF skips six more 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 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.

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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.

3.2.3.2 Remote-Handled Waste Streams

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.

3.2.3.3 Mobilized Radionuclides

Mobilized radionuclides are either dissolved or sorbed to colloids. The concentration of mobilized radionuclides is used to calculate 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 in Salado and Castile brines, assigned to the logicals PNL_CON_S1$INP and PNL_CON_S2$INP, respectively. 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. In Scenarios S4 and S5 (E2 intrusions) mobilized radionuclide concentrations are equal to those for Scenario S1 (E0 conditions), and in Scenario S3 and S6 (E1 intrusion and E1E2 intrusion, respectively) mobilized radionuclide concentrations are equal to those for Scenario S2 (E1 intrusion.)

Each mobilized radionuclide file contains a header as described in Section 3.2.2. Figure 8 shows an example of the header for these files.

Each file contains one block of data for each vector; blocks are separated by a single text line. Each block of data contains seven columns and nine rows of data, one row for each of the following times: 100, 125, 175, 350, 1000, 3000, 5000, 7500, and 10000 years. 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.

Figure 8. Example of a Header for a Radionuclide Concentration File

```
        8         9         5
vector time          CLEAM241        CLEPU239        CLEU234         CLETH230        CNETOTAL
                     [H]             [H]             [H]             [H]             [H]
```

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3.2.3.4 Colloidal Mobilization

Releases to the Culebra are provided to PRECCDFGF in the Salado transport data files. These releases are reported as the total mass (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 a colloidal mobilization fraction data file assigned to each of the logicals COLLOID_S1$INP and COLLOID_S2$INP in the map file (Section 3.2.1.1).

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.)

The colloidal mobilization fraction input files have three header rows followed by four blank lines and then a data block. Figure 9 contains the header for these files; the headers are used to identify the data that appears in the data block. The first line of the header contains three integers: the number of vectors, an unused flag, and the number of data columns in the data block. The second line contains column headings and the third line records the CDB variable from which the data originate.

The data block contains 14 columns, with one row for each vector. The first column is the vector and the second column is the time in years. 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.

Figure 9. Example of a Header for a Colliod Mobilization File

```
       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]
```

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3.2.4 Parameter Data Input Files

3.2.4.1 Sampled Parameter Values

PRECCDFGF requires one sampled parameter, GLOBAL:PBRINE, which is the probability that a drilling intrusion encounters a brine pocket below the repository. PRECCDFGF reads a set of CDB files, one for each vector, that are generated by the code POSTLHS. If the GLOBAL:PBRINE parameter is not found in the CDB file, PRECCDFGF will produce an error message and abort the run. PRECCDFGF requires that a template for the names of these files be entered in a command line argument using the keyword "-lhs". For example, a valid template is "`ccgf1_lhs_test_v###.cdb`" where "`###`" is a placeholder for the vector numbers.

3.2.4.2 Constant Parameter Values

PRECCDFGF Version 3.01 requires constant parameter values obtained from the WIPP PA Parameter Database (PAPDB). PRECCDFGF reads these parameters from an input file in the CDB format produced by the code MATSET. Table 3-3 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. If a required parameter is not found in the CDB file, PRECCDFGF will produce an error and abort the run.

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Table 3-3. 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

3.3 Output File

PRECCDFGF generates a single ASCII file containing the parameter values and the release information consolidated from the various input files for input to the CCDFGF code. This file is referred to as the release table file, or the RELTAB file.

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

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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 the number of Culebra release points per vector.

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. The RELTAB file produced with PRECCDFGF Version 3.00 and above is only compatible with CCDFGF Version 8.00 and above (Brunell, 2022a).

3.3.1.1 Sampled Parameters Section

The RELTAB file lists the values of sampled parameters for each vector. In Version 3.01, the only sampled parameter is the probability of a drilling intrusion encountering a brine pocket below the repository.

3.3.1.2 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 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 (m^2) 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 (m^2) of a drilling intrusion into CH waste with cavings included. PRECCDFGF uses the drill diameter (m) 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 waste stream 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.

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3.3.1.3 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 (L), middle (M), upper (U), and other (O) 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.

The E1 and E2 intrusion blocks contain three 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.

