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Sandia National Laboratories

Carlsbad Programs Group

Waste Isolation Pilot Plant

Execution of Performance Assessment Codes for the CRA-2014 Performance Assessment

Revision 0

Task Number 1.2.5

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1 INTRODUCTION

1.1 BACKGROUND

The Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, has been developed by the U.S. Department of Energy (DOE) for the geologic (deep underground) disposal of transuranic (TRU) 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), Part 191. The DOE demonstrates compliance with the containment requirements according to the Certification Criteria in Title 40 CFR Part 194 by means of performance assessment (PA) calculations performed by Sandia National Laboratories (SNL). WIPP PA calculations estimate the probability and consequence of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure. The models used in PA are maintained and updated with new information as part of an ongoing process. Improved information regarding important WIPP features, events, and processes typically results in refinements and modifications to PA models and the parameters used in them. Planned changes to the repository and/or the components therein also result in updates to WIPP PA models. WIPP PA models are used to support the repository recertification process that occurs at five-year intervals following the receipt of the first waste shipment at the site in 1999.

PA calculations were included in the 1996 Compliance Certification Application (CCA) (U.S. DOE 1996), and in a subsequent Performance Assessment Verification Test (PAVT) (MacKinnon and Freeze 1997a, 1997b and 1997c). Based in part on the CCA and PAVT PA calculations, the EPA certified that the WIPP met the regulatory containment criteria. The facility was approved for disposal of transuranic waste in May 1998 (U.S. EPA 1998). PA calculations were an integral part of the 2004 Compliance Recertification Application (CRA-2004) (U.S. DOE 2004). During their review of the CRA-2004, the EPA requested an additional PA calculation, referred to as the CRA-2004 Performance Assessment Baseline Calculation (PABC) (Leigh et al. 2005), be conducted with modified assumptions and parameter values (Cotsworth 2005). Following review of the CRA-2004 and the CRA-2004 PABC, the EPA recertified the WIPP in March 2006 (U.S. EPA 2006).

PA calculations were completed for the second WIPP recertification and documented in the 2009 Compliance Recertification Application (CRA-2009). The CRA-2009 PA resulted from continued review of the CRA-2004 PABC, including a number of technical changes and corrections, as well as updates to parameters and improvements to the PA computer codes (Clayton et al. 2008). To incorporate additional information which was received after the CRA-2009 PA was completed, but before the submittal of the CRA-2009, the EPA requested an additional PA calculation, referred to as the 2009 Compliance Recertification Application Performance Assessment Baseline Calculation (PABC-2009) (Clayton et al. 2010), be undertaken which included updated information (Cotsworth 2009). Following the completion and submission of the PABC-2009, the WIPP was recertified in 2010 (U.S. EPA 2010).

The Land Withdrawal Act (U.S. Congress 1992) requires that the DOE apply for WIPP recertification every five years following the initial 1999 waste shipment. The 2014 Compliance

Recertification Application (CRA-2014) is the third WIPP recertification application submitted by the DOE for EPA approval. The PA executed by SNL in support of the CRA-2014 is detailed in AP-164 (Camphouse 2013). The CRA-2014 PA includes a number of technical changes and parameter refinements, as well as a redesigned WIPP panel closure system. Results found in the CRA-2014 PA are compared to those obtained in the PABC-2009 in order to assess repository performance in terms of the current regulatory baseline. This report documents the Run Control component of the CRA-2014 PA analysis.

The aim of the CRA-2014 PA is to quantify regulatory compliance impacts associated with changes made since the PABC-2009. Impacts will be determined by a direct comparison of CRA-2014 PA and PABC-2009 results. Changes incorporated into the CRA-2014 PA include planned changes as well as parameter and implementation changes. The approach taken in the CRA-2014 PA is to reasonably isolate impacts associated with these changes, and then to assess the combined impact when all are included in the PA. To that end, a number of individual cases will be investigated in the CRA-2014 PA. The first case considered in the CRA-2014 PA will be used to compare the impact of a baseline set of changes relative to the PABC-2009. The name given to this case is CRA14-BL (for CRA-2014 Baseline). With the results of case CRA14-BL in hand, two parameter updates will be added to the set of baseline changes so that their impacts can be determined. The addition of these changes, and their impact on regulatory compliance, will be captured in the second case CRA14-TP (for CRA-2014 (T)AUFAIL (P)BRINE). The focus of the third case CRA14-BV (for CRA-2014 (B)rine (V)olumes) is to assess the impact of the variable brine volume implementation on results calculated in case CRA14-TP. The fourth and final case CRA14-0 will incorporate all changes included in the CRA-2014 PA. For any codes not run for a particular case, the results obtained from the previous case will be used. The details associated with each case are detailed in AP-164 (Camphouse 2013).

A single replicate (Replicate 1) will be executed for Case CRA14-BL, CRA14-TP, and CRA14-BV. Three replicates will be executed for Case CRA14-0. 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-2014 Run Control Team

Function	**Personnel**
Performance Assessment Team Lead	Chris Camphouse
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-2014 are shown in Table 1.2.

Table 1.2 CRA-2014 Analysts

Major WIPP PA Codes	**Analyst(s)**
EPAUNI	Dwayne Kicker
LHS	Tom Kirchner
BRAGFLO	Chris Camphouse
NUTS	Sungtae Kim
PANEL	Sungtae Kim
CUTTINGS_S	Dwayne Kicker
BRAGFLO_DBR	Bwalya Malama
CCDFGF	Todd Zeitler
STEPWISE	Tom Kirchner

2 WIPP PA ALPHA CLUSTER

The CRA-2014 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-2014

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

3 WIPP PA SOFTWARE CONFIGURATION MANAGEMENT AND RUN CONTROL SYSTEMS

The computer simulations that form the core of the CRA-2014 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 or archive 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 cluster. 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 3.2.3.

3.1 LIBRARY SYSTEM

An essential element of the Software Configuration Management System (SCMS) on the WIPP PA Alpha Cluster is the Configuration 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-2014:

1. A Software Configuration Management System 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.

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

CMS Version 4.5-2 was used for the CRA-2014. Consult the CMS User Guide (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) for further information.

3.2 RUN CONTROL SYSTEMS

3.2.1 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 and all parameters from the Performance Assessment Parameter Database (PAPDB). Executables are handled in two ways: 1) the executable is fetched from an access-controlled CMS library; or 2) a copy of the executable 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
- 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-2014 are stored in CMS library LIBCRA14_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.

3.2.2 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 CRA-2014 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_CRA14.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.
CRA14	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".

3.2.3 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 (Kirchner 2012) for more information. PAPDB Version 2.00 was used for the CRA-2014.

Codes that access the PAPDB require that Digital Command Language (DCL) logicals for the database name, analysis name, computational code name, computational code version, and analysis revision be set. These items are set by the run control script (and are specified in the run control script input file). The production PAPDB, "ParamDB", was used in the CRA-2014.

It should be noted that the WIPP PA codes only retrieve parameter values from the PAPDB and have no capability to modify the parameter values in 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 2006).

3.3 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 Coordinator 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 addition, only the CCA_MASTER account can write to the CRA-2014 libraries.

4 WIPP PA CODES

The major WIPP PA codes used in the CRA-2014 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 (Long 2012).

Table 4.1 WIPP PA VMS Software Used in the CRA-2014

Code	Version	Executable	Build Date	CMS Library	CMS Class
ALGEBRACDB	2.35	ALGEBRACDB_PA96.EXE	31-01-96	LIBALG	PA96
BRAGFLO (for case CRA14-BL)	6.0	BRAGFLO_QB0600.EXE	12-02-07	LIBBF	QB0600
BRAGFLO (for case CRA14-0)	6.02	BRAGFLO_QB0602.EXE	29-11-12	LIBBF	QB0602
PREBRAG (for case CRA14-BL)	8.00	PREBRAG_QA0800.EXE	08-03-07	LIBBF	QA0800
PREBRAG (for case CRA14-0)	8.02	PREBRAG_QA0802.EXE	29-11-12	LIBBF	QA0802
POSTBRAG	4.00A	POSTBRAG_QA0400A.EXE	28-03-07	LIBBF	QA0400A
CCDFGF	6.0	CCDFGF_QC0600.EXE	23-02-10	LIBCCGF	QC0600
PRECCDFGF	2.0	PRECCDFGF_QA0200.EXE	06-04-10	LIBCCGF	QA0200
CUTTINGS_S	6.02	CUTTINGS_S_QA0602.EXE	09-06-05	LIBCUSP	QA0602
EPAUNI	1.15A	EPAUNI_QA0115A.EXE	03-07-03	LIBEPU	QA0115A
GENMESH	6.08	GM_PA96.EXE	31-01-96	LIBGM	PA96
ICSET	2.22	ICSET_PA96.EXE	01-02-96	LIBIC	PA96
LHS	2.42	LHS_QA0242.EXE	18-01-05	LIBLHS	QA0242
PRELHS	2.40	PRELHS_QA0240.EXE	04-01-12	LIBLHS	QA0240
POSTLHS	4.07A	POSTLHS_QA0407A.EXE	25-04-05	LIBLHS	QA0407A
MATSET	9.20	MATSET_QA0920.EXE	04-01-12	LIBMS	QA0920
NUTS	2.05C	NUTS_QA0205C.EXE	24-05-06	LIBNUT	QA0205C
PANEL	4.03	PANEL_QA0403.EXE	25-04-05	LIBPANEL	QA0403
PCCSRC	2.21	PCCSRC_PA96.EXE	23-05-96	LIBPCC	PA96
RELATE	1.43	RELATE_PA96.EXE	06-03-96	LIBREL	PA96
STEPWISE	2.21	STEPWISE_PA96_2.EXE	02-12-96	LIBSTP	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 (Safley 2012). 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-2014

Utility	Executable	CMS Library	CMS Class	Section
SCREEN	SCREEN.EXE	LIBCRA1BC_NUT	SCREEN_V1.0	5.5.1.2
LHS_EDIT	LHS_EDIT.EXE	LIBCRA09_LHS	LHS_EDIT_V1.0	5.2

5 CALCULATION FLOW

The following sections describe the calculation flow for the CRA-2014. 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 INVENTORY DECAY CALCULATIONS (EPAUNI)

The EPAUNI code calculates the decay of the radionuclide components in each inventory waste stream over the 10,000-year regulatory period (for use in calculating direct solids releases). These calculations are deterministic, so multiple replicates and vectors of uncertain parameters are not used. Calculations are performed for both contact-handled (CH) and remote-handled (RH) waste. The DCL script used to control the inventory decay calculations is shown in Table 5.1. The EPAUNI input and output files, along with the script input and log files are shown in Table 5.2.

Table 5.1 Inventory Decay Run Control Script

Code	Script Name	CMS Library	CMS Class
EPAUNI	EVAL_EPU.COM	LIBCRA14_EVAL	CRA14-BL

Table 5.2 Inventory Decay Input and Output Files for CRA14-BL

	File Names[1]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_EPU_CRA14BL.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_EPU_CRA14BL.LOG	LIBCRA14_EPU	CRA14-BL
EPAUNI			
Input	EPU_CRA14_*h*H.INP	LIBCRA14_EPU	CRA14-BL
Input	EPU_CRA14_*h*H_MISC.INP	LIBCRA14_EPU	CRA14-BL
Output	EPU_CRA14BL_*h*H.DAT	LIBCRA14_EPU	CRA14-BL, CRA14-TP, CRA14-BV, CRA14-0
Output	EPU_CRA14BL_*h*H.OUT	LIBCRA14_EPU	CRA14-BL
Output	EPU_CRA14BL_*h*H.OUT2	LIBCRA14_EPU	CRA14-BL
Output	EPU_CRA14BL_*h*H.DIA	LIBCRA14_EPU	CRA14-BL
Output	EPU_CRA14BL_*h*H_ACTIVITY.DIA	LIBCRA14_EPU	CRA14-BL

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

5.2 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 for CRA14-0 and one replicate each for CRA14-BL and CRA14-TP).

PRELHS and LHS are executed in sequence by the DCL script EVAL_LHS.COM shown in Table 5.3. The input and output files for PRELHS and LHS, as well as the input and log files for the script are shown in Table 5.4, 5.5, and 5.6.

Table 5.3 Parameter Sampling Run Control Script

Codes	Script	CMS Library	CMS Class
PRELHS, LHS	EVAL_LHS.COM	LIBCRA14_EVAL	CRA14-BL, CRA14-TP, CRA14-0

Table 5.4 Parameter Sampling Input and Output Files for CRA14-BL

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_LHS_CRA14BL_R1.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_LHS_CRA14BL_R1.LOG	LIBCRA14_LHS	CRA14-BL
PRELHS			
Input	LHS1_CRA14BL_R1.INP	LIBCRA14_LHS	CRA14-BL
Output	LHS1_CRA14BL_R1.TRN	LIBCRA14_LHS	CRA14-BL
Output	LHS1_CRA14BL_R1.DBG	LIBCRA14_LHS	CRA14-BL
LHS			
Input	LHS1_CRA14BL_R1.TRN	LIBCRA14_LHS	CRA14-BL
Output	LHS2_CRA14BL_R1.TRN	LIBCRA14_LHS	CRA14-BL
Output	LHS2_CRA14BL_R1.DBG	LIBCRA14_LHS	CRA14-BL
LHS Edit			
Input	LHS_CONTROL_R1.INP	NOT KEPT	NOT KEPT
Input	LHS2_CRA14BL_R1.TRN	LIBCRA14_LHS	CRA14-BL
Output	LHS2_CRA14BL_R1_CON.TRN	LIBCRA14_LHS	CRA14-BL

Table 5.5 Parameter Sampling Input and Output Files for CRA14-TP

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_LHS_CRA14TP_R1.INP	LIBCRA14_EVAL	CRA14-TP
Log	EVAL_LHS_CRA14TP_R1.LOG	LIBCRA14_LHS	CRA14-TP

PRELHS			
Input	LHS1_CRA14TP_R1.INP	LIBCRA14_LHS	CRA14-TP
Output	LHS1_CRA14TP_R1.TRN	LIBCRA14_LHS	CRA14-TP
Output	LHS1_CRA14TP_R1.DBG	LIBCRA14_LHS	CRA14-TP
LHS			
Input	LHS1_CRA14TP_R1.TRN	LIBCRA14_LHS	CRA14-TP
Output	LHS2_CRA14TP_R1.TRN	LIBCRA14_LHS	CRA14-TP
Output	LHS2_CRA14TP_R1.DBG	LIBCRA14_LHS	CRA14-TP
LHS Edit			
Input	LHS_CONTROL_R1.INP	NOT KEPT	NOT KEPT
Input	LHS2_CRA14TP_R1.TRN	LIBCRA14_LHS	CRA14-TP
Output	LHS2_CRA14TP_R1_CON.TRN	LIBCRA14_LHS	CRA14-TP

Table 5.6 Parameter Sampling Input and Output Files for CRA14-0

	File Names[1]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_LHS_CRA14_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_LHS_CRA14_R*r*.LOG	LIBCRA14_LHS	CRA14-0
PRELHS			
Input	LHS1_CRA14_R*r*.INP	LIBCRA14_LHS	CRA14-0
Output	LHS1_CRA14_R*r*.TRN	LIBCRA14_LHS	CRA14-0
Output	LHS1_CRA14_R*r*.DBG	LIBCRA14_LHS	CRA14-0
LHS			
Input	LHS1_CRA14_R*r*.TRN	LIBCRA14_LHS	CRA14-0
Output	LHS2_CRA14_R*r*.TRN	LIBCRA14_LHS	CRA14-0
Output	LHS2_CRA14_R*r*.DBG	LIBCRA14_LHS	CRA14-0
LHS Edit			
Input	LHS_CONTROL_R*r*.INP	NOT KEPT	NOT KEPT
Input	LHS2_CRA14_R*r*.TRN	LIBCRA14_LHS	CRA14-0
Output	LHS2_CRA14_R*r*_CON.TRN	LIBCRA14_LHS	CRA14-0

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

5.3 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 for CRA14-0 and only one replicate for CRA14-BL. Each replicate includes six scenarios (S1-S6) designed to cover a range of drilling intrusion types and times, as shown in Table 5.7. For each replicate/scenario combination, calculations are performed for 100 vectors of uncertain model input parameters.

Table 5.7 BRAGFLO Scenarios

BRAGFLO Scenario	Description[1,2]
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 5.8.

Table 5.8 Salado Flow Run Control Scripts

Step	Codes in Step	Script(s)	CMS Library	CMS Class
1	GENMESH MATSET	EVAL_GENERIC_STEP1.COM	LIBCRA14_EVAL	CRA14-BL CRA14-0
2	POSTLHS	EVAL_GENERIC_STEP2.COM	LIBCRA14_EVAL	CRA14-BL CRA14-0
3	ICSET ALGEBRACDB	EVAL_BF_STEP3.COM	LIBCRA14_EVAL	CRA14-BL CRA14-0
4	PREBRAG	EVAL_BF_STEP4.COM	LIBCRA14_EVAL	CRA14-BL CRA14-0
5	BRAGFLO POSTBRAG ALGEBRACDB	EVAL_BF_STEP5_MASTER.COM EVAL_BF_STEP5_SLAVE.COM	LIBCRA14_EVAL LIBCRA14_EVAL	CRA14-BL CRA14-0 CRA14-BL CRA14-0
6	ALGEBRACDB	EVAL_BF_STEP6_MASTER.COM EVAL_BF_STEP6_SLAVE.COM	LIBCRA14_EVAL LIBCRA14_EVAL	ANALYSIS ANALYSIS

5.3.1 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 5.9 and 5.10.

