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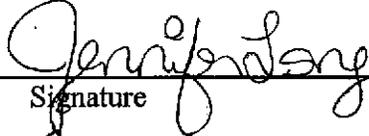
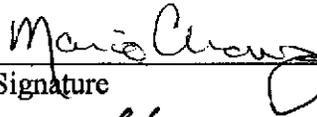
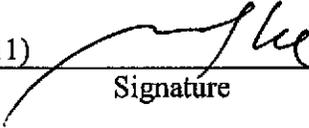
**Sandia National Laboratories  
Carlsbad Programs Group**

**Waste Isolation Pilot Plant**

**Execution of Performance Assessment Codes  
for the  
2009 Compliance Recertification Application Performance Assessment**

**Revision 0**

**Task Number 1.2.5**

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# 1 INTRODUCTION

The Waste Isolation Pilot Plant (WIPP) is a deep geologic repository developed by the U.S. Department of Energy (DOE) for the disposal of transuranic (TRU) radioactive waste. Containment of TRU waste at the WIPP is regulated by the U.S. Environmental Protection Agency (EPA) according to the regulations set forth in Title 40 of the Code of Federal Regulations (CFR), Parts 191 (U.S. DOE, 2004) and 194 (EPA 1998). The DOE demonstrates compliance with the containment requirements in the regulations by means of a performance assessment (PA) that estimates releases from the repository for the regulatory period of 10,000 years after facility closure.

This report documents the hardware, software, access control and run control systems as well as the procedures used to perform the WIPP 2009 Compliance Recertification Application Performance Assessment Baseline Calculation (CRA-2009 PA).

The CRA-2009 PA work reported here was conducted under the Analysis Plan for the 2009 Compliance Recertification Application Performance Assessment Rev. 0 (AP-137, Clayton 2007). The inventory comparison task was revised to include more detail which resulted in the Analysis Plan for the 2009 Compliance Recertification Application Performance Assessment Rev.1 (AP-137, Clayton 2008). There is no impact on run control and so this document is valid for both revisions.

## 1.1 BACKGROUND

PA calculations were included in DOE's 1996 WIPP Compliance Certification Application (CCA, DOE 1996), and in a subsequent Performance Assessment Verification Test (PAVT, MacKinnon and Freeze 1997a, 1997b, 1997c). Based in part on the CCA and PAVT PA calculations, the EPA certified that the WIPP met the containment criteria in the regulations and was approved for disposal of transuranic waste in May 1998 (EPA 1998). PA calculations were also an integral part of DOE's 2004 WIPP Compliance Recertification Application (CRA-2004, DOE 2004). During their review of the CRA-2004, the EPA requested an additional performance assessment calculation be conducted with modified assumptions and parameter values (Cotsworth 2005). This PA is referred to as the WIPP 2004 Compliance Recertification Application Performance Assessment Baseline Calculation (CRA-2004 PABC, Leigh et al. 2005a). With the EPA's recertification decision in 2006, the CRA-2004 PABC was established as the PA baseline. Continued review of the CRA-2004 PABC has shown that a number of technical changes and corrections are necessary. Furthermore, updates to parameters and improvements to the PA computer codes have been developed since the recertification.

The Land Withdrawal Act (U.S. Congress 1992) requires that the DOE apply for recertification every five years from the first receipt of waste. Thus, the DOE is required to submit no later than March 2009. The results of the analysis described herein will be included in the 2009 Compliance Recertification Application (CRA-2009) to demonstrate compliance with the containment requirements according to the Certification Criteria in Title 40 CFR Part 194.

The changes from the CRA-2004 PABC that will be implemented in the CRA-2009 PA can be grouped into three areas which include:

1. Modification and improvements to:
  - a. the parameter representing the maximum flow duration for DBRs
  - b. the sampling method applied to the humid and inundated CPR degradation rates
  - c. include additional chemistry parameters
  - d. capillary pressure and relative permeability models
  - e. computer codes used in the PA.
2. Update of the drilling rate (GLOBAL:LAMBDAD) as required by Title 40 CFR 194.15.
3. Error corrections:
  - a. to account for cellulose, plastic and rubber (CPR) contents in emplacement materials in the inventory
  - b. to halite/disturbed rock zone porosity parameters
  - c. to the fraction of repository volume occupied by waste
  - d. to the input files for the direct brine release (DBR) calculations and the NUTS code.

It is expected that all of the changes do not significantly impact releases and are minor, but need to be incorporated for completeness and correctness. The results of the CRA-2009 PA will be used to show the impacts.

In general, three replicates are performed for most types of calculations (i.e., those process models which explicitly account for uncertainty). Each replicate typically includes several scenarios designed to cover an appropriate range of conditions. For calculations designed to model the consequences of drilling intrusions, multiple intrusion times and/or drilling locations are included in several scenarios. For a given replicate/scenario or replicate/scenario/intrusion time or replicate/scenario/intrusion time/intrusion location combination, calculations are typically performed for 100 sets (vectors) of uncertain model parameters.

The CCDFs are constructed for each replicate/vector combination. CCDFs are constructed for several individual release mechanisms as well as for total releases.

## ***1.2 KEY PERSONNEL***

The Run Control Coordinator modified and maintained the scripts used to run WIPP PA codes, created and maintained the libraries used to archive calculation results, and performed the calculations. The run control team members are listed in Table 1.1.

**Table 1.1 CRA-2009 PA Run Control Team**

<b>Function</b>	<b>Personnel</b>
Performance Assessment Team Lead	Daniel Clayton
Run Control Coordinator	Jennifer Long
PA Parameter Database Administrator	Jennifer Long

The WIPP PA analysts were responsible for preparing input for the various WIPP PA codes and performing data analysis and interpretation of the calculation results. The PA analysts for the CRA-2009 PA are shown in Table 1.2.

**Table 1.2 CRA-2009 PA Analysts**

<b>Major WIPP PA Code(s)</b>	<b>Analyst(s)</b>
LHS	Tom Kirchner
BRAGFLO	Martin Nemer
NUTS	Ahmed Ismail
PANEL	James Garner
CUTTINGS_S	Ahmed Ismail
BRAGFLO DBR	Daniel Clayton
CCDFGF	Sean Dunagan

## 2 WIPP PA COMPUTING SYSTEMS

The CRA-2009 PA was performed using the WIPP PA Alpha Cluster. The WIPP PA Alpha Cluster consists of 8 Hewlett Packard (HP) AlphaServer nodes configured to share the same disk array (using Storage Area Network (SAN) technology for efficient disk utilization and data storage/management). This allows for highly distributed processing, while providing for integrated data access. The WIPP PA Alpha Cluster runs the OpenVMS operating system (Version 8.2). The node name and hardware description for the nodes used are provided in Table 2.1.

**Table 2.1 WIPP PA Alpha Cluster Nodes Used in CRA-2009 PA**

<b>Node</b>	<b>Hardware Type</b>	<b># of CPUs</b>	<b>CPU</b>	<b>Operating System</b>
TBB	HP AlphaServer ES47	4	Alpha EV7	Open VMS 8.2
TRS	HP AlphaServer ES47	4	Alpha EV7	Open VMS 8.2
GNR	HP AlphaServer ES47	4	Alpha EV7	Open VMS 8.2
MC5	HP AlphaServer ES47	4	Alpha EV7	Open VMS 8.2
CCR	HP AlphaServer ES45 Model 2	4	Alpha EV68	Open VMS 8.2
TDN	HP AlphaServer ES45 Model 2	4	Alpha EV68	Open VMS 8.2
BTO	HP AlphaServer ES45 Model 2	4	Alpha EV68	Open VMS 8.2
CSN	HP AlphaServer ES45 Model 2	4	Alpha EV68	Open VMS 8.2

### **3 WIPP PA SOFTWARE CONFIGURATION MANAGEMENT AND RUN CONTROL SYSTEMS**

The computer simulations that form the core of the CRA-2009 PA are made fully traceable and reproducible through three key elements: 1) An archive or library system for controlling, tracking changes, and monitoring user access for source code, executables, simulation input and output files; 2) a scripting tool that interacts with the library to fetch input files, execute codes, and store output files; and 3) an access control capability to allow only approved individuals to run official calculations and have write access to areas where official inputs and/or results are stored. The following sections briefly describe how these elements are implemented on the WIPP PA computing clusters. Additional information is available in Long (2002).

Most calculations performed on the WIPP PA Alpha Cluster can also take advantage of the WIPP PA Parameter Database (PAPDB) to control the use of key modeling parameters. The PAPDB is discussed in section 3.5.

#### **3.1 LIBRARIES**

An essential element of the run control system on the WIPP PA Alpha Cluster is the HP Code Management System (CMS) for OpenVMS. CMS is a library system originally designed for software development and maintenance. CMS stores files called elements in an online library, keeps track of changes made to these files, and monitors user access to the files. CMS was used in two ways in the CRA-2009 PA.

A Software Configuration Management System (SCMS) has been implemented on the WIPP PA Alpha Cluster using (CMS). The source code, build scripts, executables, and test files for WIPP PA software are archived in access-controlled CMS libraries.

CMS is also used in conjunction with run control scripts to archive input files and output files from WIPP PA calculations.

CMS Version 4.5-1 was used for the CRA-2009 PA. Consult the CMS User Guide ([http://h71000.www7.hp.com/doc/73FINAL/5822/5822\\_.htm](http://h71000.www7.hp.com/doc/73FINAL/5822/5822_.htm)) and the CMS User's Manual ([http://h71000.www7.hp.com/doc/73FINAL/5607/5607\\_.htm](http://h71000.www7.hp.com/doc/73FINAL/5607/5607_.htm)) for further information.

#### **3.2 RUN CONTROL SCRIPTS**

The execution of WIPP PA codes on the Alpha Cluster for regulatory calculations is orchestrated using a collection of Digital Command Language (DCL) scripts. The DCL run control scripts fetch all input files from access-controlled CMS libraries. Executables are handled in two ways: 1) the executable is fetched from an access-controlled CMS library; or 2) a copy residing in an access-

controlled directory is used. The run control scripts also store all important output files to access-controlled CMS libraries. The run control scripts read from input files that specify:

- Analysis ID (CRA09)
- Analysis directory
- Replicate, scenario, intrusion times, intrusion locations and vector information, as appropriate
- Names and locations of all codes (executables) used in the run
- Code input files and their storage location
- Code output files and their post-run destination
- Log file name and post-run disposition

All DCL scripts used in the CRA-2009 PA are stored in CMS library LIBCRA09\_EVAL. The scripts were modified and maintained by the Run Control Coordinator. All CMS elements in the EVAL library conform to a naming convention imposed by the PA Team Lead and the Run Control Coordinator.

Some DCL run control scripts finish very quickly. Others run for a very long time, so they are submitted to a batch queue on the Alpha Cluster. For these cases, a small DCL utility is used to submit the script to the batch queue. The submit utilities are mainly a convenience to save the Run Control Coordinator from having to type out the long and complicated submit commands.

In general, each type of calculation is separated into several steps according to the number of times a particular code is run (and to allow for timely inspection of intermediate results). For example, utility codes used to set up the mesh and assign material properties to element blocks are typically run once. Codes used to sample subjectively uncertain parameters and assign those parameters values to model parameters are typically run once per replicate. Process model codes are typically run once per replicate/scenario/vector combination or once per replicate/scenario/vector/intrusion time or once per replicate/scenario/vector/intrusion time/intrusion location combination.

