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SANDIA NATIONAL LABORATORIES
WASTE ISOLATION PILOT PLANT

Summary Report and Run Control for the 2012 WIPP Panel Closure System Performance Assessment

Revision 0

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Table of Contents

List of Figures

List of Tables

EXECUTIVE SUMMARY

Waste panel closures comprise a repository feature that has been represented in WIPP PA since the original Compliance Certification Application of 1996. The 1998 rulemaking that certified WIPP to receive transuranic waste placed conditions on the panel closure design to be implemented in the repository. The mandated "Option D" design consists of a concrete block wall, an open drift section, and a concrete monolith. The engineering of the panel closure has been re-assessed, and a revised design is proposed that is simpler, cheaper, and easier to construct. The revised panel closure design, termed the Run-of-Mine Panel Closure System (ROMPCS), is comprised of 100 feet of run-of-mine (ROM) salt with barriers at each end. The PCS-2012 PA quantifies WIPP repository performance impacts associated with the replacement of the currently approved Option D panel closure design with the ROMPCS. Impacts are assessed via a direct comparison of results obtained in the 2009 Performance Assessment Baseline Calculation (PABC-2009) to those calculated in the PCS-2012 PA with the ROMPCS.

Total normalized releases calculated in the PCS-2012 PA are greater than those found in the PABC-2009, but continue to remain below their regulatory limits. As a result, replacement of the Option D panel closure with the ROMPCS design would not result in WIPP non-compliance with the containment requirements of 40 CFR Part 191. Cuttings and cavings releases and direct brine releases (DBRs) were the two primary release components contributing to total releases in the PABC-2009, and continue to be so in the PCS-2012 PA. Cuttings and cavings releases are not impacted by the change in panel closure design, and so remain unchanged from those calculated in the PABC-2009.

For both undisturbed and intruded repository conditions, implementation of the ROMPCS yields higher long-term waste panel pressure (on average) than was seen in the PABC-2009. Pressure increases translate to increases in spallings volumes and their frequency. As a result, increased spallings releases are seen in the PCS-2012 PA results when compared to the PABC-2009. These increases do not have a significant impact on total normalized releases found in the PCS-2012 PA.

Increased direct brine releases are also seen in the PCS-2012 PA results. DBRs depend on waste panel pressure and brine saturation at the time of intrusion. In addition to increases in waste panel pressure, implementation of the ROMPCS design results in increased mean waste panel brine saturation for undisturbed conditions as well as intrusion scenarios that do not intersect a Castile brine pocket. For intrusion scenarios that intersect a region of pressurized Castile brine, increases in pressure are accompanied by only slight reductions in the mean waste panel brine saturation in the PCS-2012 PA as compared to PABC-2009 results. The combined effect of these impacts is an increase to normalized direct brine releases in the PCS-2012 PA. The increase in total normalized releases seen in the PCS-2012 PA as compared to the PABC-2009 is primarily due to the increase in DBRs calculated in the PCS-2012 PA.

1 INTRODUCTION

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. 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 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.

Waste panel closures comprise a repository feature that has been represented in WIPP PA since the original Compliance Certification Application (CCA) of 1996. Panel closures are included in WIPP PA models principally because they are a part of the disposal system, not because they play a substantive role in inhibiting the release of radionuclides to the outside environment. The DOE stated in the CCA (DOE 1996) that *"The panel closure system was not designed or intended to support long-term repository performance."* The 1998 rulemaking that certified WIPP to receive transuranic waste placed conditions on the panel closure design to be implemented in the repository. The mandated design consists of a concrete block wall, an open drift section, and a concrete monolith, and was termed the "Option D" panel closure. Following the selection of the Option D design in 1998, the engineering of the panel closure has been re-assessed, and a revised design has been established that is simpler, cheaper, and easier to construct. The revised panel closure design, termed the Run-of-Mine Panel Closure System (ROMPCS), is comprised of 100 feet of run-of-mine (ROM) salt with barriers at each end. The ROM salt is generated from ongoing mining operations at the WIPP and may be compacted and/or moistened as it is emplaced in a panel entry. The barriers consist of ventilation bulkheads, similar to those currently used in the panels as room closures.

The DOE has submitted a planned change request (PCR) to the EPA requesting that EPA modify Condition 1 of the Final Certification Rulemaking for 40 CFR Part 194 (EPA, 1998) for the WIPP. The PCR submitted to EPA requests that Condition 1 be changed, and that the ROMPCS design be approved for use in all panels (DOE, 2011). In support of this rulemaking change, a PA has been completed that incorporates the ROMPCS design into the current PA baseline established by the 2009 Performance Assessment Baseline Calculation (PABC-2009) (Clayton et al., 2010). The name given to this new panel closure PA is PCS-2012, and the plan for its execution is detailed in AP-161 (Camphouse 2012a). PCS-2012 PA results are compared to PABC-2009 results as a means to quantify potential panel closure redesign impacts. This document provides the summary report of the PCS-2012 PA analysis.

2 RUN-OF-MINE PANEL CLOSURE SYSTEM

The goal of the PCS-2012 PA is to quantify regulatory compliance impacts resulting from the replacement of the Option D panel closure with the ROMPCS. Figure 2-1 shows the Option D panel closure is 40 meters long and consists of three components, namely a concrete explosion wall, an open drift section, and a concrete monolith. This panel closure has been implemented in PA analyses done in support of WIPP re-certification since the CRA-2004 PA (Stein & Zelinski 2003).

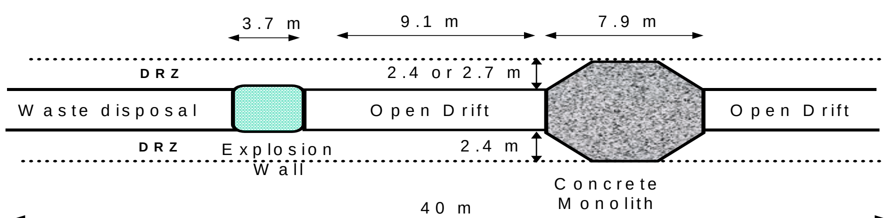
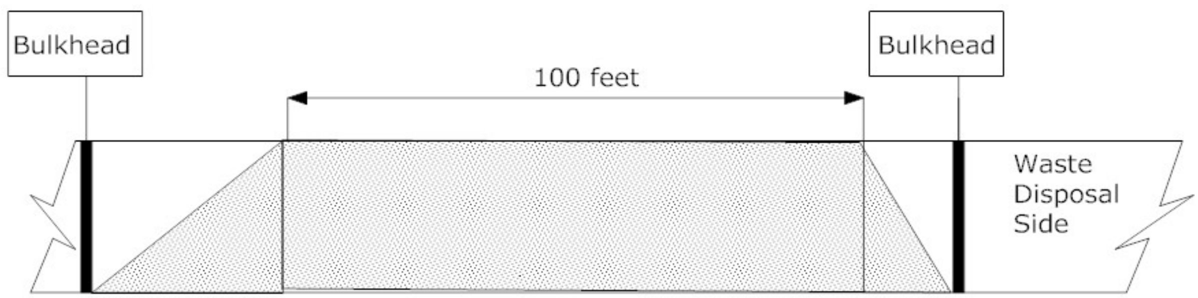
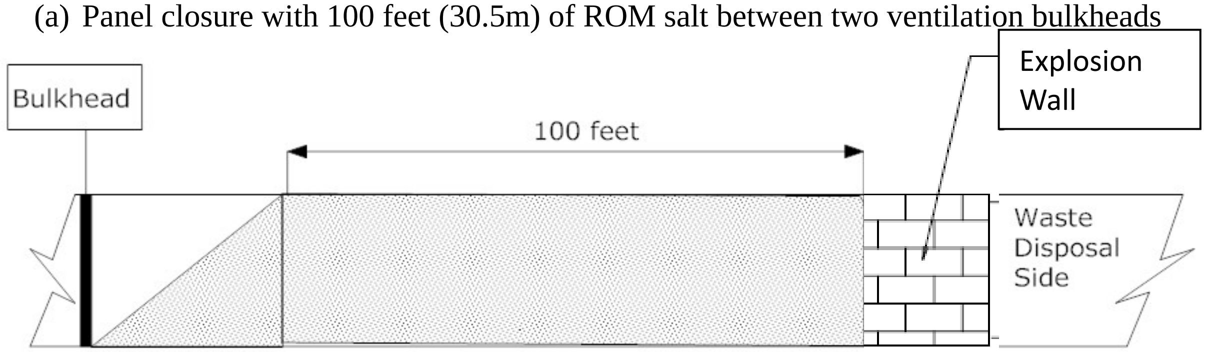


Figure 2-1: A Schematic of the “Option D” Panel Closure

The ROMPCS is comprised of 100 feet of run-of-mine salt with barriers at each end, and is illustrated in Figure 2-2. The ROM salt is generated from ongoing mining operations at the WIPP and may be compacted and/or moistened as it is emplaced in a panel entry. The barriers consist of ventilation bulkheads, similar to those currently used in the panels as room closures. The ventilation bulkheads are designed to restrict air flows and prevent personnel access into waste-filled areas during the WIPP operational phase. In Panels 1, 2, and 5, where explosion walls fabricated from concrete blocks have already been emplaced in the panel entries, an explosion wall is the inner barrier and a ventilation bulkhead will be the outer barrier, as shown in Figure 2-2(b). Explosion walls are inspected on a regular basis, and their anticipated condition is also assessed through numerical modeling (e.g. RockSol, 2006). Installed explosion walls show surface spalling or slabbing of the concrete blocks as a result of the loading caused by inward creep of the salt. Numerical stress analysis of the concrete explosion wall has demonstrated that the free faces and the rib contacts will be in a condition of plastic yield with an unyielded core by 7 years after emplacement (Rocksol, 2006, Figures 7 and 10). No long term stress analyses have been carried out; however, it is expected that the spalling and yield will be progressive, and that the walls will not be significant structures after the initial 100 year time period, due to the brittle, non-plastic behavior of concrete. The ventilation bulkheads and explosion walls are therefore expected to have no significant impact on long-term performance of the panel closures and are therefore not included in the PCS-2012 PA representation of the ROMPCS. Consequently, the ROMPCS is modeled as consisting of 100 feet of ROM salt in the PCS-2012 PA.



(a) Panel closure with 100 feet (30.5m) of ROM salt between two ventilation bulkheads



(b) Panel closure with 100 feet (30.5m) of ROM salt between a ventilation bulkhead & explosion wall

Figure 2-2: Schematic of the ROMPCS

2.1 ROMPCS Modeling and Parameterization

The modeling approach and parameter developments undertaken to represent the ROMPCS in the PCS-2012 PA are documented in Camphouse et al. (2012a), Patterson (2012), and Camphouse (2012b). These aspects of the PCS-2012 PA are now discussed. For the sake of clarity in the discussion that follows, select parameters used to model the Option D panel closure in the PABC-2009 are shown in Table 2-1.

Table 2-1: Option D Panel Closure Parameters Used in the PABC-2009

Material	Property	Distribution	Statistics
CONC_PCS	Porosity	Constant	0.05
	PRMX (m^2)	Triangular	Min = 2.0×10^{-21}
	PRMY (m^2)		Mean = 1.53×10^{-19}
	PRMZ (m^2)		Max = 1.0×10^{-17}
DRZ_1	Porosity	Cumulative	Min = 0.0039
			Mean = 0.0211
			Max = 0.0548
	PRMX (m^2)	Uniform	Min = 3.98×10^{-20}
	PRMY (m^2)		Mean = 1.0×10^{-16}
	PRMZ (m^2)		Max = 3.16×10^{-13}
DRZ_PCS	Porosity	Cumulative	Min = 0.0039
			Mean = 0.0211
			Max = 0.0548
	PRMX (m^2)	Triangular	Min = 2.0×10^{-21}
	PRMY (m^2)		Mean = 1.53×10^{-19}
	PRMZ (m^2)		Max = 1.0×10^{-17}

ROMPCS properties in the PCS-2012 PA are based on three time periods: from 0 to 100 years, from 100 years to 200 years, and from 200 years to 10,000 years. Three time periods are appropriate because the process to consolidate the ROM salt occurs over a primary time scale of approximately 100 years, while the process to heal fractures in the DRZ surrounding the PCS occurs over a longer time scale of approximately 200 years. The ROM salt comprising the ROMPCS is therefore represented by three materials, denoted as PCS_T1 for the first 100 years, PCS_T2 from 100 to 200 years, and PCS_T3 for 200 to 10,000 years. Analyses and calculations have shown (Camphouse et al. 2012a) that the time-dependent back stress imposed on the DRZ by the re-consolidated ROM salt panel closure does not become appreciable until roughly 200 years after emplacement of the ROM salt in the drift. As a result, it is reasonable and appropriate to maintain the same properties for the DRZ above and below the ROMPCS for the first 200 years after closure as are specified to the DRZ surrounding the disposal rooms. After 200 years, the DRZ above and below the ROMPCS is modeled as having healed, and this sub-region of the DRZ is represented by material DRZ_PCS. Material DRZ_PCS has the same property values in the PCS-2012 PA as were assigned to it in the PABC-2009.