3.3.1.4 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.

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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.

3.3.1.5 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.

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 and each intrusion scenario.

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.

3.3.1.6 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.

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The remainder of the Culebra transport data section is repeated for each vector. The first line designates the culebra release point number and the text CULEBRA RELEASE POINT. Next, 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. These data are repeated for each Culebra release point designated at run time.

4.0 MODELS AND METHODS

PRECCDFGF serves to collate the numerous output files from other WIPP PA codes into a single release table file (RELTAB file) that can be used by CCDFGF. PRECCDFGF collates the output from the following WIPP PA codes:

- BRAGFLO (for DBR release volumes)
- CUTTINGS_S (for cuttings, cavings, and spallings release volumes)
- NUTS (for Salado transport and releases to the Culebra)
- PANEL (for radionuclide concentrations in solution and for releases to the Culebra)
- SECOTP2D (for radionuclide transport through the Culebra)
- EPAUNI (for radionuclide concentrations in solid materials)

With the exceptions of EPAUNI and CUTTINGS_S, PRECCDFGF reads the output of the code SUMMARIZE after SUMMARIZE extracts the appropriate interpolated values from the output of each WIPP PA code. PRECCDFGF reads the output of EPAUNI and CUTTINGS_S directly.

PRECCDFGF reads a set of CDB files to obtain sampled values for the PBRINE parameter. Typically, these CDB files are created by using the POSTLHS code. If the PBRINE parameter is not present in any of the set of CDB files, PRECCDFGF stops execution.

PRECCDFGF reads one CDB file to obtain constant parameter values. Typically, this CDB file is created by using MATSET or a combination of MATSET and POSTLHS. If a parameter is not present in the CDB file, PRECCDFGF stops execution.

PRECCDFGF calculates each radionuclide's decay constant (yr^{-1}) and specific activity (Ci/kg). PRECCDFGF also computes the repository scale CH waste concentration (EPA units/m^3) for use in spalling releases. PRECCDFGF does not perform any other calculations on the data it reads.

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5.0 CONTROL FLOW AND LOGIC

PRECCDFGF executes a fixed sequence of major subroutines to read control information, read input data and write the RELTAB. The major subroutines are (in order):

1. CDBINIT – reads command line arguments.
2. ReadControlParameters – contructs logical variable names for mobilized radionuclide files (Section 3.2.3.3) and colloid mobilization files (Section 3.2.3.4).
3. MapFiles – reads the map file
4. LoadDataFromDatabase – reads the constant parameter values (Section 3.2.4.2).
5. CreateRad – calculates decay constant and specific activity for radionuclides Am241, Pu239, U234 and Th230 from input data.
6. PRECUT – reads inventory files (Section 3.2.3) and direct solid release files (Section 3.2.2.1).
7. PREBS – reads direct brine release files (Section 3.2.2.2).
8. PRENUT – reads Salado transport files (Section 3.2.2.3).
9. PRESEC – reads Culebra transport files (Section 3.2.2.4).
10. RELTAB – writes the release table (RELTAB) file (Section 3.3).

5.1 Data Structures

PRECCDFGF uses standard FORTRAN data types for all variables. To group radionuclide properties by radionuclide, PRECCDFGF defines one derived data type, Radionuclide, that contains a pointer to any daughter species.

5.2 Allowable/Prescribed Ranges for Input and Output

PRECCDFGF requires that the headers of the release data files match the format described in Section 3.2.2. PRECCDFGF requires each release data file's header to have the same number of vectors as provided on the command line (see Section 8.0). 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.

Variable names and types that appear in the headers of release data input files must match hardwired values, as indicated in Figure 3, Figure 4, Figure 5, Figure 6, Figure 7, Figure 8 and Figure 9.
Logical variable names must be those listed in the example map file (Figure 1). Logical variable names include specific scenarios (S1 through S6), panel group (L, M, U, O) and intrusion times (integer preceding $INP). PRECCDFGF Version 3.01 requires the specific values shown by logical variable names in the example map file.

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6.0 REQUIRED USER TRAINING AND/OR BACKGROUND

In order to run and interpret the results of the PRECCDFGF code successfully, the user will need a basic knowledge of Sandia's CAMDAT database.

