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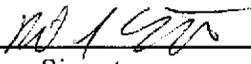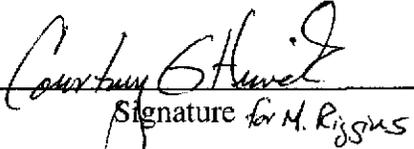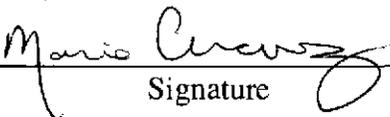# Sandia National Laboratories
Waste Isolation Pilot Plant

Impact Analysis of Decreased Duration of Direct Brine Release in WIPP Performance Assessment

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WIPP:1.4.1.2:PA:QA-L:PKG545750

Table of Contents

Tables

Figures

Information Only

1 Introduction

This report presents the results of an impact analysis conducted as described in AP-131, "Analysis Plan for the Modification of the Waste Shear Strength and Direct Brine Release Parameters," (Kirkes and Herrick 2006). Specifically, this report responds to activities 5 and 6 of Table 1 in AP-131 (reproduced below). Note that activities 1 through 4 are complete and have been documented in Kirkes (2007). The results of activities 1 through 4 recommend a new value for the maximum duration of a direct brine release (DBR), as represented in the input parameter "MAXFLOW." Therefore, this analysis compares and documents DBR calculations using the new MAXFLOW parameter with current baseline DBR calculations.

Table 1: Task list and estimated schedule for DBR changes (Modified from Kirkes and Herrick 2006).

Task	Description
1	Request new data from WRES (Update of Leonard, 1996)
2	Re-evaluate supporting documentation in parameter records package 231034 for DBR MINFLOW and MAXFLOW
3	Document results of information review for DBR in Parameter Justification Report
4	Implement NP 9-2 for MINFLOW and MAXFLOW
5	Perform impact analysis using DBR_BRAGFLO
6	Document results of DBR_BRAGFLO impact analysis in final analysis report

2 Background for the Duration of DBRs

DBRs are releases of contaminated brine originating in the repository and flowing up an intrusion borehole during the period of drilling. In order for a DBR to occur, two criteria must be met (Stoelzel and O'Brien 1996).

1. Volume averaged pressure in the vicinity of the repository encountered by drilling must exceed drilling mud hydrostatic pressure (assumed to be 8 megapascals [MPa]).

2. Brine saturation in the repository must exceed the residual saturation of the waste material (sampled from a uniform distribution ranging from 0.0 to 0.552).

If both of these criteria are met, DBR is calculated using the code BRAGFLO with a two dimensional, semi-horizontally oriented grid, which represents the vicinity of the waste panels. If either of these conditions is not satisfied, no DBR is calculated (Stein et al. 2005). The current model is constrained to flow for at least 3 days (represented in BRAGFLO as the parameter MINFLOW), or for as long as 11 days (represented in BRAGFLO as the parameter MAXFLOW), if conditions within the model support continued flow.

3 Recommended Maximum Durations for DBRs

Based on analyses presented in Kirkes (2007), the newly recommended value for the maximum duration of a DBR (MAXFLOW parameter) is 4.5 days. This new value is based on a review of historic data, new data, and interviews with drilling personnel in the area (Kirkes 2007). This

Information Only

value is justified according to NP 9-2, "*Parameters.*" The updated value for the MAXFLOW parameter is more consistent with drilling data and current drilling practices.

4   Comparison of Releases using New Value for MAXFLOW

To determine the effects and impacts of using a MAXFLOW parameter value of 4.5 days, BRAGFLO_DBR calculations using the new value have been conducted and compared to the most recent approved baseline calculations, the Performance Assessment Baseline Calculations (PABC). Calculations have been constructed such that only the parameter MAXFLOW is varied from those of the PABC. The sequence of calculations as well as the input and output files are described in Appendix A. These results are compared to those presented in the "Analysis Package for Direct Brine Releases: Compliance Recertification Application – 2004 PABC" (Stein et al. 2005).