The 200-year delay of DRZ healing in the PCS-2012 PA is an important distinction between the Option D panel closure representation used in the PABC-2009 and the ROMPCS representation used in the PCS-2012 PA. The Option D panel closure was modeled in the PABC-2009 (and prior analyses) as having an immediate healing effect on the DRZ above it, with material DRZ_PCS being in place at t = 0. In contrast, the ROMPCS in the PCS-2012 PA is modeled as having no healing effect on the DRZ until 200 years after panel closure emplacement. For the first 200 years, the DRZ above and below the ROMPCS is indistinguishable from the DRZ above and below the waste panels. The DRZ overall (PA parameter DRZ_1 in Table 2-1) has a permeability range varying from a minimum value of 3.98×10^{-20} m^2 to a maximum value of 3.16×10^{-13} m^2 in the x, y, and z directions. Material DRZ_PCS has a permeability range varying from a minimum of 2.0×10^{-21} m^2 to a maximum of 1.0×10^{-17} m^2 in the x, y, and z directions. As a result, there is a path of increased permeability (on average) above and below panel closures in the PCS-2012 PA for the first 200 years as compared to the PABC-2009. An expected consequence of this increased permeability is an increase in brine and gas flow through the DRZ and around the panel closure for the first 200 years. In effect, the panel closures in the PCS-2012 PA are “looser” than those implemented in the PABC-2009 for the first 200 years due to the higher permeability (on average) of the DRZ material above and below them.

The complete set of parameters used to model the ROMPCS in the PCS-2012 PA is shown in Table 2-2 and Table 2-3. As developed in Camphouse et al. (2012a) and Patterson (2012), permeability and porosity values are obtained through sampling for ROMPCS material PCS_T1. However, only porosity is sampled for materials PCS_T2 and PCS_T3. Sampled porosity values are then used to calculate permeability values for these materials according to the algorithm developed on page 15 of Camphouse et al. (2012a). At 200 years, the ROMPCS material transitions from PCS_T2 to PCS_T3 with the DRZ region above and below PCS_T3 represented as healed by material DRZ_PCS. Under this configuration, the range of calculated permeabilities for PCS_T3 is comparable to the permeability range assigned to the Option D monolith (material CONC_PCS in Table 2-1), with the minimum value calculated for PCS_T3 being roughly an order of magnitude less than the minimum CONC_PCS permeability value. As material DRZ_PCS represents regions of healed DRZ for both the ROMPCS and the Option D closure (with equal DRZ_PCS property values prescribed for both panel closure cases), the final ROMPCS configuration comprises a panel closure that is slightly “tighter” (on average) than the Option D case.

The algorithm used to calculate permeability from a sampled porosity value depends on an additional sampled parameter, quantity α in the algorithm developed in Camphouse et al. (2012a). The name given to this additional parameter in the PCS-2012 PA is POR2PERM. Porosity and permeability ranges used for materials PCS_T1, PCS_T2, and PCS_T3 are shown in Table 2-2. As can be seen in that table, there is overlap in the porosity ranges specified for PCS_T1 and PCS_T2. This overlap could potentially result in an increase in panel closure porosity during the transition from PCS_T1 to PCS_T2 at 100 years, a non-physical result. To prevent this possibility, the porosity for PCS_T2 is conditionally sampled (Kirchner 2012a) in the PCS-2012 PA. Using the MATERIAL:PROPERTY parameter naming convention used in WIPP PA, the porosity for material PCS_T2 is conditionally sampled such that PCS_T2:POROSITY $\leq$ PCS_T1:POROSITY. There is also overlap in the porosity ranges specified for PCS_T2 and PCS_T3. To prevent physically unrealistic increases in porosity during the transition from PCS_T2 to PCS_T3 at 200 years, the porosity for PCS_T3 is conditionally sampled so that PCS_T3:POROSITY ≤ PCS_T2:POROSITY. Similar constraints are placed on the calculated permeability values for PCS_T2 and PCS_T3. As can be seen in Table 2-2, a low sampled permeability value for PCS_T1 could be followed by a higher calculated permeability value for PCS_T2, dependent on the sampled PCS_T2 porosity and POR2PERM values. An instantaneous increase in panel closure permeability after 100 years of creep closure is an unrealistic occurrence. To prevent this non-physical result, the calculated permeability value for PCS_T2 is constrained in the PCS-2012 PA such that PCS_T2:PRMX ≤ PCS_T1:PRMX. If a higher permeability value is calculated for material PCS_T2 than was sampled for material PCS_T1, then material PCS_T2 retains the permeability value for PCS_T1. The same is true for the calculated permeabilities in the y and z directions. A similar constraint is placed on the calculated permeability for PCS_T3 in order to prevent non-physical instantaneous increases in panel closure permeability at 200 years. The constraint placed on the calculated permeability for PCS_T3 is that PCS_T3:PRMX ≤ PCS_T2:PRMX, and likewise in the x and y directions. If the calculated permeability for PCS_T3 is greater than that obtained for PCS_T2, then PCS_T3 retains the permeabilities assigned to PCS_T2.

Table 2-2: Sampled Panel Closure Parameters for the PCS-2012 PA

Parameter	Units	Description	Distribution Type	Distribution Parameters	Default Value	Source
PCS_T1:POROSITY	none	Porosity of run-of-mine panel closure, years 0 to 100	Uniform	Min = 0.066 Max = 0.187 Mean = 0.1265	0.1265	Camphouse et al. (2012a) Table 2 and page 15
PCS_T2:POROSITY[1]	none	Porosity of run-of-mine panel closure, years 100 to 200	Uniform	Min = 0.025 Max = 0.075 Mean = 0.05	0.05	Camphouse et al. (2012a) Table 2 and page 15
PCS_T3:POROSITY[2]	none	Porosity of run-of-mine panel closure, years 200 to 10,000	Uniform	Min = 0.001 Max = 0.0519 Mean = 0.0265	0.0265	Camphouse et al. (2012a) Table 2 and page 15
PCS_T1:PRMX_LOG[3] PCS_T1:PRMY_LOG PCS_T1:PRMZ_LOG	$\log(m^2)$	$\log_{10}$ of intrinsic permeability, X, Y, and Z directions.	Uniform	Min = -21.0 Max = -12.0 Mean = -16.5	-16.5	Patterson (2012) Page 13
PCS_T2:POR2PERM[4] PCS_T3:POR2PERM	none	Distribution used to calculate permeability from sampled porosity values	Normal	Min = -1.72 Max = 1.72 Mean = 0.0 SD = 0.86	0.0	Camphouse et al. (2012a) Page 15 (sampled α value)
PCS_T1:SAT_IBRN	none	Initial brine saturation of run-of-mine panel closure	Uniform	Min = 0.04 Max = 0.16 Mean = 0.1	0.1	Camphouse (2012b)

[1] PCS_T2:POROSITY is constrained such that PCS_T2:POROSITY ≤ PCS_T1:POROSITY for a given vector in order to avoid non-physical instantaneous increases in ROMPCS porosity at 100 years.
[2] PCS_T3:POROSITY is constrained such that PCS_T3:POROSITY ≤ PCS_T2:POROSITY for a given vector in order to avoid non-physical instantaneous increases in ROMPCS porosity at 200 years.
[3] Parameter values are sampled for PCS_T1:PRMX_LOG. PCS_T1:PRMY_LOG and PCS_T1:PRMZ_LOG inherit the sampled value obtained for PCS_T1:PRMX_LOG for each vector.
[4] Parameter values are sampled for PCS_T2:POR2PERM. PCS_T3:POR2PERM inherits the sampled value obtained for PCS_T2:POR2PERM for each vector.

Table 2 (cont): Sampled Panel Closure Parameters for the PCS-2012 PA

PCS_T1:SAT_RBRN[5] PCS_T2:SAT_RBRN PCS_T3:SAT_RBRN	none	Residual Brine Saturation	Cumulative	(Prob,Value): (0,0) (0.5,0.2) (1.0,0.6)	0.2	Camphouse et al. (2012a) Table 6
PCS_T1:SAT_RGAS[6] PCS_T2:SAT_RGAS PCS_T3:SAT_RGAS	none	Residual Gas Saturation	Uniform	Min = 0.0 Max = 0.4 Mean = 0.2	0.2	Camphouse et al. (2012a) Table 6
PCS_T1:PORE_DIS[7] PCS_T2:PORE_DIS PCS_T3:PORE_DIS	none	Brooks-Corey pore distribution parameter	Cumulative	(Prob,Value): (0,0.11) (0.5,0.94) (1.0,8.1)	0.94	Camphouse et al. (2012a) Table 8

[5] Parameter values are sampled for PCS_T1:SAT_ RBRN. PCS_T2: SAT_ RBRN and PCS_T3: SAT_ RBRN inherit the sampled value obtained for PCS_T1:SAT_ RBRN for each vector.
[6] Parameter values are sampled for PCS_T1:SAT_ RGAS. PCS_T2: SAT_ RGAS and PCS_T3: SAT_ RGAS inherit the sampled value obtained for PCS_T1:SAT_ RGAS for each vector.
[7] Parameter values are sampled for PCS_T1:PORE_DIS. PCS_T2: PORE_DIS and PCS_T3: PORE_DIS inherit the sampled value obtained for PCS_T1: PORE_DIS for each vector.

Table 2-3: Constant Panel Closure Parameters for the PCS-2012 PA

Parameter	Units	Description	Value	Source
PCS_T2:PRMX_LOG[8] PCS_T2:PRMY_LOG PCS_T2:PRMZ_LOG	log(m^2)	$\log_{10}$ of intrinsic permeability, X, Y, and Z directions.	-18.6	See Footnote
PCS_T3:PRMX_LOG[9] PCS_T3:PRMY_LOG PCS_T3:PRMZ_LOG	log(m^2)	$\log_{10}$ of intrinsic permeability, X, Y, and Z directions.	-19.1	See Footnote
PCS_T1:RELP_MOD PCS_T2:RELP_MOD PCS_T3:RELP_MOD	none	Relative Permeability Model Number	4 (a modified Brooks-Corey Model)	Camphouse et al. (2012a) Table 7
PCS_T1:CAP_MOD PCS_T2:CAP_MOD PCS_T3:CAP_MOD	none	Capillary Pressure Model Number	1 (unbounded capillary pressure)	Camphouse (2012b) Camphouse (2012c)
PCS_T1:KPT PCS_T2:KPT PCS_T3:KPT	none	Flag to Enable Dynamic Updating of Threshold Capillary Pressure as a Function of Permeability	0.0	Camphouse et al. (2012a) Table 8
PCS_T1:PCT_A PCS_T2:PCT_A PCS_T3:PCT_A	Pa	Threshold Capillary Pressure Linear Parameter	0.0	Camphouse (2012b) Camphouse (2012c)
PCS_T1:PCT_EXP PCS_T2:PCT_EXP PCS_T3:PCT_EXP	none	Threshold Capillary Pressure Exponential Parameter	0.0	Camphouse (2012b) Camphouse (2012c)
PCS_T1:PC_MAX PCS_T2:PC_MAX PCS_T3:PC_MAX	Pa	Maximum Allowable Capillary Pressure	1×10^8	Camphouse et al. (2012a) Table 8

[8] Permeabilities of PCS_T2 in the X, Y, and Z directions are calculated from the sampled PCS_T2:POROSITY values as described in Camphouse et al. (2012a). A constant default log-permeability is specified, however, to allow for parameter traceability in PCS-2012 PA input files as compared to those used in the PABC-2009. The specified default value is the average of the minimum and maximum values listed in Table 5 of Camphouse et al. (2012a).

[9] Permeabilities of PCS_T3 in the X, Y, and Z directions are calculated from the sampled PCS_T3:POROSITY values as described in Camphouse et al. (2012a). The specified constant default value is the average of the minimum and maximum values listed in Table 5 of Camphouse et al. (2012a).