Table 5.9 Salado Flow Step 1 Input and Output Files for CRA14-BL

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_BF_CRA14BL_STEP1.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_BF_CRA14BL_STEP1.LOG	LIBCRA14_BF	CRA14-BL
GENMESH			
Input	GM_BF_CRA14BL.INP	LIBCRA14_BF	CRA14-BL
Output	GM_BF_CRA14BL.CDB	LIBCRA14_BF	CRA14-BL
Output	GM_BF_CRA14BL.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_BF_CRA14BL.INP	LIBCRA14_BF	CRA14-BL
Input	GM_BF_CRA14BL.CDB	LIBCRA14_BF	CRA14-BL
Output	MS_BF_CRA14BL.CDB	LIBCRA14_BF	CRA14-BL
Output	MS_BF_CRA14BL.DBG	NOT KEPT	NOT KEPT

Table 5.10 Salado Flow Step 1 Input and Output Files for CRA14-0

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_BF_CRA14_STEP1.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_BF_CRA14_STEP1.LOG	LIBCRA14_BF	CRA14-0
GENMESH			
Input	GM_BF_CRA14.INP	LIBCRA14_BF	CRA14-0
Output	GM_BF_CRA14.CDB	LIBCRA14_BF	CRA14-0
Output	GM_BF_CRA14.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_BF_CRA14.INP	LIBCRA14_BF	CRA14-0
Input	GM_BF_CRA14.CDB	LIBCRA14_BF	CRA14-0
Output	MS_BF_CRA14.CDB	LIBCRA14_BF	CRA14-0
Output	MS_BF_CRA14.DBG	NOT KEPT	NOT KEPT

5.3.2 SALADO FLOW STEP 2

Step 2 uses POSTLHS to assign the sampled parameter values used by BRAGFLO (generated by LHS, see Section 5.12) 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 5.11 and 5.12.

Table 5.11 Salado Flow Step 2 Input and Output Files for CRA14-BL

	File Names[1]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_BF_CRA14BL_STEP2_R1.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_BF_CRA14BL_STEP2_R1.LOG	LIBCRA14_BF	CRA14-BL
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA14_LHS	CRA14-BL
Input	LHS2_CRA14BL_R1_CON.TRN	LIBCRA14_LHS	CRA14-BL
Input	MS_BF_CRA14BL.CDB	LIBCRA14_BF	CRA14-BL
Output	LHS3_BF_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_BF	CRA14-BL
Output	LHS3_BF_CRA14BL_R1.DBG	LIBCRA14_BF	CRA14-BL

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

Table 5.12 Salado Flow Step 2 Input and Output Files for CRA14-0

	File Names[1,2]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_BF_CRA14_STEP2_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_BF_CRA14_STEP2_R*r*.LOG	LIBCRA14_BF	CRA14-0
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA14_LHS	CRA14-0
Input	LHS2_CRA14_R*r*_CON.TRN	LIBCRA14_LHS	CRA14-0
Input	MS_BF_CRA14.CDB	LIBCRA14_BF	CRA14-0
Output	LHS3_BF_CRA14_R*r*_V*vvv*.CDB	LIBCRA14_BF	CRA14-0
Output	LHS3_BF_CRA14_R*r*.DBG	LIBCRA14_BF	CRA14-0

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

5.3.3 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 5.13 and 5.14.

Table 5.13 Salado Flow Step 3 Input and Output Files for CRA14-BL

	File Names[1]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_BF_CRA14BL_STEP3_R1.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_BF_CRA14BL_STEP3_R1.LOG	LIBCRA14_BF	CRA14-BL
ICSET			
Input	IC_BF_CRA14BL.INP	LIBCRA14_BF	CRA14-BL
Input	LHS3_BF_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_BF	CRA14-BL
Output	IC_BF_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_BF	CRA14-BL
Output	IC_BF_CRA14BL_R1_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG1_BF_CRA14BL.INP	LIBCRA14_BF	CRA14-BL
Input	IC_BF_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_BF	CRA14-BL
Output	ALG1_BF_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_BF	CRA14-BL
Output	ALG1_BF_CRA14BL_R1_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

Table 5.14 Salado Flow Step 3 Input and Output Files for CRA14-0

	File Names[1,2]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_BF_CRA14_STEP3_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_BF_CRA14_STEP3_R*r*.LOG	LIBCRA14_BF	CRA14-0
ICSET			
Input	IC_BF_CRA14.INP	LIBCRA14_BF	CRA14-0
Input	LHS3_BF_CRA14_R*r*_V*vvv*.CDB	LIBCRA14_BF	CRA14-0
Output	IC_BF_CRA14_R*r*_V*vvv*.CDB	LIBCRA14_BF	CRA14-0
Output	IC_BF_CRA14_R*r*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG1_BF_CRA14.INP	LIBCRA14_BF	CRA14-0
Input	IC_BF_CRA14_R*r*_V*vvv*.CDB	LIBCRA14_BF	CRA14-0
Output	ALG1_BF_CRA14_R*r*_V*vvv*.CDB	LIBCRA14_BF	CRA14-0
Output	ALG1_BF_CRA14_R*r*_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

5.3.4 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 5.15 and 5.16.

Table 5.15 Salado Flow Step 4 Input and Output Files for CRA14-BL

	File Names[1,2]	CMS Library[1]	CMS Class
SCRIPT			
Script Input	EVAL_BF_CRA14BL_STEP4_R1_S*s*.INP	LIBCRA14_EVAL	CRA14-BL
Script Log	EVAL_BF_CRA14BL_STEP4_R1_S*s*.LOG	LIBCRA14_BFR1S*s*	CRA14-BL
PREBRAG			
Input	BF1_CRA14BL_S*s*.INP	LIBCRA14_BF	CRA14-BL
Input	ALG1_BF_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_BF	CRA14-BL
Output	BF2_CRA14BL_R1_S*s*_V*vvv*.INP	LIBCRA14_BFR1S*s*	CRA14-BL
Output	BF1_CRA14BL_R1_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

Table 5.16 Salado Flow Step 4 Input and Output Files for CRA14-0

	File Names[1,2,3]	CMS Library[1,2]	CMS Class
SCRIPT			
Script Input	EVAL_BF_CRA14_STEP4_R*r*_S*s*.INP	LIBCRA14_EVAL	CRA14-BL
Script Log	EVAL_BF_CRA14_STEP4_R*r*_S*s*.LOG	LIBCRA14_BFR*r*S*s*	CRA14-BL
PREBRAG			
Input	BF1_CRA14_S*s*.INP	LIBCRA14_BF	CRA14-BL
Input	ALG1_BF_CRA14_R*r*_V*vvv*.CDB	LIBCRA14_BF	CRA14-BL
Output	BF2_CRA14_R*r*_S*s*_V*vvv*.INP	LIBCRA14_BFR*r*S*s*	CRA14-BL
Output	BF1_CRA14_R*r*_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

5.3.5 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.

5.3.5.1 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 5.17 and 5.18.

Table 5.17 Salado Flow Step 5 Input and Output Files (Generic Case) for CRA14-BL

	File Names[1,2,3]	CMS Library[1]	CMS Class
MASTER SCRIPT			
Input	EVAL_BF_CRA14BL_STEP5_R1_S*s*.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_BF_CRA14BL_STEP5_R1_S*s*.LOG	LIBCRA14_BFR1S*s*	CRA14-BL
SLAVE SCRIPT			
Log[3]	EVAL_BF_CRA14BL_STEP5_R1_S*s*_V*vvv*.LOG	LIBCRA14_BFR1S*s*	CRA14-BL
BRAGFLO			
Input	BF2_CRA14BL_R1_S*s*_V*vvv*.INP	LIBCRA14_BFR1S*s*	CRA14-BL
Input	BF2_CRA14_CLOSURE.DAT	LIBCRA14_BF	CRA14-BL
Output	BF2_CRA14BL_R1_S*s*_V*vvv*.OUT	NOT KEPT	NOT KEPT
Output	BF2_CRA14BL_R1_S*s*_V*vvv*.SUM	LIBCRA14_BFR1S*s*	CRA14-BL
Output	BF2_CRA14BL_R1_S*s*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Output	BF2_CRA14BL_R1_S*s*_V*vvv*.ROT	NOT KEPT	NOT KEPT
Output	BF2_CRA14BL_R1_S*s*_V*vvv*.RIN	NOT KEPT	NOT KEPT
POSTBRAG			
Input	BF2_CRA14BL_R1_S*s*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Input	ALG1_BF_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_BF	CRA14-BL
Output	BF3_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_BFR1S*s*	CRA14-BL CRA14-TP
Output	BF3_CRA14BL_R1_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG2_BF_CRA14BL.INP	LIBCRA14_BF	CRA14-BL
Input	BF3_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_BFR1S*s*	CRA14-BL
Output	ALG2_BF_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_BFR1S*s*	CRA14-BL
Output	ALG2_BF_CRA14BL_R1_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

1. $s \in \{1, 2, 3, 4, 5, 6\}$
2. $vvv \in \{001, 002, ..., 100\}$ for each s
3. The script inputs are echoed into the log file, so the input file is not kept.

Table 5.18 Salado Flow Step 5 Input and Output Files (Generic Case) for CRA14-0

	File Names[1,2,3,4]	CMS Library[1,2]	CMS Class
MASTER SCRIPT			
Input	EVAL_BF_CRA14_STEP5_R*r*_S*s*.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_BF_CRA14_STEP5_R*r*_S*s*.LOG	LIBCRA14_BFR*r*S*s*	CRA14-0
SLAVE SCRIPT			
Log[4]	EVAL_BF_CRA14_STEP5_R*r*_S*s*_V*vvv*.LOG	LIBCRA14_BFR*r*S*s*	CRA14-0
BRAGFLO			
Input	BF2_CRA14_R*r*_S*s*_V*vvv*.INP	LIBCRA14_BFR*r*S*s*	CRA14-0
Input	BF2_CRA14_CLOSURE.DAT	LIBCRA14_BF	CRA14-0
Output	BF2_CRA14_R*r*_S*s*_V*vvv*.OUT	NOT KEPT	NOT KEPT
Output	BF2_CRA14_R*r*_S*s*_V*vvv*.SUM	LIBCRA14_BFR*r*S*s*	CRA14-0
Output	BF2_CRA14_R*r*_S*s*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Output	BF2_CRA14_R*r*_S*s*_V*vvv*.ROT	NOT KEPT	NOT KEPT
Output	BF2_CRA14_R*r*_S*s*_V*vvv*.RIN	NOT KEPT	NOT KEPT
POSTBRAG			
Input	BF2_CRA14_R*r*_S*s*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Input	ALG1_BF_CRA14_R*r*_V*vvv*.CDB	LIBCRA14_BF	CRA14-0
Output	BF3_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_BFR*r*S*s*	CRA14-0
Output	BF3_CRA14_R*r*_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG2_BF_CRA14.INP	LIBCRA14_BF	CRA14-0
Input	BF3_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_BFR*r*S*s*	CRA14-0
Output	ALG2_BF_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_BFR*r*S*s*	CRA14-0
Output	ALG2_BF_CRA14_R*r*_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

1. $r \in \{1, 2, 3\}$
2. $s \in \{1, 2, 3, 4, 5, 6\}$ for each r
3. $vvv \in \{001, 002, ..., 100\}$ for each s
4. The script inputs are echoed into the log file, so the input file is not kept

5.3.5.2 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 5.3.5.1. 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 5.19 for CRA14-BL and in Table 5.21 for CRA14-0. The modified file names are shown in Table 5.20 for CRA14-BL and Table 5.22 for CRA14-0. 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 5.19 Salado Flow Step 5 Modified Input Runs for CRA14-BL

Replicate	Scenario	Vectors
R1	S1	51
	S2	51
	S3	51
	S4	51
	S5	51
	S6	51

Table 5.20 Salado Flow Step 5 Modified Input Runs File Names for CRA14-BL

	File Names[1]	CMS Library[1]	CMS Class
MASTER SCRIPT			
Input	EVAL_BF_CRA14BL_STEP5_R1_S*s*_V051_MOD.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_BF_CRA14BL_STEP5_R1_S*s*_V051_MOD.LOG	LIBCRA14_BFR1S*s*	CRA14-BL
BRAGFLO			
Input	BF2_CRA14BL_R1_S*s*_V051_MOD.INP	LIBCRA14_BFR1S*s*	CRA14-BL

1. s∈{1, 2, 3, 4, 5, 6} as shown in Table 5.19

Table 5.21 Salado Flow Step 5 Modified Input Run for CRA14-0

Replicate	Scenario	Vectors
R2	S3	99

Table 5.22 Salado Flow Step 5 Modified Input Runs File Names for CRA14-0

	File Names	CMS Library	CMS Class
MASTER SCRIPT			
Input	EVAL_BF_CRA14_STEP5_R2_S3_V099_MOD.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_BF_CRA14_STEP5_R2_S3_V099_MOD.LOG	LIBCRA14_BFR2S3	CRA14-0
BRAGFLO			
Input	BF2_CRA14_R2_S3_V099_MOD.INP	LIBCRA14_BFR2S3	CRA14-0

5.3.6 SALADO FLOW STEP 6

Step 6 re-runs ALGEBRACDB (ALG2) with a modified input file. The file names are the same as the ALGEBRACDB files in Tables 5.17 and 5.18 but are in a different class. This step was added to produce additional files needed for a gas generation analysis. Two DCL run control scripts are used in Step 6. 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 ALGEBRACDB. The input and log files for the Step 6 script as well as the input and output files for ALGEBRACDB are shown in Tables 5.23 and 5.24.

Table 5.23 Salado Flow Step 6 Input and Output Files for CRA14-BL

	File Names[1,2,3]	CMS Library[1]	CMS Class
MASTER SCRIPT			
Input	EVAL_BF_CRA14BL_STEP6_R1_S*s*.INP	LIBCRA14_EVAL	ANALYSIS
Log	EVAL_BF_CRA14BL_STEP6_R1_S*s*.LOG	LIBCRA14_BFR1S*s*	ANALYSIS
SLAVE SCRIPT			
Log[3]	EVAL_BF_CRA14BL_STEP6_R1_S*s*_V*vvv*.LOG	LIBCRA14_BFR1S*s*	ANALYSIS
ALGEBRACDB			
Input	ALG2_BF_CRA14BL.INP	LIBCRA14_BF	ANALYSIS
Input	BF3_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_BFR1S*s*	ANALYSIS
Output	ALG2_BF_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_BFR1S*s*	ANALYSIS
Output	ALG2_BF_CRA14BL_R1_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

1. $s \in \{1, 2, 3, 4, 5, 6\}$
2. $vvv \in \{001, 002, ..., 100\}$ for each s
3. The script inputs are echoed into the log file, so the input file is not kept.

Table 5.24 Salado Flow Step 6 Input and Output Files for CRA14-0

	File Names[1,2,3,4]	CMS Library[1,2]	CMS Class
MASTER SCRIPT			
Input	EVAL_BF_CRA14_STEP6_R*r*_S*s*.INP	LIBCRA14_EVAL	ANALYSIS
Log	EVAL_BF_CRA14_STEP6_R*r*_S*s*.LOG	LIBCRA14_BFR*r*S*s*	ANALYSIS
SLAVE SCRIPT			
Log[4]	EVAL_BF_CRA14_STEP6_R*r*_S*s*_V*vvv*.LOG	LIBCRA14_BFR*r*S*s*	ANALYSIS
ALGEBRACDB			
Input	ALG2_BF_CRA14.INP	LIBCRA14_BF	ANALYSIS
Input	BF3_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_BFR*r*S*s*	ANALYSIS
Output	ALG2_BF_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_BFR*r*S*s*	ANALYSIS
Output	ALG2_BF_CRA14_R*r*_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

1. $r \in \{1, 2, 3\}$
2. $s \in \{1, 2, 3, 4, 5, 6\}$ for each r
3. $vvv \in \{001, 002, ..., 100\}$ for each s
4. The script inputs are echoed into the log file, so the input file is not kept

5.4 ACTINIDE MOBILIZATION CALCULATIONS (PANEL)

Actinide mobilization in WIPP brines as dissolved species and sorbed to colloids is calculated with the PANEL code, run in "concentration" mode (referred to here as PANEL_CON). This information is needed to compute the amount of radionuclides available for transport away from the repository (in direct brine releases to the surface, or in brines migrating to the accessible environment via subsurface pathways).

Three replicates of the mobilization calculations are performed for CRA14-0 and one replicate each for CRA14-BL and CRA14-BV. Five scenarios, nominally corresponding to BRAGFLO scenarios S1-S5, are performed for each replicate. For CRA14-BV and CRA14-0, the file names for steps 4-7 are identical and are distinguished by the class they reside in. However, the only difference between scenarios as far as actinide mobilization is concerned is the actinide solubility associated with the brine type. Actinide solubilities in Salado brine are appropriate for the BRAGFLO S1 (undisturbed) scenario as well as scenarios S4 and S5 (where intrusions penetrate the repository only). Actinide solubilities in Castile brine are appropriate for BRAGFLO scenarios S2 and S3 (where intrusions penetrate the Castile brine pocket). Thus, only S1 and S2 are required. However, S3-S5 are calculated for the sake of convenience in performing Salado transport calculations with the NUTS code (see Section 5.5.1). The Step 8 calculations are documented in Section 5.5.2 after the NUTS code information.

The steps in the calculation, the codes run in each step, and the DCL script used to perform the step are shown in Table 5.25.