Five scenarios or repository states (S1-S5) are considered in the BRAGFLO_DBR modeling for the WIPP PA. These scenarios are the same that were used for the PABC. The scenarios include one undisturbed scenario (S1) and four scenarios with a single drilling intrusion into the repository (S2-S5). Two types of intrusion are modeled; an E1 intrusion, which assumes the borehole passes through both a waste panel and a pressurized brine pocket under the repository, and an E2 intrusion, which assumes the borehole only passes through the waste panel. Scenarios S2 and S4 model the effect of an E1 and E2 intrusion at 350 years, respectively, while scenarios S3 and S5 model the effect of an E1 and E2 intrusion at 1,000 years, respectively.

The scenarios indicate the state of the repository when the intrusion occurs. The initial conditions, such as waste panel pressure and saturation are used in the DBR calculations and are based on the state of the repository. For example, scenario S1 calculations use the pressure and saturation values of an undisturbed repository, while scenario S2 calculations assume the repository had a previous E1 intrusion at 350 years and use the associated pressure and saturation values. The S1 scenario calculates the DBR due to the first intrusion into the repository, while scenarios S2-S5 calculate the DBR due to the second intrusion into the repository. The results from the S2-S5 scenarios are also used for the third, fourth, etc. intrusion into the repository.

Each analysis generated 7,800 separate results for all the vector-scenario-time-drilling location combinations. To compare the results, some summary statistics for each analysis are compared and grouped by scenario. Table 2 shows the number of non-zero DBR volumes for the AP-131 and PABC analyses. For consistency with the PABC analysis, non-zero DBR volumes are defined as volumes that are greater than 10^{-7} m^3. As seen in Table 2, there are no differences between the number of non-zero DBR volumes between the AP-131 and PABC analyses for any of the scenarios. This is due to the fact that the parameter MAXFLOW is not a used as criteria to determine if there is a DBR, but rather is used in the calculation of the volume of the DBR.

Table 3 shows the maximum DBR volumes from the AP-131 and PABC analyses. There was no change in the maximum DBR volumes for scenarios S1, S4 and S5 for the AP-131 analysis from the PABC, as the corresponding vectors used in the minimum DBR duration (3 days) and so the change in the maximum DBR duration had no effect. For scenarios S2 and S3 the maximum DBR volumes decreased to ~60% of the PABC values for the AP-131 analysis. The maximum remained in scenario S2 for both analyses.

Table 4 shows that the average DBR volumes for the AP-131 and PABC analyses. As seen in Table 4, the average DBR volume decreased ~15% from the PABC to the AP-131 analysis in all scenarios.

Table 2: Number of non-zero DBR volumes calculated by scenario for the AP-131 and PABC analyses.

Scenario	AP-131	PABC
S1	57	57
S2	357	357
S3	237	237
S4	27	27
S5	43	43
Total	721	721

Table 3: Maximum DBR volumes (in m^3) calculated by scenario for the AP-131 and PABC analyses.

Scenario	AP-131	PABC
S1	18.0	18.0
S2	41.5	68.9
S3	36.5	64.0
S4	14.1	14.1
S5	14.1	14.1
Maximum	41.5	68.9

Table 4: Average DBR volumes (in m^3) calculated by scenario for the AP-131 and PABC analyses.

Scenario	AP-131	PABC
S1	0.014	0.017
S2	2.53	3.00
S3	1.30	1.60
S4	0.012	0.014
S5	0.013	0.015

Part of the DBR analysis includes addressing the sensitivity of the DBR volume to input parameters. Sensitivity analyses determined that waste pressure is one of the most important variables that controlled DBR volumes (Helton et al. 1998). For this impact assessment, the sensitivity of the DBR volumes to the waste pressure is analyzed by generating a scatter plot of pressure versus DBR volumes.