Table 3 (cont): Constant Panel Closure Parameters for the PCS-2012 PA				
PCS_T1:P0_MIN PCS_T2:P0_MIN PCS_T3:P0_MIN	Pa	Minimum Brine Pressure for Capillary Model 3 (CAP_MOD = 3 has never been used in PA)	1.01325×10^{5}	Camphouse et al. (2012a) Table 8
PCS_T1:COMP_RCK PCS_T2:COMP_RCK PCS_T3:COMP_RCK	Pa^{-1}	Bulk Compressibility	8.0×10^{-11}	Camphouse et al. (2012a) Table 8

2.2 FEPs Assessment

The PCS-2012 PA began with an assessment that identified and evaluated the features, events, and processes (FEPs) that are related to the changes introduced by the proposed panel closure design. The purpose of the FEPs evaluation was to determine if the current FEPs baseline (currently the PABC-2009 FEPs baseline) is suitable to evaluate the new closure design, or if changes to FEPs descriptions, screening arguments, or decisions are necessary. The results of this assessment concluded that no changes are needed to the FEPs baseline (Kirkes 2011) [10]. It should be pointed out that the FEPs analysis only determines that the WIPP design features are appropriately identified, described, and screened according to established FEPs screening methods. WIPP FEPs W109 *Panel Closure Geometry* and W110, *Panel Closure Properties*, are directly related to the changes proposed by the new PCS design and were the focus of the FEPs assessment. These two FEPs have been screened in (represented) as part of previous performance assessments in all scenarios, and continue to be so in the PCS-2012 PA.

3 METHODOLOGY

The PA methodology accommodates both aleatory (i.e. stochastic) and epistemic (i.e. subjective) uncertainty in its constituent models. Aleatory uncertainty pertains to unknowable future events such as intrusion times and locations that may affect repository performance. It is accounted for by the generation of random sequences of future events. Epistemic uncertainty concerns parameter values that are assumed to be constants and the constants' true values are uncertain due to a lack of knowledge about the system. An example of a parameter with epistemic uncertainty is the permeability of a material. Epistemic uncertainty is accounted for by sampling of parameter values from assigned distributions. One set of sampled values required to run a WIPP PA calculation is termed a vector. In the PCS-2012 PA, models were executed for three replicates of 100 vectors. Parameter sampling performed in the PCS-2012 PA is documented in Kirchner (2012a), and the sensitivities of variable output to sampled parameters are documented in Kirchner (2012b). A sample size of 10,000 possible sequences of future events is used in PA calculations to address aleatory uncertainty. The releases for each of 10,000 possible sequences of future events are tabulated for each of the 300 vectors, totaling 3,000,000 possible sequences.

For a random variable, the complementary cumulative distribution function (CCDF) provides the probability of the variable being greater than a particular value. By regulation, PA results are presented as a distribution of CCDFs of releases (EPA 1996). Each individual CCDF summarizes the likelihood of releases across all futures for one vector of parameter values. The uncertainty in parameter values results in a distribution of CCDFs.

[10] Kirkes (2011) also evaluated changes associated with a proposed reconfiguration of the repository layout; the PCS changes are a subset of this FEP evaluation. Only the elements (and FEPs) relating to the PCS redesign are germane to the PCS-2012 PA analyses.

Releases are quantified in terms of "EPA units". Releases in EPA units result from a normalization by radionuclide and the total inventory. For each radionuclide, the ratio of its 10,000 year cumulative release (in curies) to its release limit is calculated. The sum of these ratios is calculated across the set of radionuclides and normalized by the transuranic inventory (in curies) of α-emitters with half-lives greater than 20 years. Mathematically, the formula used to calculate releases in terms of EPA units is of the form

$$R = \frac{1 \times 10^6 \text{ curies}}{C} \sum_i \frac{Q_i}{L_i}$$

where R is the normalized release in EPA units. Quantity Q_i is the 10,000 year cumulative release (in curies) of radionuclide i. Quantity L_i is the release limit for radionuclide i, and C is the total transuranic inventory (in curies) of α-emitters with half-lives greater than 20 years.

The PCS-2012 PA was developed so that the structure of calculations performed therein was as similar as possible to that used in the PABC-2009. PABC-2009 calculated results potentially impacted by the panel closure redesign were updated, while the results from previous PAs were used for individual numerical codes not affected by these changes. The PCS-2012 PA utilized the same waste inventory information, drilling rate and plugging pattern parameters, and radionuclide solubility parameters as were used in the PABC-2009. Separate documentation was prepared describing calculations performed and results obtained for each code executed in the PCS-2012 PA. Citations for this additional documentation are included in the references section of this summary report, and are indicated in the list below.

- Parameter Sampling (Kirchner 2012a)
- Sensitivity Analysis (Kirchner 2012b)
- Salado Flow (Camphouse 2012d)
- Cuttings, Cavings, and Spallings (Kicker 2012)
- Direct Brine Releases (Malama 2012)
- CCDF Normalized Releases (Zeitler 2012)

4 RUN CONTROL

Run control documentation of codes executed in the PCS-2012 PA is provided in APPENDIX Appendix A. This documentation contains:

1. A description of the hardware platform and operating system used to perform the calculations.
2. A listing of the codes and versions used to perform the calculations.
3. A listing of the scripts used to run each calculation.
4. A listing of the input and output files for each calculation.
5. A listing of the library and class where each file is stored.
6. File naming conventions.

As described previously, PABC-2009 results were used for individual numerical codes primarily unaffected by the panel closure redesign. Documentation of run control for results calculated in the PABC-2009 is provided in Long (2010).

5 RESULTS

Replacement of the Option D panel closure with the ROMPCS design has no impact on cuttings and cavings releases resulting from drilling intrusions in repository waste areas. Cuttings and cavings results obtained in the PCS-2012 PA are identical to those found in the PABC-2009. In addition, Culebra transport results calculated in the PABC-2009 are also used in the PCS-202 PA calculations. Discussions of cuttings and cavings releases, as well as Culebra transport releases, calculated in the PABC-2009 can be found in Clayton et al. (2010) and the references therein. The primary focus of the PCS-2012 PA is a determination of pressure and brine saturation changes in waste-containing repository regions, and the impacts these changes have on spallings releases and DBRs. Spallings releases and DBRs are two of the release components used to calculate total normalized releases. As a result, the impact of pressure and brine saturation changes on total normalized releases is of interest as well.

Summary results obtained in the PCS-2012 PA are broken out in sections below, and are compared to PABC-2009 results. Salado flow modeling results are presented in Section 5.1. The use of PABC-2009 Culebra transport results for the PCS-2012 PA is justified in Section 5.1.4. Spallings results are presented in Section 5.2. Direct brine releases are presented in Section 5.3. The impact of the ROMPCS design on regulatory compliance is discussed in terms of total normalized releases in Section 5.4. As the CCDF is the regulatory metric used to demonstrate compliance, CCDFs obtained in the PCS-2012 PA and the PABC-2009 are compared for each component of release in the appropriate section.

Following the completion of the PCS-2012 PA calculations, but prior to the completion of the summary report, a transcription error was discovered in the ALG1 input file for BRAGFLO. This error has a negligible impact on results obtained in the PCS-2012 PA, and is discussed in Appendix B.

5.1 Salado Flow Results

PA code BRAGFLO calculates the flow of brine and gas in the vicinity of the WIPP repository over the 10,000-year regulatory compliance period. During BRAGFLO calculations, stochastic uncertainty is addressed by defining a set of six scenarios for which brine and gas flow is calculated for each of the vectors generated via parameter sampling. The total number of BRAGFLO simulations executed in the PCS-2012 PA is 1,800 (300 vectors times 6 scenarios).

The six scenarios used in the PCS-2012 PA are unchanged from those used for the PABC-2009. The scenarios include one undisturbed scenario (S1-BF), four scenarios that include a single inadvertent future drilling intrusion into the repository during the 10,000 year regulatory period (S2-BF to S5-BF), and one scenario investigating the effect of two intrusions into a single waste panel (S6-BF). Two types of intrusions, denoted as E1 and E2, are considered. An E1 intrusion assumes the borehole passes through a waste-filled panel and into a pressurized brine pocket that may exist under the repository in the Castile formation. An E2 intrusion assumes that the borehole passes through the repository but does not encounter a brine pocket. Scenarios S2-BF and S3-BF model the effect of an E1 intrusion occurring at 350 years and 1000 years, respectively, after the repository is closed. Scenarios S4-BF and S5-BF model the effect of an E2 intrusion at 350 and 1000 years. Scenario S6-BF models an E2 intrusion occurring at 1000 years, followed by an E1 intrusion into the same panel at 2000 years. Calculated brine flows up the intrusion borehole obtained in scenario S6-BF are used in PA code PANEL to determine the radionuclide source term to the Culebra. Transport releases from the Culebra obtained in the PABC-2009 are also used in the PCS-2012 PA. PCS-2012 PA results from BRAGFLO scenario S6-BF are briefly discussed to justify the appropriateness of PABC-2009 Culebra transport calculations for the PCS-2012 PA. Table 5-1 summarizes the six scenarios used in this analysis.

Table 5-1: BRAGFLO Modeling Scenarios

Scenario	**Description**
S1-BF	Undisturbed Repository
S2-BF	E1 intrusion at 350 years
S3-BF	E1 intrusion at 1000 years
S4-BF	E2 intrusion at 350 years
S5-BF	E2 intrusion at 1000 years
S6-BF	E2 intrusion at 1000 years; E1 intrusion at 2000 years.

Computed results are presented for the PCS-2012 PA and compared with those obtained in the PABC-2009. Results are discussed in terms of overall means. Overall means are obtained by forming the average of the 300 realizations calculated for a given quantity and scenario. Results are presented for undisturbed scenario S1-BF. Intruded results are presented for scenarios S2-BF and S4-BF, as these are representative of the intrusion types considered in scenarios S2-BF to S5-BF with the only differences being the timing of drilling intrusions. Results from scenario S6-BF are also briefly discussed.

Option D panel closures were implemented in the PABC-2009. The computational grid and material map used in the PABC-2009 Salado flow calculations are shown in Figure 5-1. A minor error has been corrected in the material map schematic shown in Figure 5-1. That figure depicts an E1 intrusion into the repository. The BRAGFLO schematic included with the PABC-2009 Salado flow analysis package (Nemer 2010) depicts the lower borehole extending only to the bottom horizon of the lower DRZ. In actuality, the lower borehole extends to the floor of the intruded waste panel. The PABC-2009 BRAGFLO grid and material map shown in Figure 5-1 has been modified so that it represents the correct extent of the lower borehole in an E1 intrusion. The analogous PCS-2012 PA BRAGFLO computational grid and material map are shown in Figure 5-2. As that figure also depicts an E1 intrusion scenario, with 350 years post-closure being the first time instance at which an intrusion occurs, materials DRZ_PCS and ROMPCS material PCS_T3 are in place at the time of all intrusions in the Salado flow calculations. The development of the PCS-2012 PA BRAGFLO grid, as well as the representation of the temporal evolution of the ROMPCS in the BRAGFLO material map, is fully discussed in Camphouse (2012d).

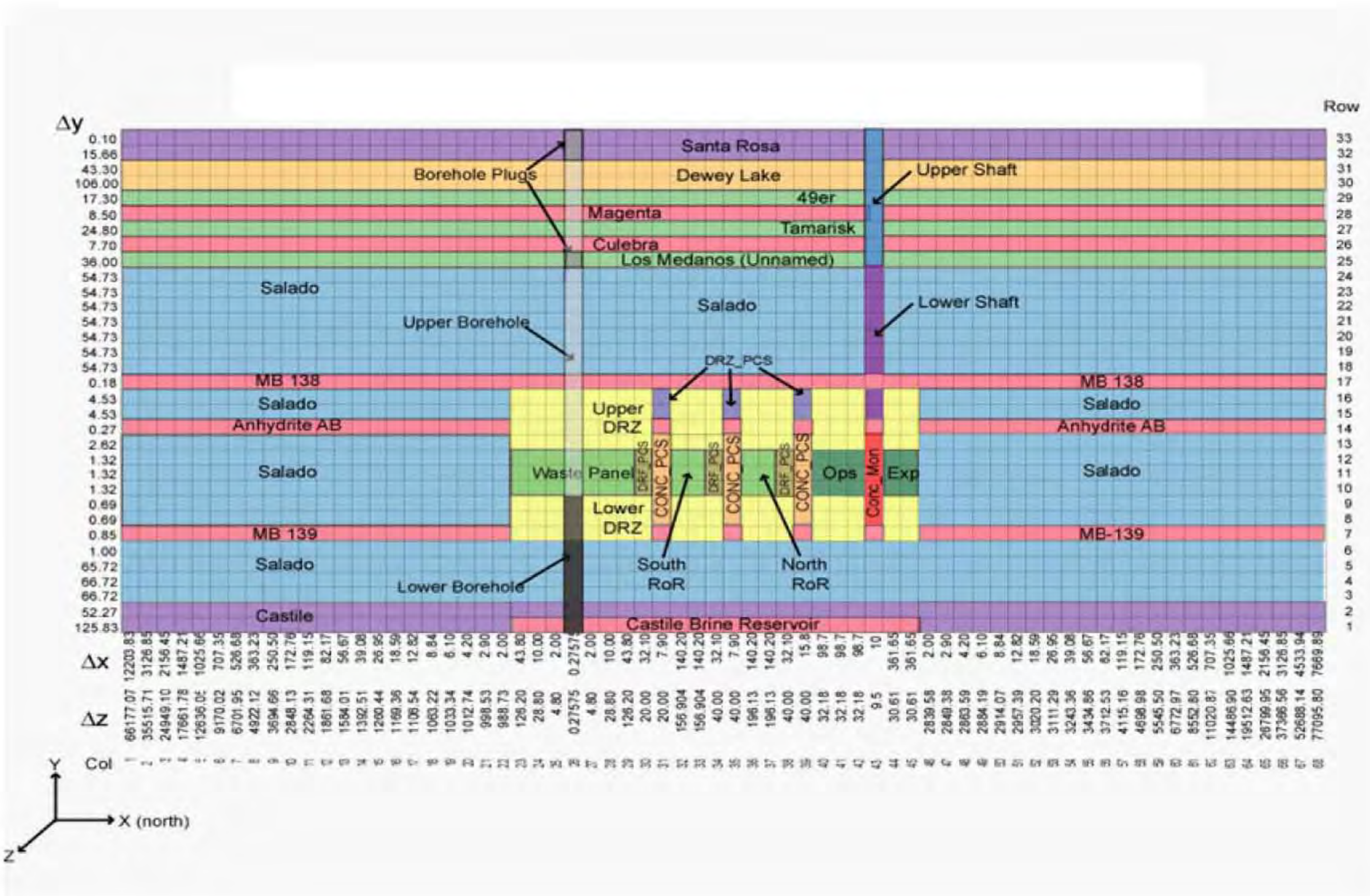


Figure 5-1: PABC-2009 BRAGFLO Grid and Material Map for an E1 Intrusion (Δx, Δy, and Δz dimensions in meters).