### ***3.3 FILE NAMING CONVENTIONS***

The PA Team Lead and Run Control Coordinator attempted to embed as much meaningful information as possible in the names of files used during calculations, while still adhering to SCMS naming conventions. This was accomplished using a naming convention that provided the following information:

- The code associated with the file.
- The calculation type, e.g. BRAGFLO.
- An identifier indicating the file is part of the CRA09 calculations.
- The replicate number.
- The scenario number.

- The vector number, if applicable.
- The time intrusion value, if applicable.
- The intrusion location (upper, lower, or middle) used, if applicable.
- The mining type (full or partial) represented, if applicable.
- The file format or file type (input text, binary, .CDB, debug, etc.,)

Underscores (   ) are normally used to separate the distinct elements of identification embedded in a file name. The first item in the file name was typically used to designate which code is reading or creating the file. The PA code prefix, defined in the SCMS Plan (Long 2002) is used as the designator. In some cases, the second item specifies the code prefix that a generic code is being run to support. The next item in the file name designates the calculation type or code flow. Again, the prefix defined by the SCMS Plan is used for unique identification.

A file with the name GM\_BF\_CRA09.INP can be decoded as follows:

GM	The file is used by the GENMESH code.
BF	This file relates to the code BRAGFLO (BF) run stream.
CRA09	This is the calculation ID.
INP	This is a code input file.

Many files also include replicate, scenario, and vector references as follows:

R1	The replicate number associated with this calculation is "1".
S3	The scenario number associated with this calculation is "3".
V007	The vector number associated with this calculation is "007".

### ***3.4 ACCESS CONTROL***

The VMS operating system supports formal access control through access control lists (ACLs). The system administrator can use ACLs to restrict access to disks, directories, files, applications, libraries, or other resources.

On the WIPP PA Alpha Cluster, a special account (CCA\_MASTER) has been set up to perform official calculations. Only the Run Control Coordinators can access this account. All official calculations are run within an access-controlled working directory specific to the code being run. Only the CCA\_MASTER account can write to this working directory. In additions, only the CCA\_MASTER account can write to the CRA-2009 PA libraries.

### ***3.5 WIPP PA PARAMETER DATABASE***

The PAPDB contains data values, associated models, source information, usage, and additional information documenting parameter information. In addition to parameter management, the PAPDB allows certain WIPP PA codes (PRELHS and MATSET) to retrieve parameter data for use in the PA computational stream on the WIPP PA Alpha Cluster. PRELHS is used to retrieve parameter data for subjectively uncertain (sampled) parameters (e.g., range, mean, distribution, etc.). MATSET is used mainly to retrieve values for constant parameters; however, it also retrieves the median values for parameters modeled with uncertainty distributions. See the PAPDB Design Document (WIPP PA 2001) and User's Manual (WIPP PA 2002) for more information. PAPDB Version 1.0 was used for the CRA-2009 PA.

Codes that access the PAPDB require that Digital Command Language (DCL) logicals for the database name, analysis name, computational code name, computational code version, retrieval number, and database password be set. These items are set by the run control script (and are specified in the run control script input file). The production PAPDB, "PARAMETER\_PROD", was used in the CRA-2009 PA.

It should be noted that the WIPP PA codes only retrieve parameter values from the PAPDB and have no capability to modify the database. Changes to the PAPDB are only made by the PAPDB Administrator in accordance with Nuclear Waste Management Procedure NP 9-2: Parameters (Chavez 2006b).

## 4 WIPP PA CODES

The major WIPP PA codes used in the CRA-2009 PA on the Alpha Cluster are shown in Table 4.1. These codes have been qualified under Nuclear Waste Management Procedure NP 19-1: Software Requirements (Chavez 2006c).

**Table 4.1 WIPP PA VMS Software Used in the CRA-2009 PA**

Code	Version	Executable	Build Date	CMS Library	CMS Class
ALGEBRACDB	2.35	ALGEBRACDB_PA96.EXE	31-01-96	LIBALG	PA96
BRAGFLO	6.00	BRAGFLO_QB0600.EXE	12-02-07	LIBBF	QB0600
PREBRAG	8.00	PREBRAG_QA0800.EXE	08-03-07	LIBBF	QA0800
POSTBRAG	4.00A	POSTBRAG_QA0400A.EXE	28-03-07	LIBBF	QA0400A
CCDFGF	5.02	CCDFGF_QB0502.EXE	13-12-04	LIBCCGF	QB0502
PRECCDFGF	1.01	PRECCDFGF_QA0101.EXE	07-07-05	LIBCCGF	QA0101
CCDFSUM	2.00	CCDFSUM_PA96_2.EXE	13-12-96	LIBCCGF	PA96_2
CUTTINGS S	6.02	CUTTINGS_S_QA0602.EXE	09-06-05	LIBCUSP	QA0602
GENMESH	6.08	GM_PA96.EXE	31-01-96	LIBGM	PA96
GROPECDB	2.12	GROPECDB_PA96.EXE	27-06-96	LIBGR	PA96
ICSET	2.22	ICSET_PA96.EXE	01-02-96	LIBIC	PA96
LHS	2.42	LHS_QA0242.EXE	18-01-05	LIBLHS	QA0242
PRELHS	2.30	PRELHS_QA0230.EXE	27-11-01	LIBLHS	QA0230
POSTLHS	4.07A	POSTLHS_QA0407A.EXE	25-04-05	LIBLHS	QA0407A
MATSET	9.10	MATSET_QA0910.EXE	29-11-01	LIBMS	QA0910
NUTS	2.05C	NUTS_QA0205C.EXE	24-05-06	LIBNUT	QA0205C
PANEL	4.03	PANEL_QA0403.EXE	25-04-05	LIBPANEL	QA0403
RELATE	1.43	RELATE_PA96.EXE	06-03-96	LIBREL	PA96
SUMMARIZE	3.01	SUMMARIZE_QB0301.EXE	21-12-05	LIBSUM	QB0301

In addition to the major codes referenced in Table 4.1, a couple of utility codes were qualified and used under Nuclear Waste Management Procedure NP 9-1: Analyses (Chavez 2006a). The VMS utility codes used on the WIPP PA Alpha Cluster are listed in Table 4.2, along with references to their storage location and to the appropriate section of this document.

**Table 4.2 VMS Utility Codes Used in the CRA-2009 PA**

Utility	Executable	CMS Library	CMS Class	Section
SCREEN	SCREEN.EXE	LIBCRA1BC_NUT	SCREEN_V1.0	5.4.1.2
LHS_EDIT	LHS_EDIT.EXE	LIBCRA09_LHS	LHS_EDIT_V1.0	5.1

## 5 CALCULATION FLOW

The following sections describe the calculation flow for the CRA-2009 PA. The codes run, code input and output file names and storage locations, scripts used, and script input and output file names and storage locations are covered. The discussion is organized according to the main groups of calculations and the codes that are used to perform them.

## 5.1 SAMPLING OF UNCERTAIN PARAMETERS (LHS)

Sampling of the uncertain parameters used by the various process model codes is performed with the PRELHS and LHS codes. PRELHS reads information about the ranges and distributions of the uncertain parameters from the PAPDB and formats this information for LHS. The LHS code implements the sampling algorithms. LHS is executed once per replicate (there are three replicates).

PRELHS and LHS are executed in sequence by the DCL script EVAL\_LHS.COM shown in Table 5.1. The input and output files for PRELHS and LHS, as well as the input and log files for the script are shown in Table 5.2.

**Table 5.1 Parameter Sampling Run Control Script**

Codes	Script	CMS Library	CMS Class
PRELHS, LHS	EVAL_LHS.COM	LIBCRA09_EVAL	CRA09-0

**Table 5.2 Parameter Sampling Input and Output Files**

	File Names <sup>1</sup>	CMS Library	CMS Class
<b>SCRIPT</b>			
Input	EVAL_LHS_CRA09_Rr.INP	LIBCRA09_EVAL	CRA09-0
Log	EVAL_LHS_CRA09_Rr.LOG	LIBCRA09_LHS	CRA09-0
<b>PRELHS</b>			
Input	LHS1_CRA09_Rr.INP	LIBCRA09_LHS	CRA09-0
Output	LHS1_CRA09_Rr.TRN	LIBCRA09_LHS	CRA09-0
Output	LHS1_CRA09_Rr.DBG	LIBCRA09_LHS	CRA09-0
<b>LHS</b>			
Input	LHS1_CRA09_Rr.TRN	LIBCRA09_LHS	CRA09-0
Output	LHS2_CRA09_Rr.TRN	LIBCRA09_LHS	CRA09-0
Output	LHS2_CRA09_Rr.DBG	LIBCRA09_LHS	CRA09-0
<b>LHS Edit</b>			
Input	LHS_CONTROL_Rr.INP	NOT KEPT	NOT KEPT
Input	LHS2_CRA09_Rr.TRN	LIBCRA09_LHS	CRA09-0
Output	LHS2_CRA09_Rr_CON.TRN	LIBCRA09_LHS	CRA09-0

1.  $r \in \{1,2,3\}$

## 5.2 SALADO FLOW CALCULATIONS (BRAGFLO)

Brine and gas flow in and around the repository and in overlying formations is calculated using the BRAGFLO suite of codes (PREBRAG, BRAGFLO, and POSTBRAG) in conjunction with several utility codes. The entire set of calculations is performed for three replicates. Each replicate includes six scenarios (S1-S6) designed to cover a range of drilling intrusion types and times, as shown in Table 5.3. For each replicate/scenario combination, calculations are performed for 100 vectors of uncertain model input parameters.

**Table 5.3 BRAGFLO Scenarios**

BRAGFLO Scenario	Description <sup>1,2</sup>
S1	Undisturbed
S2	E1 intrusion at 350 years
S3	E1 intrusion at 1000 years
S4	E2 intrusion at 350 years
S5	E2 intrusion at 1000 years
S6	E2 intrusion at 1000 years, E1 intrusion at 2000 years

1. E1 intrusion penetrates the repository and intersects a brine pocket in the underlying Castile Formation.
2. E2 intrusion penetrates the repository but does not encounter a Castile brine pocket

The brine and gas flow calculations are divided into several steps. The steps, the codes run in each step, and the DCL script(s) used to perform the step are shown in Table 5.4.

**Table 5.4 Salado Flow Run Control Scripts**

Step	Codes in Step	Script(s)	CMS Library	CMS Class
1	GENMESH MATSET	EVAL_GENERIC_STEP1.COM	LIBCRA09_EVAL	CRA09-0
2	POSTLHS	EVAL_GENERIC_STEP2.COM	LIBCRA09_EVAL	CRA09-0
3	ICSET ALGEBRACDB	EVAL_BF_STEP3.COM	LIBCRA09_EVAL	CRA09-0
4	PREBRAG	EVAL_BF_STEP4.COM	LIBCRA09_EVAL	CRA09-0
5	BRAGFLO POSTBRAG ALGEBRACDB	EVAL_BF_STEP5_MASTER.COM EVAL_BF_STEP5_SLAVE.COM	LIBCRA09_EVAL LIBCRA09_EVAL	CRA09-0 CRA09-0
6	ALGEBRACDB	EVAL_BF_STEP6.COM SUB_BF_STEP6.COM	LIBCRA09_EVAL LIBCRA09_EVAL	CRA09-0 CRA09-0

### 5.2.1 SALADO FLOW STEP 1

Step 1 uses GENMESH and MATSET to generate the computational grid and assign material properties to element blocks. Step 1 is run once. The input and log files for the Step 1 script as well as the input and output files for GENMESH and MATSET are shown in Table 5.5.