Table 5.25 Actinide Mobilization Calculation (PANEL) Run Control Scripts

Step	Codes in Step	Script[1]	CMS Library	CMS Class
1	GENMESH, MATSET	EVAL_GENERIC_STEP1.COM	LIBCRA14_EVAL	CRA14-BL CRA14-BV CRA14-0
2	PANEL_DECAY	EVAL_PANEL_STEP2.COM	LIBCRA14_EVAL	CRA14-BL CRA14-BV CRA14-0
3	ALGEBRACDB	EVAL_PANEL_STEP3.COM	LIBCRA14_EVAL	CRA14-BL CRA14-BV CRA14-0
4	ALGEBRACDB	EVAL_PANEL_STEP4.COM	LIBCRA14_EVAL	CRA14-BL CRA14-BV CRA14-0
5	POSTLHS	EVAL_PANEL_STEP5.COM	LIBCRA14_EVAL	CRA14-BL CRA14-BV CRA14-0
6	ALGEBRACDB	EVAL_PANEL_STEP6.COM	LIBCRA14_EVAL	CRA14-BL
6	ALGEBRACDB	EVAL_PANEL_CRA14BV_STEP6.COM	LIBCRA14_EVAL	CRA14-BV CRA14-0
7	PANEL_CON	EVAL_PANEL_STEP7.COM	LIBCRA14_EVAL	CRA14-BL CRA14-BV CRA14-0
8	PANEL_INT	EVAL_PANEL_CRA14BL_STEP8.COM	LIBCRA14_EVAL	CRA14-BL
8	PANEL_INT	EVAL_PANEL_CRA14BV*b*_STEP8.COM	LIBCRA14_EVAL	CRA14-0

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

5.4.1 ACTINIDE MOBILIZATION 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 5.26, 5.27, and 5.28.

Table 5.26 Actinide Mobilization Step 1 Input and Output Files for CRA14-BL

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BL_STEP1.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_PANEL_CRA14BL_STEP1.LOG	LIBCRA14_PANEL	CRA14-BL
GENMESH			
Input	GM_PANEL_CRA14BL.INP	LIBCRA14_PANEL	CRA14-BL
Output	GM_PANEL_CRA14BL.CDB	LIBCRA14_PANEL	CRA14-BL
Output	GM_PANEL_CRA14BL.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_PANEL_CRA14BL.INP	LIBCRA14_PANEL	CRA14-BL
Input	GM_PANEL_CRA14BL.CDB	LIBCRA14_PANEL	CRA14-BL
Output	MS_PANEL_CRA14BL.CDB	LIBCRA14_PANEL	CRA14-BL
Output	MS_PANEL_CRA14BL.DBG	NOT KEPT	NOT KEPT

Table 5.27 Actinide Mobilization Step 1 Input and Output Files for CRA14-BV

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BV_STEP1.INP	LIBCRA14_EVAL	CRA14-BV
Log	EVAL_PANEL_CRA14BV_STEP1.LOG	LIBCRA14_PANEL	CRA14-BV
GENMESH			
Input	GM_PANEL_CRA14BV.INP	LIBCRA14_PANEL	CRA14-BV
Output	GM_PANEL_CRA14BV.CDB	LIBCRA14_PANEL	CRA14-BV
Output	GM_PANEL_CRA14BV.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_PANEL_CRA14BV.INP	LIBCRA14_PANEL	CRA14-BV
Input	GM_PANEL_CRA14BV.CDB	LIBCRA14_PANEL	CRA14-BV
Output	MS_PANEL_CRA14BV.CDB	LIBCRA14_PANEL	CRA14-BV
Output	MS_PANEL_CRA14BV.DBG	NOT KEPT	NOT KEPT

Table 5.28 Actinide Mobilization Step 1 Input and Output Files for CRA14-0

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14_STEP1.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_PANEL_CRA14_STEP1.LOG	LIBCRA14_PANEL	CRA14-0
GENMESH			

Input	GM_PANEL_CRA14.INP	LIBCRA14_PANEL	CRA14-0
Output	GM_PANEL_CRA14.CDB	LIBCRA14_PANEL	CRA14-0
Output	GM_PANEL_CRA14.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_PANEL_CRA14.INP	LIBCRA14_PANEL	CRA14-0
Input	GM_PANEL_CRA14.CDB	LIBCRA14_PANEL	CRA14-0
Output	MS_PANEL_CRA14.CDB	LIBCRA14_PANEL	CRA14-0
Output	MS_PANEL_CRA14.DBG	NOT KEPT	NOT KEPT

5.4.2 ACTINIDE MOBILIZATION STEP 2

Step 2 uses PANEL in DECAY mode to produce decayed radionuclide information. Step 2 is run once. The output file is used for all replicates, scenarios, and vectors and is only denoted by R1_S1_V001 as required by the PANEL code. The input and log files for the Step 2 script as well as the input and output files for PANEL DECAY are shown in Table 5.29, 5.30, and 5.31.

Table 5.29 Actinide Mobilization Step 2 Input and Output Files for CRA14-BL

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BL_STEP2.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_PANEL_CRA14BL_STEP2.LOG	LIBCRA14_PANEL	CRA14-BL
PANEL DECAY			
Input	MS_PANEL_CRA14BL.CDB	LIBCRA14_PANEL	CRA14-BL
Output	PANEL_DECAY_CRA14BL_R1_S1_V001.CDB	LIBCRA14_PANEL	CRA14-BL
Output	PANEL_DECAY_CRA14BL_R1_S1_V001.DBG	NOT KEPT	NOT KEPT

Table 5.30 Actinide Mobilization Step 2 Input and Output Files for CRA14-BV

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BV_STEP2.INP	LIBCRA14_EVAL	CRA14-BV
Log	EVAL_PANEL_CRA14BV_STEP2.LOG	LIBCRA14_PANEL	CRA14-BV
PANEL DECAY			
Input	MS_PANEL_CRA14BV.CDB	LIBCRA14_PANEL	CRA14-BV
Output	PANEL_DECAY_CRA14BV_R1_S1_V001.CDB	LIBCRA14_PANEL	CRA14-BV
Output	PANEL_DECAY_CRA14BV_R1_S1_V001.DBG	NOT KEPT	NOT KEPT

Table 5.31 Actinide Mobilization Step 2 Input and Output Files for CRA14-0

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14_STEP2.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_PANEL_CRA14_STEP2.LOG	LIBCRA14_PANEL	CRA14-0
PANEL DECAY			
Input	MS_PANEL_CRA14.CDB	LIBCRA14_PANEL	CRA14-0

Output	PANEL_DECAY_CRA14_R1_S1_V001.CDB	LIBCRA14_PANEL	CRA14-0
Output	PANEL_DECAY_CRA14_R1_S1_V001.DBG	NOT KEPT	NOT KEPT

5.4.3 ACTINIDE MOBILIZATION STEP 3

Step 3 performs pre-processing of input data with ALGEBRACDB. The Step 3 script is run once. The input and log files for the Step 3 script as well as the input and output files for ALGEBRACDB are shown in Table 5.32, 5.33, and 5.34.

Table 5.32 Actinide Mobilization Step 3 Input and Output Files for CRA14-BL

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BL_STEP3.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_PANEL_CRA14BL_STEP3.LOG	LIBCRA14_PANEL	CRA14-BL
ALGEBRACDB			
Input	ALG1_PANEL_CRA14BL.INP	LIBCRA14_PANEL	CRA14-BL
Input	PANEL_DECAY_CRA14BL_R1_S1_V001.CDB	LIBCRA14_PANEL	CRA14-BL
Output	ALG1_PANEL_CRA14BL.CDB	LIBCRA14_PANEL	CRA14-BL
Output	ALG1_PANEL_CRA14BL.DBG	NOT KEPT	NOT KEPT

Table 5.33 Actinide Mobilization Step 3 Input and Output Files for CRA14-BV

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BV_STEP3.INP	LIBCRA14_EVAL	CRA14-BV
Log	EVAL_PANEL_CRA14BV_STEP3.LOG	LIBCRA14_PANEL	CRA14-BV
ALGEBRACDB			
Input	ALG1_PANEL_CRA14BV.INP	LIBCRA14_PANEL	CRA14-BV
Input	PANEL_DECAY_CRA14BV_R1_S1_V001.CDB	LIBCRA14_PANEL	CRA14-BV
Output	ALG1_PANEL_CRA14BV.CDB	LIBCRA14_PANEL	CRA14-BV
Output	ALG1_PANEL_CRA14BV.DBG	NOT KEPT	NOT KEPT

Table 5.34 Actinide Mobilization Step 3 Input and Output Files for CRA14-0

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14_STEP3.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_PANEL_CRA14_STEP3.LOG	LIBCRA14_PANEL	CRA14-0
ALGEBRACDB			
Input	ALG1_PANEL_CRA14.INP	LIBCRA14_PANEL	CRA14-0
Input	PANEL_DECAY_CRA14_R1_S1_V001.CDB	LIBCRA14_PANEL	CRA14-0
Output	ALG1_PANEL_CRA14.CDB	LIBCRA14_PANEL	CRA14-0
Output	ALG1_PANEL_CRA14.DBG	NOT KEPT	NOT KEPT

5.4.4 ACTINIDE MOBILIZATION STEP 4

The script for Step 4 performs pre-processing of input data with ALGEBRACDB. The Step 4 script is run once for the CRA14-BL case and once for each Brine Volume (BV*b*) for CRA14-BV and CRA14-0. The input and log files for the script as well as the input and output files for ALGEBRACDB are shown in Table 5.35, 5.36, and 5.37.

Table 5.35 Actinide Mobilization Step 4 Input and Output Files for CRA14-BL

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BL_STEP4.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_PANEL_CRA14BL_STEP4.LOG	LIBCRA14_PANEL	CRA14-BL
ALGEBRACDB			
Input	ALG2_PANEL_CRA14BL.INP	LIBCRA14_PANEL	CRA14-BL
Input	ALG1_PANEL_CRA14BL.CDB	LIBCRA14_PANEL	CRA14-BL
Output	ALG2_PANEL_CRA14BL.CDB	LIBCRA14_PANEL	CRA14-BL
Output	ALG2_PANEL_CRA14BL.DBG	NOT KEPT	NOT KEPT

Table 5.36 Actinide Mobilization Step 4 Input and Output Files for CRA14-BV

	File Names[1]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BV*b*_STEP4.INP	LIBCRA14_EVAL	CRA14-BV
Log	EVAL_PANEL_CRA14BV*b*_STEP4.LOG	LIBCRA14_PANEL	CRA14-BV
ALGEBRACDB			
Input	ALG2_PANEL_CRA14BV*b*.INP	LIBCRA14_PANEL	CRA14-BV
Input	ALG1_PANEL_CRA14BV.CDB	LIBCRA14_PANEL	CRA14-BV
Output	ALG2_PANEL_CRA14BV*b*.CDB	LIBCRA14_PANEL	CRA14-BV
Output	ALG2_PANEL_CRA14BV*b*.DBG	NOT KEPT	NOT KEPT

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

Table 5.37 Actinide Mobilization Step 4 Input and Output Files for CRA14-0

	File Names[1]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BV*b*_STEP4.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_PANEL_CRA14BV*b*_STEP4.LOG	LIBCRA14_PANEL	CRA14-0
ALGEBRACDB			
Input	ALG2_PANEL_CRA14BV*b*.INP	LIBCRA14_PANEL	CRA14-0
Input	ALG1_PANEL_CRA14BV.CDB	LIBCRA14_PANEL	CRA14-0
Output	ALG2_PANEL_CRA14BV*b*.CDB	LIBCRA14_PANEL	CRA14-0
Output	ALG2_PANEL_CRA14BV*b*.DBG	NOT KEPT	NOT KEPT

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

5.4.5 ACTINIDE MOBILIZATION STEP 5

Step 5 uses POSTLHS to assign the sampled parameter values used by PANEL (generated by LHS, see Section 5.2) to the appropriate materials and element block properties. Step 5 is run once for CRA14-BL and once per replicate/brine volume combination for CRA14-BV and CRA14-0. POSTLHS loops over all 100 vectors in the replicate. The input and log files for the Step 5 script as well as the input and output files for POSTLHS are shown in Table 5.38, 5.39 and 5.40.

Table 5.38 Actinide Mobilization Step 5 Input and Output Files for CRA14-BL

	File Names[1]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_PANEL_CRA14BL_STEP5_R1.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_PANEL_CRA14BL_STEP5_R1.LOG	LIBCRA14_PANEL	CRA14-BL
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA14_LHS	CRA14-BL
Input	LHS2_CRA14BL_R1_CON.TRN	LIBCRA14_LHS	CRA14-BL
Input	ALG2_PANEL_CRA14BL.CDB	LIBCRA14_PANEL	CRA14-BL
Output	LHS3_PANEL_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BL
Output	LHS3_PANEL_CRA14BL_R1.DBG	LIBCRA14_PANEL	CRA14-BL

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

Table 5.39 Actinide Mobilization Step 5 Input and Output Files for CRA14-BV

	File Names[1,2]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_PANEL_CRA14BV*b*_STEP5_R1.INP	LIBCRA14_EVAL	CRA14-BV
Log	EVAL_PANEL_CRA14BV*b*_STEP5_R1.LOG	LIBCRA14_PANEL	CRA14-BV
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA14_LHS	CRA14-BV
Input	LHS2_CRA14TP_R1_CON.TRN	LIBCRA14_LHS	CRA14-BV
Input	ALG2_PANEL_CRA14BV*b*.CDB	LIBCRA14_PANEL	CRA14-BV
Output	LHS3_PANEL_CRA14BV*b*_R1_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BV
Output	LHS3_PANEL_CRA14BV*b*_R1.DBG	LIBCRA14_PANEL	CRA14-BV

1. $vvv \in \{001, 002, ..., 100\}$
2. $b \in \{1, 2, 3, 4, 5\}$

Table 5.40 Actinide Mobilization Step 5 Input and Output Files for CRA14-0

	File Names[1,2,3]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_PANEL_CRA14BV*b*_STEP5_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_PANEL_CRA14BV*b*_STEP5_R*r*.LOG	LIBCRA14_PANEL	CRA14-0
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA14_LHS	CRA14-0
Input	LHS2_CRA14_R*r*_CON.TRN	LIBCRA14_LHS	CRA14-0
Input	ALG2_PANEL_CRA14BV*b*.CDB	LIBCRA14_PANEL	CRA14-0

Output	LHS3_PANEL_CRA14BV*b*_R*r*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-0
Output	LHS3_PANEL_CRA14BV*b*_R*r*.DBG	LIBCRA14_PANEL	CRA14-0

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

5.4.6 ACTINIDE MOBILIZATION STEP 6

The script for Step 6 performs processing of input data with ALGEBRACDB. The Step 6 script is run once for CRA14-BL and once per replicate/brine volume combination for CRA14-BV and CRA14-0. ALGEBRACDB 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 ALGEBRACDB are shown in Table 5.41, 5.42, and 5.43.

Table 5.41 Actinide Mobilization Step 6 Input and Output Files for CRA14-BL

	File Names[1]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BL_STEP6_R1.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_PANEL_CRA14BL_STEP6_R1.LOG	LIBCRA14_PANEL	CRA14-BL
ALGEBRACDB			
Input	ALG3_PANEL_CRA14BL.INP	LIBCRA14_PANEL	CRA14-BL
Input	LHS3_PANEL_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BL
Output	ALG3_PANEL_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BL
Output	ALG3_PANEL_CRA14BL_R1_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

Table 5.42 Actinide Mobilization Step 6 Input and Output Files for CRA14-BV

	File Names[1,2]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BV*b*_STEP6_R1.INP	LIBCRA14_EVAL	CRA14-BV
Log	EVAL_PANEL_CRA14BV*b*_STEP6_R1.LOG	LIBCRA14_PANEL	CRA14-BV
ALGEBRACDB			
Input	ALG3_PANEL_CRA14BV*b*.INP	LIBCRA14_PANEL	CRA14-BV
Input	LHS3_PANEL_CRA14BV*b*_R1_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BV
Output	ALG3_PANEL_CRA14BV*b*_R1_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BV
Output	ALG3_PANEL_CRA14BV*b*_R1_V*vvv*.DBG	NOT KEPT	NOT KEPT

1. $vvv \in \{001, 002, ..., 100\}$
2. $b \in \{1, 2, 3, 4, 5\}$

Table 5.43 Actinide Mobilization Step 6 Input and Output Files for CRA14-0

	File Names[1,2,3]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BV*b*_STEP6_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_PANEL_CRA14BV*b*_STEP6_R*r*.LOG	LIBCRA14_PANEL	CRA14-0

ALGEBRACDB			
Input	ALG3_PANEL_CRA14BV*b*.INP	LIBCRA14_PANEL	CRA14-0
Input	LHS3_PANEL_CRA14BV*b*_R*r*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-0
Output	ALG3_PANEL_CRA14BV*b*_R*r*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-0
Output	ALG3_PANEL_CRA14BV*b*_R*r*_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

5.4.7 ACTINIDE MOBILIZATION STEP 7

The script for Step 7 orchestrates the actinide mobilization calculations using PANEL_CON. The Step 7 script is run once for CRA14-BL and once per replicate/brine volume combination for CRA14-BV and CRA14-0. The script loops over scenarios S1 through S5, and all 100 vectors for each scenario, invoking PANEL_CON for each scenario/vector combination. The input and log files for the script as well as the input and output files for PANEL_CON are shown in Table 5.44, 5.45, and 5.46.

Table 5.44 Actinide Mobilization Step 4 Input and Output Files for CRA14-BL

	File Names[1,2]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_PANEL_CRA14BL_STEP7_R1.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_PANEL_CRA14BL_STEP7_R1.LOG	LIBCRA14_PANEL	CRA14-BL
PANEL_CON			
Input	ALG3_PANEL_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BL
Output	PANEL_CON_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BL
Output	PANEL_CON_CRA14BL_R1_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

Table 5.45 Actinide Mobilization Step 4 Input and Output Files for CRA14-BV

	File Names[1,2,3]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_PANEL_CRA14BV*b*_STEP7_R1.INP	LIBCRA14_EVAL	CRA14-BV
Log	EVAL_PANEL_CRA14BV*b*_STEP7_R1.LOG	LIBCRA14_PANEL	CRA14-BV
PANEL_CON			
Input	ALG3_PANEL_CRA14BV*b*_R1_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BV
Output	PANEL_CON_CRA14BV*b*_R1_S*s*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BV
Output	PANEL_CON_CRA14BV*b*_R1_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

Table 5.46 Actinide Mobilization Step 4 Input and Output Files for CRA14-0

	File Names[1,2,3,4]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_PANEL_CRA14BV*b*_STEP7_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_PANEL_CRA14BV*b*_STEP7_R*r*.LOG	LIBCRA14_PANEL	CRA14-0
PANEL_CON			
Input	ALG3_PANEL_CRA14BV*b*_R*r*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-0
Output	PANEL_CON_CRA14BV*b*_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-0
Output	PANEL_CON_CRA14BV*b*_R*r*_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

5.5 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 E2E1 multiple intrusion condition is calculated using the PANEL code.

5.5.1 SALADO TRANSPORT CALCULATIONS (NUTS)

Radionuclide transport in the Salado for single intrusion conditions is calculated using the NUTS code. Three replicate calculations are performed for CRA14-0 and one replicate for CRA14-BL. Five scenarios, corresponding to BRAGFLO scenarios S1-S5, are included in each replicate.

The steps, the codes run in each step, and the DCL scripts used to perform the step are shown in Table 5.47. Corresponding to each run control script is a small utility used to submit the script to a batch queue.

Table 5.47 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	LIBCRA14_EVAL	CRA14-BL CRA14-0
2	SUMMARIZE SCREEN	EVAL_NUT_STEP2.COM SUB_NUT_STEP2.COM	LIBCRA14_EVAL	CRA14-BL CRA14-0
3	MATSET NUTS ALGEBRACDB	EVAL_NUT_STEP3.COM SUB_NUT_STEP3.COM	LIBCRA14_EVAL	CRA14-BL CRA14-0
4	NUTS ALGEBRACDB	EVAL_NUT_STEP4.COM SUB_NUT_STEP4.COM	LIBCRA14_EVAL	CRA14-BL CRA14-0

5.5.1.1 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. 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 5.48 and 5.49.