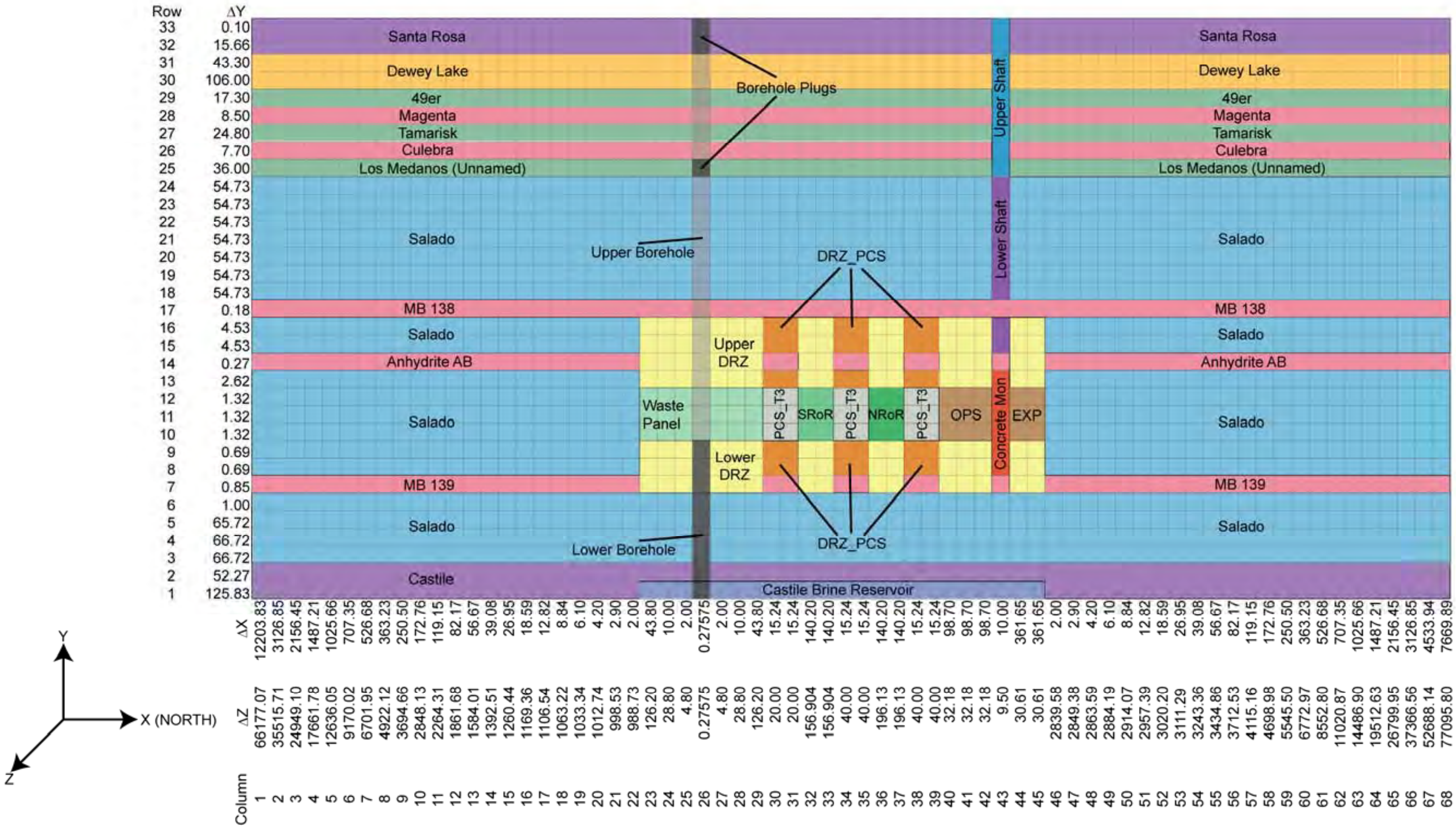


Figure 5-2: PCS-2012 BRAGFLO Grid and Material Map for an E1 Intrusion (Δx, Δy, and Δz dimensions in meters).

5.1.1 Results for an Undisturbed Repository (Scenario S1-BF)

Results are now presented for undisturbed scenario S1-BF. For the sake of brevity in what follows, waste area results are discussed in terms of the waste panel. Trends discussed for the waste panel also apply to other repository waste areas.

The PCS-2012 PA overall mean of cumulative brine flow into the waste panel, denoted by quantity BRNWASIC, is compared to the PABC-2009 overall mean of the same quantity in Figure 5-3. As seen in that figure, there is an increase in the mean cumulative brine flow into the waste panel in the PCS-2012 PA as compared to the PABC-2009. The majority of the increase in quantity BRNWASIC for the PCS-2012 PA occurs during the first 200 years. The increase during the first 200 years is readily apparent in Figure 5-4, where the time scale used to plot BRNWASIC overall means is restricted to the first 1,000 years. As seen in that figure, the difference in the overall means obtained in the two analyses increases steadily until 200 years. At 200 years, the ROMPCS assumes its long-term properties with the DRZ healed above and below it. At 200 years in the PCS-2012 PA BRNWASIC overall mean in Figure 5-4, the rate of increase decreases sharply. At 200 years, the difference between the BRNWASIC overall means obtained in the two analyses is roughly 600 m^3, and this difference between the overall means remains fairly constant for the remainder of the regulatory period.

The increase of brine flow into the waste panel results in a corresponding increase in the waste panel brine saturation, denoted by quantity WAS_SATB. The overall means for WAS_SATB obtained in the PCS-2012 PA and the PABC-2009 are plotted together in Figure 5-5. As seen in that figure, there is an increase in the mean for WAS_SATB in the PCS-2012 PA as compared to the PABC-2009. The increase in brine inflow to the waste panel during the first 200 years translates to an increase in the waste panel brine saturation. Beyond 200 years, the WAS_SATB overall means obtained in the two analyses are qualitatively very similar with differences seen in the magnitude of the respective curves primarily due to increases seen in the PCS-2012 PA during the first 200 years.

Increases in waste panel brine inflow and brine saturation potentially impact waste panel gas generation, denoted by quantity GASMOL_W. Overall means of waste panel gas generation obtained in the PCS-2012 PA and the PABC-2009 are plotted together in Figure 5-6. As seen in that figure, the overall mean for gas generated in the waste panel increased in the PCS-2012 PA. The increases seen in the mean waste panel brine inflow and mean waste panel brine saturation in the PCS-2012 PA result in a corresponding increase in waste panel gas generation.

Overall means of waste panel pressure obtained in the PCS-2012 PA and the PABC-2009 are shown together in Figure 5-7. As seen in that figure, there is a long-term increase in the mean waste panel pressure obtained in the PCS-2012 PA as compared to the PABC-2009. The increase in waste panel gas generation seen in the PCS-2012 PA translates to a long-term increase in the waste panel mean pressure.

Pressure is released from repository waste areas to other repository regions before the ROMPCS and the surrounding DRZ assume their long-term properties at 200 years. The overall means of pressure in the operations area, denoted by quantity OPS_PRES, obtained in the PCS-2012 PA and the PABC-2009 are shown together in Figure 5-8. As seen in Figure 5-8, the mean pressure in the operations area is greater in the PCS-2012 PA at early times when compared to the PABC-2009. After the ROMPCS and the DRZ above and below it assume their long-term properties at 200 years, the rate of pressure release from repository waste areas into the operations area decreases. The "tighter" characteristics of the ROMPCS after 200 years results in less pressure being released to the operations region as compared to Option D. The result is an eventual decrease in the mean pressure in this region when compared to PABC-2009 results. Results obtained for the experimental region are virtually identical to those found for the operations area.

The base of the repository shaft is modeled in WIPP PA as being directly between the operations and experimental regions. Consequently, the pressure in these two regions impacts the volume of brine moved up the shaft toward the ground surface. The overall means of brine flow up the shaft, denoted by quantity BNSHUDRZ, obtained in the PCS-2012 PA and the PABC-2009 are shown together in Figure 5-9. As seen in that figure, the trends for brine flow up the shaft correspond closely to pressure trends in the operations and experimental areas. At early times, an increase is seen in the mean volume of brine flow up the shaft in the PCS-2012 PA. Eventually, however, the mean brine flow up the shaft is reduced in the PCS-2012 PA results, primarily due to the reductions in the mean pressure seen in the operations and experimental areas after the ROMPCS and surrounding DRZ assume their long-term properties.

Summary statistics for scenario S1-BF are shown in Table 5-2.

Table 5-2: Summary Statistics for Scenario S1-BF

Quantity (units)	**Mean Value**		**Maximum Value**	
	PABC-2009	**PCS-2012 PA**	**PABC-2009**	**PCS-2012 PA**
BRNWASIC ($x10^3$ m^3)	1.78	2.38	12.46	16.67
WAS_SATB (none)	0.16	0.20	0.99	0.99
GASMOL_W ($x10^6$ moles)	29.09	30.84	148.40	149.00
WAS_PRES (MPa)	6.52	6.77	16.19	16.29
BNSHUDRZ (m^3)	2.74	2.46	34.76	32.11

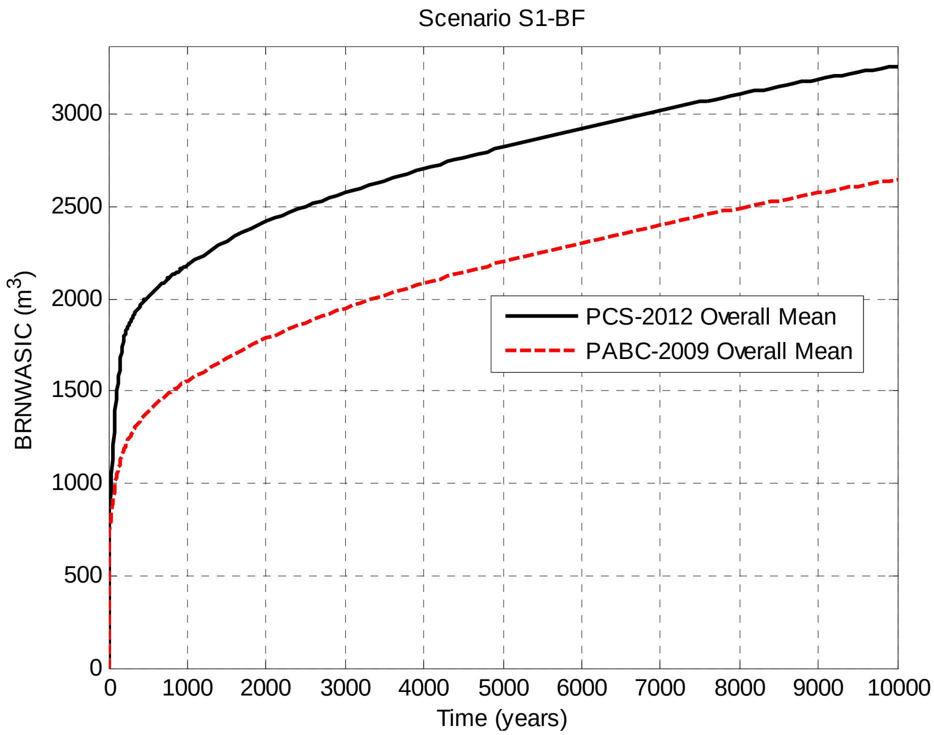


Figure 5-3: Overall Means of Cumulative Brine Inflow to the Waste Panel, Scenario S1-BF.