**Table 5.5 Salado Flow Step 1 Input and Output Files**

	File Names	CMS Library	CMS Class
<b>SCRIPT</b>			
Input	EVAL BF CRA09 STEP1.INP	LIBCRA09 EVAL	CRA09-0
Log	EVAL BF CRA09 STEP1.LOG	LIBCRA09 BF	CRA09-0
<b>GENMESH</b>			
Input	GM BF CRA09.INP	LIBCRA09 BF	CRA09-0
Output	GM BF CRA09.CDB	LIBCRA09 BF	CRA09-0
Output	GM BF CRA09.DBG	NOT KEPT	NOT KEPT
<b>MATSET</b>			
Input	MS BF CRA09.INP	LIBCRA09 BF	CRA09-0
Input	GM BF CRA09.CDB	LIBCRA09 BF	CRA09-0
Output	MS BF CRA09.CDB	LIBCRA09 BF	CRA09-0
Output	MS BF CRA09.DBG	NOT KEPT	NOT KEPT

### 5.2.2 SALADO FLOW STEP 2

Step 2 uses POSTLHS to assign the sampled parameter values used by BRAGFLO (generated by LHS, see Section 5.1) to the appropriate materials and element block properties. Step 2 is run once per replicate. POSTLHS loops over all 100 vectors in the replicate. The input and log files for the Step 2 script as well as the input and output files for POSTLHS are shown in Table 5.6.

**Table 5.6 Salado Flow Step 2 Input and Output Files**

	File Names <sup>1,2</sup>	CMS Library	CMS Class
<b>SCRIPT</b>			
Input	EVAL BF CRA09 STEP2 R <sub>r</sub> .INP	LIBCRA09 EVAL	CRA09-0
Log	EVAL BF CRA09 STEP2 R <sub>r</sub> .LOG	LIBCRA09 BF	CRA09-0
<b>POSTLHS</b>			
Input	LHS3 DUMMY.INP	LIBCRA09 LHS	CRA09-0
Input	LHS2 CRA09 R <sub>r</sub> CON.TRN	LIBCRA09 LHS	CRA09-0
Input	MS BF CRA09.CDB	LIBCRA09 BF	CRA09-0
Output	LHS3 BF CRA09 R <sub>r</sub> V <sub>vvv</sub> .CDB	LIBCRA09 BF	CRA09-0
Output	LHS3 BF CRA09 R <sub>r</sub> .DBG	LIBCRA09 BF	CRA09-0

1.  $r \in \{1, 2, 3\}$

2.  $vvv \in \{001, 002, \dots, 100\}$  for each  $r$

### 5.2.3 SALADO FLOW STEP 3

Step 3 assigns initial conditions with ICSET and performs some pre-processing of input data with ALGEBRACDB. Since ALGEBRACDB is used in multiple BRAGFLO steps, this use is referred to as ALG1. Step 3 is run once for each replicate. The script loops over all 100 vectors in the replicate. The input and log files for the Step 3 script as well as the input and output files for ICSET and ALGEBRACDB are shown in Table 5.7.

**Table 5.7 Salado Flow Step 3 Input and Output Files**

	File Names <sup>1,2</sup>	CMS Library	CMS Class
<b>SCRIPT</b>			
Input	EVAL BF CRA09 STEP3 R <sub>r</sub> .INP	LIBCRA09_EVAL	CRA09-0
Log	EVAL BF CRA09 STEP3 R <sub>r</sub> .LOG	LIBCRA09_BF	CRA09-0
<b>ICSET</b>			
Input	IC BF CRA09.INP	LIBCRA09_BF	CRA09-0
Input	LHS3 BF CRA09 R <sub>r</sub> V <sub>vvv</sub> .CDB	LIBCRA09_BF	CRA09-0
Output	IC BF CRA09 R <sub>r</sub> V <sub>vvv</sub> .CDB	LIBCRA09_BF	CRA09-0
Output	IC BF CRA09 R <sub>r</sub> V <sub>vvv</sub> .DBG	NOT KEPT	NOT KEPT
<b>ALGEBRACDB</b>			
Input	ALG1 BF CRA09.INP	LIBCRA09_BF	CRA09-0
Input	IC BF CRA09 R <sub>r</sub> V <sub>vvv</sub> .CDB	LIBCRA09_BF	CRA09-0
Output	ALG1 BF CRA09 R <sub>r</sub> V <sub>vvv</sub> .CDB	LIBCRA09_BF	CRA09-0
Output	ALG1 BF CRA09 R <sub>r</sub> V <sub>vvv</sub> .DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$

2.  $vvv \in \{001, 002, \dots, 100\}$  for each  $r$

### 5.2.4 SALADO FLOW STEP 4

Step 4 consists of running the pre-processing code PREBRAG. Step 4 is repeated for each replicate/scenario combination. The script loops over all 100 vectors in the replicate/scenario combination. The input and log files for the Step 4 script as well as the input and output files for PREBRAG are shown in Table 5.8.

**Table 5.8 Salado Flow Step 4 Input and Output Files**

	File Names <sup>1,2,3</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Script Input	EVAL BF CRA09 STEP4 R <sub>r</sub> S <sub>s</sub> .INP	LIBCRA09 EVAL	CRA09-0
Script Log	EVAL BF CRA09 STEP4 R <sub>r</sub> S <sub>s</sub> .LOG	LIBCRA09 BFR <sub>r</sub> S <sub>s</sub>	CRA09-0
<b>PREBRAG</b>			
Input	BF1 CRA09 S <sub>s</sub> .INP	LIBCRA09 BF	CRA09-0
Input	ALG1 BF CRA09 R <sub>r</sub> V <sub>vvv</sub> .CDB	LIBCRA09 BF	CRA09-0
Output	BF2 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .INP	LIBCRA09 BFR <sub>r</sub> S <sub>s</sub>	CRA09-0
Output	BF1 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{1, 2, 3, 4, 5, 6\}$  for each  $r$
3.  $vvv \in \{001, 002, \dots, 100\}$  for each  $s$

## 5.2.5 SALADO FLOW STEP 5

Step 5 runs BRAGFLO, POSTBRAG, and ALGEBRACDB (ALG2). This step has been separated from Step 4 to allow the analysts to edit/modify the BRAGFLO input file in cases where the generic numerical control parameters are not sufficient to obtain a converged solution.

In the paragraphs that follow, the procedure for the general case is described first and then the procedure followed to re-run certain replicate/scenario/vector combinations that were run with modified BRAGFLO input files due to convergence problems.

### 5.2.5.1 GENERAL CASE

Two DCL run control scripts are used in Step 5. The master script is invoked once for each replicate/scenario combination. The master script loops over all 100 vectors in the replicate/scenario combination. For each vector, the master script writes an input file for the slave script, and then calls the slave script with that input file to run BRAGFLO, POSTBRAG, and ALGEBRACDB. The input and log files for the Step 5 script as well as the input and output files for BRAGFLO, POSTBRAG, and ALGEBRACDB are shown in Table 5.9.

**Table 5.9 Salado Flow Step 5 Input and Output Files (Generic Case)**

	File Names <sup>1,2,3,4</sup>	CMS Library <sup>1,2,5</sup>	CMS Class
<b>MASTER SCRIPT</b>			
Input	EVAL BF CRA09 STEP5 R <sub>r</sub> S <sub>s</sub> .INP	LIBCRA09_EVAL	CRA09-0
Log	EVAL BF CRA09 STEP5 R <sub>r</sub> S <sub>s</sub> .LOG	LIBCRA09_BFR <sub>r</sub> S <sub>s</sub>	CRA09-0
<b>SLAVE SCRIPT</b>			
Log <sup>4</sup>	EVAL BF CRA09 STEP5 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .LOG	LIBCRA09_BFR <sub>r</sub> S <sub>s</sub>	CRA09-0
<b>BRAGFLO</b>			
Input	BF2 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .INP	LIBCRA09_BFR <sub>r</sub> S <sub>s</sub>	CRA09-0
Input	BF2 CRA1BC CLOSURE.DAT	LIBCRA1BC_BF	CRA09-0
Output	BF2 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .OUT	NOT KEPT	NOT KEPT
Output	BF2 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .SUM <sup>5</sup>	LIBCRA09_BF	CRA09-0
Output	BF2 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .BIN	NOT KEPT	NOT KEPT
Output	BF2 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .ROT	NOT KEPT	NOT KEPT
Output	BF2 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .RIN	NOT KEPT	NOT KEPT
<b>POSTBRAG</b>			
Input	BF2 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .BIN	NOT KEPT	NOT KEPT
Input	ALG1 BF CRA09 R <sub>r</sub> V <sub>vvv</sub> .CDB	LIBCRA09_BF	CRA09-0
Output	BF3 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .CDB	LIBCRA09_BFR <sub>r</sub> S <sub>s</sub>	CRA09-0
Output	BF3 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .DBG	NOT KEPT	NOT KEPT
<b>ALGEBRACDB</b>			
Input	ALG2 BF CRA09.INP	LIBCRA09_BF	CRA09-0
Input	BF3 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .CDB	LIBCRA09_BFR <sub>r</sub> S <sub>s</sub>	CRA09-0
Output	ALG2 BF CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .CDB	LIBCRA09_BFR <sub>r</sub> S <sub>s</sub>	CRA09-0
Output	ALG2 BF CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{1, 2, 3, 4, 5, 6\}$  for each  $r$
3.  $vvv \in \{001, 002, \dots, 100\}$  for each  $s$
4. The script inputs are echoed into the log file, so the input file is not kept
5. Due to an error in the master script input file, the \*.SUM output files for replicate R1 were placed in CMS library LIBCRA09\_BF instead of the library for the replicate/scenario combination. Note that output files for simulations reported in Table 5.10 (modified input runs) were archived in the correct libraries (LIBCRA09\_BFR<sub>r</sub>S<sub>s</sub>).

### 5.2.5.2 MODIFIED BRAGFLO INPUT CASE

In the few instances when BRAGFLO failed to converge using the generic numerical control parameters, a new BRAGFLO input file was submitted by the analysts and the case was re-run in a manner similar to that described above in Section 5.2.5.1. In order to track these cases a special tag

(“MOD”) was inserted into the BRAGFLO input file name, as well as the master script input file and log file names.

The replicate/scenario/vectors requiring modified BRAGFLO input files are shown in Table 5.10. The modified file names are shown in Table 5.11. All other files have the same names as for the generic case. Files in the libraries from the un-converged runs were replaced with files from the re-run.

**Table 5.10 Salado Flow Step 5 Modified Input Runs**

Replicate	Scenario	Vectors
R1	S1	28, 46
	S2	28, 46
	S3	22, 28, 46
	S4	22, 28, 46
	S5	28, 46
	S6	22, 28, 46
R2	S1	99
	S2	95
	S4	99
R3	S1	32
	S2	32, 71
	S3	35, 75
	S4	35
	S6	35

**Table 5.11 Salado Flow Step 5 Modified Input Runs File Names**

	File Names <sup>1,2,3</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>MASTER SCRIPT</b>			
Input	EVAL BF CRA09 STEP5 R <sub>r</sub> S <sub>s</sub> MOD.INP	LIBCRA09_EVAL	CRA09-0
Log	EVAL BF CRA09 STEP5 R <sub>r</sub> S <sub>s</sub> MOD.LOG	LIBCRA09_BFR <sub>r</sub> S <sub>s</sub>	CRA09-0
<b>BRAGFLO</b>			
Input	BF2 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> MOD.INP	LIBCRA09_BFR <sub>r</sub> S <sub>s</sub>	CRA09-0

1.  $r \in \{1, 2, 3\}$  as shown in Table 5.10
2.  $s \in \{1, 2, 3, 4, 5, 6\}$  as shown in Table 5.10
3. vectors as shown in Table 5.10

### 5.2.6 SALADO FLOW STEP 6

Step 6 runs ALGEBRACDB (ALG2). This step has been separated from Step 5 to allow for a rerun to correct a problem with the previous run of ALGEBRACDB (ALG2).