The scatter plot of pressure in the intruded panel versus DBR volume for the S2 scenario, lower intrusion for AP-131 analysis is shown in Figure 1. The analogous plot from the PABC analysis (Stein et al. 2005) is shown in Figure 2. Both figures show that there are no calculated volumes until pressures exceed 8 MPa as indicated by the vertical line in the figures.
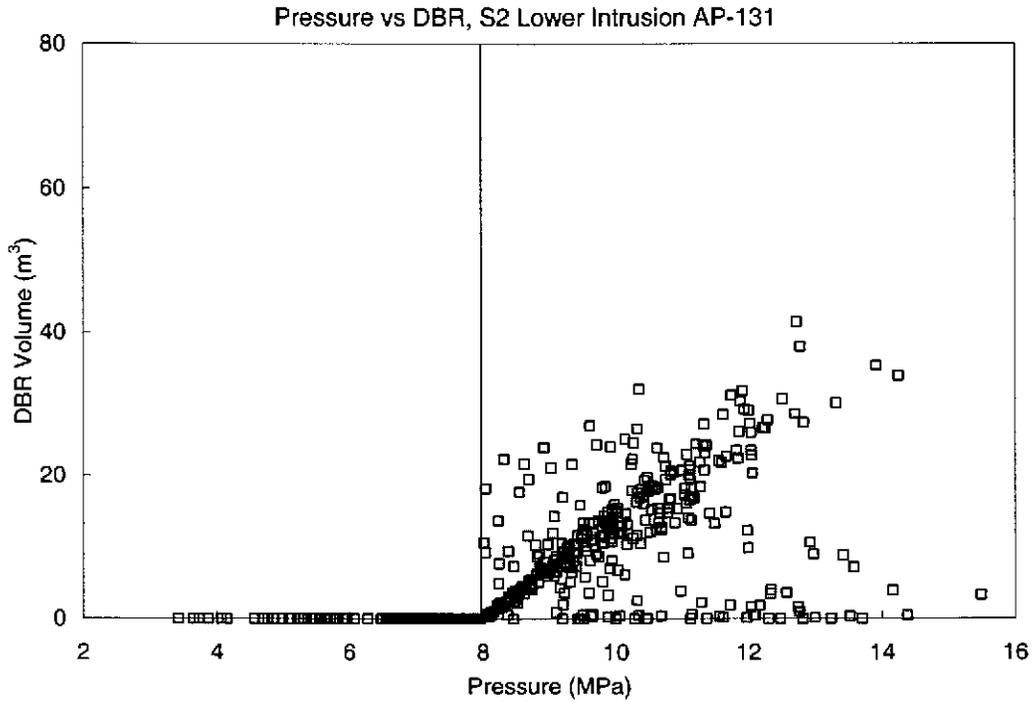
Figure 1: Scatter plot of pressure in the intruded panel vs. direct brine release volume for the S2 scenario, lower intrusion AP-131 analysis.
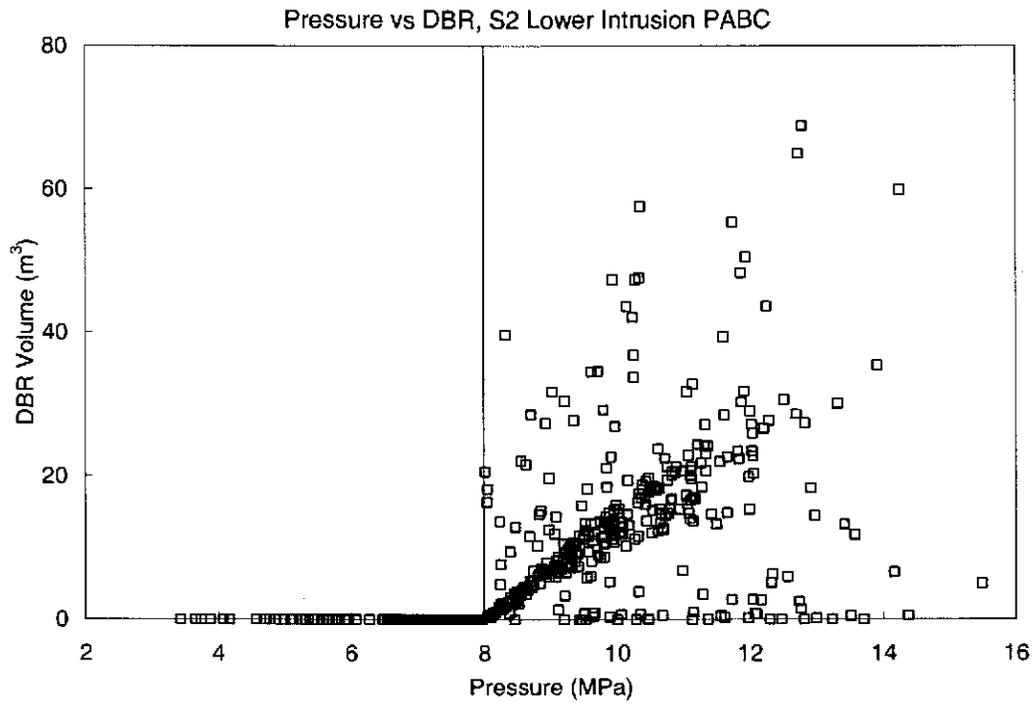