Table 5.48 Salado Transport (NUTS) Step 1 Input and Output Files for CRA14-BL

	File Names[1,2]	CMS Library[1]	CMS Class
SCRIPT			
Script Input	EVAL_NUT_CRA14BL_STEP1_R1_S*s*.INP	LIBCRA14_EVAL	CRA14-BL
Script Log	EVAL_NUT_CRA14BL_STEP1_R1_S*s*.LOG	LIBCRA14_NUTR1S*s*	CRA14-BL
NUTS_SCN			
Input	NUT_SCN_CRA14BL_S*s*.INP	LIBCRA14_NUT	CRA14-BL
Input	BF2_CRA14BL_R1_S*s*_V*vvv*.INP	LIBCRA14_BFR1S*s*	CRA14-BL
Input	BF3_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_BFR1S*s*	CRA14-BL
Output	NUT_SCN_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	NUT_SCN_CRA14BL_R1_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG_NUT_SCN_CRA14BL.INP	LIBCRA14_NUT	CRA14-BL
Input	NUT_SCN_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	ALG_NUT_SCN_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	ALG_NUT_SCN_CRA14BL_R1_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

Table 5.49 Salado Transport (NUTS) Step 1 Input and Output Files for CRA14-0

	File Names[1,2,3]	CMS Library[1,2]	CMS Class
SCRIPT			
Script Input	EVAL_NUT_CRA14_STEP1_R*r*_S*s*.INP	LIBCRA14_EVAL	CRA14-0
Script Log	EVAL_NUT_CRA14_STEP1_R*r*_S*s*.LOG	LIBCRA14_NUTR*r*S*s*	CRA14-0
NUTS_SCN			
Input	NUT_SCN_CRA14_S*s*.INP	LIBCRA14_NUT	CRA14-0
Input	BF2_CRA14_R*r*_S*s*_V*vvv*.INP	LIBCRA14_BFR*r*S*s*	CRA14-0
Input	BF3_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_BFR*r*S*s*	CRA14-0
Output	NUT_SCN_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	NUT_SCN_CRA14_R*r*_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG_NUT_SCN_CRA14.INP	LIBCRA14_NUT	CRA14-0
Input	NUT_SCN_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	ALG_NUT_SCN_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	ALG_NUT_SCN_CRA14_R*r*_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

5.5.1.2 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. 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 5.50 for CRA14-BL and in Table 5.52 for CRA14-0. Lists of "screened-in" vectors for each replicate/scenario combination are shown in Table 5.51 for CRA14-BL and Table 5.53 for CRA14-0. 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 5.50 Salado Transport (NUTS) Step 2 Input and Output Files for CRA14-BL

	File Names[1,2]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_NUT_CRA14BL_STEP2_R1.INP	LIBCRA14_EVAL	CRA14-BL
Input	SUM_NUT_SCN_CRA14BL.TMPL	LIBCRA14_NUT	CRA14-BL
Output	SUM_NUT_SCN_CRA14BL_R1_S*s*.INP	LIBCRA14_NUTR1S*s*	CRA14-BL
Log	EVAL_NUT_CRA14BL_STEP2_R1.LOG	LIBCRA14_NUT	CRA14-BL
SUMMARIZE			
Input	ALG_NUT_SCN_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Input	SUM_NUT_SCN_CRA14BL_R1_S*s*.INP	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	SUM_NUT_SCN_CRA14BL_R1_S*s*.TBL	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	SUM_NUT_SCN_CRA14BL_R1_S*s*.LOG	NOT KEPT	NOT KEPT
SCREEN			
Input	SCREEN_NUT_SCN_CRA14BL_R1.INP	LIBCRA14_NUT	CRA14-BL
Input	SUM_NUT_SCN_CRA14BL_R1_S*s*.TBL	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	SCREEN_NUT_SCN_CRA14BL_R1_S*s*.OUT	LIBCRA14_NUTR1S*s*	CRA14-BL

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

Table 5.51 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 5.51 Screened-in Vectors by Replicate/Scenario for CRA14-BL

Replicate	Scenario	Vectors	Vector Count
R1	1	None	0
	2	2, 3, 5, 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, 39, 41, 43, 45, 46, 47, 48, 49, 50, 51, 52, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 69, 70, 71, 72, 74, 76, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 91, 92, 93, 94, 98	71
	3	2, 3, 7, 8, 9, 10, 12, 13, 14, 16, 17, 20, 22, 23, 24, 25, 27, 28, 29, 30, 34, 35, 36, 38, 41, 43, 45, 46, 47, 49, 50, 51, 52, 54, 55, 58, 59, 60, 61, 62, 63, 66, 67, 69, 70, 72, 76, 78, 79, 80, 82, 83, 86, 89, 90, 93, 98	57
	4	2, 7, 9, 12, 16, 17, 27, 28, 30, 36, 45, 50, 55, 67, 76, 78, 79, 83, 93, 98	20
	5	2, 7, 9, 12, 16, 17, 27, 28, 30, 36, 45, 50, 55, 67, 76, 78, 79, 83, 93, 98	20

Table 5.52 Salado Transport (NUTS) Step 2 Input and Output Files for CRA14-0

	File Names[1,2,3]	CMS Library[1,2]	CMS Class
SCRIPT			
Input	EVAL_NUT_CRA14_STEP2_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Input	SUM_NUT_SCN_CRA14.TMPL	LIBCRA14_NUT	CRA14-0
Output	SUM_NUT_SCN_CRA14_R*r*_S*s*.INP	LIBCRA14_NUTR*r*S*s*	CRA14-0
Log	EVAL_NUT_CRA14_STEP2_R*r*.LOG	LIBCRA14_NUT	CRA14-0
SUMMARIZE			
Input	ALG_NUT_SCN_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Input	SUM_NUT_SCN_CRA14_R*r*_S*s*.INP	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	SUM_NUT_SCN_CRA14_R*r*_S*s*.TBL	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	SUM_NUT_SCN_CRA14_R*r*_S*s*.LOG	NOT KEPT	NOT KEPT
SCREEN			
Input	SCREEN_NUT_SCN_CRA14_R*r*.INP	LIBCRA14_NUT	CRA14-0
Input	SUM_NUT_SCN_CRA14_R*r*_S*s*.TBL	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	SCREEN_NUT_SCN_CRA14_R*r*_S*s*.OUT	LIBCRA14_NUTR*r*S*s*	CRA14-0

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

Table 5.53 Screened-in Vectors by Replicate/Scenario for CRA14-0

Replicate	Scenario	Vectors	Vector Count
R1	1	None	0
	2	1, 2, 3, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 33, 34, 35, 36, 37, 38, 39, 41, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 68, 69, 70, 71, 72, 74, 75, 76, 77, 78, 79, 80, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 100	87
	3	1, 2, 3, 5, 6, 7, 8, 9, 11, 12, 13, 14, 16, 17, 19, 20, 22, 23, 24, 25, 26, 27, 28, 29, 30, 34, 35, 36, 37, 38, 39, 41, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 54, 55, 58, 59, 60, 61, 62, 63, 64, 66, 67, 69, 70, 71, 72, 74, 75, 76, 77, 78, 79, 80, 82, 83, 84, 86, 88, 89, 90, 92, 93, 94, 95, 96, 97, 98, 100	79
	4	2, 7, 9, 12, 16, 17, 20, 27, 28, 30, 36, 45, 50, 63, 66, 67, 76, 78, 98	19
	5	7, 9, 12, 16, 17, 27, 28, 30, 36, 45, 50, 63, 66, 67, 76, 78, 98	17
R2	1	None	0
	2	1, 2, 3, 4, 6, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 77, 79, 80, 81, 82, 83, 84, 86, 87, 88, 89, 90, 92, 93, 94, 95, 96, 98, 99, 100	88
	3	1, 2, 3, 4, 6, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 19, 20, 21, 22, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 61, 62, 63, 65, 66, 67, 68, 70, 71, 72, 74, 75, 77, 79, 80, 81, 83, 84, 86, 87, 89, 90, 92, 94, 95, 96, 98, 99, 100	81
	4	4, 17, 21, 24, 25, 28, 30, 34, 36, 40, 53, 55, 59, 63, 67, 68, 79, 90, 92, 95, 96, 98	22
	5	4, 17, 21, 24, 25, 28, 30, 34, 36, 40, 53, 55, 59, 63, 67, 68, 79, 90, 92, 95, 96, 98	22
R3	1	None	0
	2	2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 77, 78, 79, 81, 83, 84, 85, 86, 87, 88, 89, 90, 91, 93, 94, 95, 96, 97, 98, 99, 100	92
	3	2, 3, 5, 7, 8, 10, 11, 13, 14, 15, 17, 18, 20, 21, 22, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 50, 51, 52, 53, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 73, 74, 75, 77, 78, 79, 81, 84, 85, 86, 88, 89, 90, 91, 93, 94, 95, 96, 97, 98, 99, 100	81
	4	30, 35, 37, 40, 42, 44, 47, 49, 53, 59, 61, 63, 66, 69, 77, 86, 91, 93, 96, 97	20
	5	30, 35, 40, 42, 44, 47, 49, 53, 59, 63, 66, 69, 77, 86, 93, 96	16

5.5.1.3 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 5.54 and 5.55.

Table 5.54 Salado Transport (NUTS) Step 3 Input and Output Files for CRA14-BL

	File Names[1,2]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_NUT_CRA14BL_STEP3_R1_S*s*.INP	LIBCRA14_EVAL	CRA14-BL
Input	SCREEN_NUT_SCN_CRA14BL_R1_S*s*.OUT	LIBCRA14_NUTR1S*s*	CRA14-BL
Log	EVAL_NUT_CRA14BL_STEP3_R1_S*s*.LOG	LIBCRA14_NUTR1S*s*	CRA14-BL
MATSET			
Input	MS_NUT_CRA14BL.INP	LIBCRA14_NUT	CRA14-BL
Input	BF3_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_BFR1S*s*	CRA14-BL
Output	MS_NUT_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	MS_NUT_CRA14BL_R1_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT
NUTS_ISO			
Input	NUT_ISO_CRA14BL_S*s*.INP	LIBCRA14_NUT	CRA14-BL
Input	BF2_CRA14BL_R1_S*s*_V*vvv*.INP	LIBCRA14_BFR1S*s*	CRA14-BL
Input	MS_NUT_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Input	PANEL_CON_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BL
Output	NUT_ISO_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	NUT_ISO_CRA14BL_R1_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG_NUT_ISO_CRA14BL.INP	LIBCRA14_NUT	CRA14-BL
Input	NUT_ISO_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	ALG_NUT_ISO_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	ALG_NUT_ISO_CRA14BL_R1_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

1. $s \in \{1, 2, 3, 4, 5\}$
2. *vvv* as indicated in Table 5.51.

Table 5.55 Salado Transport (NUTS) Step 3 Input and Output Files for CRA14-0

	File Names[1,2,3]	CMS Library[1,2]	CMS Class
SCRIPT			
Input	EVAL_NUT_CRA14_STEP3_R*r*_S*s*.INP	LIBCRA14_EVAL	CRA14-0
Input	SCREEN_NUT_SCN_CRA14_R*r*_S*s*.OUT	LIBCRA14_NUTR*r*S*s*	CRA14-0
Log	EVAL_NUT_CRA14_STEP3_R*r*_S*s*.LOG	LIBCRA14_NUTR*r*S*s*	CRA14-0
MATSET			
Input	MS_NUT_CRA14.INP	LIBCRA14_NUT	CRA14-0
Input	BF3_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_BFR*r*S*s*	CRA14-0
Output	MS_NUT_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	MS_NUT_CRA14_R*r*_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT
NUTS_ISO			
Input	NUT_ISO_CRA14_S*s*.INP	LIBCRA14_NUT	CRA14-0
Input	BF2_CRA14_R*r*_S*s*_V*vvv*.INP	LIBCRA14_BFR*r*S*s*	CRA14-0
Input	MS_NUT_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Input	PANEL_CON_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-0
Output	NUT_ISO_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	NUT_ISO_CRA14_R*r*_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG_NUT_ISO_CRA14.INP	LIBCRA14_NUT	CRA14-0
Input	NUT_ISO_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	ALG_NUT_ISO_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	ALG_NUT_ISO_CRA14_R*r*_S*s*_V*vvv*.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 5.515.53.

5.5.1.4 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 5.56 and 5.57.

Table 5.56 Salado Transport (NUTS) Step 4 Input and Output Files for CRA14-BL

	File Names[1,2,3]	**CMS Library[1]**	**CMS Class**
SCRIPT			
Input	EVAL_NUT_CRA14BL_STEP4_R1_Ss.INP	LIBCRA14_EVAL	CRA14-BL
Input	SCREEN_NUT_SCN_CRA14BL_R1_Ss.OUT	LIBCRA14_NUTR1Ss	CRA14-BL
Log	EVAL_NUT_CRA14BL_STEP4_R1_Ss.LOG	LIBCRA14_NUTR1Ss	CRA14-BL
NUTS_INT			
Input	NUT_INT_CRA14BL_Ss_Tttttt.INP	LIBCRA14_NUT	CRA14-BL
Input	BF2_CRA14BL_R1_Ss_Vvvv.INP	LIBCRA14_BFR1Ss	CRA14-BL
Input	MS_NUT_CRA14BL_R1_Ss_Vvvv.CDB	LIBCRA14_NUTR1Ss	CRA14-BL
Input	PANEL_CON_CRA14BL_R1_Ss_Vvvv.CDB	LIBCRA14_PANEL	CRA14-BL
Input	NUT_ISO_CRA14BL_R1_S1_Vvvv.CDB	LIBCRA14_NUTR1S1	CRA14-BL
Output	NUT_INT_CRA14BL_R1_Ss_Ttttt_Vvvv.CDB	LIBCRA14_NUTR1Ss	CRA14-BL
Output	NUT_INT_CRA14BL_R1_Ss_Ttttt_Vvvv.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG_NUT_ISO_CRA14BL.INP	LIBCRA14_NUT	CRA14-BL
Input	NUT_INT_CRA14BL_R1_Ss_Ttttt_Vvvv.CDB	LIBCRA14_NUTR1Ss	CRA14-BL
Output	ALG_NUT_INT_CRA14BL_R1_Ss_Ttttt_Vvvv.CDB	LIBCRA14_NUTR1Ss	CRA14-BL
Output	ALG_NUT_INT_CRA14BL_R1_Ss_Ttttt_Vvvv.DGB	NOT KEPT	NOT KEPT

1. $s \in \{2, 3, 4, 5\}$
2. $ttttt \in \begin{cases} \{00100\} & \text{for S2, S4} \\ \{03000, 05000, 07000, 09000\} & \text{for S3, S5} \end{cases}$
3. *vvv* as specified in Table 5.51.

Table 5.57 Salado Transport (NUTS) Step 4 Input and Output Files for CRA14-0

	File Names[1,2,3,4]	CMS Library[1,2]	CMS Class
SCRIPT			
Input	EVAL_NUT_CRA14_STEP4_R*r*_S*s*.INP	LIBCRA14_EVAL	CRA14-0
Input	SCREEN_NUT_SCN_CRA14_R*r*_S*s*.OUT	LIBCRA14_NUTR*r*S*s*	CRA14-0
Log	EVAL_NUT_CRA14_STEP4_R*r*_S*s*.LOG	LIBCRA14_NUTR*r*S*s*	CRA14-0
NUTS_INT			
Input	NUT_INT_CRA14_S*s*_T*ttttt*.INP	LIBCRA14_NUT	CRA14-0
Input	BF2_CRA14_R*r*_S*s*_V*vvv*.INP	LIBCRA14_BFR*r*S*s*	CRA14-0
Input	MS_NUT_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Input	PANEL_CON_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-0
Input	NUT_ISO_CRA14_R*r*_S1_V*vvv*.CDB	LIBCRA14_NUTR*r*S1	CRA14-0
Output	NUT_INT_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	NUT_INT_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG_NUT_ISO_CRA14.INP	LIBCRA14_NUT	CRA14-0
Input	NUT_INT_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	ALG_NUT_INT_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	ALG_NUT_INT_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.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 5.513.

5.5.2 SALADO TRANSPORT CALCULATIONS (PANEL)

Radionuclide transport to the Culebra for the E2E1 intrusion combination (BRAGFLO scenario S6; see Table 5.7) is calculated by running the PANEL code in "intrusion mode" (PANEL_INT). This calculation is Step 8 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 5.58 and 5.59.

Table 5.58 Salado Transport (PANEL_INT) Input and Output Files for CRA14-BL

	File Names[1,2]	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_PANEL_CRA14BL_STEP8_R1.INP	LIBCRA14_EVAL	CRA14-BL
Script Log	EVAL_PANEL_CRA14BL_STEP8_R1.LOG	LIBCRA14_PANEL	CRA14-BL
PANEL_INT			
Input	ALG3_PANEL_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BL
Input	ALG2_BF_CRA14BL_R1_S6_V*vvv*.CDB	LIBCRA14_BFR1S6	CRA14-BL
Output	PANEL_INT_CRA14BL_R1_S6_TI*tttt*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BL
Output	PANEL_INT_CRA14BL_R1_S6_TI*tttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

Table 5.59 Salado Transport (PANEL_INT) Input and Output Files for CRA14-0

	File Names[1,2,3,4]	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_PANEL_CRA14_STEP8_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Script Log	EVAL_PANEL_CRA14_STEP8_R*r*.LOG[5]	LIBCRA14_PANEL	CRA14-0
PANEL_INT			
Input	ALG3_PANEL_CRA14BV*b*_R*r*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-0
Input	ALG2_BF_CRA14_R*r*_S6_V*vvv*.CDB	LIBCRA14_BFR*r*S6	CRA14-0
Output	PANEL_INT_CRA14BV*b*_R*r*_S6_TI*tttt*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-0
Output	PANEL_INT_CRA14BV*b*_R*r*_S6_TI*tttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT

1. $r \in \{1, 2, 3\}$
2. $tttt \in \{0100, 0350, 1000, 2000, 4000, 6000, 9000\}$ for each r
3. $vvv \in \{001, 002, ..., 100\}$ for each intrusion time
4. $b \in \{1, 2, 3, 4, 5\}$
5. The log files for each run have the same name. The generation of the log file corresponds to the Brine Volume for which it was output for.