**Table 5.12 Salado Flow Step 6 Input and Output Files**

	File Names <sup>1,2,3</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>MASTER SCRIPT</b>			
Input	EVAL BF CRA09 STEP6 Rr.INP	LIBCRA09 EVAL	CRA09-0
Log	EVAL BF CRA09 STEP6 Rr.LOG	LIBCRA09 BFRrSs	CRA09-0
<b>ALGEBRACDB</b>			
Input	ALG2 BF CRA09.INP	LIBCRA09 BF	CRA09-0
Input	BF3 CRA09 Rr Ss Vvvv.CDB	LIBCRA09 BFRrSs	CRA09-0
Output	ALG2 BF CRA09 Rr Ss Vvvv.CDB	LIBCRA09 BFRrSs	CRA09-0
Output	ALG2 BF CRA09 Rr Ss Vvvv.DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{1, 2, 3, 4, 5, 6\}$  for each  $r$
3.  $vvv \in \{001, 002, \dots, 100\}$  for each  $s$

### 5.3 ACTINIDE MOBILIZATION CALCULATIONS (PANEL)

The PANEL code calculates the quantities of actinides mobilized by colloids and as dissolved species in WIPP brines. PANEL uses actinide solubilities from the parameter database which are derived from Fracture-Matrix Transport (FMT) results. As the CRA-2009 PA will use the same inventory as was used for the CRA-2004 PABC and no changes to the geochemistry conceptual model have been made, no FMT calculations will be performed for the CRA-2009 PA. The CRA-2009 PA will use the same actinide solubilities and uncertainties that were used in the CRA-2004 PABC. Consequently, the actinide mobilization calculations for the CRA-2009 PA will be identical to CRA-2004 PABC results since their conceptual models and parameters are not affected by any of the PA updates or corrections. The CRA-2004 PABC PANEL results are documented in Garner and Leigh (2005).

### 5.4 SALADO TRANSPORT CALCULATIONS (NUTS AND PANEL)

Radionuclide transport in the Salado for single intrusion conditions is calculated using the NUTS code. Salado transport for the E1E2 multiple intrusion condition is calculated using the PANEL code.

## 5.4.1 SALADO TRANSPORT CALCULATIONS (NUTS)

Radionuclide transport in the Salado for single intrusion conditions is calculated using the NUTS code. Three replicate calculations are performed. Five scenarios, corresponding to BRAGFLO scenarios S1-S5, are included in each replicate.

The steps, the codes run in each step, and the DCL script(s) used to perform the step are shown in Table 5.13. Corresponding to each run control script is a small utility used to submit the script to a batch queue.

**Table 5.13 Salado Transport (NUTS) Run Control Scripts**

Step	Codes Run in Step	Scripts	CMS Library	CMS Class
1	NUTS ALGEBRACDB	EVAL_NUT_STEP1.COM SUB_NUT_STEP1.COM	LIBCRA09_EVAL	CRA09-0
2	SUMMARIZE SCREEN	EVAL_NUT_STEP2.COM SUB_NUT_STEP2.COM	LIBCRA09_EVAL	CRA09-0
3	NUTS ALGEBRACDB	EVAL_NUT_STEP3.COM SUB_NUT_STEP3.COM	LIBCRA09_EVAL	CRA09-0
4	NUTS ALGEBRACDB	EVAL_NUT_STEP4.COM SUB_NUT_STEP4.COM	LIBCRA09_EVAL	CRA09-0

### 5.4.1.1 SALADO TRANSPORT (NUTS) –STEP 1 (NUTS\_SCN)

Step 1 invokes NUTS in “screening mode” (referred to here as NUTS\_SCN) to compute the transport of a conservative tracer for BRAGFLO scenarios S1-S5. Scenario S1 corresponds to undisturbed conditions. Scenario S2-S5 corresponds to single-intrusion conditions. Step 1 is run for each replicate for each of these scenarios. The script loops over all 100 vectors for each replicate/scenario combination. The input and log files for the script as well as the input and output files for NUTS\_SCN are shown in Table 5.14.

**Table 5.14 Salado Transport (NUTS) Step 1 Input and Output Files**

	File Names <sup>1,2,3</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Script Input	EVAL_NUT_CRA09_STEP1_Rr_Ss.INP	LIBCRA09_EVAL	CRA09-0
Script Log	EVAL_NUT_CRA09_STEP1_Rr_Ss.LOG	LIBCRA09_NUTRrSs	CRA09-0
<b>NUTS_SCN</b>			
Input	NUT_SCN_CRA09_Ss.INP	LIBCRA09_NUT	CRA09-0
Input	BF2_CRA09_Rr_Ss_Vvvv.INP	LIBCRA09_BFRrSs	CRA09-0
Input	BF3_CRA09_Rr_Ss_Vvvv.CDB	LIBCRA09_BFRrSs	CRA09-0
Output	NUT_SCN_CRA09_Rr_Ss_Vvvv.CDB	LIBCRA09_NUTRrSs	CRA09-0
Output	NUT_SCN_CRA09_Rr_Ss_Vvvv.DBG	NOT KEPT	NOT KEPT
<b>ALGEBRACDB</b>			
Input	ALG_NUT_SCN_CRA09.INP	LIBCRA09_NUT	CRA09-0
Input	NUT_SCN_CRA09_Rr_Ss_Vvvv.CDB	LIBCRA09_NUTRrSs	CRA09-0

Output	ALG_NUT_SCN_CRA09_Rr_Ss_Vvvv.CDB	LIBCRA09_NUTRrSs	CRA09-0
Output	ALG_NUT_SCN_CRA09_Rr_Ss_Vvvv.DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{1, 2, 3, 4, 5\}$  for each  $r$
3.  $vvv \in \{001, 002, \dots, 100\}$  for each  $s$

### 5.4.1.2 SALADO TRANSPORT (NUTS) –STEP 2 (SCREEN)

Step 2 uses the SUMMARIZE and SCREEN utilities to “screen-in” vectors for inclusion in the full transport simulations. Step 2 is run for each replicate for scenarios S1-S5. For each replicate/scenario combination, the script writes an input control file for SUMMARIZE (by filling in pieces of information in a control file template), then runs SUMMARIZE to tabulate transport of the conservative tracer at key locations. The script then runs the SCREEN utility on the SUMMARIZE table. The SCREEN utility output file lists vectors that are “screened-in” for use in the full transport simulations. The input and log files for the script as well as the input and output files for Step 2 are shown in Table 5.15. Lists of “screened-in” vectors for each replicate/scenario combination are shown in Table 5.16. One should note that for each replicate, a vector is automatically “screened in” for scenario S1 if it was “screened in” for any of scenarios S2-S5, regardless of the tracer transport results. This is done because the undisturbed simulation results are needed as initial conditions to compute the consequences of intrusions.

The SCREEN output files have two sections: UNION and NONUNION. The NONUNION section lists those vectors that have transport of the conservative tracer vector greater than the tolerance. The UNION section is used only in S1. For each replicate, if a vector is screened for S2-S5, it is automatically screened in for S1. It then gets listed in the UNION section for S1, along with any S1 vectors that were greater than the conservative tracer transport criteria (which are listed in the NONUNION section).

**Table 5.15 Salado Transport (NUTS) Step 2 Input and Output Files**

	File Names <sup>1,2,3</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Input	EVAL_NUT_CRA09_STEP2_Rr.INP	LIBCRA09_EVAL	CRA09-0
Input	SUM_NUT_SCN_CRA09.TMPL	LIBCRA09_NUT	CRA09-0
Output	SUM_NUT_SCN_CRA09_Rr_Ss.INP	LIBCRA09_NUTRrSs	CRA09-0
Log	EVAL_NUT_CRA09_STEP2_Rr.LOG	LIBCRA09_NUT	CRA09-0
<b>SUMMARIZE</b>			
Input	ALG_NUT_SCN_CRA09_Rr_Ss_Vvvv.CDB	LIBCRA09_NUTRrSs	CRA09-0
Input	SUM_NUT_SCN_CRA09_Rr_Ss.INP	LIBCRA09_NUTRrSs	CRA09-0
Output	SUM_NUT_SCN_CRA09_Rr_Ss.TBL	LIBCRA09_NUTRrSs	CRA09-0
Output	SUM_NUT_SCN_CRA09_Rr_Ss.LOG	NOT KEPT	NOT KEPT
<b>SCREEN</b>			

Input	SCREEN NUT SCN CRA09 Rr.INP	LIBCRA09 NUT	CRA09-0
Input	SUM NUT SCN CRA09 Rr Ss.TBL	LIBCRA09 NUTRrSs	CRA09-0
Output	SCREEN NUT SCN CRA09 Rr Ss.OUT	LIBCRA09 NUTRrSs	CRA09-0

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{1, 2, 3, 4, 5\}$  for each  $r$
3.  $vv \in \{001, 002, \dots, 100\}$  for each  $s$

Table 5.16 lists screened-in vectors for each scenario/replicate combination. All vectors in S1 for each replicate were run only to provide the conditions at the time of intrusion for the ISO and TI runs.

**Table 5.16 Screened-in Vectors by Replicate/Scenario**

Replicate	Scenario	Vectors	Number of Vectors
1	1	2, 3, 6, 7, 8, 9, 10, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 34, 35, 36, 38, 41, 43, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 69, 70, 71, 72, 73, 74, 76, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 92, 93, 94, 98	70
	2	2, 3, 6, 7, 8, 9, 10, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 34, 35, 36, 38, 41, 43, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 69, 70, 71, 72, 73, 74, 76, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 92, 93, 94, 98	70
	3	2, 3, 7, 8, 9, 10, 12, 13, 14, 16, 17, 20, 22, 23, 24, 25, 27, 28, 29, 30, 34, 35, 36, 41, 43, 45, 46, 47, 49, 50, 54, 55, 58, 59, 60, 61, 62, 63, 66, 67, 70, 71, 76, 78, 79, 80, 82, 83, 84, 86, 89, 90, 93, 94, 98	55
	4	2, 7, 9, 12, 16, 17, 27, 36, 45, 50, 53, 55, 76, 78, 82	15
	5	7, 9, 12, 16, 17, 27, 36, 45, 50, 53, 55, 76, 78, 82	14
2	1	2, 3, 4, 6, 8, 9, 10, 11, 12, 14, 16, 17, 18, 19, 20, 21, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 64, 65, 66, 67, 68, 69, 71, 72, 74, 75, 77, 79, 80, 81, 83, 84, 87, 89, 90, 91, 92, 95, 96, 98, 99, 100	76
	2	2, 3, 4, 6, 8, 9, 10, 11, 12, 14, 16, 17, 18, 19, 20, 21, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 64, 65, 66, 67, 68, 69, 71, 72, 74, 75, 77, 79, 80, 81, 83, 84, 87, 89, 90, 91, 92, 95, 96, 98, 99, 100	76
	3	3, 4, 6, 8, 9, 12, 14, 16, 17, 18, 20, 21, 24, 25, 26, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 39, 40, 41, 44, 48, 50, 51, 52, 53, 54, 55, 59, 63, 65, 66, 67, 68, 71, 72, 74, 75, 77, 79, 80, 84, 87, 89, 90, 92, 95, 96, 98, 99	58
	4	4, 17, 24, 28, 34, 36, 40, 53, 55, 63, 68, 79, 92, 95	14
	5	4, 17, 24, 28, 34, 40, 53, 55, 63, 68, 79, 92, 95	13
3	1	2, 3, 4, 7, 10, 11, 13, 14, 15, 17, 18, 19, 21, 22, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 50, 52, 53, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 73, 74, 76, 77, 78, 79, 84, 85, 86, 88, 89, 90, 91, 93, 94, 95, 96, 97, 98, 99, 100	77
	2	2, 3, 4, 7, 10, 11, 13, 14, 15, 17, 18, 19, 21, 22, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 50, 52, 53, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 73, 74, 76, 77, 78, 79, 84, 85, 86, 88, 89, 90, 91, 93, 94, 95, 96, 97, 98, 99, 100	77
	3	2, 10, 11, 14, 15, 18, 21, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 37, 38, 39, 40, 42, 43, 44, 45, 46, 47, 49, 50, 53, 56, 58, 59, 60, 61, 63, 64, 65, 66, 67, 68, 69, 73, 74, 77, 78, 79, 84, 85, 86, 88, 89, 91, 93, 94, 95, 96, 97, 98	60
	4	30, 35, 37, 42, 44, 47, 49, 53, 59, 66, 77, 79, 86, 93, 96	15