Figure 2: Scatter plot of pressure in the intruded panel vs. direct brine release volume for the S2 scenario, lower intrusion PABC analysis.

Comparison of Figure 1 to Figure 2 shows that the decrease in the parameter MAXFLOW decreased the DBR volume at all pressures for the higher DBR volumes. Figure 2 shows many vector-scenario-time-drilling location combinations with calculated volumes greater than 40 m^3, which have all significantly reduced, as seen in Figure 1.

Both analyses show a high concentration of results that are near a line extending from 0 m^3 and 8 MPa to 30 m^3 and 12 MPa. This correlation does not appear to vary with time as values from the five different times are all present in this area. The decrease in the parameter MAXFLOW does not appear to have affected the relationship between the DBR volume and pressure from the PABC analysis, as the same high concentration of results are present in both Figure 1 and Figure 2.

Using the DBR results for AP-131, a complementary cumulative distribution function (CCDF) of the DBRs was generated. The sequence of calculations as well as the input and output files are described in Appendix A. The DBR CCDF for AP-131 is then compared with the DBR CCDF for the PABC (Vugrin and Dunagan 2005) and both are shown in Figure 3. As seen in Figure 3, the two CCDFs are similar. Reducing the parameter MAXFLOW slightly decreases the DBR CCDF for all probabilities. This is consistent with the summary statistics presented above. As the number of non-zero DBR volumes is the same between the AP-131 and PABC analysis, the probability of the DBR CCDF should not change between the two analyses. The maximum and average DBR volumes decreased for the AP-131 analysis, which correlates with the small decrease in the AP-131 DBR CCDF compared with the PABC DBR CCDF.
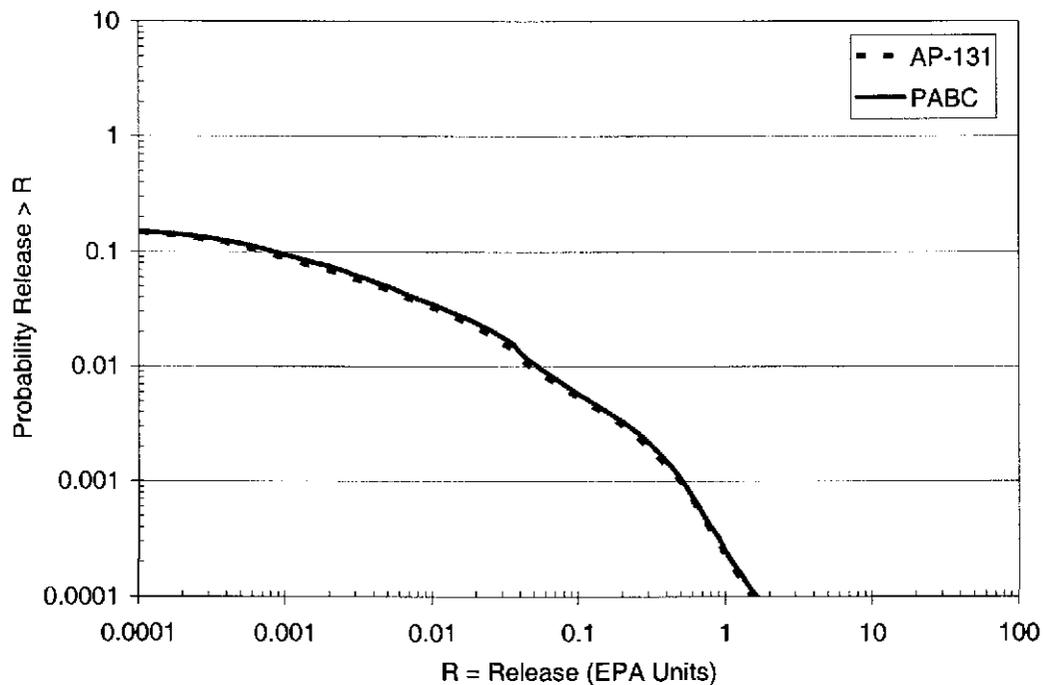
Figure 3: DBR CCDF for the AP-131 and PABC analyses.