5.6 SINGLE-INTRUSION SPALLINGS VOLUME CALCULATIONS (DRSPALL)

Implementation of the PA updates or corrections do not affect the CRA-2014 PA DRSPALL calculations, thus, the spallings results calculated by DRSPALL for the CRA-2004 PABC will be used for the CRA-2014. The CRA-2004 PABC DRSPALL results are documented in Vugrin (2005).

5.7 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 5.60. Step 3 also includes a small utility used to submit the script to a batch queue.

Table 5.60 Solids Volume (CUTTINGS_S) Run Control Scripts

Step	Codes Run in Step	Scripts	Script CMS Library	Script CMS Class
1	GENMESH MATSET	EVAL_CUSP_STEP1.COM	LIBCRA14_EVAL	CRA14-BL, CRA14-TP, CRA14-0
2	POSTLHS	EVAL_CUSP_STEP2.COM	LIBCRA14_EVAL	CRA14-BL, CRA14-TP, CRA14-0
3	CUTTINGS_S	EVAL_CUSP_STEP3.COM SUB_CUSP_STEP3.COM	LIBCRA14_EVAL	CRA14-BL, CRA14-TP, CRA14-0

Three replicate calculations are performed for CRA14-0 and one replicate each for CRA14-BL and CRA14-TP. 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 CUTTINGS_S 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 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.

5.7.1 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 are shown in Table 5.61, 5.62, and 5.63.

Table 5.61 Solids Volume Step 1 Input and Output Files for CRA14-BL

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_CUSP_CRA14BL_STEP1.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_CUSP_CRA14BL_STEP1.LOG	LIBCRA14_CUSP	CRA14-BL
GENMESH			
Input	GM_CUSP_CRA14BL.INP	LIBCRA14_CUSP	CRA14-BL
Output	GM_CUSP_CRA14BL.CDB	LIBCRA14_CUSP	CRA14-BL
Output	GM_CUSP_CRA14BL.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_CUSP_CRA14BL.INP	LIBCRA14_CUSP	CRA14-BL
Input	GM_CUSP_CRA14BL.CDB	LIBCRA14_CUSP	CRA14-BL
Output	MS_CUSP_CRA14BL.CDB	LIBCRA14_CUSP	CRA14-BL
Output	MS_CUSP_CRA14BL.DBG	NOT KEPT	NOT KEPT

Table 5.62 Solids Volume Step 1 Input and Output Files for CRA14-TP

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_CUSP_CRA14TP_STEP1.INP	LIBCRA14_EVAL	CRA14-TP
Log	EVAL_CUSP_CRA14TP_STEP1.LOG	LIBCRA14_CUSP	CRA14-TP
GENMESH			
Input	GM_CUSP_CRA14TP.INP	LIBCRA14_CUSP	CRA14-TP
Output	GM_CUSP_CRA14TP.CDB	LIBCRA14_CUSP	CRA14-TP
Output	GM_CUSP_CRA14TP.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_CUSP_CRA14TP.INP	LIBCRA14_CUSP	CRA14-TP
Input	GM_CUSP_CRA14TP.CDB	LIBCRA14_CUSP	CRA14-TP
Output	MS_CUSP_CRA14TP.CDB	LIBCRA14_CUSP	CRA14-TP
Output	MS_CUSP_CRA14TP.DBG	NOT KEPT	NOT KEPT

Table 5.63 Solids Volume Step 1 Input and Output Files for CRA14-0

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_CUSP_CRA14_STEP1.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_CUSP_CRA14_STEP1.LOG	LIBCRA14_CUSP	CRA14-0
GENMESH			
Input	GM_CUSP_CRA14.INP	LIBCRA14_CUSP	CRA14-0
Output	GM_CUSP_CRA14.CDB	LIBCRA14_CUSP	CRA14-0
Output	GM_CUSP_CRA14.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_CUSP_CRA14.INP	LIBCRA14_CUSP	CRA14-0
Input	GM_CUSP_CRA14.CDB	LIBCRA14_CUSP	CRA14-0
Output	MS_CUSP_CRA14.CDB	LIBCRA14_CUSP	CRA14-0
Output	MS_CUSP_CRA14.DBG	NOT KEPT	NOT KEPT

5.7.2 SOLIDS VOLUME STEP 2

Step 2 uses POSTLHS to assign the sampled parameter values used by CUTTINGS_S (generated by LHS, see Section 5.2) 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 5.64, 5.65, and 5.66.

Table 5.64 Solids Volume Step 2 Input and Output Files for CRA14-BL

	File Names[1]	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CUSP_CRA14BL_STEP2_R1.INP	LIBCRA14_EVAL	CRA14-BL
Script Log	EVAL_CUSP_CRA14BL_STEP2_R1.LOG	LIBCRA14_CUSP	CRA14-BL
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA14_LHS	CRA14-BL
Input	LHS2_CRA14BL_R1_CON.TRN	LIBCRA14_LHS	CRA14-BL
Input	MS_CUSP_CRA14BL.CDB	LIBCRA14_CUSP	CRA14-BL
Output	LHS3_CUSP_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_CUSP	CRA14-BL
Output	LHS3_CUSP_CRA14BL_R1.DBG	LIBCRA14_CUSP	CRA14-BL

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

Table 5.65 Solids Volume Step 2 Input and Output Files for CRA14-TP

	File Names[1]	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CUSP_CRA14TP_STEP2_R1.INP	LIBCRA14_EVAL	CRA14-TP
Script Log	EVAL_CUSP_CRA14TP_STEP2_R1LOG	LIBCRA14_CUSP	CRA14-TP
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA14_LHS	CRA14-TP
Input	LHS2_CRA14TP_R1_CON.TRN	LIBCRA14_LHS	CRA14-TP
Input	MS_CUSP_CRA14TP.CDB	LIBCRA14_CUSP	CRA14-TP
Output	LHS3_CUSP_CRA14TP_R1_V*vvv*.CDB	LIBCRA14_CUSP	CRA14-TP
Output	LHS3_CUSP_CRA14TP_R1.DBG	LIBCRA14_CUSP	CRA14-TP

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

Table 5.66 Solids Volume Step 2 Input and Output Files for CRA14-0

	File Names[1,2]	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CUSP_CRA14_STEP2_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Script Log	EVAL_CUSP_CRA14_STEP2_R*r*.LOG	LIBCRA14_CUSP	CRA14-0
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA14_LHS	CRA14-0
Input	LHS2_CRA14_R*r*_CON.TRN	LIBCRA14_LHS	CRA14-0
Input	MS_CUSP_CRA14.CDB	LIBCRA14_CUSP	CRA14-0
Output	LHS3_CUSP_CRA14_R*r*_V*vvv*.CDB	LIBCRA14_CUSP	CRA14-0
Output	LHS3_CUSP_CRA14_R*r*.DBG	LIBCRA14_CUSP	CRA14-0

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

5.7.3 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 5.67, 5.68, and 5.69.

Table 5.67 Solids Volume Step 3 Input and Output Files for CRA14-BL

	File Names[1,2,3,4]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_CUSP_CRA14BL_STEP3_R1.INP	LIBCRA14_EVAL	CRA14-BL
Output	CUSP_CRA14BL_MASTER_R1.INP	LIBCRA14_CUSP	CRA14-BL
Log	EVAL_CUSP_CRA14BL_STEP3_R1.LOG	LIBCRA14_CUSP	CRA14-BL
CUTTINGS_S			
Input	CUSP_CRA14BL_MASTER_R1.INP	LIBCRA14_CUSP	CRA14-BL
Input	CUSP_CRA14BL.INP	LIBCRA14_CUSP	CRA14-BL
Input	LHS3_CUSP_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_CUSP	CRA14-BL
Input	BF3_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_BFR1S*s*	CRA14-BL
Input	MSPALL_DRS_CRA1BC_R1.OUT	LIBCRA1BC_DRS	CRA14-BL
Output	CUSP_CRA14BL_R1.TBL	LIBCRA14_CUSP	CRA14-BL
Output	CUSP_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.CDB	LIBCRA14_CUSPR1S*s*	CRA14-BL
Output	CUSP_CRA14BL_R1.DBG	LIBCRA14_CUSP	CRA14-BL

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

Table 5.68 Solids Volume Step 3 Input and Output Files for CRA14-TP

	File Names[1,2,3,4]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_CUSP_CRA14TP_STEP3_R1.INP	LIBCRA14_EVAL	CRA14-TP
Output	CUSP_CRA14TP_MASTER_R1.INP	LIBCRA14_CUSP	CRA14-TP
Log	EVAL_CUSP_CRA14TP_STEP3_R1.LOG	LIBCRA14_CUSP	CRA14-TP
CUTTINGS_S			
Input	CUSP_CRA14TP_MASTER_R1.INP	LIBCRA14_CUSP	CRA14-TP
Input	CUSP_CRA14TP.INP	LIBCRA14_CUSP	CRA14-TP
Input	LHS3_CUSP_CRA14TP_R1_V*vvv*.CDB	LIBCRA14_CUSP	CRA14-TP
Input	BF3_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_BFR1S*s*	CRA14-TP
Input	MSPALL_DRS_CRA1BC_R1.OUT	LIBCRA1BC_DRS	CRA14-TP
Output	CUSP_CRA14TP_R1.TBL	LIBCRA14_CUSP	CRA14-TP
Output	CUSP_CRA14TP_R1_S*s*_T*tttt*_*c*_V*vvv*.CDB	LIBCRA14_CUSPR1S*s*	CRA14-TP
Output	CUSP_CRA14TP_R1.DBG	LIBCRA14_CUSP	CRA14-TP

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

Table 5.69 Solids Volume Step 3 Input and Output Files for CRA14-0

	File Names[1,2,3,4,5]	CMS Library[1,2]	CMS Class
SCRIPT			
Input	EVAL_CUSP_CRA14_STEP3_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Output	CUSP_CRA14_MASTER_R*r*.INP	LIBCRA14_CUSP	CRA14-0
Log	EVAL_CUSP_CRA14_STEP3_R*r*.LOG	LIBCRA14_CUSP	CRA14-0
CUTTINGS_S			
Input	CUSP_CRA14_MASTER_R*r*.INP	LIBCRA14_CUSP	CRA14-0
Input	CUSP_CRA14.INP	LIBCRA14_CUSP	CRA14-0
Input	LHS3_CUSP_CRA14_R*r*_V*vvv*.CDB	LIBCRA14_CUSP	CRA14-0
Input	BF3_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_BFR*r*S*s*	CRA14-0
Input	MSPALL_DRS_CRA1BC_R*r*.OUT	LIBCRA1BC_DRS	CRA14-0
Output	CUSP_CRA14_R*r*.TBL	LIBCRA14_CUSP	CRA14-0
Output	CUSP_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBCRA14_CUSPR*r*S*s*	CRA14-0
Output	CUSP_CRA14_R*r*.DBG	LIBCRA14_CUSP	CRA14-0

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

5.8 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 5.70.

Three replicates are performed for CRA14-0 and one replicate for CRA14-BL. 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 L, middle M and upper U) 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 5.70 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	LIBCRA14_EVAL	CRA14-BL CRA14-0
2	ALGEBRACDB RELATE ICSET	EVAL_DBR_STEP2.COM SUB_DBR_STEP2.COM	LIBCRA14_EVAL	CRA14-BL CRA14-0
3	PREBRAG BRAGFLO POSTBRAG ALGEBRACDB	EVAL_DBR_STEP3.COM SUB_DBR_STEP3.COM	LIBCRA14_EVAL	CRA14-BL CRA14-0

5.8.1 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 5.71 and 5.72.

Table 5.71 Direct Brine Release Step 1 Input and Output Files for CRA14-BL

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_DBR_CRA14BL_STEP1.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_DBR_CRA14BL_STEP1.LOG	LIBCRA14_DBR	CRA14-BL
GENMESH			
Input	GM_DBR_CRA14BL.INP	LIBCRA14_DBR	CRA14-BL
Output	GM_DBR_CRA14BL.CDB	LIBCRA14_DBR	CRA14-BL
Output	GM_DBR_CRA14BL.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_DBR_CRA14BL.INP	LIBCRA14_DBR	CRA14-BL
Input	GM_DBR_CRA14BL.CDB	LIBCRA14_DBR	CRA14-BL
Output	MS_DBR_CRA14BL.CDB	LIBCRA14_DBR	CRA14-BL
Output	MS_DBR_CRA14BL.DBG	NOT KEPT	NOT KEPT

Table 5.72 Direct Brine Release Step 1 Input and Output Files for CRA14-0

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_DBR_CRA14_STEP1.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_DBR_CRA14_STEP1.LOG	LIBCRA14_DBR	CRA14-0
GENMESH			
Input	GM_DBR_CRA14.INP	LIBCRA14_DBR	CRA14-0
Output	GM_DBR_CRA14.CDB	LIBCRA14_DBR	CRA14-0
Output	GM_DBR_CRA14.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_DBR_CRA14.INP	LIBCRA14_DBR	CRA14-0
Input	GM_DBR_CRA14.CDB	LIBCRA14_DBR	CRA14-0
Output	MS_DBR_CRA14.CDB	LIBCRA14_DBR	CRA14-0
Output	MS_DBR_CRA14.DBG	NOT KEPT	NOT KEPT

5.8.2 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 5.73 and 5.74.

Table 5.73 Direct Brine Release Step 2 Input and Output Files for CRA14-BL

	File Names[1,2,3]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_DBR_CRA14BL_STEP2_R1_S*s*.INP	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_DBR_CRA14BL_STEP2_R1_S*s*.LOG	LIBCRA14_DBRR1S*s*	CRA14-BL
ALGEBRACDB			
Input	ALG1_DBR_CRA14BL.INP	LIBCRA14_DBR	CRA14-BL
Input	CUSP_CRA14BL_R1_S*s*_T*ttttt*_L_V*vvv*.CDB[4]	LIBCRA14_CUSPR1S*s*	CRA14-BL
Output	ALG1_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	ALG1_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
RELATE_1			
Input	REL1_DBR_CRA14BL.INP	LIBCRA14_DBR	CRA14-BL
Input	MS_DBR_CRA14BL.CDB	LIBCRA14_DBR	CRA14-BL
Input	ALG1_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	REL1_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	REL1_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
RELATE_2			
Input	REL2_DBR_CRA14BL_S*s*.INP	LIBCRA14_DBR	CRA14-BL
Input	REL1_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Input	BF3_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_BFR1S*s*	CRA14-BL
Output	REL2_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	REL2_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ICSET			
Input	IC_DBR_CRA14BL_S*s*.INP	LIBCRA14_DBR	CRA14-BL
Input	REL2_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	IC_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	IC_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG2_DBR_CRA14BL_S*s*.INP	LIBCRA14_DBR	CRA14-BL
Input	IC_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	ALG2_DBR_CRA14BL_R1_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	ALG2_DBR_CRA14BL_R1_S*s*_T*ttttt*_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. $vvv \in \{001, 002, ..., 100\}$ for each intrusion

4. The files CUSP_CRA14_R1_S*s*_T*ttttt*_L_V*vvv*.CDB do not have leading zeros in front of the intrusion time *ttttt*.

Table 5.74 Direct Brine Release Step 2 Input and Output Files for CRA14-0

	File Names[1,2,3,4]	CMS Library[1,2]	CMS Class
SCRIPT			
Input	EVAL_DBR_CRA14_STEP2_R*r*_S*s*.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_DBR_CRA14_STEP2_R*r*_S*s*.LOG	LIBCRA14_DBRR*r*S*s*	CRA14-0
ALGEBRACDB			
Input	ALG1_DBR_CRA14.INP	LIBCRA14_DBR	CRA14-0
Input	CUSP_CRA14_R*r*_S*s*_T*ttttt*_L_V*vvv*.CDB[5]	LIBCRA14_CUSPR*r*S*s*	CRA14-0
Output	ALG1_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	ALG1_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
RELATE_1			
Input	REL1_DBR_CRA14.INP	LIBCRA14_DBR	CRA14-0
Input	MS_DBR_CRA14.CDB	LIBCRA14_DBR	CRA14-0
Input	ALG1_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	REL1_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	REL1_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
RELATE_2			
Input	REL2_DBR_CRA14_S*s*.INP	LIBCRA14_DBR	CRA14-0
Input	REL1_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Input	BF3_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_BFR*r*S*s*	CRA14-0
Output	REL2_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	REL2_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ICSET			
Input	IC_DBR_CRA14_S*s*.INP	LIBCRA14_DBR	CRA14-0
Input	REL2_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	IC_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	IC_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG2_DBR_CRA14_S*s*.INP	LIBCRA14_DBR	CRA14-0
Input	IC_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	ALG2_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	ALG2_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT

1. $r \in \{1, 2, 3\}$
2. $s \in \{1, 2, 3, 4, 5\}$ for each r
3. $ttttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} & \text{for S1} \\ \{00550, 00750, 02000, 04000, 10000\} & \text{for S2, S4} \\ \{01200, 01400, 03000, 05000, 10000\} & \text{for S3, S5} \end{cases}$
4. $vvv \in \{001, 002, ..., 100\}$ for each intrusion
5. The files CUSP_CRA14_R*r*_S*s*_T*ttttt*_L_V*vvv*.CDB do not have leading zeros in front of the intrusion time *ttttt*.

5.8.3 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 5.75 and 5.76.