5	30, 35, 42, 47, 49, 53, 59, 66, 77, 79, 86, 93, 96	13
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### 5.4.1.3 SALADO TRANSPORT (NUTS) - STEP 3 (NUTS\_ISO)

Step 3 invokes NUTS in “isotope mode” (referred to here as NUTS\_ISO) to compute radionuclide transport for BRAGFLO scenarios S1-S5. Scenario S1 corresponds to undisturbed conditions. Scenario S2-S5 corresponds to single-intrusion conditions. Step 3 is run for each replicate for each of these scenarios. The script loops over the screened-in vectors specified in the SCREEN output file for each replicate/scenario combination. The input and log files for the script as well as the input and output files for NUTS\_ISO are shown in Table 5.17.

**Table 5.17 Salado Transport (NUTS) Step 3 Input and Output Files**

	File Names <sup>1,2,3</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Input	EVAL NUT CRA09 STEP3 R <sub>r</sub> S <sub>s</sub> .INP	LIBCRA09 EVAL	CRA09-0
Input	SCREEN NUT SCN CRA09 R <sub>r</sub> S <sub>s</sub> .OUT	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
Log	EVAL NUT CRA09 STEP3 R <sub>r</sub> S <sub>s</sub> .LOG	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
<b>NUTS_ISO</b>			
Input	NUT ISO CRA09 S <sub>s</sub> .INP	LIBCRA09 NUT	CRA09-0
Input	BF2 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .INP	LIBCRA09 BFR <sub>r</sub> S <sub>s</sub>	CRA09-0
Input	BF3 CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .CDB	LIBCRA09 BFR <sub>r</sub> S <sub>s</sub>	CRA09-0
Input	PANEL CON CRA1BC R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .CDB	LIBCRA1BC PANEL	CRA1BC-0
Output	NUT ISO CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .CDB	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
Output	NUT ISO CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .DBG	NOT KEPT	NOT KEPT
<b>ALGEBRACDB</b>			
Input	ALG NUT ISO CRA09 S <sub>s</sub> .INP	LIBCRA09 NUT	CRA09-0
Input	NUT ISO CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .CDB	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
Output	ALG NUT ISO CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .CDB	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
Output	ALG NUT ISO CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{1, 2, 3, 4, 5\}$  for each  $r$
3.  $vvv$  as indicated in Table 5.16.

### 5.4.1.4 SALADO TRANSPORT (NUTS) - STEP 4 (NUTS\_INT)

Step 4 invokes NUTS in “intrusion mode” (referred to here as NUTS\_INT) to compute radionuclide transport for single intrusions (BRAGFLO scenarios S2-S5, but at times different from the intrusion times in the BRAGFLO scenarios). Step 4 is run for each replicate for scenarios S2-S5. The script loops over the screened-in vectors specified in the SCREEN output file for each replicate/scenario combination. The input and log files for the script as well as the input and output files for NUTS\_INT are shown in Table 5.18.

**Table 5.18 Salado Transport (NUTS) Step 4 Input and Output Files**

	File Names <sup>1,2,3,4</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Input	EVAL_NUT_CRA09_STEP4_Rr_Ss.INP	LIBCRA09_EVAL	CRA09-0
Input	SCREEN_NUT_SCN_CRA09_Rr_Ss.OUT	LIBCRA09_NUTRrSs	CRA09-0
Log	EVAL_NUT_CRA09_STEP4_Rr_Ss.LOG	LIBCRA09_NUTRrSs	CRA09-0
<b>NUTS_INT</b>			
Input	NUT_INT_CRA09_Ss_Tttttt.INP	LIBCRA09_NUT	CRA09-0
Input	BF2_CRA09_Rr_Ss_Vvvv.INP	LIBCRA09_BFRrSs	CRA09-0
Input	BF3_CRA09_Rr_Ss_Vvvv.CDB	LIBCRA09_BFRrSs	CRA09-0
Input	PANEL_CON_CRA1BC_Rr_Ss_Vvvv.CDB	LIBCRA1BC_PANEL	CRA1BC-0
Input	NUT_ISO_CRA09_Rr_S1_Vvvv.CDB	LIBCRA09_NUTRrS1	CRA09-0
Output	NUT_INT_CRA09_Rr_Ss_Tttttt_Vvvv.CDB	LIBCRA09_NUTRrSs	CRA09-0
Output	NUT_INT_CRA09_Rr_Ss_Tttttt_Vvvv.DBG	NOT KEPT	NOT KEPT
<b>ALGEBRACDB</b>			
Input	ALG_NUT_ISO_CRA09_Ss.INP	LIBCRA09_NUT	CRA09-0
Input	NUT_INT_CRA09_Rr_Ss_Tttttt_Vvvv.CDB	LIBCRA09_NUTRrSs	CRA09-0
Output	ALG_NUT_INT_CRA09_Rr_Ss_Tttttt_Vvvv.CDB	LIBCRA09_NUTRrSs	CRA09-0
Output	ALG_NUT_INT_CRA09_Rr_Ss_Tttttt_Vvvv.DGB	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{2, 3, 4, 5\}$  for each  $r$
3.  $ttttt \in \begin{cases} \{00100\} & \text{for S2, S4} \\ \{03000, 05000, 07000, 09000\} & \text{for S3, S5} \end{cases}$
4.  $vvv$  as specified in Table 5.16.

### 5.4.2 SALADO TRANSPORT CALCULATIONS (PANEL)

Radionuclide transport to the Culebra for the E1E2 intrusion combination (BRAGFLO scenario S6; see Table 5.3) is calculated by running the PANEL code in “intrusion mode” (PANEL\_INT). This calculation is Step 5 in the PANEL run control. The script for PANEL\_INT is run once per replicate. The script loops over intrusion times and vectors, invoking panel PANEL\_INT for each intrusion/vector combination. The input and log files for the script as well as the input and output files for PANEL\_INT are shown in Table 5.19.

**Table 5.19 Salado Transport (PANEL\_INT) Input and Output Files**

	File Names <sup>1,2,3</sup>	CMS Library	CMS Class
<b>SCRIPT</b>			
Script Input	EVAL PANEL CRA09 STEP5 R <sub>r</sub> .INP	LIBCRA09 EVAL	CRA09-0
Script Log	EVAL PANEL CRA09 STEP5 R <sub>r</sub> .LOG	LIBCRA09 PANEL	CRA09-0
<b>PANEL_INT</b>			
Input	ALG PANEL CRA1BC R <sub>r</sub> V <sub>vvv</sub> .CDB	LIBCRA1BC PANEL	CRA1BC-0
Input	ALG2 BF CRA09 R <sub>r</sub> S6 V <sub>vvv</sub> .CDB	LIBCRA09 BFR+S6	CRA09-0
Output	PANEL INT CRA09 R <sub>r</sub> S6 T <sub>tttt</sub> V <sub>vvv</sub> .CDB	LIBCRA09 PANEL	CRA09-0
Output	PANEL INT CRA09 R <sub>r</sub> S6 T <sub>tttt</sub> V <sub>vvv</sub> .DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $ttt \in \{0100, 0350, 1000, 2000, 4000, 6000, 9000\}$  for each  $r$
3.  $vvv \in \{001, 002, \dots, 100\}$  for each intrusion time

### 5.5 SINGLE-INTRUSION SPALLINGS VOLUME CALCULATIONS (DRSPALL)

Implementation of the PA updates or corrections do not affect the CRA-2004 PABC DRSPALL calculations, thus, the spallings results calculated by DRSPALL for the CRA-2004 PABC will be used for the CRA-2009 PA. The CRA-2004 PABC DRSPALL results are documented in Vugrin (2005).

### 5.6 SINGLE-INTRUSION SOLIDS VOLUME CALCULATIONS (CUTTINGS\_S)

The total volume of radionuclide-contaminated solids that may reach the surface during a drilling intrusion event is calculated by the CUTTINGS\_S code. The single intrusion solids volume calculations are divided into 3 steps. The codes run in each step, and the DCL script(s) used to perform the steps are shown in Table 5.20. Step 3 also includes a small utility used to submit the script to a batch queue.

**Table 5.20 Solids Volume (CUTTINGS\_S) Run Control Scripts**

Step	Codes in Step	Scripts	Script CMS Library	Script CMS Class
1	GENMESH MATSET	EVAL_CUSP_STEP1.COM	LIBCRA09_EVAL	CRA09-0
2	POSTLHS	EVAL_CUSP_STEP2.COM	LIBCRA09_EVAL	CRA09-0
3	CUTTINGS_S	EVAL_CUSP_STEP3.COM SUB_CUSP_STEP3.COM	LIBCRA09_EVAL	CRA09-0

Three replicate calculations are performed. Five scenarios, S1-S5 are included in each replicate. Here the scenario indicates which BRAGFLO scenario provides the input conditions for the

simulation (i.e., CUTTINGS\_S scenario S1 means that CUTTINGS\_S uses BRAGFLO scenario S1 results as the inputs for the solids release calculations, CUTTINGS\_S scenario S2 means that it CUTTINGS uses BRAGFLO scenario S2 results as the inputs for the solids release calculations, etc.). A number of intrusion times are considered for each scenario. For the CUTTINGS\_S S1 scenario, these are intrusions into an undisturbed repository. For other the scenarios, these intrusions are considered subsequent to the intrusion contained in the BRAGFLO simulation. An intrusion time of 550 years in CUTTINGS\_S scenario S2 calculates the volume of solids released by an intrusion 200 years after the E1 intrusion at 350 years modeled in BRAGFLO scenario S2. An intrusion time of 1200 years in CUTTINGS\_S scenario S3 calculates the volume of solids released by an intrusion 200 years after the E1 intrusion at 1000 years modeled in BRAGFLO scenario S3.

Three drilling locations (upper, lower and middle) are considered for each replicate/scenario/intrusion time combination. See Stein et al. (2005) for an explanation of the drilling locations. Calculations are performed for a set of 100 uncertain input parameter vectors for each replicate/scenario/intrusion time/intrusion location combination.

### 5.6.1 SOLIDS VOLUME STEP 1

Step 1 uses GENMESH and MATSET to generate the computational grid and assign material properties to element blocks. Step1 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 5.21.