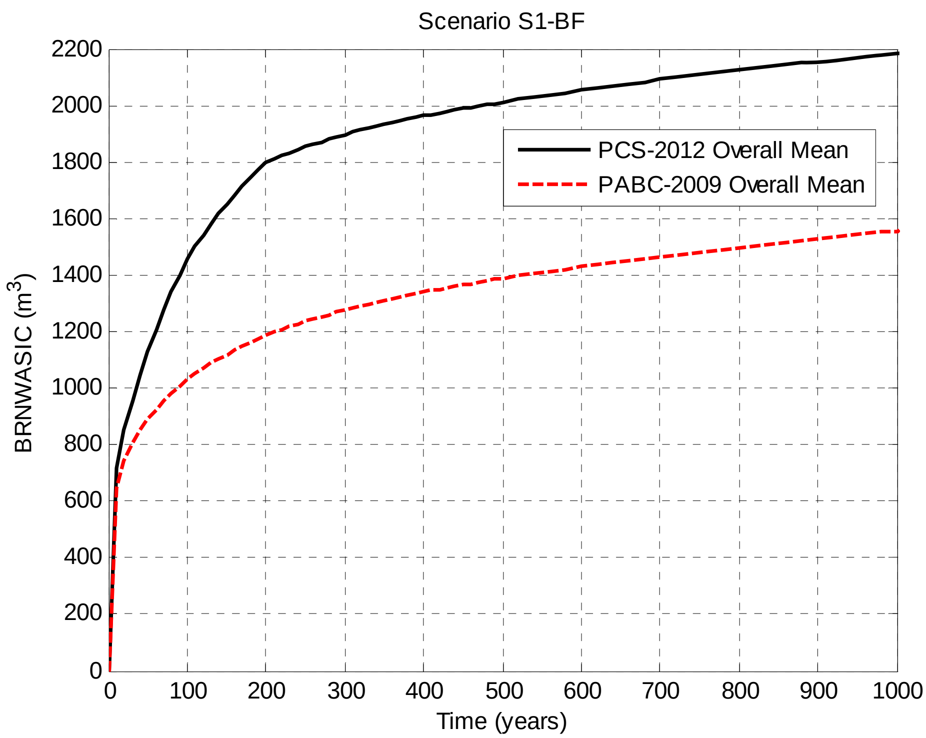


Figure 5-4: Overall Means of Cumulative Brine Inflow to the Waste Panel, Scenario S1-BF and Years 0 to 1,000.

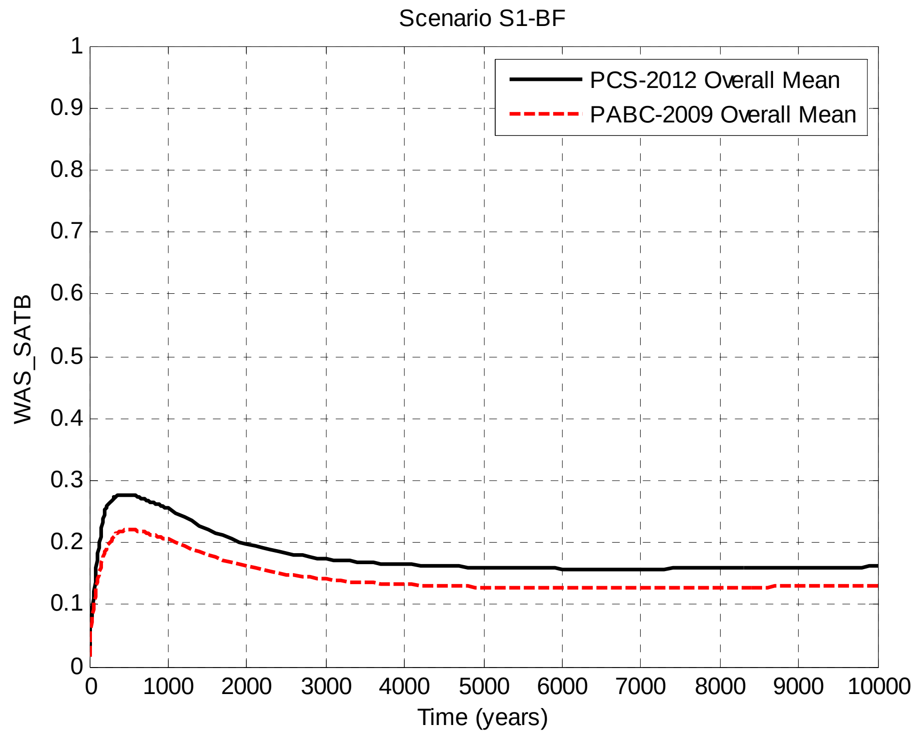


Figure 5-5: Overall Means of Waste Panel Brine Saturation, Scenario S1-BF.

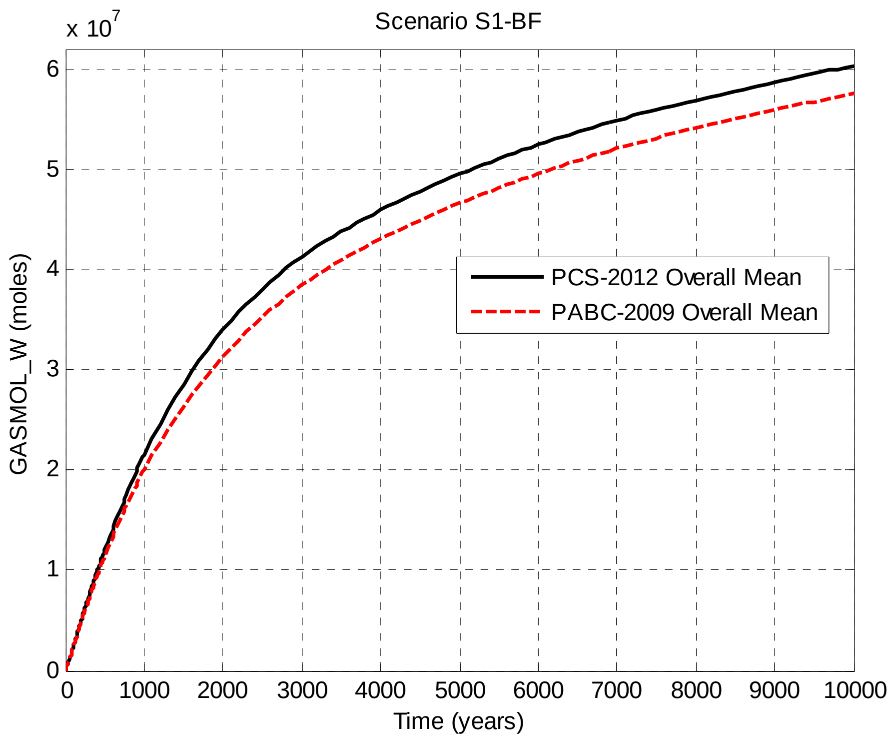


Figure 5-6: Overall Means of Waste Panel Gas Generation (in moles), Scenario S1-BF.

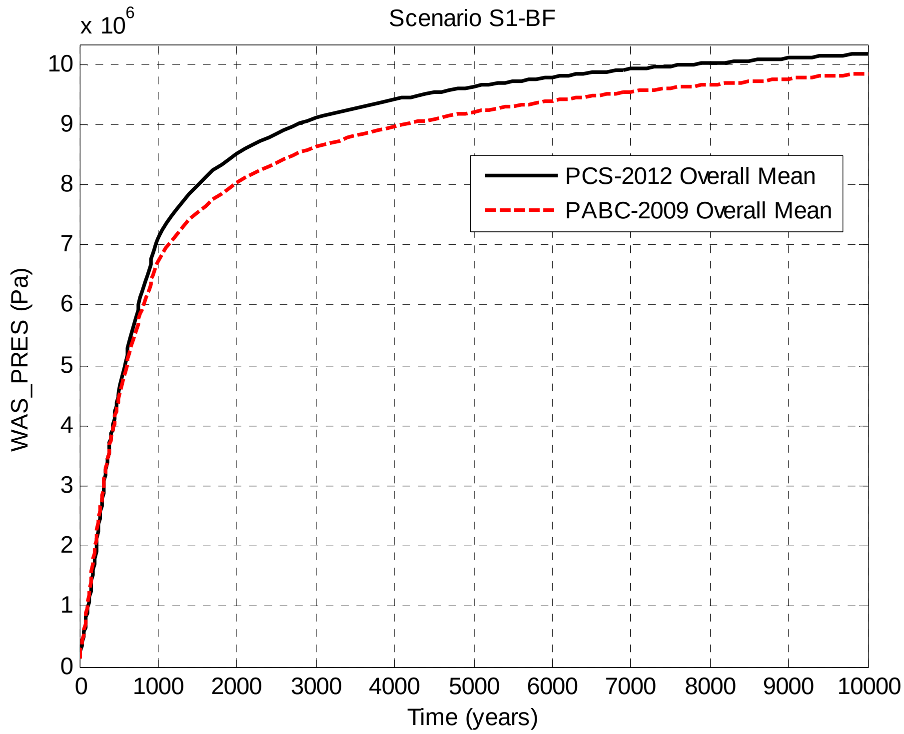


Figure 5-7: Overall Means of Waste Panel Pressure, Scenario S1-BF.

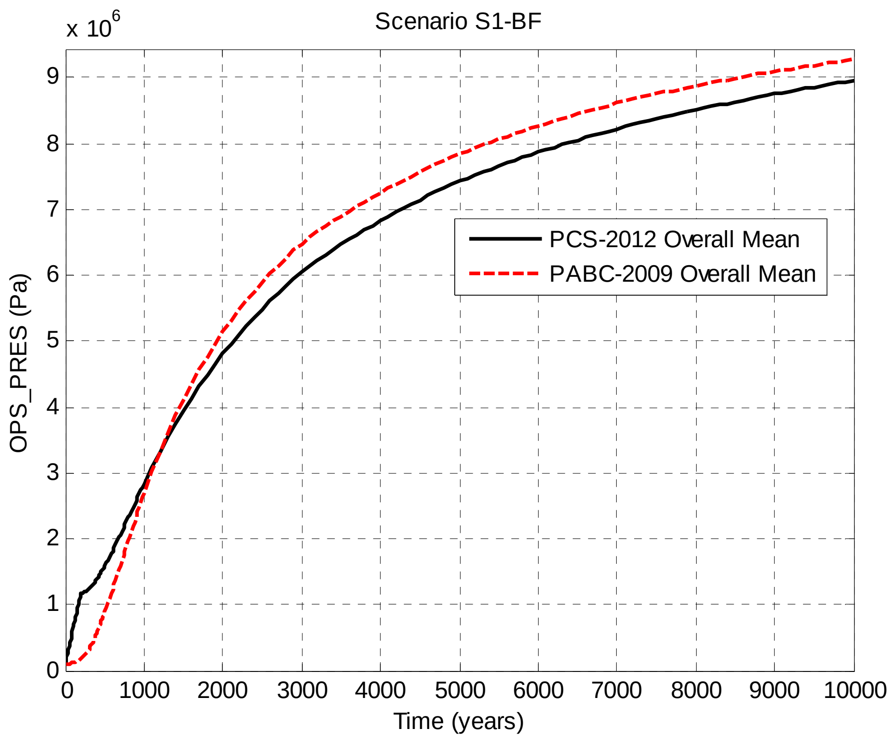


Figure 5-8: Overall Means of Pressure in the Operations Region, Scenario S1-BF.

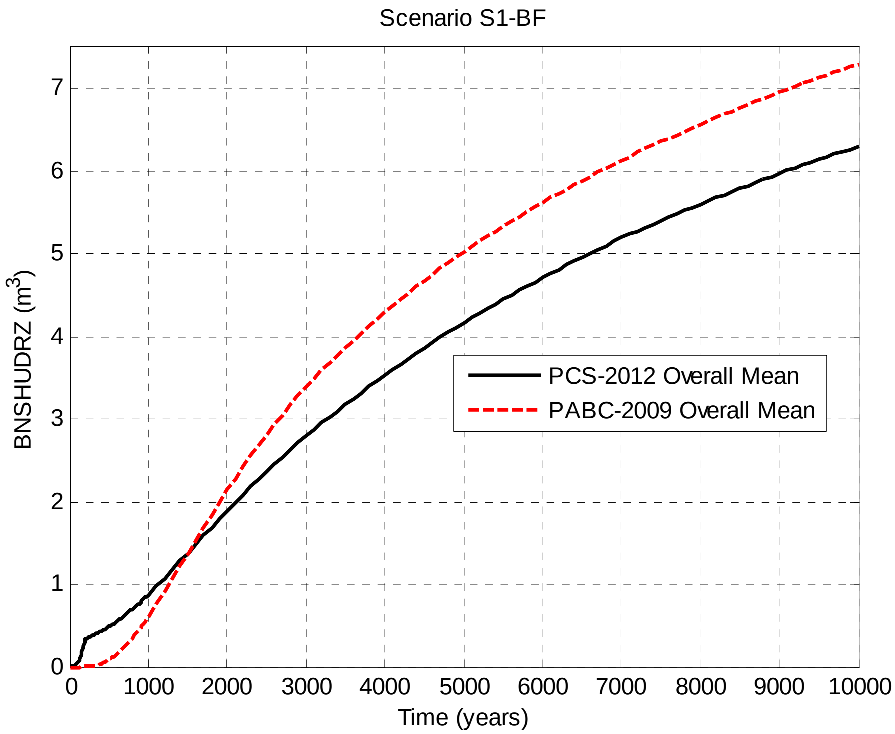


Figure 5-9: Overall Means of Brine Flow up the Shaft, Scenario S1-BF.