Table 5.75 Direct Brine Release Step 3 Input and Output Files for CRA14-BL

	File Names[1,2,3,4]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_DBR_CRA14BL_STEP3_R1_S*s*.INP[5]	LIBCRA14_EVAL	CRA14-BL
Log	EVAL_DBR_CRA14BL_STEP3_R1_S*s*.LOG[5]	LIBCRA14_DBRR1S*s*	CRA14-BL
PREBRAG			
Input	BF1_DBR_CRA14BL_*c*.INP	LIBCRA14_DBR	CRA14-BL
Input	ALG2_DBR_CRA14BL_R1_S*s*_T*tttt*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	BF2_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.INP	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	BF1_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.DBG	NOT KEPT	NOT KEPT
BRAGFLO			
Input	BF2_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.INP	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	BF2_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.OUT	NOT KEPT	NOT KEPT
Output	BF2_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.SUM	NOT KEPT	NOT KEPT
Output	BF2_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Output	BF2_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.ROT	NOT KEPT	NOT KEPT
Output	BF2_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.RIN	NOT KEPT	NOT KEPT
POSTBRAG			
Input	ALG2_DBR_CRA14BL_R1_S*s*_T*tttt*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Input	BF2_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Output	BF3_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	BF3_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG3_DBR_CRA14BL_*c*.INP	LIBCRA14_DBR	CRA14-BL
Input	BF3_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	ALG3_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	ALG3_DBR_CRA14BL_R1_S*s*_T*tttt*_*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

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

5. A script input and a log file for R1S1 T100 are separate from the other script input and log files. EVAL_DBR_CRA14BL_STEP3_R1_S1_T100.INP and EVAL_DBR_CRA14BL_STEP3_R1_S1_T100.LOG

Table 5.76 Direct Brine Release Step 3 Input and Output Files for CRA14-0

	File Names[1,2,3,4,5]	CMS Library[1,2]	CMS Class
SCRIPT			
Input	EVAL_DBR_CRA14_STEP3_R*r*_S*s*.INP[6]	LIBCRA14_EVAL	CRA14-0
Log	EVAL_DBR_CRA14_STEP3_R*r*_S*s*.LOG[6]	LIBCRA14_DBRR*r*S*s*	CRA14-0
PREBRAG			
Input	BF1_DBR_CRA14_*c*.INP	LIBCRA14_DBR	CRA14-0
Input	ALG2_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	BF2_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.INP	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	BF1_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.DBG	NOT KEPT	NOT KEPT
BRAGFLO			
Input	BF2_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.INP	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	BF2_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.OUT	NOT KEPT	NOT KEPT
Output	BF2_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.SUM	NOT KEPT	NOT KEPT
Output	BF2_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Output	BF2_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.ROT	NOT KEPT	NOT KEPT
Output	BF2_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.RIN	NOT KEPT	NOT KEPT
POSTBRAG			
Input	ALG2_DBR_CRA14_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Input	BF2_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Output	BF3_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	BF3_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG3_DBR_CRA14_*c*.INP	LIBCRA14_DBR	CRA14-0
Input	BF3_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	ALG3_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	ALG3_DBR_CRA14_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.DBG	NOT KEPT	NOT KEPT

1. $r \in \{1, 2, 3\}$
2. $s \in \{1, 2, 3, 4, 5\}$ for each r
3. $ttttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} & \text{for S1} \\ \{00550, 00750, 02000, 04000, 10000\} & \text{for S2, S4} \\ \{01200, 01400, 03000, 05000, 10000\} & \text{for S3, S5} \end{cases}$
4. $c \in \{\text{L, M, U}\}$ for each intrusion
5. $vvv \in \{001, 002, ..., 100\}$ for each c
6. A script input and a log file for R1S1 T100 are separate from the other script input and log files. EVAL_DBR_CRA14_STEP3_R1_S1_T100.INP and EVAL_DBR_CRA14_STEP3_R1_S1_T100.LOG

5.9 CULEBRA TRANSPORT CALCULATIONS

The same transmissivity fields as were developed in the PABC-2009 will be used for the CRA-2014 PA. As a result, the Culebra flow and transport results obtained in the PABC-2009 will be used for the CRA-2014 PA. These results are documented in Kuhlman (2010).

5.10 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 (Camphouse 2010). The run control scripts used to process the CDB data for the various process models are shown in Table 5.77. 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 5.77 CCDF Input Tabulation Run Control Scripts

Code	Script	Script CMS Library	Script CMS Class
SUMMARIZE	EVAL_SUM.COM SUB_SUM.COM	LIBCRA14_EVAL	CRA14-BL CRA14-BV CRA14-0

5.10.1 CCDF INPUT TABULATION FOR ACTINIDE MOBILIZATION

SUMMARIZE is used to extract and tabulate mobilized actinide concentrations from PANEL_CON output CDB files (see Section 5.4). The DCL run control script is run for scenarios S1 and S2 for each replicate/brine volume combination. The script uses the same SUMMARIZE input control file template for all runs, generating a SUMMARIZE input control file for each replicate/scenario/brine volume combination. The script input and log files along with the SUMMARIZE input and output files are shown in Table 5.78, 5.79, and 5.80.

Table 5.78 CCDF Input Tabulation Input and Output Files (Actinide Mobilization) for CRA14-BL

	File Names[1,2]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_SUM_PANEL_CON_CRA14BL_R1_S*s*.INP	LIBCRA14_EVAL	CRA14-BL
Input	SUM_PANEL_CON_CRA14BL.TMPL	LIBCRA14_SUM	CRA14-BL
Output	SUM_PANEL_CON_CRA14BL_R1_S*s*.INP	LIBCRA14_SUM	CRA14-BL
Log	EVAL_SUM_PANEL_CON_CRA14BL_R1_S*s*.LOG	LIBCRA14_SUM	CRA14-BL
SUMMARIZE			
Input	SUM_PANEL_CON_CRA14BL_R1_S*s*.INP	LIBCRA14_SUM	CRA14-BL
Input	PANEL_CON_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BL
Output	SUM_PANEL_CON_CRA14BL_R1_S*s*.TBL	LIBCRA14_SUM	CRA14-BL
Output	SUM_PANEL_CON_CRA14BL_R1_S*s*.DBG	NOT KEPT	NOT KEPT

1. $s \in \{1, 2\}$
2. $vvv \in \{001, 002, ..., 100\}$ for each s

Table 5.79 CCDF Input Tabulation Input and Output Files (Actinide Mobilization) for CRA14-BV

	File Names[1,2,3]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_SUM_PANEL_CON_CRA14BV*b*_R1_S*s*.INP	LIBCRA14_EVAL	CRA14-BV
Input	SUM_PANEL_CON_CRA14BV.TMPL	LIBCRA14_SUM	CRA14-BV
Output	SUM_PANEL_CON_CRA14BV*b*_R1_S*s*.INP	LIBCRA14_SUM	CRA14-BV
Log	EVAL_SUM_PANEL_CON_CRA14BV*b*_R1_S*s*.LOG	LIBCRA14_SUM	CRA14-BV
SUMMARIZE			
Input	SUM_PANEL_CON_CRA14BV*b*_R1_S*s*.INP	LIBCRA14_SUM	CRA14-BV
Input	PANEL_CON_CRA14BV*b*_R1_S*s*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BV
Output	SUM_PANEL_CON_CRA14BV*b*_R1_S*s*.TBL	LIBCRA14_SUM	CRA14-BV
Output	SUM_PANEL_CON_CRA14BV*b*_R1_S*s*.DBG	NOT KEPT	NOT KEPT

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

Table 5.80 CCDF Input Tabulation Input and Output Files (Actinide Mobilization) for CRA14-0

	File Names[1,2,3,4]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_SUM_PANEL_CON_CRA14BV*b*_R*r*_S*s*.INP	LIBCRA14_EVAL	CRA14-0
Input	SUM_PANEL_CON_CRA14BV.TMPL	LIBCRA14_SUM	CRA14-0
Output	SUM_PANEL_CON_CRA14BV*b*_R*r*_S*s*.INP	LIBCRA14_SUM	CRA14-0
Log	EVAL_SUM_PANEL_CON_CRA14BV*b*_R*r*_S*s*.LOG	LIBCRA14_SUM	CRA14-0
SUMMARIZE			
Input	SUM_PANEL_CON_CRA14BV*b*_R*r*_S*s*.INP	LIBCRA14_SUM	CRA14-0
Input	PANEL_CON_CRA14BV*b*_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-0
Output	SUM_PANEL_CON_CRA14BV*b*_R*r*_S*s*.TBL	LIBCRA14_SUM	CRA14-0
Output	SUM_PANEL_CON_CRA14BV*b*_R*r*_S*s*.DBG	NOT KEPT	NOT KEPT

1. $r \in \{1, 2, 3\}$
2. $s \in \{1, 2\}$ for each r

3. *vvv*∈{001, 002, ..., 100} for each *s*

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

5.10.2 CCDF INPUT TABULATION FOR COLLOID SOURCE TERM

SUMMARIZE is used to extract and tabulate the colloid fractions data from PANEL_CON output CDB files (see Section 5.4). As with the actinide mobilization data, the DCL run control script is run for scenarios S1 and S2 for each replicate/brine volume combination. The script uses the same SUMMARIZE input control file template for all runs, generating a SUMMARIZE input control file for each replicate/scenario/brine volume combination. For CRA14-BV and CRA14-0, the file names are identical and are distinguished by the class they reside in. The script input and log files along with the SUMMARIZE input and output files are shown in Table 5.81, 5.82, and 5.83.

Table 5.81 CCDF Input Tabulation Input and Output Files (Colloid Source Term) for CRA14-BL

	File Names[1,2]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_SUM_PANEL_ST_CRA14BL_R1_S*s*.INP	LIBCRA14_EVAL	CRA14-BL
Input	SUM_PANEL_ST_CRA14BL.TMPL	LIBCRA14_SUM	CRA14-BL
Output	SUM_PANEL_ST_CRA14BL_R1_S*s*.INP	LIBCRA14_SUM	CRA14-BL
Log	EVAL_SUM_PANEL_ST_CRA14BL_R1_S*s*.LOG	LIBCRA14_SUM	CRA14-BL
SUMMARIZE			
Input	SUM_PANEL_ST_CRA14BL_R1_S*s*.INP	LIBCRA14_SUM	CRA14-BL
Input	PANEL_CON_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BL
Output	SUM_PANEL_ST_CRA14BL_R1_S*s*.TBL	LIBCRA14_SUM	CRA14-BL
Output	SUM_PANEL_ST_CRA14BL_R1_S*s*.DBG	NOT KEPT	NOT KEPT

1. $s \in \{1, 2\}$

2. *vvv*∈{001, 002, ..., 100} for each *s*

Table 5.82 CCDF Input Tabulation Input and Output Files (Colloid Source Term) for CRA14-BV

	File Names[1,2,3]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_SUM_PANEL_ST_CRA14BV*b*_R1_S*s*.INP	LIBCRA14_EVAL	CRA14-BV
Input	SUM_PANEL_ST_CRA14BV.TMPL	LIBCRA14_SUM	CRA14-BV
Output	SUM_PANEL_ST_CRA14BV*b*_R1_S*s*.INP	LIBCRA14_SUM	CRA14-BV
Log	EVAL_SUM_PANEL_ST_CRA14BV*b*_R1_S*s*.LOG	LIBCRA14_SUM	CRA14-BV
SUMMARIZE			
Input	SUM_PANEL_ST_CRA14BV*b*_R1_S*s*.INP	LIBCRA14_SUM	CRA14-BV
Input	PANEL_CON_CRA14BV*b*_R1_S*s*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-BV
Output	SUM_PANEL_ST_CRA14BV*b*_R1_S*s*.TBL	LIBCRA14_SUM	CRA14-BV
Output	SUM_PANEL_ST_CRA14BV*b*_R1_S*s*.DBG	NOT KEPT	NOT KEPT

1. $s \in \{1, 2\}$

2. *vvv*∈{001, 002, ..., 100} for each *s*

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

Table 5.83 CCDF Input Tabulation Input and Output Files (Colloid Source Term) for CRA14-0

	File Names[1,2,3,4]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_SUM_PANEL_ST_CRA14BV*b*_R*r*_S*s*.INP	LIBCRA14_EVAL	CRA14-0
Input	SUM_PANEL_ST_CRA14BV.TMPL	LIBCRA14_SUM	CRA14-0
Output	SUM_PANEL_ST_CRA14BV*b*_R*r*_S*s*.INP	LIBCRA14_SUM	CRA14-0
Log	EVAL_SUM_PANEL_ST_CRA14BV*b*_R*r*_S*s*.LOG	LIBCRA14_SUM	CRA14-0
SUMMARIZE			
Input	SUM_PANEL_ST_CRA14BV*b*_R*r*_S*s*.INP	LIBCRA14_SUM	CRA14-0
Input	PANEL_CON_CRA14BV*b*_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_PANEL	CRA14-0
Output	SUM_PANEL_ST_CRA14BV*b*_R*r*_S*s*.TBL	LIBCRA14_SUM	CRA14-0
Output	SUM_PANEL_ST_CRA14BV*b*_R*r*_S*s*.DBG	NOT KEPT	NOT KEPT

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

5.10.3 CCDF INPUT TABULATION FOR SALADO TRANSPORT FOR 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-NUTS ALGEBRACDB output CDB files (see Section 5.5.1). The script uses the output file from the SCREEN utility (see Section 5.5.1.2) 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 5.84 and 5.85. 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 5.5.1.3. Although there are no intrusions, the t=100 SUMMARIZE input control file template file can still be used for this scenario.

Table 5.84 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S1) for CRA14-BL

	File Names[1]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_SUM_NUT_CRA14BL_R1_S1.INP	LIBCRA14_EVAL	CRA14-BL
Input	SCREEN_NUT_SCN_CRA14BL_R1_S1.OUT	LIBCRA14_NUTR1S1	CRA14-BL
Input	SUM_NUT_CRA14BL_T00100.TMPL	LIBCRA14_SUM	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_S1.INP	LIBCRA14_SUM	CRA14-BL
Log	EVAL_SUM_NUT_CRA14BL_R1_S1.LOG	LIBCRA14_SUM	CRA14-BL
SUMMARIZE			
Input	SUM_NUT_CRA14BL_R1_S1.INP	LIBCRA14_SUM	CRA14-BL
Input	ALG_NUT_ISO_CRA14BL_R1_S1_V*vvv*.CDB	LIBCRA14_NUTR1S1	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_S1.TBL	LIBCRA14_SUM	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_S1.DBG	NOT KEPT	NOT KEPT

1. *vvv* as indicated in Table 5.51.

Table 5.85 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S1) for CRA14-0

	File Names[1,2]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_SUM_NUT_CRA14_R*r*_S1.INP	LIBCRA14_EVAL	CRA14-0
Input	SCREEN_NUT_SCN_CRA14_R*r*_S1.OUT	LIBCRA14_NUTR*r*S1	CRA14-0
Input	SUM_NUT_CRA14_T00100.TMPL	LIBCRA14_SUM	CRA14-0
Output	SUM_NUT_CRA14_R*r*_S1.INP	LIBCRA14_SUM	CRA14-0
Log	EVAL_SUM_NUT_CRA14_R*r*_S1.LOG	LIBCRA14_SUM	CRA14-0
SUMMARIZE			
Input	SUM_NUT_CRA14_R*r*_S1.INP	LIBCRA14_SUM	CRA14-0
Input	ALG_NUT_ISO_CRA14_R*r*_S1_V*vvv*.CDB	LIBCRA14_NUTR*r*S1	CRA14-0
Output	SUM_NUT_CRA14_R*r*_S1.TBL	LIBCRA14_SUM	CRA14-0
Output	SUM_NUT_CRA14_R*r*_S1.DBG	NOT KEPT	NOT KEPT

1. $r \in \{1, 2, 3\}$
2. *vvv* as indicated in Table 5.513.

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 5.5.1.4. Category B includes t=350 years and the appropriate output CDB file comes from the S2 or S4 ISO runs described in Section 5.5.1.3. 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 5.86 and Table 5.87, respectively for CRA14-BL and Table 5.88 and Table 5.89, respectively for CRA14-0.

Table 5.86 CCDF Input Tabulation Input and Output Files (Salado Transport–NUTS S2A,S4A) for CRA14-BL

	File Names[1,2]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_SUM_NUT_CRA14BL_R1_S*s*A.INP	LIBCRA14_EVAL	CRA14-BL
Input	SCREEN_NUT_SCN_CRA14BL_R1_S*s*.OUT	LIBCRA14_NUTR1S*s*	CRA14-BL
Input	SUM_NUT_CRA14BL_T00100.TMPL	LIBCRA14_SUM	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_S*s*_T00100.INP	LIBCRA14_SUM	CRA14-BL
Log	EVAL_SUM_NUT_CRA14BL_R1_S*s*A.LOG	LIBCRA14_SUM	CRA14-BL
SUMMARIZE			
Input	SUM_NUT_CRA14BL_R1_S*s*_T00100.INP	LIBCRA14_SUM	CRA14-BL
Input	ALG_NUT_INT_CRA14BL_R1_S*s*_T00100_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_Ss_T00100.TBL	LIBCRA14_SUM	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_Ss_T00100.DBG	NOT KEPT	NOT KEPT

1. $s \in \{2, 4\}$
2. *vvv* as indicated in Table 5.51.

Table 5.87 CCDF Input Tabulation Input and Output Files (Salado Transport–NUTS S2B,S4B) for CRA14-BL

	File Names[1,2]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_SUM_NUT_CRA14BL_R1_S*s*B.INP	LIBCRA14_EVAL	CRA14-BL
Input	SCREEN_NUT_SCN_CRA14BL_R1_S*s*.OUT	LIBCRA14_NUTR1S*s*	CRA14-BL
Input	SUM_NUT_CRA14BL_T00350.TMPL	LIBCRA14_SUM	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_S*s*_T00350.INP	LIBCRA14_SUM	CRA14-BL
Log	EVAL_SUM_NUT_CRA14BL_R1_S*s*B.LOG	LIBCRA14_SUM	CRA14-BL
SUMMARIZE			
Input	SUM_NUT_CRA14BL_R1_S*s*_T00350.INP	LIBCRA14_SUM	CRA14-BL
Input	ALG_NUT_1SO_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_Ss_T00350.TBL	LIBCRA14_SUM	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_Ss_T00350.DBG	NOT KEPT	NOT KEPT

1. $s \in \{2, 4\}$
2. *vvv* as indicated in Table 5.51.

Table 5.88 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S2A,S4A) for CRA14-0

	File Names[1,2,3]	CMS Library[1,2]	CMS Class
SCRIPT			
Input	EVAL_SUM_NUT_CRA14_R*r*_S*s*A.INP	LIBCRA14_EVAL	CRA14-0
Input	SCREEN_NUT_SCN_CRA14_R*r*_S*s*.OUT	LIBCRA14_NUTR*r*S*s*	CRA14-0
Input	SUM_NUT_CRA14_T00100.TMPL	LIBCRA14_SUM	CRA14-0
Output	SUM_NUT_CRA14_R*r*_S*s*_T00100.INP	LIBCRA14_SUM	CRA14-0
Log	EVAL_SUM_NUT_CRA14_R*r*_S*s*A.LOG	LIBCRA14_SUM	CRA14-0
SUMMARIZE			
Input	SUM_NUT_CRA14_R*r*_S*s*_T00100.INP	LIBCRA14_SUM	CRA14-0
Input	ALG_NUT_INT_CRA14_R*r*_S*s*_T00100_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	SUM_NUT_CRA14_R*r*_Ss_T00100.TBL	LIBCRA14_SUM	CRA14-0
Output	SUM_NUT_CRA14_R*r*_Ss_T00100.DBG	NOT KEPT	NOT KEPT

1. $r \in \{1, 2, 3\}$
2. $s \in \{2, 4\}$ for each *r*
3. *vvv* as indicated in Table 5.513.