**Table 5.21 Solids Volume Step 1 Input and Output Files**

	File Names	CMS Library	CMS Class
<b>SCRIPT</b>			
Input	EVAL_CUSP_CRA09_STEP1.INP	LIBCRA09_EVAL	CRA09-0
Log	EVAL_CUSP_CRA09_STEP1.LOG	LIBCRA09_CUSP	CRA09-0
<b>GENMESH</b>			
Input	GM_CUSP_CRA09.INP	LIBCRA09_CUSP	CRA09-0
Output	GM_CUSP_CRA09.CDB	LIBCRA09_CUSP	CRA09-0
Output	GM_CUSP_CRA09.DBG	NOT KEPT	NOT KEPT
<b>MATSET</b>			
Input	MS_CUSP_CRA09.INP	LIBCRA09_CUSP	CRA09-0
Input	GM_CUSP_CRA09.CDB	LIBCRA09_CUSP	CRA09-0
Output	MS_CUSP_CRA09.CDB	LIBCRA09_CUSP	CRA09-0
Output	MS_CUSP_CRA09.DBG	NOT KEPT	NOT KEPT

### 5.6.2 SOLIDS VOLUME STEP 2

Step 2 uses POSTLHS to assign the sampled parameter values used by CUTTINGS\_S (generated by LHS, see Section 5.1) to the appropriate materials and element block properties. Step 2 is run

once per replicate. 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 5.22.

**Table 5.22 Solids Volume Step 2 Input and Output Files**

	File Names <sup>1,2</sup>	CMS Library	CMS Class
<b>SCRIPT</b>			
Script Input	EVAL_CUSP_CRA09_STEP2_Rr.INP	LIBCRA09_EVAL	CRA09-0
Script Log	EVAL_CUSP_CRA09_STEP2_Rr.LOG	LIBCRA09_CUSP	CRA09-0
<b>POSTLHS</b>			
Input	LHS3_DUMMY.INP	LIBCRA09_LHS	CRA09-0
Input	LHS2_CRA09_Rr_CON.TRN	LIBCRA09_LHS	CRA09-0
Input	MS_CUSP_CRA09.CDB	LIBCRA09_CUSP	CRA09-0
Output	LHS3_CUSP_CRA09_Rr_Vvvv.CDB	LIBCRA09_CUSP	CRA09-0
Output	LHS3_CUSP_CRA09_Rr.DBG	LIBCRA09_CUSP	CRA09-0

1.  $r \in \{1, 2, 3\}$
2.  $vvv \in \{001, 002, \dots, 100\}$  for each  $r$

### 5.6.3 SOLIDS VOLUME STEP 3

Step 3 runs the CUTTINGS\_S code, and is invoked for each replicate. The script generates the CUTTINGS\_S master input control file. The CUTTINGS\_S code itself loops over scenarios, intrusion times, intrusion locations, and vectors. The input and log files for the Step 3 script as well as the input and output files for CUTTINGS\_S are shown in Table 5.23.

**Table 5.23 Solids Volume Step 3 Input and Output Files**

	File Names <sup>1,2,3,4,5</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Input	EVAL_CUSP_CRA09_STEP3_Rr.INP	LIBCRA09_EVAL	CRA09-0
Output	CUSP_CRA09_MASTER_Rr.INP	LIBCRA09_CUSP	CRA09-0
Log	EVAL_CUSP_CRA09_STEP3_Rr.LOG	LIBCRA09_CUSP	CRA09-0
<b>CUTTINGS_S</b>			
Input	CUSP_CRA09_MASTER_Rr.INP	LIBCRA09_CUSP	CRA09-0
Input	CUSP_CRA09.INP	LIBCRA09_CUSP	CRA09-0
Input	LHS3_CUSP_CRA09_Rr_Vvvv.CDB	LIBCRA09_CUSP	CRA09-0
Input	BF3_CRA09_Rr_Ss_Vvvv.CDB	LIBCRA09_BFRrSs	CRA09-0
Input	MSPALL_DRS_CRA1BC_Rr.OUT	LIBCRA1BC_DRS	CRA09-0
Output	CUSP_CRA09_Rr.TBL	LIBCRA09_CUSP	CRA09-0
Output	CUSP_CRA09_Rr_Ss_Ttttt_c_Vvvv.CDB	LIBCRA09_CUSPRrSs	CRA09-0
Output	CUSP_CRA09_Rr.DBG	LIBCRA09_CUSP	CRA09-0

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{1, 2, 3, 4, 5\}$  for each  $r$
3.  $tttt \in \begin{cases} \{100, 350, 1000, 3000, 5000, 10000\} & \text{for S1} \\ \{550, 750, 2000, 4000, 10000\} & \text{for S2, S4} \\ \{1200, 1400, 3000, 5000, 10000\} & \text{for S3, S5} \end{cases}$
4.  $c \in \{L, U, M\}$  for each intrusion time
5.  $vvv \in \{001, 002, \dots, 100\}$  for each  $c$

## 5.7 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 5.24.

Three replicates are performed. Each replicate includes five scenarios (S1-S5). The scenario designations for the direct brine release calculations have the same meanings as those for the direct solids volume calculations. 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 replicate/scenario/intrusion time/intrusion location combination.

**Table 5.24 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	LIBCRA09_EVAL	CRA09-0
2	ALGEBRACDB RELATE ICSET	EVAL_DBR_STEP2.COM SUB_DBR_STEP2.COM	LIBCRA09_EVAL	CRA09-0
3	PREBRAG BRAGFLO POSTBRAG ALGEBRACDB	EVAL_DBR_STEP3.COM SUB_DBR_STEP3.COM	LIBCRA09_EVAL	CRA09-0

### 5.7.1 DIRECT BRINE RELEASE STEP 1

Step 1 uses GENMESH and MATSET 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 are shown in Table 5.25.

**Table 5.25 Direct Brine Release Step 1 Input and Output Files**

	File Names	CMS Library	CMS Class
<b>SCRIPT</b>			
Input	EVAL_DBR_CRA09_STEP1.INP	LIBCRA09_EVAL	CRA09-0
Log	EVAL_DBR_CRA09_STEP1.LOG	LIBCRA09_DBR	CRA09-0
<b>GENMESH</b>			
Input	GM_DBR_CRA09.INP	LIBCRA09_DBR	CRA09-0
Output	GM_DBR_CRA09.CDB	LIBCRA09_DBR	CRA09-0
Output	GM_DBR_CRA09.DBG	NOT KEPT	NOT KEPT
<b>MATSET</b>			

Input	MS_DBR_CRA09.INP	LIBCRA09_DBR	CRA09-0
Input	GM_DBR_CRA09.CDB	LIBCRA09_DBR	CRA09-0
Output	MS_DBR_CRA09.CDB	LIBCRA09_DBR	CRA09-0
Output	MS_DBR_CRA09.DBG	NOT KEPT	NOT KEPT

### 5.7.2 DIRECT BRINE RELEASE STEP 2

Step 2 performs pre-processing of input data with ALGEBRACDB (because ALGEBRACDB is used in multiple steps, this use is referred to as ALG1). The RELATE code is used to assign material properties to element blocks. RELATE is run twice (RELATE\_1 and RELATE\_2). Finally, ICSET is used to assign initial conditions. The Step 2 script is run for each replicate/scenario combination. The script loops over the appropriate intrusion times for the scenario. For each intrusion time, the script loops over all 100 vectors. The input and log files for the Step 2 script as well as the input and output files for ALGEBRACDB, RELATE, and ICSET are shown in Table 5.26.

**Table 5.26 Direct Brine Release Step 2 Input and Output Files**

	File Names <sup>1,2,3,4</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Input	EVAL_DBR_CRA09_STEP2_Rr_Ss.INP	LIBCRA09_EVAL	CRA09-0
Log	EVAL_DBR_CRA09_STEP2_Rr_Ss.LOG	LIBCRA09_DBRrSs	CRA09-0
<b>ALGEBRACDB</b>			
Input	ALG1_DBR_CRA09.INP	LIBCRA09_DBR	CRA09-0
Input	CUSP_CRA09_Rr_Ss_Ttttt_L_Vvvv.CDB	LIBCRA09_CUSPRrSs	CRA09-0
Output	ALG1_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.CDB	LIBCRA09_DBRrSs	CRA09-0
Output	ALG1_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.DBG	NOT KEPT	NOT KEPT
<b>RELATE_1</b>			
Input	REL1_DBR_CRA09.INP	LIBCRA09_DBR	CRA09-0
Input	MS_DBR_CRA09.CDB	LIBCRA09_DBR	CRA09-0
Input	ALG1_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.CDB	LIBCRA09_DBRrSs	CRA09-0
Output	REL1_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.CDB	LIBCRA09_DBRrSs	CRA09-0
Output	REL1_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.DBG	NOT KEPT	NOT KEPT
<b>RELATE_2</b>			
Input	REL2_DBR_CRA09_Ss.INP	LIBCRA09_DBR	CRA09-0
Input	REL1_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.CDB	LIBCRA09_DBRrSs	CRA09-0
Input	BF3_CRA09_Rr_Ss_Vvvv.CDB	LIBCRA09_BFRrSs	CRA09-0
Output	REL2_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.CDB	LIBCRA09_DBRrSs	CRA09-0
Output	REL2_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.DBG	NOT KEPT	NOT KEPT
<b>ICSET</b>			
Input	IC_DBR_CRA09_Ss.INP	LIBCRA09_DBR	CRA09-0
Input	REL2_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.CDB	LIBCRA09_DBRrSs	CRA09-0

Output	IC_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.CDB	LIBCRA09_DBRRrSs	CRA09-0
Output	IC_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.DBG	NOT KEPT	NOT KEPT
<b>ALGEBRACDB</b>			
Input	ALG2_DBR_CRA09_Ss.INP	LIBCRA09_DBR	CRA09-0
Input	IC_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.CDB	LIBCRA09_DBRRrSs	CRA09-0
Output	ALG2_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.CDB	LIBCRA09_DBRRrSs	CRA09-0
Output	ALG2_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{1, 2, 3, 4, 5\}$  for each  $r$
3.  $tttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} & \text{for S1} \\ \{00550, 00750, 02000, 04000, 10000\} & \text{for S2, S4} \\ \{01200, 01400, 03000, 05000, 10000\} & \text{for S3, S5} \end{cases}$
4.  $vvv \in \{001, 002, \dots, 100\}$  for each intrusion

### 5.7.3 DIRECT BRINE RELEASE STEP 3

Step 3 runs PREBRAG, BRAGFLO, POSTBRAG, and ALGEBRACDB (ALG2). The Step 3 script is invoked for each replicate/scenario combination. 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 PREBRAG, BRAGFLO, POSTBRAG, ALGEBRACDB sequence is run for each replicate/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 PREBRAG, BRAGFLO, POSTBRAG, ALGEBRACDB are shown in Table 5.27.