5   Conclusion

An impact analysis was conducted using the newly recommended value for the maximum duration of a DBR (MAXFLOW parameter) of 4.5 days. This new value is based on a review of historic data, new data, and interviews with drilling personnel in the area (Kirkes 2007). The updated value for the MAXFLOW parameter is more consistent with drilling data and current drilling practices.

The analysis shows that there are no changes incurred for the number of non-zero DBR volumes by changing the MAXFLOW parameter, while the maximum and average DBR volumes decreased. Reducing the parameter MAXFLOW slightly decreases the DBR CCDF for all probabilities. Although minimal changes result from using the updated MAXFLOW parameter, its inclusion is still necessary to be consistent with current drilling data and practices.

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Appendix A

The calculation flow used for the AP-131 calculation is similar to that used for PABC (Kanney and Leigh 2005), except the calculation flow is significantly reduced to only incorporate the codes used for DBR calculations. All other input and output files that were used are the same as were used for the PABC. The calculation flow for AP-131 is discussed below.

SINGLE-INTRUSION DIRECT BRINE RELEASE CALCULATIONS (BRAGFLO_DBR)

Single-intrusion direct brine release volumes are calculated using the BRAGFLO suite of codes (PREBRAG, BRAGFLO, POSTBRAG), in conjunction with several utility codes. The steps, the codes run in each step, and the DCL script(s) used to perform the step are shown in Table A.1.

The calculations include five scenarios (S1-S5). A number of intrusion times are considered for each scenario. For each intrusion time, intrusions into three locations (lower, middle and upper) are modeled. See Stein et al. (2005) for a detailed discussion of the drilling locations. A set of 100 vectors is run for each scenario/intrusion time/intrusion location combination. One replicate was performed. For this calculation only ALGEBRACDB of step 3 was run.

Table A.1: Direct Brine Release Run Control Scripts

Step	Codes in Step	Script(s)	Script CMS Library	Script CMS Class
1	GENMESH MATSET	EVAL_DBR_STEP1.COM	NA	NA
2	ALGEBRACDB RELATE ICSET	EVAL_DBR_STEP2.COM SUB_DBR_STEP2.COM	NA	NA
3	PREBRAG BRAGFLO POSTBRAG ALGEBRACDB	EVAL_DBR_STEP3.COM SUB_DBR_STEP3.COM	LIBAP131_EVAL	AP131-0

DIRECT BRINE RELEASE STEP 3

Step 3 usually runs PREBRAG, BRAGFLO, POSTBRAG, and ALGEBRACDB (ALG3). However, for this calculation only ALGEBRACDB (ALG3) was run. The Step 3 script is invoked for each scenario. The script loops over the appropriate intrusion times for the scenario. For each intrusion time, the script loops over all three intrusion locations. For each intrusion location, the script loops over all 100 vectors. The ALGEBRACDB sequence is run for each scenario/intrusion time/intrusion location/vector combination. The input and log files for the Step 3 script as well as the input and output files for ALGEBRACDB are shown in Table A.2.