Users should be familiar with the purpose and output from of the following WIPP PA codes, as used in WIPP PA: BRAGFLO, CUTTINGS_S, PANEL, NUTS, SECOTP2D, and EPAUNI. Users should understand how to use the code SUMMARIZE to obtain interpolated output listing from these WIPP PA codes. Users should be familiar with the codes MATSET and POSTLHS and should understand how to use these codes to obtain parameter values from the WIPP PA Parameter Database (PAPDB).

7.0 CAPABILITIES AND LIMITATIONS

PRECCDFGF requires all of the various input files to be properly formatted and to contain data as described in each file's header. The lack of data in an input file will cause PRECCDFGF to cease execution with errors.

The radionuclides expected in the input data are fixed: Am241, Pu239, U234 and Th230.

For the S1 scenario, the intrusion times for DBR and spallings releases are fixed in the source code at 100, 350, 1000, 3000, 5000 and 1000 years. The intrusion times for other scenarios are also fixed in the sense that the intrusion times are embedded in the logical variable names (Figure 1) which are fixed in the source code. The three panel groups (denoted by L, M, U, and O) are fixed in the same manner.

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8.0 USER INTERACTIONS WITH THE SOFTWARE

PRECCDFGF Version 3.01 executes on a Solaris platform. To execute PRECCDFGF, the program executable name (preccdfgf) must be in the user's current PATH or referenced by its path name.

PRECCDFGF 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 "–"; they 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.

PRECCDFGF expects the following command line arguments:

1. –input The name of the input CAMDAT file containing constant parameter values from the PAPDB.

2. –nvec The number of vectors for which the input files contain data. The default is 100 for this optional argument.

3. –tend The time period in years to be calculated by CCDFGF. The default is 10000 for this optional argument.

4. –nbrine The number of brine volumes to be used to assemble direct brine release data. The default is 1.

5. -crp The number of Culebra release points to be used to assemble Culebra transport data. The default value is 1.

6. –lhs The template for the names of the set of CAMDAT files that contain the sampled value for the probability of hitting a brine pocket. The template must contain "###", which will be replaced with the three-digit vector number 001 to the number of vectors supplied in the "–nvec" argument. For example, "lhs3_ccgf_CRA14BL_r1_v###.cdb", where ### would be replaced with 001 .. 100.

7. –map The name of the map file.

8. –times The name of the text file listing the times for which direct brine release (DBR) and spallings release volumes will be interpolated.

9. –output The name of the output release table (RELTAB).

10. –error The name of the text file to contain the error log.

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9.0 ERROR MESSAGES

PRECCDFGF Version 3.01 checks for a limited number of errors in the input data. Error-checking is not comprehensive. PRECCDFGF Version 3.01 may produce the following error messages:

`Incorrect file assignments`

Subroutine: CDBINIT

Occurs when an error results from reading command line inputs.

`Error with number of vectors`

Subroutine: CDBINIT

Occurs when an invalid value is provided on the command line as the value of '-nvec'

`Error with time period`

Subroutine: CDBINIT

Occurs when an invalid value is provided on the command line as the value of '-tend'

`Error with number of Culebra release points`

Subroutine: CDBINIT

Occurs when an invalid value is provided on the command line as the value of '-crp'

`Error with number of brine volumes`

Subroutine: CDBINIT

Occurs when an invalid value is provided on the command line as the value of '-nbrine'

`LHS Template file <filename> does not contain ### as required.`

Subroutine: CDBINIT

Occurs when the placeholder text "###" is not found in the template for LHS file names provided on the command line as the value of '-lhs'.

`Error closing CDB file`

Subroutine: CloseCDB

Occurs if an error occurs when closing any CDB file.

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`Could not get CDB size info`

Function: DBVALUE

Occurs if an error occurs when reading sizes from any CDB file.

`IN DBIELBK`

Function: DBVALUE

Occurs if an error occurs when reading element block names and numbers from any CDB file.

`OVER 50 PROPERTIES IN DBVALUE`

Function: DBVALUE

Occurs if more than 50 property names are found in any CDB file.

`ERROR LOADING VALUE FROM DATABASE`

Function: DBVALUE

Occurs if specified parameter name is not found in a CDB file.