5.1.2 Results for an E1 Intrusion at 350 Years (Scenario S2-BF)

Results are now presented for disturbance scenario S2-BF. Results presented for this scenario are representative of those calculated for E1 intrusion scenarios (scenarios S2-BF and S3-BF), with the only difference being the time of the intrusion. In the results that follow, PCS-2012 PA trends discussed for scenario S2-BF also apply to scenario S3-BF.

The fundamental characteristic of an E1 intrusion is the creation of a connected pathway between the repository waste panel and a region of pressurized brine in the Castile. Castile brine moves upward into the waste panel immediately after the intrusion, increasing waste panel pressure, brine saturation, and impacting other waste panel quantities.

The overall means of waste panel pressure obtained in the PCS-2012 PA and the PABC-2009 for scenario S2-BF are plotted together in Figure 5-10. As seen in that figure, the mean waste panel pressure calculated in the PCS-2012 PA is greater than that found in the PABC-2009 for a period of time after the intrusion. The long-term permeability range of the ROMPCS is lower than that prescribed to the Option D design in the PABC-2009. This reduction results in less long-term brine and gas flow through the ROMPCS, away from the waste panel, as compared to Option D. Following the E1 intrusion at 350 years, the “tighter” ROMPCS design results in a period of increased waste panel pressurization as compared to the PABC-2009 results.

An increase in waste panel pressure potentially impacts the volume of cumulative brine inflow to the waste panel, denoted by quantity BRNWASIC. The overall means of BRNWASIC obtained in the PCS-2012 PA and the PABC-2009 are shown together in Figure 5-11. As seen in that figure, the increased permeability range of the ROMPCS at early times results in greater brine inflow to the waste panel before the ROMPCS attains its long-term properties at 200 years. Following the intrusion time of 350 years, an increase in mean waste panel pressure occurs in the PCS-2012 PA results. This pressure increase slightly inhibits brine flow into the waste panel, resulting in a reduction in cumulative waste panel brine inflow as compared to the PABC-2009 results.

The reduction of brine flowing into the waste panel in the PCS-2012 PA impacts the waste panel brine saturation, denoted by quantity WAS_SATB. The overall means of quantity WAS_SATB obtained in the PCS-2012 PA and the PABC-2009 are shown together in Figure 5-12. As is evident in that figure, the mean waste panel brine saturation obtained in the PCS-2012 PA is reduced slightly from that calculated in the PABC-2009 after the intrusion at 350 years. The reduction of brine inflow to the waste panel translates to a reduction in waste panel brine saturation.

The overall means of waste panel gas generation (quantity GASMOL_W) obtained in the PCS-2012 PA and the PABC-2009 are shown together in Figure 5-13. The overall means obtained for quantity GASMOL_W obtained in the two analyses are nearly identical, with a very slight reduction seen in the PCS-2012 PA mean. This slight reduction in gas generation is most likely due to the reduction in waste panel brine inflow and brine saturation seen in the PCS-2012 PA results.

The volume of brine flow up the intrusion borehole is denoted by quantity BNBHUDRZ. Overall means of BNBHUDRZ obtained in the PCS-2012 PA and the PABC-2009 are shown together in Figure 5-14. The overall means obtained in the two analyses are almost identical, with a very slight increase seen in the PCS-2012 PA result.

Summary statistics for scenario S2-BF are shown in Table 5-3.

Table 5-3: Summary Statistics for Scenario S2-BF

Quantity (units)	**Mean Value**		**Maximum Value**	
	PABC-2009	**PCS-2012 PA**	**PABC-2009**	**PCS-2012 PA**
BRNWASIC ($x10^3$ m^3)	14.03	13.68	182.15	182.08
WAS_SATB (none)	0.68	0.67	0.99	0.99
GASMOL_W ($x10^6$ moles)	54.75	54.57	149.00	149.00
WAS_PRES (MPa)	7.39	7.50	15.63	16.40
BNBHUDRZ ($x10^3$ m^3)	3.25	3.28	166.84	169.54

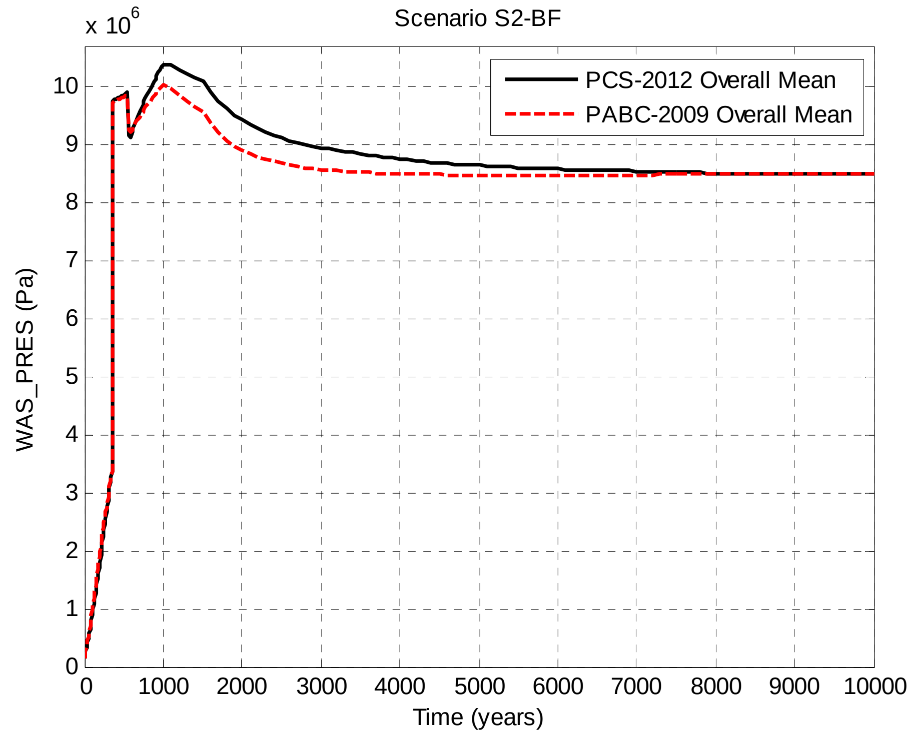


Figure 5-10: Overall Means of Waste Panel Pressure, Scenario S2-BF.

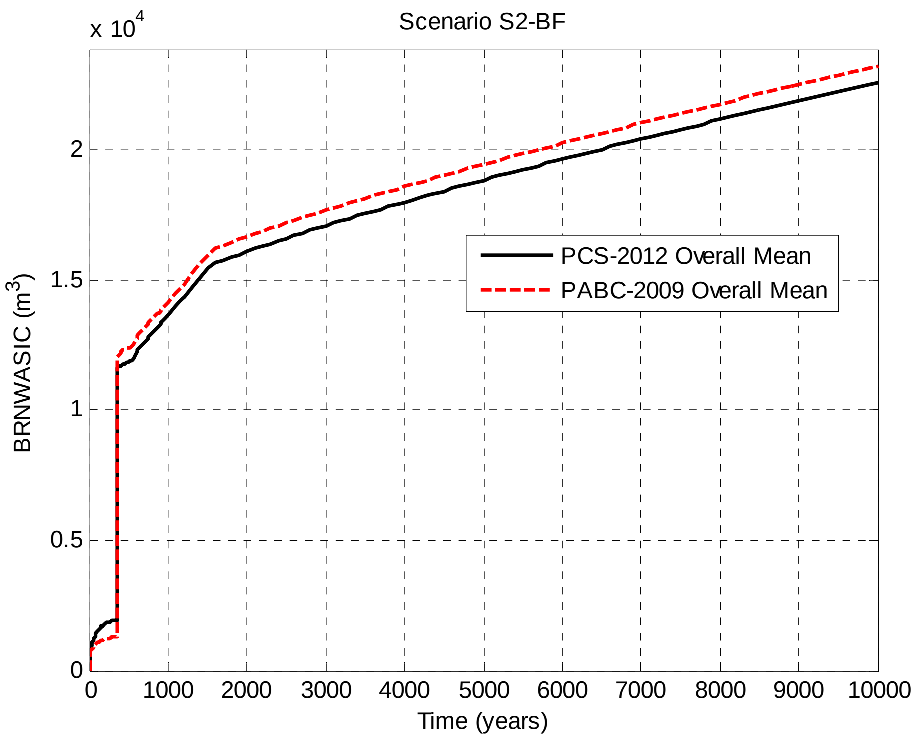


Figure 5-11: Overall Means of Cumulative Brine Inflow to the Waste Panel, Scenario S2-BF.

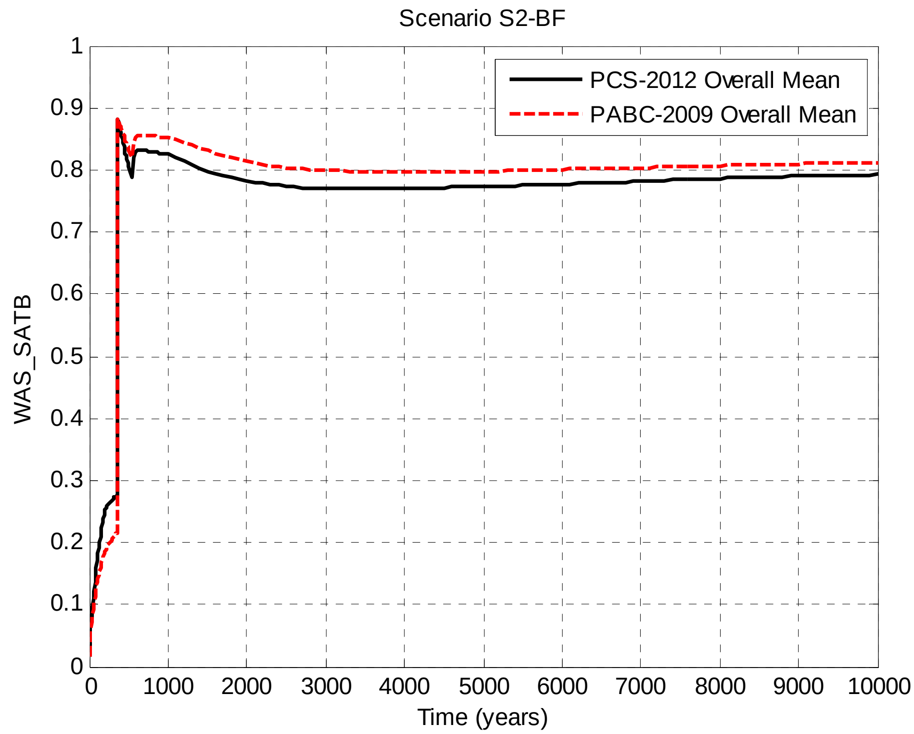


Figure 5-12: Overall Means of Waste Panel Brine Saturation, Scenario S2-BF.