Table 5.89 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S2B,S4B) for CRA14-0

	File Names[1,2,3]	CMS Library[1,2]	CMS Class
SCRIPT			
Input	EVAL_SUM_NUT_CRA14_R*r*_S*s*B.INP	LIBCRA14_EVAL	CRA14-0
Input	SCREEN_NUT_SCN_CRA14_R*r*_S*s*.OUT	LIBCRA14_NUTR*r*S*s*	CRA14-0
Input	SUM_NUT_CRA14_T00350.TMPL	LIBCRA14_SUM	CRA14-0
Output	SUM_NUT_CRA14_R*r*_S*s*_T00350.INP	LIBCRA14_SUM	CRA14-0
Log	EVAL_SUM_NUT_CRA14_R*r*_S*s*B.LOG	LIBCRA14_SUM	CRA14-0
SUMMARIZE			
Input	SUM_NUT_CRA14_R*r*_S*s*_T00350.INP	LIBCRA14_SUM	CRA14-0
Input	ALG_NUT_ISO_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	SUM_NUT_CRA14_R*r*_Ss_T00350.TBL	LIBCRA14_SUM	CRA14-0
Output	SUM_NUT_CRA14_R*r*_Ss_T00350.DBG	NOT KEPT	NOT KEPT

1. $r \in \{1, 2, 3\}$
2. $s \in \{2, 4\}$ for each *r*
3. *vvv* as indicated in Table 5.513.

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 5.5.1.3. 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 5.5.1.4. For category B, the script 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 5.90 and Table 5.91, respectively for CRA14-BL and Table 5.92 and Table 5.93, respectively for CRA14-0.

Table 5.90 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S3A,S5A) for CRA14-BL

	File Names[1,2]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_SUM_NUT_CRA14BL_R1_S*s*A.INP	LIBCRA14_EVAL	CRA14-BL
Input	SCREEN_NUT_SCN_CRA14BL_R1_S*s*.OUT	LIBCRA14_NUTR1S*s*	CRA14-BL
Input	SUM_NUT_CRA14BL_T01000.TMPL	LIBCRA14_SUM	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_S*s*_T01000.INP	LIBCRA14_SUM	CRA14-BL
Log	EVAL_SUM_NUT_CRA14BL_R1_S*s*A.LOG	LIBCRA14_SUM	CRA14-BL
SUMMARIZE			
Input	SUM_NUT_CRA14BL_R1_S*s*_T01000.INP	LIBCRA14_SUM	CRA14-BL
Input	ALG_NUT_ISO_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_Ss_T01000.TBL	LIBCRA14_SUM	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_Ss_T01000.DBG	NOT KEPT	NOT KEPT

1. $s \in \{3, 5\}$
2. *vvv* as indicated in Table 5.51.

Table 5.91 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S3B,S5B) for CRA14-BL

	File Names[1,2,3]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_SUM_NUT_CRA14BL_R1_S*s*B.INP	LIBCRA14_EVAL	CRA14-BL
Input	SCREEN_NUT_SCN_CRA14BL_R1_S*s*.OUT	LIBCRA14_NUTR1S*s*	CRA14-BL
Input	SUM_NUT_CRA14BL_T*tttt*.TMPL	LIBCRA14_SUM	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_S*s*_T*tttt*.INP	LIBCRA14_SUM	CRA14-BL
Log	EVAL_SUM_NUT_CRA14BL_R1_S*s*B.LOG	LIBCRA14_SUM	CRA14-BL
SUMMARIZE			
Input	SUM_NUT_CRA14BL_R1_S*s*_T*tttt*.INP	LIBCRA14_SUM	CRA14-BL
Input	ALG_NUT_INT_CRA14BL_R1_S*s*_V*vvv*.CDB	LIBCRA14_NUTR1S*s*	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_Ss_T*tttt*.TBL	LIBCRA14_SUM	CRA14-BL
Output	SUM_NUT_CRA14BL_R1_Ss_T*tttt*.DBG	NOT KEPT	NOT KEPT

1. $s \in \{3, 5\}$
2. $tttt \in \{03000, 05000, 07000, 09000\}$ for each s
3. *vvv* as indicated in Table 5.51.

Table 5.92 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S3A,S5A) for CRA14-0

	File Names[1,2,3]	CMS Library[1,2]	CMS Class
SCRIPT			
Input	EVAL_SUM_NUT_CRA14_R*r*_S*s*A.INP	LIBCRA14_EVAL	CRA14-0
Input	SCREEN_NUT_SCN_CRA14_R*r*_S*s*.OUT	LIBCRA14_NUTR*r*S*s*	CRA14-0
Input	SUM_NUT_CRA14_T01000.TMPL	LIBCRA14_SUM	CRA14-0
Output	SUM_NUT_CRA14_R*r*_S*s*_T01000.INP	LIBCRA14_SUM	CRA14-0
Log	EVAL_SUM_NUT_CRA14_R*r*_S*s*A.LOG	LIBCRA14_SUM	CRA14-0
SUMMARIZE			
Input	SUM_NUT_CRA14_R*r*_S*s*_T01000.INP	LIBCRA14_SUM	CRA14-0
Input	ALG_NUT_ISO_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	SUM_NUT_CRA14_R*r*_S*s*_T01000.TBL	LIBCRA14_SUM	CRA14-0
Output	SUM_NUT_CRA14_R*r*_S*s*_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 5.513.

Table 5.93 CCDF Input Tabulation Input and Output Files (Salado Transport – NUTS S3B,S5B) for CRA14-0

	File Names[1,2,3,4]	CMS Library[1,2]	CMS Class
SCRIPT			
Input	EVAL_SUM_NUT_CRA14_R*r*_S*s*B.INP	LIBCRA14_EVAL	CRA14-0
Input	SCREEN_NUT_SCN_CRA14_R*r*_S*s*.OUT	LIBCRA14_NUTR*r*S*s*	CRA14-0
Input	SUM_NUT_CRA14_T*ttttt*.TMPL	LIBCRA14_SUM	CRA14-0
Output	SUM_NUT_CRA14_R*r*_S*s*_T*ttttt*.INP	LIBCRA14_SUM	CRA14-0
Log	EVAL_SUM_NUT_CRA14_R*r*_S*s*B.LOG	LIBCRA14_SUM	CRA14-0
SUMMARIZE			
Input	SUM_NUT_CRA14_R*r*_S*s*_T*ttttt*.INP	LIBCRA14_SUM	CRA14-0
Input	ALG_NUT_INT_CRA14_R*r*_S*s*_V*vvv*.CDB	LIBCRA14_NUTR*r*S*s*	CRA14-0
Output	SUM_NUT_CRA14_R*r*_S*s*_T*ttttt*.TBL	LIBCRA14_SUM	CRA14-0
Output	SUM_NUT_CRA14_R*r*_S*s*_T*ttttt*.DBG	NOT KEPT	NOT KEPT

1. $r \in \{1, 2, 3\}$
2. $s \in \{3, 5\}$ for each r
3. $ttttt \in \{03000, 05000, 07000, 09000\}$ for each s
4. *vvv* as indicated in Table 5.513.

5.10.4 CCDF INPUT TABULATION FOR SALADO TRANSPORT FOR PANEL

SUMMARIZE is used to extract and tabulate radionuclide transport data for the multiple-intrusion (E2E1) conditions from the appropriate PANEL_INT output CDB files (see Section 5.5.2). 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/brine volume combination. The script uses the appropriate template to generate a SUMMARIZE input control file for each replicate/scenario/intrusion/brine volume combination. The script input and log files along with the SUMMARIZE input and output files are shown in Table 5.94 and 5.95.

Table 5.94 CCDF Input Tabulation Input and Output Files (Salado Transport - PANEL_INT) for CRA14-BL

	File Names[1,2]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_SUM_PANEL_INT_CRA14BL_R1_S6.INP	LIBCRA14_EVAL	CRA14-BL
Input	SUM_PANEL_INT_CRA14BL_T*tttt*.TMPL	LIBCRA14_SUM	CRA14-BL
Output	SUM_PANEL_INT_CRA14BL_R1_S6_*Ttttt*.INP	LIBCRA14_SUM	CRA14-BL
Log	EVAL_SUM_PANEL_INT_CRA14BL_R1_S6.LOG	LIBCRA14_SUM	CRA14-BL
SUMMARIZE			
Input	SUM_PANEL_INT_CRA14BL_R1_S6_*Ttttt*.INP	LIBCRA14_SUM	CRA14-BL
Input	PANEL_INT_CRA14BL_R1_S6_TI*tttt*_V*vvv*.CDB[3]	LIBCRA14_PANEL	CRA14-BL
Output	SUM_PANEL_INT_CRA14BL_R1_S6_T*tttt*.TBL	LIBCRA14_SUM	CRA14-BL
Output	SUM_PANEL_INT_CRA14BL_R1_S6_T*tttt*.DBG	NOT KEPT	NOT KEPT

1. *ttttt*∈{00100, 00350, 01000, 02000, 04000, 06000, 09000}
2. *vvv* ∈ {001, 002, ..., 100}
3. The PANEL INT CDB files time intrusions only have four digits.

Table 5.95 CCDF Input Tabulation Input and Output Files (Salado Transport - PANEL_INT) for CRA14-0

	File Names[1,2,3,4]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_SUM_PANEL_INT_CRA14BV*b*_R*r*_S6.INP	LIBCRA14_EVAL	CRA14-0
Input	SUM_PANEL_INT_CRA14BV*b*_T*tttt*.TMPL	LIBCRA14_SUM	CRA14-0
Output	SUM_PANEL_INT_CRA14BV*b*_R*r*_S6_*Ttttt*.INP	LIBCRA14_SUM	CRA14-0
Log	EVAL_SUM_PANEL_INT_CRA14BV*b*_R*r*_S6.LOG	LIBCRA14_SUM	CRA14-0
SUMMARIZE			
Input	SUM_PANEL_INT_CRA14BV*b*_R*r*_S6_*Ttttt*.INP	LIBCRA14_SUM	CRA14-0
Input	PANEL_INT_CRA14BV*b*_R*r*_S6_TI*tttt*_V*vvv*.CDB[5]	LIBCRA14_PANEL	CRA14-0
Output	SUM_PANEL_INT_CRA14BV*b*_R*r*_S6_T*tttt*.TBL	LIBCRA14_SUM	CRA14-0
Output	SUM_PANEL_INT_CRA14BV*b*_R*r*_S6_T*tttt*.DBG	NOT KEPT	NOT KEPT

1. *r*∈{1, 2, 3}
2. *ttttt*∈{00100, 00350, 01000, 02000, 04000, 06000, 09000} for each r
3. *vvv* ∈ {001, 002, ..., 100}
4. *b* ∈ {1, 2, 3, 4, 5}
5. The PANEL INT CDB files time intrusions only have four digits.

5.10.5 CCDF INPUT TABULATION FOR 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 5.8). 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 5.96 and 5.97.

Table 5.96 CCDF Input Tabulation Input and Output Files (Direct Brine Release) for CRA14-BL

	File Names[1,2,3,4]	CMS Library[1]	CMS Class
SCRIPT			
Input	EVAL_SUM_DBR_CRA14BL_R1_S*s*.INP	LIBCRA14_EVAL	CRA14-BL
Input	SUM_DBR_CRA14BL.TMPL	LIBCRA14_SUM	CRA14-BL
Output	SUM_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*.INP	LIBCRA14_SUM	CRA14-BL
Log	EVAL_SUM_DBR_CRA14BL_R1_S*s*.LOG	LIBCRA14_SUM	CRA14-BL
SUMMARIZE			
Input	SUM_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*.INP	LIBCRA14_SUM	CRA14-BL
Input	ALG3_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*_V*vvv*.CDB	LIBCRA14_DBRR1S*s*	CRA14-BL
Output	SUM_DBR_CRA14BL_R1_S*s*_Ttttt_*c*.TBL	LIBCRA14_SUM	CRA14-BL
Output	SUM_DBR_CRA14BL_R1_S*s*_Ttttt_*c*.DBG	NOT KEPT	NOT KEPT

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

Table 5.97 CCDF Input Tabulation Input and Output Files (Direct Brine Release) for CRA14-0

	File Names[1,2,3,4,5]	CMS Library[1,2]	CMS Class
SCRIPT			
Input	EVAL_SUM_DBR_CRA14_R*r*_S*s*.INP	LIBCRA14_EVAL	CRA14-0
Input	SUM_DBR_CRA14.TMPL	LIBCRA14_SUM	CRA14-0
Output	SUM_DBR_CRA14_R*r*_S*s*_T*tttt*_*c*.INP	LIBCRA14_SUM	CRA14-0
Log	EVAL_SUM_DBR_CRA14_R*r*_S*s*.LOG	LIBCRA14_SUM	CRA14-0
SUMMARIZE			
Input	SUM_DBR_CRA14_R*r*_S*s*_T*tttt*_*c*.INP	LIBCRA14_SUM	CRA14-0
Input	ALG3_DBR_CRA14_R*r*_S*s*_T*tttt*_*c*_V*vvv*.CDB	LIBCRA14_DBRR*r*S*s*	CRA14-0
Output	SUM_DBR_CRA14_R*r*_S*s*_Ttttt_*c*.TBL	LIBCRA14_SUM	CRA14-0
Output	SUM_DBR_CRA14_R*r*_S*s*_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. $vvv \in \{001, 002, ..., 100\}$ for each c

5.11 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 5.98.

Table 5.98 CCDF Construction Run Control Scripts

Step	Codes in Step	Scripts	CMS Library	CMS Class
1	GENMESH MATSET	EVAL_CCGF_STEP1.COM	LIBCRA14_EVAL	CRA14-BL CRA14-TP CRA14-BV CRA14-0
2	POSTLHS	EVAL_CCGF_STEP2.COM	LIBCRA14_EVAL	CRA14-BL CRA14-TP CRA14-BV CRA14-0
3	PRECCDFGF CCDFGF	EVAL_CCGF_STEP3.COM SUB_CCGF_STEP3.COM	LIBCRA14_EVAL	CRA14-BL CRA14-TP
3	PRECCDFGF CCDFGF	EVAL_CCGF_STEP3_CRA14BV.COM SUB_CCGF_STEP3_CRA14BV.COM	LIBCRA14_EVAL	CRA14-BV CRA14-0

5.11.1 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 5.99, 5.100, 5.101, and 5.102.

Table 5.99 CCDF Construction Step 1 Input and Output Files for CRA14-BL

	File Names	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CCGF_CRA14BL_STEP1.INP	LIBCRA14_EVAL	CRA14-BL
Script Log	EVAL_CCGF_CRA14BL_STEP1.LOG	LIBCRA14_CCGF	CRA14-BL
GENMESH			
Input	GM_CCGF_CRA14BL.INP	LIBCRA14_CCGF	CRA14-BL
Output	GM_CCGF_CRA14BL.CDB	LIBCRA14_CCGF	CRA14-BL
Output	GM_CCGF_CRA14BL.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_CCGF_CRA14BL.INP	LIBCRA14_CCGF	CRA14-BL
Input	GM_CCGF_CRA14BL.CDB	LIBCRA14_CCGF	CRA14-BL
Output	MS_CCGF_CRA14BL.CDB	LIBCRA14_CCGF	CRA14-BL
Output	MS_CCGF_CRA14BL.DBG	NOT KEPT	NOT KEPT

Table 5.100 CCDF Construction Step 1 Input and Output Files for CRA14-TP

	File Names	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CCGF_CRA14TP_STEP1.INP	LIBCRA14_EVAL	CRA14-TP
Script Log	EVAL_CCGF_CRA14TP_STEP1.LOG	LIBCRA14_CCGF	CRA14-TP
GENMESH			
Input	GM_CCGF_CRA14TP.INP	LIBCRA14_CCGF	CRA14-TP
Output	GM_CCGF_CRA14TP.CDB	LIBCRA14_CCGF	CRA14-TP
Output	GM_CCGF_CRA14TP.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_CCGF_CRA14TP.INP	LIBCRA14_CCGF	CRA14-TP
Input	GM_CCGF_CRA14TP.CDB	LIBCRA14_CCGF	CRA14-TP
Output	MS_CCGF_CRA14TP.CDB	LIBCRA14_CCGF	CRA14-TP
Output	MS_CCGF_CRA14TP.DBG	NOT KEPT	NOT KEPT

Table 5.101 CCDF Construction Step 1 Input and Output Files for CRA14-BV

	File Names	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CCGF_CRA14BV_STEP1.INP	LIBCRA14_EVAL	CRA14-BV
Script Log	EVAL_CCGF_CRA14BV_STEP1.LOG	LIBCRA14_CCGF	CRA14-BV
GENMESH			
Input	GM_CCGF_CRA14BV.INP	LIBCRA14_CCGF	CRA14-BV
Output	GM_CCGF_CRA14BV.CDB	LIBCRA14_CCGF	CRA14-BV
Output	GM_CCGF_CRA14BV.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_CCGF_CRA14BV.INP	LIBCRA14_CCGF	CRA14-BV
Input	GM_CCGF_CRA14BV.CDB	LIBCRA14_CCGF	CRA14-BV
Output	MS_CCGF_CRA14BV.CDB	LIBCRA14_CCGF	CRA14-BV
Output	MS_CCGF_CRA14BV.DBG	NOT KEPT	NOT KEPT

Table 5.102 CCDF Construction Step 1 Input and Output Files for CRA14-0

	File Names	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CCGF_CRA14_STEP1.INP	LIBCRA14_EVAL	CRA14-0
Script Log	EVAL_CCGF_CRA14_STEP1.LOG	LIBCRA14_CCGF	CRA14-0
GENMESH			
Input	GM_CCGF_CRA14.INP	LIBCRA14_CCGF	CRA14-0
Output	GM_CCGF_CRA14.CDB	LIBCRA14_CCGF	CRA14-0
Output	GM_CCGF_CRA14.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_CCGF_CRA14.INP	LIBCRA14_CCGF	CRA14-0
Input	GM_CCGF_CRA14.CDB	LIBCRA14_CCGF	CRA14-0
Output	MS_CCGF_CRA14.CDB	LIBCRA14_CCGF	CRA14-0
Output	MS_CCGF_CRA14.DBG	NOT KEPT	NOT KEPT

5.11.2 CCDF CONSTRUCTION STEP 2

Step 2 uses POSTLHS to assign the sampled parameter values used by CCDFGF (generated by LHS, see Section 5.2) 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 5.103, 5.104, 5.105, and 5.106.