`PROBLEM OPENING LHS CDB`

Function: LoadLHSRecord

Occurs if an LHS CDB file cannot be opened.

`Number of realizations, <N> in <fName> doesn't match the expected <nObs> Execution stopped.`

Function: nTimesAndObs

Occurs the number of vectors <N> read from file <fName> doesn't match the number of vectors input on the command line <nObs>.

`Reading <fName> expected <nTimes> times but found <nT>.`

Function: nTimesAndObs

Occurs the number of times <nT> read from file <fName> doesn't match the number of expected times <nTimes>.

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```
Error opening <fName> Execution stopped.
```

Function: nTimesAndObs

Occurs if <fName> could not be opened.

```
Unexpected end-of-file in <fName> Execution stopped.
```

Function: nTimesAndObs

Occurs if the header record could not be read from <fName>.

```
Error in spallings input file header:
    <Spall_in>
    <NTimes>    <NVectors>    <NCavities>
```

Function: OpenSpallings

Occurs if the header record from spallings file <Spall_in> has any of these errors:

- <Ntimes> is not equal to 5
- <NVectors> is not equal to <nObs> which is input on the command line
- <NCavities> is not equal to 3

```
Error in spallings input file header:
    Number of subsequent times: <values appear here>
    Expected: 6 5 5 5 5'
```

Function: OpenSpallings

Occurs if the second line of the header record from spallings file <Spall_in> contains other than the expected values.

```
Error in spallings input file header:
    Expected SCN, CAV, TIME, VEC, DRILDIAM, AREA_C, VOL_S
    But found <values appear here>
```

Function: OpenSpallings

Occurs if the third line of the header record from spallings file <Spall_in> contains other than the expected values.

```
The number of fields, <nF> does not match the number of variables
expected, <nvariables> in <FileName>
```

Subroutine: OpenSummarizeFile

Occurs if the number of columns in a SUMMARIZE file does not match the number read from the file's header.

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```
Error in input file header for <FileName>
    Expected <VariableName> : <VariableType> but found <Name> <Type>
```

Subroutine: OpenSummarizeFile

Occurs if the variable names and type in the header in a SUMMARIZE file do not match the expected values.

```
The number of observations in the file <colloid_in> (<nRealFrac>)
does not equal the expected <NOBS>
```

Subroutine: PRENUT

Occurs if the number of vectors in a colloidal mobilization file does not match the number of vectors specified in the command line input.

```
The number of observations in the file <colloid_in> (<nRealFrac>)
does not equal the expected <NOBS>
```

Subroutine: PRENUT

Occurs if the number of vectors in the colloidal mobilization file for the S1 scenario does not match the number of vectors in the colloidal mobilization file for the S2 scenario.

```
Time <TIME> not equal to <time>
```

Subroutine: PRENUT

Occurs if a formatting or other error in the data in a Salado transport release file causes misalignment of times read from the file.

```
DBR times are not in order
```

Subroutine: RWBLW

Occurs if times within a time group in the Intrusion times file are not increasing.

```
DBR release table does not span potential intrusion times
```

Subroutine: RWBLW

Occurs if the first or last time in INTRUSIONTIMES.IN is outside the range from the end of active institutional controls (parameter GLOBAL/TA) to the end of the regulatory period (10,000 years)

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`End-of-File reading unit <unit>. Execution Aborted.`

Subroutine: Skip

Can occur for multiple I/O units. SKIP is a generic subroutine that moves the current record pointer forward a specified number of records. This error occurs if the end of file is encountered before moving the specified number of records.

10.0 REFERENCES

Brunell, S. 2022a. Design Document and User's Manual for CCDFGF Version 8.01. Sandia National Laboratories. Carlsbad, NM. ERMS 577625.

Brunell, S. 2022b. Requirements Document, Verification and Validation Plan, and Validation Document for PRECCDFGF Version 3.01. Sandia National Laboratories. Carlsbad, NM. ERMS 577630.

Long, J. J. 2020. Nuclear Waste Management Procedure NP 19-1 Software Requirements, Revision 19. Sandia National Laboratories. Carlsbad, NM. ERMS 573707.

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