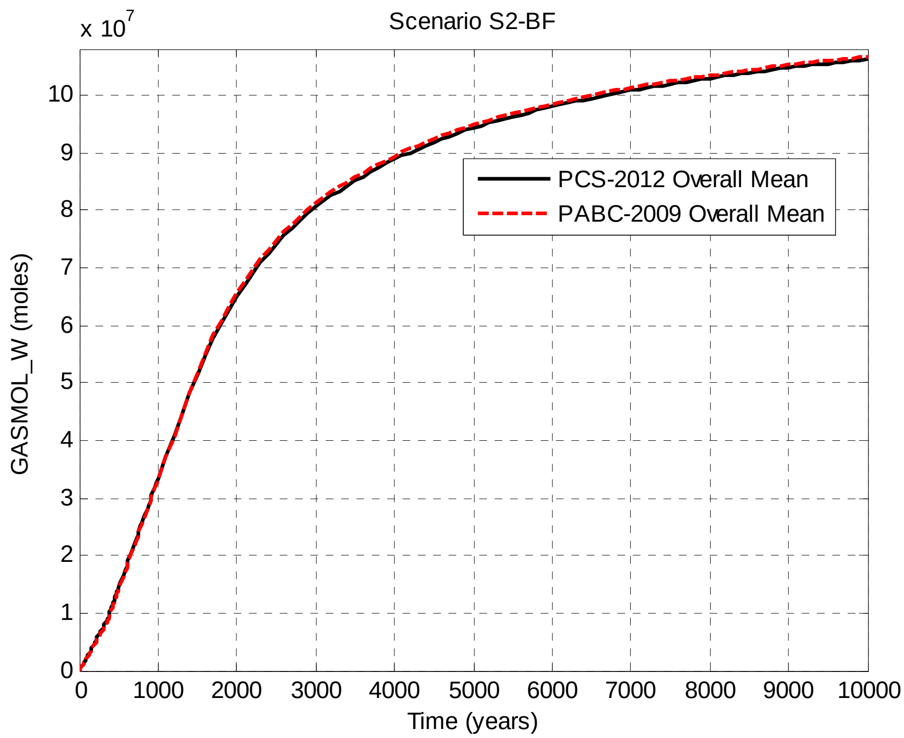


Figure 5-13: Overall Means of Waste Panel Gas Generation (in moles), Scenario S2-BF.

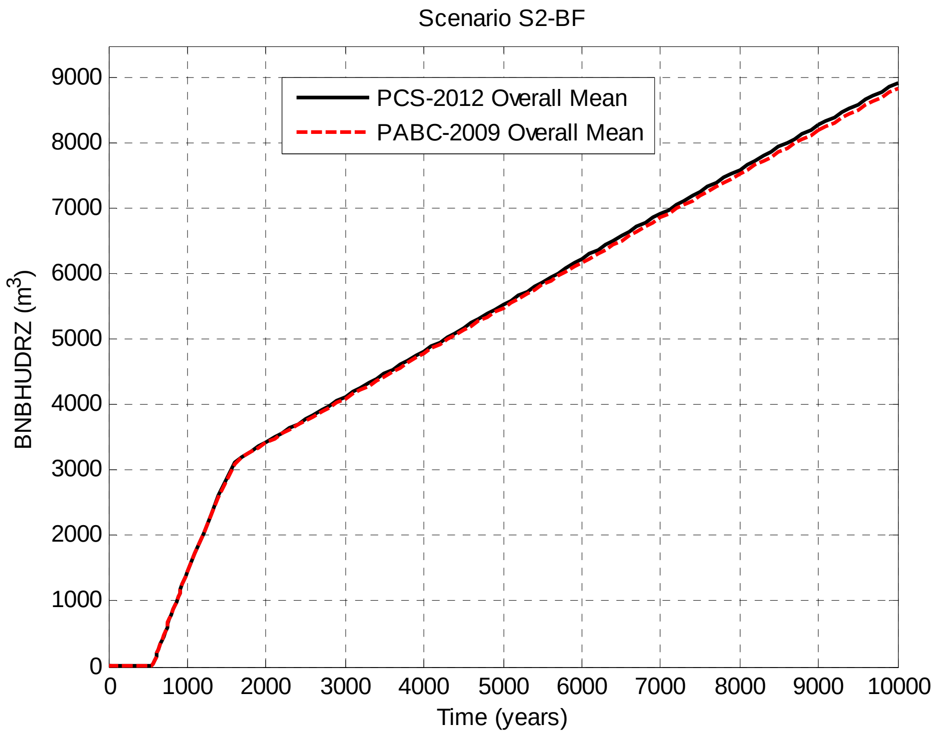


Figure 5-14: Overall Means of Brine Flow up the Borehole, Scenario S2-BF.

5.1.3 Results for an E2 Intrusion at 350 Years (Scenario S4-BF)

Results are now presented for disturbance scenario S4-BF. Results presented for this scenario are representative of those calculated for E2 intrusion scenarios (scenarios S4-BF and S5-BF), with the only difference being the time of the intrusion. In the results that follow, PCS-2012 PA trends discussed for scenario S4-BF also apply to scenario S5-BF.

As seen in the previous section, an E1 intrusion scenario results in an immediate influx of pressurized Castile brine to the waste panel, resulting in an increase is waste panel pressure when compared to undisturbed conditions. An E2 intrusion typically has the opposite effect. For the E2 intrusion scenario, no connected pathway is created between pressurized Castile brine and the repository waste panel. Following the intrusion, concrete plugs are immediately emplaced in the borehole near the ground surface. Consequently, an E2 intrusion does not typically have a significant impact on waste panel quantities *at the time of intrusion*. 200 years after the time of intrusion, concrete plugs emplaced in the borehole are modeled as failing, with the entire borehole assuming properties equivalent to sand. The result is a depressurization of the waste panel, beginning 200 years after the intrusion. Whereas an E1 intrusion typically results in an immediate increase in waste panel pressure, an E2 intrusion typically results in a *reduction* in waste panel pressure 200 years after the intrusion as compared to undisturbed conditions. The impact of the E2 intrusion on waste panel pressure is more closely seen in Figure 5-15. In that figure, PCS-2012 PA overall means of waste panel pressure obtained in scenarios S1-BF and S4-BF are plotted together with the time scale restricted to the first 1,000 years. As seen in that figure, no noticeable impact is seen in the mean waste panel pressure when the E2 intrusion occurs at 350 years. For the period of 350 years to 550 years, there is a slight increase in the mean pressure for scenario S4-BF as compared to undisturbed results. The borehole plugs fail at 550 years, creating a pathway for waste panel pressure release through the borehole and toward the ground surface. Consequently, the mean waste panel pressure for scenario S4-BF is reduced sharply at 550 years when compared to undisturbed results. The overall means of waste panel pressure obtained for scenario S4-BF in the PCS-2012 PA and the PABC-2009 are shown together in Figure 5-16. As seen in that figure, the mean waste panel pressure obtained in the PCS-2012 PA is slightly greater than the PABC-2009 result. As already discussed, the PCS-2012 PA mean waste panel pressure is greater than that seen in the PABC-2009 for undisturbed conditions (Figure 5-7). Consequently, at the time of the E2 intrusion, the mean waste panel pressure is greater in the PCS-2012 PA, and is also greater 200 years later when the borehole plugs fail. The result is a slightly higher mean pressure in the PCS-2012 PA scenario S4-BF result when compared to the PABC-2009.

The impact of the E2 intrusion on cumulative waste panel brine inflow can be clearly seen in Figure 5-17. At the intrusion time of 350 years until the borehole plugs fail at 550 years, there is only a very slight increase in quantity BRNWASIC as compared to undisturbed conditions. After the borehole plugs fail, a decrease in the waste panel pressure occurs. This pressure reduction yields in an increase in brine flow into the waste panel at 550 years compared to the undisturbed case. The overall means for quantity BRNWASIC in the PCS-2012 PA and the PABC-2009 are plotted together in Figure 5-18. As evident in that figure, an increase to the mean waste panel cumulative brine inflow is seen in the PCS-2012 PA results. This increase is due to the increased waste panel brine inflow seen for undisturbed conditions (Figure 5-4). Very little impact is seen in the mean curve for quantity BRNWASIC as compared to undisturbed conditions, until the borehole plugs fail at 550 years. The PCS-2012 PA mean waste panel brine inflow curve is already greater than that obtained in the PABC-2009 when the borehole plugs fail at 550 years. The increase in brine inflow seen after the borehole plugs fail results in a PCS-2012 PA mean waste panel brine inflow curve that remains greater than that seen in the PABC-2009.

The change to cumulative waste panel brine inflow seen in the PCS-2012 PA impacts the waste panel brine saturation. The impact of the E2 intrusion on quantity WAS_SATB is similar to that seen for cumulative brine flow into the waste panel. As seen in Figure 5-19, the mean waste panel brine saturation is changed very little as compared to undisturbed conditions for the time period of 350 to 550 years. After the borehole plugs fail at 550 years, an increase of brine inflow to the waste panel translates to a corresponding increase in brine saturation. The result is a PCS-2012 PA mean waste brine saturation curve that is greater than that seen in the PABC-2009 results (Figure 5-20). The increase in the mean cumulative brine inflow to the waste panel seen in the PCS-2012 PA translates to an increase in the mean waste panel brine saturation.

The increase in waste panel brine saturation impacts gas generation in the waste panel. More brine flows into the waste panel (on average) in PCS-2012 PA scenario S4-BF as compared to the PABC-2009, resulting in an overall mean for quantity GASMOL_W in the PCS-2012 PA that is greater than that seen in the PABC-2009 (Figure 5-21).

The volume of brine flowing up the borehole toward the ground surface is denoted by quantity BNBHUDRZ. The increase in the mean waste panel pressure seen in the PCS-2012 PA yields a slight long-term increase in the means of quantity BNBHUDRZ. The overall mean of this quantity is greater in the PCS-2012 PA, as shown in Figure 5-22.

Summary statistics for scenario S4-BF are shown in Table 5-4.

Table 5-4: Summary Statistics for Scenario S4-BF

Quantity (units)	**Mean Value**		**Maximum Value**	
	PABC-2009	**PCS-2012 PA**	**PABC-2009**	**PCS-2012 PA**
BRNWASIC ($x10^3$ m^3)	2.73	3.29	23.81	19.39
WAS_SATB (none)	0.28	0.33	0.99	0.99
GASMOL_W ($x10^6$ moles)	36.40	38.35	149.00	149.00
WAS_PRES (MPa)	4.64	4.70	14.92	15.21
BNBHUDRZ (m^3)	34.76	43.76	4876.89	5287.28

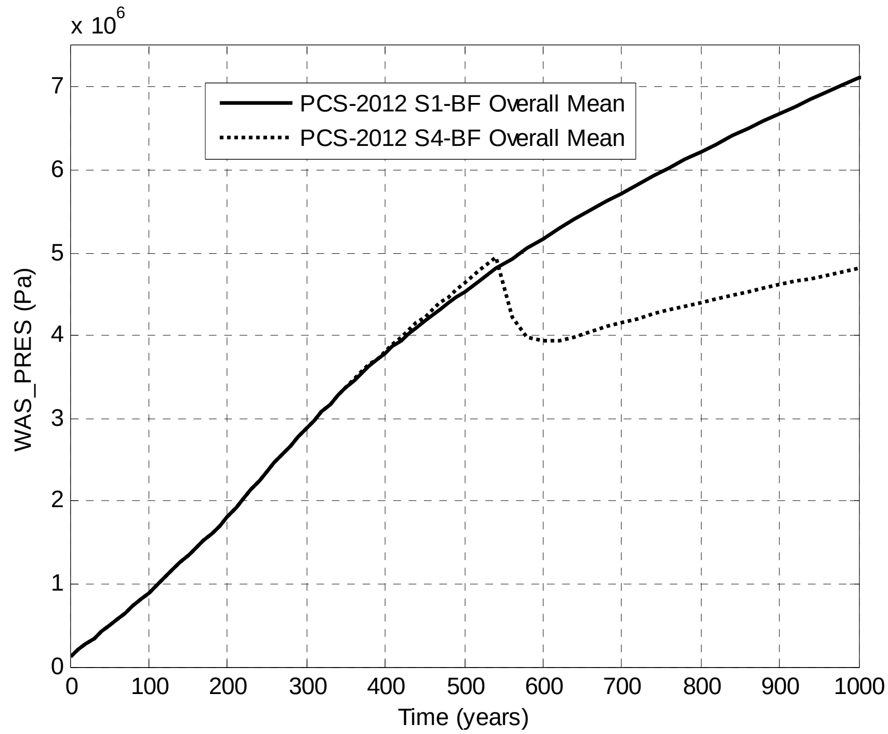


Figure 5-15: Overall Means of Waste Panel Pressure, Scenarios S1-BF and S4-BF for Years 0 to 1,000.