Table A.2: Direct Brine Release Step 3 Input and Output Files

	File Names[1,2,3,4]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_DBR_AP131_STEP3_R1_S*s*.INP	LIBAP131_EVAL	AP131-0
Log	EVAL_DBR_AP131_STEP3_R1_S*s*.LOG	LIBAP131_DBRR1S*s*	AP131-0
ALGEBRACDB			
Input	ALG3_DBR_AP131.INP	LIBAP131_DBR	AP131-0
Input	BF3_DBR_CRA1BC_R1_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBCRA1BC_DBRR1S*s*	CRA1BC-0
Output	ALG3_DBR_AP131_R1_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBAP131_DBRR1S*s*	AP131-0
Output	ALG3_DBR_AP131_R1_S*s*_T*ttttt*_*c*_V*vvv*.DBG	NOT KEPT	NOT KEPT

1. $s \in \{1, 2, 3, 4, 5\}$

2. $ttttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} & \text{for S1} \\ \{00550, 00750, 02000, 04000, 10000\} & \text{for S2, S4} \\ \{01200, 01400, 03000, 05000, 10000\} & \text{for S3, S5} \end{cases}$

3. $c \in \{L, M, U\}$ for each intrusion time, $ttttt$

4. $vvv \in \{001, 002, ..., 100\}$ for each c

CCDF INPUT TABULATION (SUMMARIZE)

The output CDB files from the various process model codes are combined into text tables by the SUMMARIZE code, for subsequent use in calculating releases to the accessible environment. The type of data extracted from each process model is described in the PRECCDFGF Design Document (WIPP PA 2005) and in Kanney and Kirchner (2005). The run control scripts used to process the CDB data for the various process models are shown in Table A.3. A single run control script is used to extract data from CDB files for all process model codes. The script performs the following steps:

- Fetch the required CDB files
- Write an input control file for SUMMARIZE by filling in items in an input control file template
- Run SUMMARIZE on the collection of CDB files

A small utility script is used to submit the main script to a batch queue.

Table A.3: CCDF Input Tabulation Run Control Scripts

Code	Script	Script CMS Library	Script CMS Class
SUMMARIZE	EVAL_SUM.COM SUB_SUM.COM	LIBAP131_EVAL	AP131-0

CCDF INPUT TABULATION (DIRECT BRINE RELEASE)

SUMMARIZE is used to extract and tabulate direct brine release volume data from the appropriate post-BRAGFLO_DBR ALGEBRACDB output CDB files.

The run control script is invoked for scenarios S1 through S5. The script loops over the appropriate intrusion times for each scenario. There is a single SUMMARIZE input control file template, which the script uses to generate a SUMMARIZE input control file for each scenario/intrusion time/intrusion location combination. The script input and log files along with the SUMMARIZE input and output files are shown in Table A.4.

Table A.4: CCDF Input Tabulation Input and Output Files (Direct Brine Release)

	File Names[1,2,3,4]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_SUM_DBR_AP131_R1_Ss.INP	LIBAP131_EVAL	AP131-0
Input	SUM_DBR_CRA1BC.TMPL	LIBCRA1BC_SUM	AP131-0
Output	SUM_DBR_AP131_R1_Ss_T$ttttt$_c.INP	LIBAP131_SUM	AP131-0
Log	EVAL_SUM_DBR_AP131_R1_Ss.LOG	LIBAP131_SUM	AP131-0
SUMMARIZE			
Input	SUM_DBR_AP131_R1_Ss_T$ttttt$_c.INP	LIBAP131_SUM	AP131-0
Input	ALG3_DBR_AP131_R1_Ss_T$ttttt$_c_Vvvv.CDB	LIBAP131_DBRR1Ss	AP131-0
Output	SUM_DBR_AP131_R1_Ss_T$ttttt$_c.TBL	LIBAP131_SUM	AP131-0
Output	SUM_DBR_AP131_R1_Ss_T$ttttt$_c.DBG	LIBAP131_SUM	AP131-0

1. $s \in \{1, 2, 3, 4, 5\}$

2. $ttttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} \text{ for S1} \\ \{00550, 00750, 02000, 04000, 10000\} \text{ for S2 and S4} \\ \{01200, 01400, 03000, 05000, 10000\} \text{ for S3 and S5} \end{cases}$

3. $c \in \{L, M, U\}$ for each intrusion time, $ttttt$

4. $vvv \in \{001, 002, ..., 100\}$ for each c

CCDF CONSTRUCTION (PRECCDFGF, CCDFGF)

The complimentary cumulative distribution functions (CCDFs) for radionuclide releases to the accessible environment are constructed using the PRECCDFGF/CCDFGF code suite. The calculations are separated into several steps according to the number of times a particular code is run and to allow for timely inspection of intermediate results. The steps, the codes run in each step, and the DCL script(s) used to perform the steps are shown in Table A.5.