Table 5.103 CCDF Construction Step 2 Input and Output Files for CRA14-BL

	File Names[1]	CMS Library	CMS Class
STEP 2			
Script Input	EVAL_CCGF_CRA14BL_STEP2_R1.INP	LIBCRA14_EVAL	CRA14-BL
Script Log	EVAL_CCGF_CRA14BL_STEP2_R1.LOG	LIBCRA14_CCGF	CRA14-BL
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA14_LHS	CRA14-BL
Input	LHS2_CRA14BL_R1_CON.TRN	LIBCRA14_LHS	CRA14-BL
Input	MS_CCGF_CRA14BL.CDB	LIBCRA14_CCGF	CRA14-BL
Output	LHS3_CCGF_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_CCGF	CRA14-BL
Output	LHS3_CCGF_CRA14BL_R1.DBG	LIBCRA14_CCGF	CRA14-BL

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

Table 5.104 CCDF Construction Step 2 Input and Output Files for CRA14-TP

	File Names[1]	CMS Library	CMS Class
STEP 2			
Script Input	EVAL_CCGF_CRA14TP_STEP2_R1.INP	LIBCRA14_EVAL	CRA14-TP
Script Log	EVAL_CCGF_CRA14TP_STEP2_R1.LOG	LIBCRA14_CCGF	CRA14-TP
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA14_LHS	CRA14-TP
Input	LHS2_CRA14TP_R1_CON.TRN	LIBCRA14_LHS	CRA14-TP
Input	MS_CCGF_CRA14TP.CDB	LIBCRA14_CCGF	CRA14-TP
Output	LHS3_CCGF_CRA14TP_R1_V*vvv*.CDB	LIBCRA14_CCGF	CRA14-TP
Output	LHS3_CCGF_CRA14TP_R1.DBG	LIBCRA14_CCGF	CRA14-TP

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

Table 5.105 CCDF Construction Step 2 Input and Output Files for CRA14-BV

	File Names[1]	CMS Library	CMS Class
STEP 2			
Script Input	EVAL_CCGF_CRA14BV_STEP2_R1.INP	LIBCRA14_EVAL	CRA14-BV
Script Log	EVAL_CCGF_CRA14BV_STEP2_R1.LOG	LIBCRA14_CCGF	CRA14-BV
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA14_LHS	CRA14-BV
Input	LHS2_CRA14TP_R1_CON.TRN	LIBCRA14_LHS	CRA14-BV
Input	MS_CCGF_CRA14BV.CDB	LIBCRA14_CCGF	CRA14-BV
Output	LHS3_CCGF_CRA14BV_R1_V*vvv*.CDB	LIBCRA14_CCGF	CRA14-BV
Output	LHS3_CCGF_CRA14BV_R1.DBG	LIBCRA14_CCGF	CRA14-BV

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

Table 5.106 CCDF Construction Step 2 Input and Output Files for CRA14-0

	File Names[1,2]	CMS Library	CMS Class
STEP 2			
Script Input	EVAL_CCGF_CRA14_STEP2_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Script Log	EVAL_CCGF_CRA14_STEP2_R*r*.LOG	LIBCRA14_CCGF	CRA14-0
POSTLHS			
Input	LHS3_DUMMY.INP	LIBCRA14_LHS	CRA14-0
Input	LHS2_CRA14_R*r*_CON.TRN	LIBCRA14_LHS	CRA14-0
Input	MS_CCGF_CRA14.CDB	LIBCRA14_CCGF	CRA14-0
Output	LHS3_CCGF_CRA14_R*r*_V*vvv*.CDB	LIBCRA14_CCGF	CRA14-0
Output	LHS3_CCGF_CRA14_R*r*.DBG	LIBCRA14_CCGF	CRA14-0

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

5.11.3 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 5.107, 5.108, 5.109, and 5.110.

Table 5.107 CCDF Construction Step 3 Input and Output Files for CRA14-BL

	File Names[1-6]	**CMS Library**	**CMS Class**
SCRIPT			
Script Input	EVAL_CCGF_STEP3_CRA14BL_R1.INP	LIBCRA14_EVAL	CRA14-BL
Script Log	EVAL_CCGF_STEP3_CRA14BL_R1.LOG	LIBCRA14_CCGF	CRA14-BL
PRECCDFGF			
Input	INTRUSIONTIMES.IN	LIBCRA14_CCGF	CRA14-BL
Input	CCGF1_CRA14BL_CONTROL.INP	LIBCRA14_CCGF	CRA14-BL
Input	MS_CCGF_CRA14BL.CDB	LIBCRA14_CCGF	CRA14-BL
Input	LHS3_CCGF_CRA14BL_R1_V*vvv*.CDB	LIBCRA14_CCGF	CRA14-BL
Input	SUM_DBR_CRA14BL_R1_S*s*_T*ttttt*_*c*.TBL	LIBCRA14_SUM	CRA14-BL
Input	CUSP_CRA14BL_R1.TBL	LIBCRA14_CUSP	CRA14-BL
Input	SUM_NUT_CRA14BL_R1_S1.TBL	LIBCRA14_SUM	CRA14-BL
Input	SUM_NUT_CRA14BL_R1_S*s*_T*ttttt*.TBL	LIBCRA14_SUM	CRA14-BL
Input	SUM_PANEL_INT_CRA14BL_R1_S6_T*ttttt*.TBL	LIBCRA14_SUM	CRA14-BL
Input	SUM_ST2D_PABC09_R1_M*m*.TBL	LIBPABC09_SUM	CRA14-BL
Input	EPU_CRA14BL_*h*H.DAT	LIBCRA14_EPU	CRA14-BL
Input	SUM_PANEL_CON_CRA14BL_R1_S*s*.TBL	LIBCRA14_SUM	CRA14-BL
Input	SUM_PANEL_ST_CRA14BL_R1_S*s*.TBL	LIBCRA14_SUM	CRA14-BL
Output	CCGF_CRA14BL_RELTAB_R1.DAT	LIBCRA14_CCGF	CRA14-BL
CCDFGF			
Input	CCGF_CRA14BL_CONTROL_R1.INP	LIBCRA14_CCGF	CRA14-BL
Input	CCGF_CRA14BL_RELTAB_R1.DAT	LIBCRA14_CCGF	CRA14-BL
Output	CCGF_CRA14BL_R1.OUT	LIBCRA14_CCGF	CRA14-BL
Output	CCGF_CRA14BL_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. $ttttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} \text{ for S1 for each } r \text{ for SUM\_DBR} \\ \{00550, 07500, 02000, 04000, 10000\} \text{ for S2, S4 for each } r \text{ for SUM\_DBR} \\ \{01200, 01400, 03000, 05000, 10000\} \text{ for S3, S5 for each } r \text{ for SUM\_DBR} \\ \{00100, 00350\} \text{ for S2, S4 for each } r \text{ for SUM\_NUT} \\ \{01000, 03000, 05000, 07000, 09000\} \text{ for S3, S5 each } r \text{ for SUM\_NUT} \\ \{00100, 00350, 01000, 02000, 04000, 06000, 09000\} \text{ for each } r \text{ for SUM\_PANEL\_INT} \end{cases}$
4. $c \in \{\text{L, M, U}\}$ for each intrusion for SUM_DBR
5. $m \in \{\text{F, P}\}$
6. $h \in \{\text{C, H}\}$

Table 5.108 CCDF Construction Step 3 Input and Output Files for CRA14-TP

	File Names[1-6]	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CCGF_STEP3_CRA14TP_R1.INP	LIBCRA14_EVAL	CRA14-TP
Script Log	EVAL_CCGF_STEP3_CRA14TP_R1.LOG	LIBCRA14_CCGF	CRA14-TP
PRECCDFGF			
Input	INTRUSIONTIMES.IN	LIBCRA14_CCGF	CRA14-TP
Input	CCGF1_CRA14TP_CONTROL.INP	LIBCRA14_CCGF	CRA14-TP
Input	MS_CCGF_CRA14TP.CDB	LIBCRA14_CCGF	CRA14-TP
Input	LHS3_CCGF_CRA14TP_R1_V*vvv*.CDB	LIBCRA14_CCGF	CRA14-TP
Input	SUM_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*.TBL	LIBCRA14_SUM	CRA14-TP
Input	CUSP_CRA14TP_R1.TBL	LIBCRA14_CUSP	CRA14-TP
Input	SUM_NUT_CRA14BL_R1_S1.TBL	LIBCRA14_SUM	CRA14-TP
Input	SUM_NUT_CRA14BL_R1_S*s*_T*tttt*.TBL	LIBCRA14_SUM	CRA14-TP
Input	SUM_PANEL_INT_CRA14BL_R1_S6_T*tttt*.TBL	LIBCRA14_SUM	CRA14-TP
Input	SUM_ST2D_PABC09_R1_M*m*.TBL	LIBPABC09_SUM	CRA14-TP
Input	EPU_CRA14BL_*h*H.DAT	LIBCRA14_EPU	CRA14-TP
Input	SUM_PANEL_CON_CRA14BL_R1_S*s*.TBL	LIBCRA14_SUM	CRA14-TP
Input	SUM_PANEL_ST_CRA14BL_R1_S*s*.TBL	LIBCRA14_SUM	CRA14-TP
Output	CCGF_CRA14TP_RELTAB_R1.DAT	LIBCRA14_CCGF	CRA14-TP
CCDFGF			
Input	CCGF_CRA14TP_CONTROL_R1.INP	LIBCRA14_CCGF	CRA14-TP
Input	CCGF_CRA14TP_RELTAB_R1.DAT	LIBCRA14_CCGF	CRA14-TP
Output	CCGF_CRA14TP_R1.OUT	LIBCRA14_CCGF	CRA14-TP
Output	CCGF_CRA14TP_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. $tttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} \text{ for S1 for each } r \text{ for SUM\_DBR} \\ \{00550, 07500, 02000, 04000, 10000\} \text{ for S2, S4 for each } r \text{ for SUM\_DBR} \\ \{01200, 01400, 03000, 05000, 10000\} \text{ for S3, S5 for each } r \text{ for SUM\_DBR} \\ \{00100, 00350\} \text{ for S2, S4 for each } r \text{ for SUM\_NUT} \\ \{01000, 03000, 05000, 07000, 09000\} \text{ for S3, S5 each } r \text{ for SUM\_NUT} \\ \{00100, 00350, 01000, 02000, 04000, 06000, 09000\} \text{ for each } r \text{ for SUM\_PANEL\_INT} \end{cases}$
4. $c \in \{L, M, U\}$ for each intrusion for SUM_DBR
5. $m \in \{F, P\}$
6. $h \in \{C, H\}$

Table 5.109 CCDF Construction Step 3 Input and Output Files for CRA14-BV

	File Names[1-7]	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CCGF_STEP3_CRA14BV_R1.INP	LIBCRA14_EVAL	CRA14-BV
Script Log	EVAL_CCGF_STEP3_CRA14BV_R1.LOG	LIBCRA14_CCGF	CRA14-BV
PRECCDFGF			
Input	INTRUSIONTIMES.IN	LIBCRA14_CCGF	CRA14-BV
Input	CCGF1_CRA14BV_CONTROL.INP	LIBCRA14_CCGF	CRA14-BV
Input	MS_CCGF_CRA14BV.CDB	LIBCRA14_CCGF	CRA14-BV
Input	LHS3_CCGF_CRA14BV_R1_V*vvv*.CDB	LIBCRA14_CCGF	CRA14-BV
Input	SUM_DBR_CRA14BL_R1_S*s*_T*tttt*_*c*.TBL	LIBCRA14_SUM	CRA14-BV
Input	CUSP_CRA14TP_R1.TBL	LIBCRA14_CUSP	CRA14-BV
Input	SUM_NUT_CRA14BL_R1_S1.TBL	LIBCRA14_SUM	CRA14-BV
Input	SUM_NUT_CRA14BL_R1_S*s*_T*tttt*.TBL	LIBCRA14_SUM	CRA14-BV
Input	SUM_PANEL_INT_CRA14BL_R1_S6_T*tttt*.TBL	LIBCRA14_SUM	CRA14-BV
Input	SUM_ST2D_PABC09_R1_M*m*.TBL	LIBPABC09_SUM	CRA14-BV
Input	EPU_CRA14BL_*h*H.DAT	LIBCRA14_EPU	CRA14-BV
Input	SUM_PANEL_CON_CRA14BV*b*_CRA14_R1_S*s*.TBL	LIBCRA14_SUM	CRA14-BV
Input	SUM_PANEL_ST_CRA14BV*b*_R1_S*s*.TBL	LIBCRA14_SUM	CRA14-BV
Output	CCGF_CRA14BV_RELTAB_R1.DAT	LIBCRA14_CCGF	CRA14-BV
CCDFGF			
Input	CCGF_CRA14BV_CONTROL_R1.INP	LIBCRA14_CCGF	CRA14-BV
Input	CCGF_CRA14BV_RELTAB_R1.DAT	LIBCRA14_CCGF	CRA14-BV
Output	CCGF_CRA14BV_R1.OUT	LIBCRA14_CCGF	CRA14-BV
Output	CCGF_CRA14BV_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. $tttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} \text{ for S1 for each } r \text{ for SUM\_DBR} \\ \{00550, 07500, 02000, 04000, 10000\} \text{ for S2, S4 for each } r \text{ for SUM\_DBR} \\ \{01200, 01400, 03000, 05000, 10000\} \text{ for S3, S5 for each } r \text{ for SUM\_DBR} \\ \{00100, 00350\} \text{ for S2, S4 for each } r \text{ for SUM\_NUT} \\ \{01000, 03000, 05000, 07000, 09000\} \text{ for S3, S5 each } r \text{ for SUM\_NUT} \\ \{00100, 00350, 01000, 02000, 04000, 06000, 09000\} \text{ for each } r \text{ for SUM\_PANEL\_INT} \end{cases}$

4. $c \in \{L, M, U\}$ for each intrusion for SUM_DBR

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

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

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

Table 5.110 CCDF Construction Step 3 Input and Output Files for CRA14-0

	File Names[1-8]	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CCGF_STEP3_CRA14_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Script Log	EVAL_CCGF_STEP3_CRA14_R*r*.LOG	LIBCRA14_CCGF	CRA14-0
PRECCDFGF			
Input	INTRUSIONTIMES.IN	LIBCRA14_CCGF	CRA14-0
Input	CCGF1_CRA14_CONTROL.INP	LIBCRA14_CCGF	CRA14-0
Input	MS_CCGF_CRA14.CDB	LIBCRA14_CCGF	CRA14-0
Input	LHS3_CCGF_CRA14_R*r*_V*vvv*.CDB	LIBCRA14_CCGF	CRA14-0
Input	SUM_DBR_CRA14_R*r*_S*s*_T*tttt*_*c*.TBL	LIBCRA14_SUM	CRA14-0
Input	CUSP_CRA14_R*r*.TBL	LIBCRA14_CUSP	CRA14-0
Input	SUM_NUT_CRA14_R*r*_S1.TBL	LIBCRA14_SUM	CRA14-0
Input	SUM_NUT_CRA14_R*r*_S*s*_T*tttt*.TBL	LIBCRA14_SUM	CRA14-0
Input	SUM_PANEL_INT_CRA14BV1_R*r*_S6_T*tttt*.TBL[9]	LIBCRA14_SUM	CRA14-0
Input	SUM_ST2D_PABC09_R*r*_M*m*.TBL	LIBPABC09_SUM	CRA14-0
Input	EPU_CRA14BL_*h*H.DAT	LIBCRA14_EPU	CRA14-0
Input	SUM_PANEL_CON_CRA14BV*b*_R*r*_S*s*.TBL	LIBCRA14_SUM	CRA14-0
Input	SUM_PANEL_ST_CRA14BV*b*_R*r*_S*s*.TBL	LIBCRA14_SUM	CRA14-0
Output	CCGF_CRA14_RELTAB_R*r*.DAT	LIBCRA14_CCGF	CRA14-0
CCDFGF			
Input	CCGF_CRA14_CONTROL_R*r*.INP	LIBCRA14_CCGF	CRA14-0
Input	CCGF_CRA14_RELTAB_R*r*.DAT	LIBCRA14_CCGF	CRA14-0
Output	CCGF_CRA14_R*r*.OUT	LIBCRA14_CCGF	CRA14-0
Output	CCGF_CRA14_R*r*.DBG	NOT KEPT	NOT KEPT

1. $r \in \{1, 2, 3\}$
2. $vvv \in \{001, 002, ..., 100\}$ 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. $h \in \{C, H\}$
8. $b \in \{1, 2, 3, 4, 5\}$
9. Only brine volume case one was used because this was the most conservative case.

5.12 *SENSITIVITY ANALYSIS (STEPWISE)*

A global sensitivity analysis was conducted on the results from CCDFGF using the linear regression code STEPWISE. STEPWISE is executed twice per replicate once for ranked data (RANK) and once for raw data (RAW). The run control script is shown in Table 5.111. The input and output files for STEPWISE, as well as the input and log files for the script are shown in Table 5.112.

Table 5.111 Sensitivity Analysis Run Control Scripts

Code	Script	Script CMS Library	Script CMS Class
STEPWISE	EVAL_STP.COM	LIBCRA14_EVAL	CRA14-0

Table 5.112 Sensitivity Analysis Input and Output Files

	File Names[1,2]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_STP_CRA14_*_ALL_R*r*.INP	LIBCRA14_EVAL	CRA14-0
Log	EVAL_STP_CRA14_*_ALL_R*r*.LOG	LIBCRA14_STPW	CRA14-0
STEPWISE			
Input	STP_CRA14_*_ALL_R*r*.INP	LIBCRA14_STPW	CRA14-0
Input	STP_CRA14_LHS_R*r*.TRN	LIBCRA14_STPW	CRA14-0
Input	STP_CRA14_MEANS_R*r*.TRN	LIBCRA14_STPW	CRA14-0
Output	STP_CRA14_*_R*r*.TXT	LIBCRA14_STPW	CRA14-0
Output	STP_CRA14_*_R*r*.SP	LIBCRA14_STPW	CRA14-0

1. $r \in \{1,2,3\}$
2. $* \in \{RANK, RAW\}$ for each r

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