**Table 5.27 Direct Brine Release Step 3 Input and Output Files**

	File Names <sup>1,2,3,4,5</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Input	EVAL_DBR_CRA09_STEP3_Rr_Ss.INP	LIBCRA09_EVAL	CRA09-0
Log	EVAL_DBR_CRA09_STEP3_Rr_Ss.LOG	LIBCRA09_DBRRrSs	CRA09-0
<b>PREBRAG</b>			
Input	BF1_DBR_CRA09_Ss_c.INP	LIBCRA09_DBR	CRA09-0
Input	ALG2_DBR_CRA09_Rr_Ss_Ttttt_Vvvv.CDB	LIBCRA09_DBRRrSs	CRA09-0
Output	BF2_DBR_CRA09_Rr_Ss_Ttttt_c_Vvvv.INP	LIBCRA09_DBRRrSs	CRA09-0
Output	BF1_DBR_CRA09_Rr_Ss_Ttttt_c_Vvvv.DBG	NOT KEPT	NOT KEPT
<b>BRAGFLO</b>			
Input	BF2_DBR_CRA09_Rr_Ss_Ttttt_c_Vvvv.INP	LIBCRA09_DBRRrSs	CRA09-0
Output	BF2_DBR_CRA09_Rr_Ss_Ttttt_c_Vvvv.OUT	NOT KEPT	NOT KEPT
Output	BF2_DBR_CRA09_Rr_Ss_Ttttt_c_Vvvv.SUM	NOT KEPT	NOT KEPT
Output	BF2_DBR_CRA09_Rr_Ss_Ttttt_c_Vvvv.BIN	NOT KEPT	NOT KEPT
Output	BF2_DBR_CRA09_Rr_Ss_Ttttt_c_Vvvv.ROT	NOT KEPT	NOT KEPT
Output	BF2_DBR_CRA09_Rr_Ss_Ttttt_c_Vvvv.RIN	NOT KEPT	NOT KEPT

<b>POSTBRAG</b>			
Input	ALG2 DBR CRA09 Rr Ss Ttttt Vvvv.CDB	LIBCRA09 DBRRrSs	CRA09-0
Input	BF2 DBR CRA09 Rr Ss Ttttt c Vvvv.BIN	NOT KEPT	NOT KEPT
Output	BF3 DBR CRA09 Rr Ss Ttttt c Vvvv.CDB	LIBCRA09 DBRRrSs	CRA09-0
Output	BF3 DBR CRA09 Rr Ss Ttttt c Vvvv.DBG	NOT KEPT	NOT KEPT
<b>ALGEBRACDB</b>			
Input	ALG3 DBR CRA09.INP	LIBCRA09 DBR	CRA09-0
Input	BF3 DBR CRA09 Rr Ss Ttttt c Vvvv.CDB	LIBCRA09 DBRRrSs	CRA09-0
Output	ALG3 DBR CRA09 Rr Ss Ttttt c Vvvv.CDB	LIBCRA09 DBRRrSs	CRA09-0
Output	ALG3 DBR CRA09 Rr Ss Ttttt c Vvvv.DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{1, 2, 3, 4, 5\}$  for each  $r$
3.  $tttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} & \text{for S1} \\ \{00550, 00750, 02000, 04000, 10000\} & \text{for S2, S4} \\ \{01200, 01400, 03000, 05000, 10000\} & \text{for S3, S5} \end{cases}$
4.  $c \in \{L, M, U\}$  for each intrusion
5.  $vvv \in \{001, 002, \dots, 100\}$  for each  $c$

## 5.8 CULEBRA FLOW AND TRANSPORT CALCULATIONS

Culebra flow and transport calculations will be identical to CRA-2004 PABC results since their conceptual models are not affected by any of the PA updates or corrections. Thus, the Culebra flow and transport results from the CRA-2004 PABC will be used for the CRA-2009 PA. These results are documented in Lowry and Kanney (2005).

## 5.9 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 5.28. 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 5.28 CCDF Input Tabulation Run Control Scripts**

Code	Script	Script CMS Library	Script CMS Class
SUMMARIZE	EVAL_SUM.COM	LIBCRA09_EVAL	CRA09-0
	SUB_SUM.COM		

### 5.9.1 CCDF INPUT TABULATION FOR SALADO TRANSPORT (NUTS)

SUMMARIZE is used to extract and tabulate radionuclide transport data for the undisturbed and single-intrusion (E1 or E2) conditions from the appropriate post-NUT ALGEBRACDB output CDB files (see section 5.4.1). The script uses the output file from the SCREEN utility (see section 5.4.1.2) to keep track of which vectors were “screened-in” and thus have an ALGEBRACDB output CDB file to process. For vectors which were not “screened-in” and thus do not have a CDB file, SUMMARIZE is instructed to write zeros to its output table file.

The run control script is invoked for scenarios S1 through S5 for each replicate. The script loops over the appropriate intrusion times for each scenario. There is a SUMMARIZE input control file template for each intrusion time. The script uses the appropriate template to generate a SUMMARIZE input control file for each replicate/scenario/intrusion time combination.

The script input and log files along with the SUMMARIZE input and output files for tabulating scenario S1 results are shown in Table 5.29. Note that scenario S1 models undisturbed conditions and therefore does not have any intrusions. In this case, the appropriate output CDB file comes from the S1 ISO runs described in section 5.4.1.3. Although there are no intrusions, the t=100 SUMMARIZE input control file template file can still be used for this scenario.

**Table 5.29 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S1)**

	File Names <sup>1,2</sup>	CMS Library <sup>1</sup>	CMS Class
<b>SCRIPT</b>			
Input	EVAL_SUM_NUT_CRA09_R <sub>r</sub> _S1.INP	LIBCRA09_EVAL	CRA09-0
Input	SCREEN_NUT_SCN_CRA09_R <sub>r</sub> _S1.OUT	LIBCRA09_NUTR <sub>r</sub> S1	CRA09-0
Input	SUM_NUT_CRA09_T00100.TMPL	LIBCRA09_SUM	CRA09-0
Output	SUM_NUT_CRA09_R <sub>r</sub> _S1.INP	LIBCRA09_SUM	CRA09-0
Log	EVAL_SUM_NUT_CRA09_R <sub>r</sub> _S1.LOG	LIBCRA09_SUM	CRA09-0
<b>SUMMARIZE</b>			
Input	SUM_NUT_CRA09_R <sub>r</sub> _S1.INP	LIBCRA09_SUM	CRA09-0
Input	ALG_NUT_ISO_CRA09_R <sub>r</sub> _S1_V <sub>vvv</sub> .CDB	LIBCRA09_NUTR <sub>r</sub> S1	CRA09-0
Output	SUM_NUT_CRA09_R <sub>r</sub> _S1.TBL	LIBCRA09_SUM	CRA09-0
Output	SUM_NUT_CRA09_R <sub>r</sub> _S1.DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$

2. vvv as indicated in Table 5.16.

CCDF input tabulation for scenarios S2 and S4 are divided into two categories depending upon the intrusion time (which determines which output CDB file needs to be used). Category A includes t=100 years and the appropriate output CDB file comes from the S2 or S4 INT runs described in section 5.4.1.4. Category B includes t=350 years and the appropriate output CDB file comes from

the S2 or S4 ISO runs described in section 5.4.1.3. The ISO run is used in this case because the BRAGFLO S2 and S4 scenarios already include an intrusion at 350 years). Input and output files for categories A and B for scenarios S2 and S4 are shown in Table 5.30 and Table 5.31, respectively.

**Table 5.30 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S2A,S4A)**

	File Names <sup>1,2,3</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Input	EVAL SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> A.INP	LIBCRA09 EVAL	CRA09-0
Input	SCREEN NUT SCN CRA09 R <sub>r</sub> S <sub>s</sub> .OUT	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
Input	SUM NUT CRA09 T00100.TMPL	LIBCRA09 SUM	CRA09-0
Output	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> T00100.INP	LIBCRA09 SUM	CRA09-0
Log	EVAL SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> A.LOG	LIBCRA09 SUM	CRA09-0
<b>SUMMARIZE</b>			
Input	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> T00100.INP	LIBCRA09 SUM	CRA09-0
Input	ALG NUT INT CRA09 R <sub>r</sub> S <sub>s</sub> T00100 V <sub>vvv</sub> .CDB	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
Output	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> T00100.TBL	LIBCRA09 SUM	CRA09-0
Output	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> T00100.DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{2, 4\}$  for each  $r$
3.  $v$  as indicated in Table 5.16.

**Table 5.31 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S2B,S4B)**

	File Names <sup>1,2,3</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Input	EVAL SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> B.INP	LIBCRA09 EVAL	CRA09-0
Input	SCREEN NUT SCN CRA09 R <sub>r</sub> S <sub>s</sub> .OUT	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
Input	SUM NUT CRA09 T00350.TMPL	LIBCRA09 SUM	CRA09-0
Output	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> T00350.INP	LIBCRA09 SUM	CRA09-0
Log	EVAL SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> B.LOG	LIBCRA09 SUM	CRA09-0
<b>SUMMARIZE</b>			
Input	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> T00350.INP	LIBCRA09 SUM	CRA09-0
Input	ALG NUT ISO CRA09 R <sub>r</sub> S <sub>s</sub> V <sub>vvv</sub> .CDB	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
Output	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> T00350.TBL	LIBCRA09 SUM	CRA09-0
Output	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> T00350.DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{2, 4\}$  for each  $r$
3.  $v$  as indicated in Table 5.16.

CCDF input tabulation for scenarios S3 and S5 are also divided into two categories depending upon the intrusion time. Category A includes  $t=1000$  years and the appropriate output CDB file comes from the S3 or S5 ISO runs described in section 5.4.1.3. The ISO run is used for this category because the BRAGFLO S3 and S5 scenarios already include an intrusion at 1000 years. Category B includes  $t=3000, 5000, 7000,$  and  $9000$  years and the appropriate output CDB file comes from the S3 or S5 INT runs described in section 5.4.1.4. For category B, the script loops over all of the

loops over all of the included intrusions. Input and output files for categories A and B for scenarios S3 and S5 are shown in Table 5.32 and Table 5.33, respectively.

**Table 5.32 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S3A,S5A)**

	File Names <sup>1,2,3</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Input	EVAL SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> A.INP	LIBCRA09 EVAL	CRA09-0
Input	SCREEN NUT SCN CRA09 R <sub>r</sub> S <sub>s</sub> .OUT	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
Input	SUM NUT CRA09 T01000.TMPL	LIBCRA09 SUM	CRA09-0
Output	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> T01000.INP	LIBCRA09 SUM	CRA09-0
Log	EVAL SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> A.LOG	LIBCRA09 SUM	CRA09-0
<b>SUMMARIZE</b>			
Input	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> T01000.INP	LIBCRA09 SUM	CRA09-0
Input	ALG NUT ISO CRA09 R <sub>r</sub> S <sub>s</sub> Vvvv.CDB	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
Output	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> T01000.TBL	LIBCRA09 SUM	CRA09-0
Output	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> T01000.DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{3, 5\}$  for each  $r$
3.  $vvv$  as indicated in Table 5.16.

**Table 5.33 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S3B,S5B)**

	File Names <sup>1,2,3,4</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Input	EVAL SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> B.INP	LIBCRA09 EVAL	CRA09-0
Input	SCREEN NUT SCN CRA09 R <sub>r</sub> S <sub>s</sub> .OUT	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
Input	SUM NUT CRA09 Ttttt.TMPL	LIBCRA09 SUM	CRA09-0
Output	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> Ttttt.INP	LIBCRA09 SUM	CRA09-0
Log	EVAL SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> B.LOG	LIBCRA09 SUM	CRA09-0
<b>SUMMARIZE</b>			
Input	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> Ttttt.INP	LIBCRA09 SUM	CRA09-0
Input	ALG NUT INT CRA09 R <sub>r</sub> S <sub>s</sub> Vvvv.CDB	LIBCRA09 NUTR <sub>r</sub> S <sub>s</sub>	CRA09-0
Output	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> Ttttt.TBL	LIBCRA09 SUM	CRA09-0
Output	SUM NUT CRA09 R <sub>r</sub> S <sub>s</sub> Ttttt.DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{3, 5\}$  for each  $r$
3.  $tttt \in \{03000, 05000, 07000, 09000\}$  for each  $s$
4.  $vvv$  as indicated in Table 5.16.