Table A.5: CCDF Construction Run Control Scripts

Step	Codes in Step	Scripts	CMS Library	CMS Class
1	GENMESH MATSET	EVAL_CCGF_STEP1.COM	LIBAP131_EVAL	AP131-0
2	POSTLHS	EVAL_CCGF_STEP2.COM	LIBAP131_EVAL	AP131-0
3	PRECCDFGF CCDFGF	EVAL_CCGF_STEP3.COM	LIBAP131_EVAL	AP131-0

CCDF CONSTRUCTION STEP 1

Step 1 uses GENMESH and MATSET codes to generate the computational grid and assign material properties to element blocks. Step 1 is run once. The input and log files for the script as well as the input and output files for GENMESH and MATSET and are shown in Table A.6.

Table A.6: CCDF Construction Step 1 Input and Output Files

	File Names	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CCGF_AP131_STEP1.INP	LIBAP131_EVAL	AP131-0
Script Log	EVAL_CCGF_AP131_STEP1.LOG	LIBAP131_CCGF	AP131-0
GENMESH			
Input	GM_CCGF_CRA1BC.INP	LIBCRA1BC_CCGF	AP131-0
Output	GM_CCGF_AP131.CDB	LIBAP131_CCGF	AP131-0
Output	GM_CCGF_AP131.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_CCGF_CRA1BC.INP	LIBCRA1BC_CCGF	AP131-0
Input	GM_CCGF_AP131.CDB	LIBAP131_CCGF	AP131-0
Output	MS_CCGF_AP131.CDB	LIBAP131_CCGF	AP131-0
Output	MS_CCGF_AP131.DBG	NOT KEPT	NOT KEPT

CCDF CONSTRUCTION STEP 2

Step 2 uses POSTLHS to assign the sampled parameter values used by CCDFGF to the appropriate materials and element block properties. Step 2 is run once. POSTLHS loops over all 100 vectors in the replicate. The input and log files for the script as well as the input and output files for POSTLHS are shown in Table A.7.

Table A.7: CCDF Construction Step 2 Input and Output Files

	File Names[1]	CMS Library	CMS Class
STEP 2			
Script Input	EVAL_CCGF_AP131_STEP2_R1.INP	LIBAP131_EVAL	AP131-0
Script Log	EVAL_CCGF_AP131_STEP2_R1.LOG	LIBAP131_CCGF	AP131-0
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA1BC_LHS	AP131-0
Input	LHS2_CRA1BC_R1.TRN	LIBCRA1BC_LHS	AP131-0
Input	MS_CCGF_AP131.CDB	LIBAP131_CCGF	AP131-0
Output	LHS3_CCGF_AP131_R1_V*vvv*.CDB	LIBAP131_CCGF	AP131-0
Output	LHS3_CCGF_AP131_R1.DBG	LIBAP131_CCGF	AP131-0

1. $vvv \in \{001, 002, ..., 100\}$

CCDF CONSTRUCTION STEP 3

Step 3 uses PRECCDFGF to organize and format output from all of the process model codes for use by CCDFGF (i.e. builds the release table file), then runs CCDFGF to compute the CCDFs. Step 3 is run once. The script loops over the appropriate scenarios and/or intrusions and/or waste types to fetch the large number of data files that are input to PRECCDFGF. The input and log files for the script as well as the input and output files for PRECCDFGF are shown in Table A.8.

Table A.8: CCDF Construction Step 3 Input and Output Files

	File Names[1-6]	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CCGF_STEP3_AP131_R1.INP	LIBAP131_EVAL	AP131-0
Script Log	EVAL_CCGF_STEP3_AP131_R1.LOG	LIBAP131_CCGF	AP131-0
PRECCDFGF			
Input	INTRUSIONTIMES.IN	LIBCRA1BC_CCGF	AP131-0
Input	MS_CCGF_AP131.CDB	LIBAP131_CCGF	AP131-0
Input	LHS3_CCGF_AP131_R1_Vvvv.CDB	LIBAP131_CCGF	AP131-0
Input	SUM_DBR_AP131_R1_Ss_T$ttttt$_c.TBL	LIBAP131_SUM	AP131-0
Input	CUSP_CRA1BC_R1.TBL	LIBCRA1BC_CUSP	AP131-0
Input	SUM_NUT_CRA1BC_R1_S1.TBL	LIBCRA1BC_SUM	AP131-0
Input	SUM_NUT_CRA1BC_R1_Ss_T$ttttt$.TBL	LIBCRA1BC_SUM	AP131-0
Input	SUM_PANEL_INT_CRA1BC_R1_S6_T$ttttt$.TBL	LIBCRA1BC_SUM	AP131-0
Input	SUM_ST2D_CRA1BC_R1_Mm.TBL	LIBCRA1BC_SUM	AP131-0
Input	EPU_CRA1BC_hH.DAT	LIBCRA1BC_EPU	AP131-0
Input	SUM_PANEL_CON_CRA1BC_R1_Ss.TBL	LIBCRA1BC_SUM	AP131-0
Input	SUM_PANEL_ST_CRA1BC_R1_Ss.TBL	LIBCRA1BC_SUM	AP131-0
Output	CCGF_AP131_RELTAB_R1.DAT	LIBAP131_CCGF	AP131-0
CCDFGF			
Input	CCGF_CRA1BC_CONTROL_R1.INP	LIBCRA1BC_CCGF	AP131-0
Input	CCGF_AP131_RELTAB_R1.DAT	LIBAP131_CCGF	AP131-0
Output	CCGF_AP131_R1.OUT	LIBAP131_CCGF	AP131-0
Output	CCGF_AP131_R1.DBG	NOT KEPT	NOT KEPT

1. $vvv \in \{001, 002, ..., 100\}$

2. $s \in \begin{cases} \{1, 2, 3, 4, 5\} \text{ for SUM\_DBR} \\ \{2, 3, 4, 5\} \text{ for SUM\_NUT} \\ \{1, 2\} \text{ for SUM\_PANEL\_CON and SUM\_PANEL\_ST} \end{cases}$

3. $ttttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} \text{ for S1 for SUM\_DBR} \\ \{00550, 07500, 02000, 04000, 10000\} \text{ for S2, S4 for SUM\_DBR} \\ \{01200, 01400, 03000, 05000, 10000\} \text{ for S3, S5 for SUM\_DBR} \\ \{00100, 00350\} \text{ for S2, S4 for SUM\_NUT} \\ \{01000, 03000, 05000, 07000, 09000\} \text{ for S3, S5 for SUM\_NUT} \\ \{00100, 00350, 01000, 02000, 04000, 06000, 09000\} \text{ for SUM\_PANEL\_INT} \end{cases}$
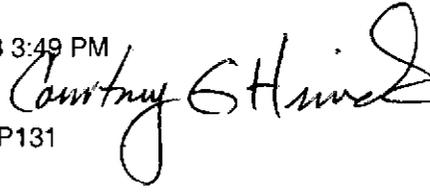
4. $c \in \{L, M, U\}$ for each intrusion time, $ttttt$ for SUM_DBR

5. $m \in \{F, P\}$

6. $h \in \{C, R\}$

From:	Riggins, Michael
Sent:	Monday, March 03, 2008 3:49 PM
To:	Herrick, Courtney Grant
Cc:	Clayton, Daniel James
Subject:	Signature authority for AP131

Importance: High

Courtney,

I give signature authority to Courtney Herrick for documents pertaining to

AP 131 - Impact Analysis of Decreased Duration of Direct Brine Release in WIPP Performance Assessment

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