## 5.9.2 CCDF INPUT TABULATION FOR SALADO TRANSPORT (PANEL\_INT)

SUMMARIZE is used to extract and tabulate radionuclide transport data for the multiple-intrusion (E1E2) conditions from the appropriate PANEL\_INT output CDB files (see section 5.4.2). The run control script is invoked for scenario S6 for each replicate. The script loops over the appropriate intrusion times. There is a SUMMARIZE input control file template for each intrusion time. The

script uses the appropriate template to generate a SUMMARIZE input control file for each replicate/scenario/intrusion combination. The script input and log files along with the SUMMARIZE input and output files are shown in Table 5.34.

**Table 5.34 CCDF Input Tabulation Input and Output Files (Salado Transport - PANEL\_INT)**

	File Names <sup>1,2,3</sup>	CMS Library	CMS Class
<b>SCRIPT</b>			
Input	EVAL SUM PANEL INT CRA09 R <sub>r</sub> S6.INP	LIBCRA09 EVAL	CRA09-0
Input	SUM PANEL INT CRA09 T <sub>tttt</sub> .TMPL	LIBCRA09 SUM	CRA09-0
Output	SUM PANEL INT CRA09 R <sub>r</sub> S6 T <sub>tttt</sub> .INP	LIBCRA09 SUM	CRA09-0
Log	EVAL SUM PANEL INT CRA09 R <sub>r</sub> S6.LOG	LIBCRA09 SUM	CRA09-0
<b>SUMMARIZE</b>			
Input	SUM PANEL INT CRA09 R <sub>r</sub> S6 T <sub>tttt</sub> .INP	LIBCRA09 SUM	CRA09-0
Input	PANEL INT CRA09 R <sub>r</sub> S6 T <sub>tttt</sub> V <sub>vvv</sub> .CDB	LIBCRA09 PANEL	CRA09-0
Output	SUM PANEL INT CRA09 R <sub>r</sub> S6 T <sub>tttt</sub> .TBL	LIBCRA09 SUM	CRA09-0
Output	SUM PANEL INT CRA09 R <sub>r</sub> S6 T <sub>tttt</sub> .DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $tttt \in \{00100, 00350, 01000, 02000, 04000, 06000, 09000\}$  for each r
3.  $vvv \in \{001, 002, \dots, 100\}$

### 5.9.3 CCDF INPUT TABULATION (DIRECT BRINE RELEASE)

SUMMARIZE is used to extract and tabulate brine release volume data from the appropriate post-BRAGFLO\_DBR ALGEBRACDB output CDB files (see section 5.7). The run control script is invoked for scenarios S2 through S5 for each replicate. 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 replicate/scenario/intrusion time/intrusion location combination. The script input and log files along with the SUMMARIZE input and output files are shown in Table 5.35.

**Table 5.35 CCDF Input Tabulation Input and Output Files (Direct Brine Release)**

	File Names <sup>1,2,3,4,5</sup>	CMS Library <sup>1,2</sup>	CMS Class
<b>SCRIPT</b>			
Input	EVAL_SUM_DBR_CRA09_Rr_Ss.INP	LIBCRA09_EVAL	CRA09-0
Input	SUM_DBR_CRA09.TMPL	LIBCRA09_SUM	CRA09-0
Output	SUM_DBR_CRA09_Rr_Ss_Ttttt_c.INP	LIBCRA09_SUM	CRA09-0
Log	EVAL_SUM_DBR_CRA09_Rr_Ss.LOG	LIBCRA09_SUM	CRA09-0
<b>SUMMARIZE</b>			
Input	SUM_DBR_CRA09_Rr_Ss_Ttttt_c.INP	LIBCRA09_SUM	CRA09-0
Input	ALG3_DBR_CRA09_Rr_Ss_Ttttt_c_Vvvv.CDB	LIBCRA09_DBRrSs	CRA09-0
Output	SUM_DBR_CRA09_Rr_Ss_Ttttt_c.TBL	LIBCRA09_SUM	CRA09-0
Output	SUM_DBR_CRA09_Rr_Ss_Ttttt_c.DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $s \in \{1, 2, 3, 4, 5\}$  for each  $r$
3.  $tttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} & \text{for S1} \\ \{00550, 00750, 02000, 04000, 10000\} & \text{for S2 and S4} \\ \{01200, 01400, 03000, 05000, 10000\} & \text{for S3 and S5} \end{cases}$
4.  $c \in \{L, M, U\}$  for each intrusion time
5.  $vvv \in \{001, 002, \dots, 100\}$  for each  $c$

## 5.10 CCDF CONSTRUCTION (PRECCDFGF, CCDFGF, CCDFSUM)

The complimentary cumulative distribution functions (CCDFs) for radionuclide releases to the accessible environment are constructed using the PRECCDFGF/CCDFGF code suite. CCDFs are plotted using the CCDFSUM code. 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 5.36.

**Table 5.36 CCDF Construction Run Control Scripts**

Step	Codes in Step	Scripts	CMS Library	CMS Class
1	GENMESH MATSET	EVAL_CCGF_STEP1.COM	LIBCRA09_EVAL	CRA09-0
2	POSTLHS	EVAL_CCGF_STEP2.COM	LIBCRA09_EVAL	CRA09-0
3	PRECCDFGF CCDFGF	EVAL_CCGF_STEP3.COM SUB_CCGF_STEP3.COM	LIBCRA09_EVAL	CRA09-0

### 5.10.1 CCDF CONSTRUCTION STEP 1

Step 1 uses GENMESH and MATSET 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 5.37.

**Table 5.37 CCDF Construction Step 1 Input and Output Files**

	File Names	CMS Library	CMS Class
<b>SCRIPT</b>			
Script Input	EVAL_CCGF_CRA09_STEP1.INP	LIBCRA09_EVAL	CRA09-0
Script Log	EVAL_CCGF_CRA09_STEP1.LOG	LIBCRA09_CCGF	CRA09-0
<b>GENMESH</b>			
Input	GM_CCGF_CRA09.INP	LIBCRA09_CCGF	CRA09-0
Output	GM_CCGF_CRA09.CDB	LIBCRA09_CCGF	CRA09-0
Output	GM_CCGF_CRA09.DBG	NOT KEPT	NOT KEPT
<b>MATSET</b>			
Input	MS_CCGF_CRA09.INP	LIBCRA09_CCGF	CRA09-0
Input	GM_CCGF_CRA09.CDB	LIBCRA09_CCGF	CRA09-0
Output	MS_CCGF_CRA09.CDB	LIBCRA09_CCGF	CRA09-0
Output	MS_CCGF_CRA09.DBG	NOT KEPT	NOT KEPT

### 5.10.2 CCDF CONSTRUCTION STEP 2

Step 2 uses POSTLHS to assign the sampled parameter values used by CCDFGF (generated by LHS, see Section 5.1) to the appropriate materials and element block properties. Step 2 is run once

per replicate. 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 5.38.

**Table 5.38 CCDF Construction Step 2 Input and Output Files**

	File Names <sup>1,2</sup>	CMS Library	CMS Class
<b>STEP 2</b>			
Script Input	EVAL CCGF CRA09 STEP2 Rr.INP	LIBCRA09 EVAL	CRA09-0
Script Log	EVAL CCGF CRA09 STEP2 Rr.LOG	LIBCRA09 CCGF	CRA09-0
<b>POSTLHS</b>			
Input	LHS3_DUMMY.INP	LIBCRA09 LHS	CRA09-0
Input	LHS2 CRA09 Rr CON.TRN	LIBCRA09 LHS	CRA09-0
Input	MS CCGF CRA09.CDB	LIBCRA09 CCGF	CRA09-0
Output	LHS3_CCGF CRA09 Rr Vvvv.CDB	LIBCRA09 CCGF	CRA09-0
Output	LHS3 CCGF CRA09 Rr.DBG	LIBCRA09 CCGF	CRA09-0

1.  $r \in \{1, 2, 3\}$
2.  $vvv \in \{001, 002, \dots, 100\}$  for each  $r$

### 5.10.3 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 per replicate. 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 5.39.

**Table 5.39 CCDF Construction Step 3 Input and Output Files**

	File Names <sup>1-7</sup>	CMS Library	CMS Class
<b>SCRIPT</b>			
Script Input	EVAL CCGF STEP3 CRA09 Rr.INP	LIBCRA09 EVAL	CRA09-0
Script Log	EVAL CCGF STEP3 CRA09 Rr.LOG	LIBCRA09 CCGF	CRA09-0
<b>PRECCDFGF</b>			
Input	INTRUSIONTIMES.IN	LIBCRA1BC CCGF	CRA09-0
Input	MS CCGF CRA09.CDB	LIBCRA09 CCGF	CRA09-0
Input	LHS3_CCGF CRA09 Rr Vvvv.CDB	LIBCRA09 CCGF	CRA09-0
Input	SUM_DBR CRA09 Rr Ss Ttttt c.TBL	LIBCRA09 SUM	CRA09-0
Input	CUSP CRA09 Rr.TBL	LIBCRA09 CUSP	CRA09-0
Input	SUM NUT CRA09 Rr S1.TBL	LIBCRA09 SUM	CRA09-0
Input	SUM NUT CRA09 Rr Ss Ttttt.TBL	LIBCRA09 SUM	CRA09-0
Input	SUM PANEL INT CRA09 Rr S6 Ttttt.TBL	LIBCRA09 SUM	CRA09-0
Input	SUM ST2D CRA1BC Rr Mm.TBL	LIBCRA1BC SUM	CRA09-0
Input	EPU CRA1BC hH.DAT	LIBCRA1BC EPU	CRA09-0
Input	SUM PANEL CON CRA1BC Rr Ss.TBL	LIBCRA1BC SUM	CRA09-0
Input	SUM PANEL ST CRA1BC Rr Ss.TBL	LIBCRA1BC SUM	CRA09-0

Output	CCGF CRA09 RELTAB Rr.DAT	LIBCRA09 CCGF	CRA09-0
<b>CCDFGF</b>			
Input	CCGF CRA09 CONTROL Rr.INP	LIBCRA09 CCGF	CRA09-0
Input	CCGF CRA09 RELTAB Rr.DAT	LIBCRA09 CCGF	CRA09-0
Output	CCGF CRA09 Rr.OUT	LIBCRA09 CCGF	CRA09-0
Output	CCGF CRA09 Rr.DBG	NOT KEPT	NOT KEPT

1.  $r \in \{1, 2, 3\}$
2.  $vvv \in \{001, 002, \dots, 100\}$  for each  $r$
3.  $s \in \begin{cases} \{1, 2, 3, 4, 5\} & \text{for SUM\_DBR} \\ \{2, 3, 4, 5\} & \text{for SUM\_NUT} \\ \{1, 2\} & \text{for SUM\_PANEL\_CON and SUM\_PANEL\_ST} \end{cases}$
4.  $tttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} & \text{for S1 for each } r \text{ for SUM\_DBR} \\ \{00550, 07500, 02000, 04000, 10000\} & \text{for S2, S4 for each } r \text{ for SUM\_DBR} \\ \{01200, 01400, 03000, 05000, 10000\} & \text{for S3, S5 for each } r \text{ for SUM\_DBR} \\ \{00100, 00350\} & \text{for S2, S4 for each } r \text{ for SUM\_NUT} \\ \{01000, 03000, 05000, 07000, 09000\} & \text{for S3, S5 each } r \text{ for SUM\_NUT} \\ \{00100, 00350, 01000, 02000, 04000, 06000, 09000\} & \text{for each } r \text{ for SUM\_PANEL\_INT} \end{cases}$
5.  $c \in \{L, M, U\}$  for each intrusion for SUM\\_DBR
6.  $m \in \{F, P\}$
7.  $h \in \{C, H\}$

## 6 REFERENCES

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