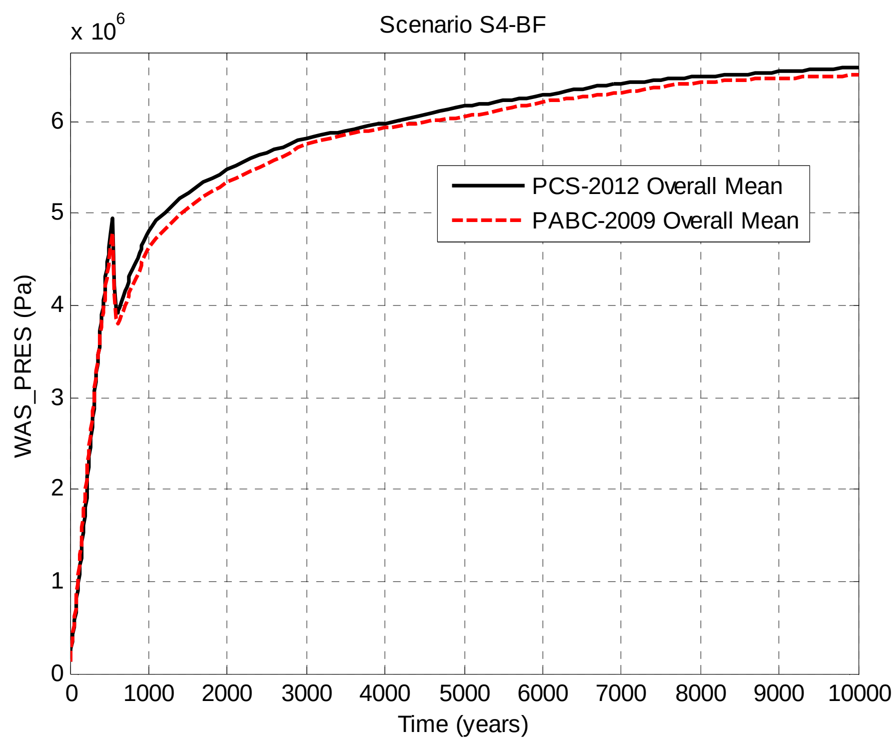


Figure 5-16: Overall Means of Waste Panel Pressure, Scenario S4-BF.

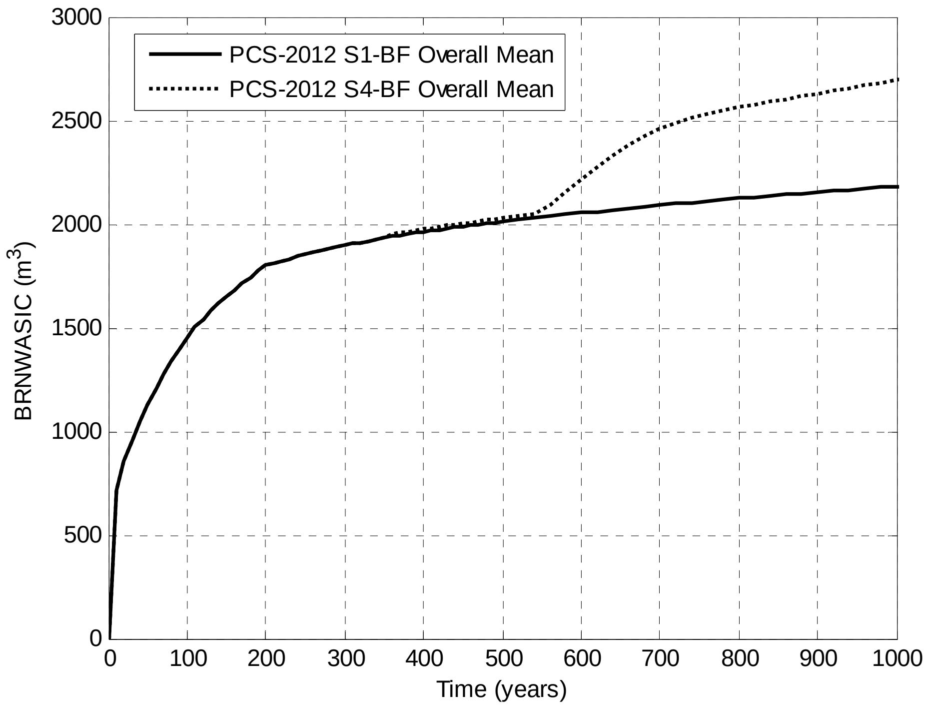


Figure 5-17: Overall Means of Cumulative Brine Inflow to the Waste Panel, Scenarios S1-BF and S4-BF for Years 0 to 1,000.

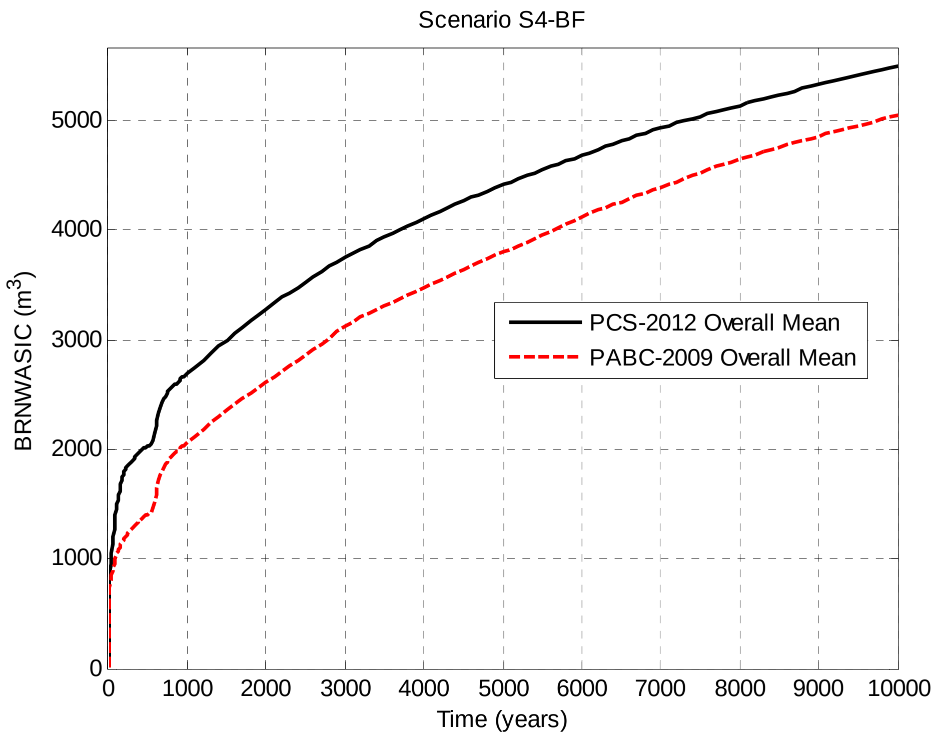


Figure 5-18: Overall Means of Cumulative Brine Inflow to the Waste Panel, Scenario S4-BF.

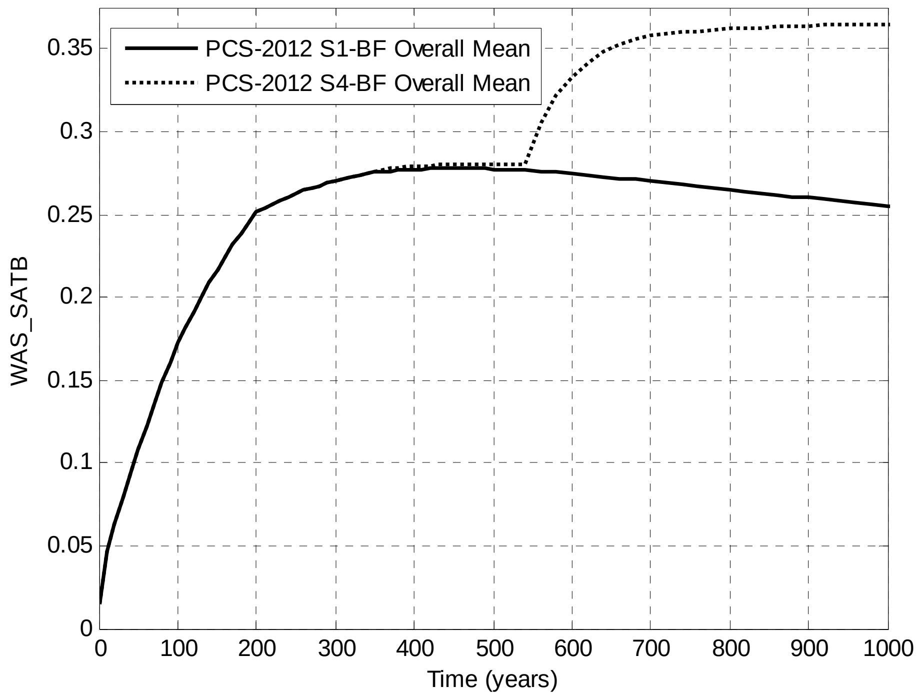


Figure 5-19: Overall Means of Waste Panel Brine Saturation, Scenarios S1-BF and S4-BF for Years 0 to 1,000.

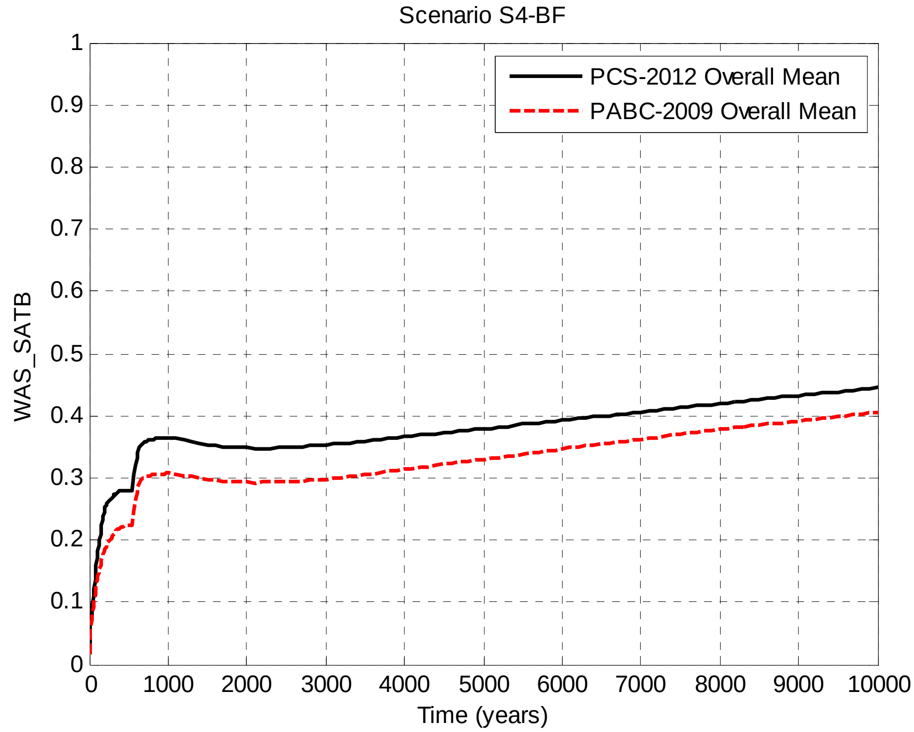


Figure 5-20: Overall Means of Waste Panel Brine Saturation, Scenario S4-BF.

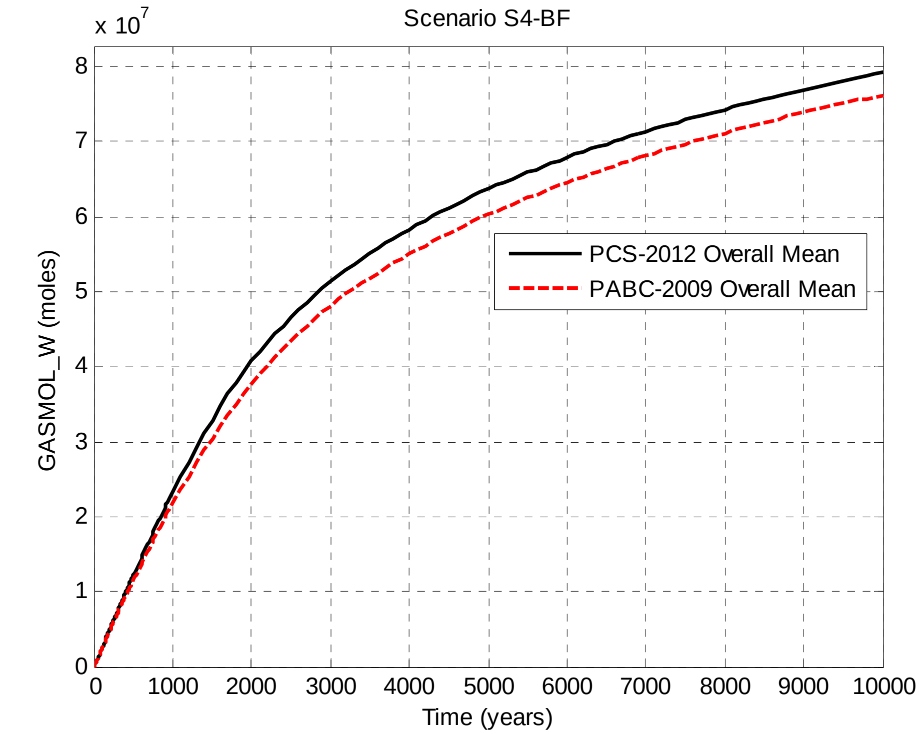


Figure 5-21: Overall Means of Waste Panel Gas Generation (in moles), Scenario S4-BF.

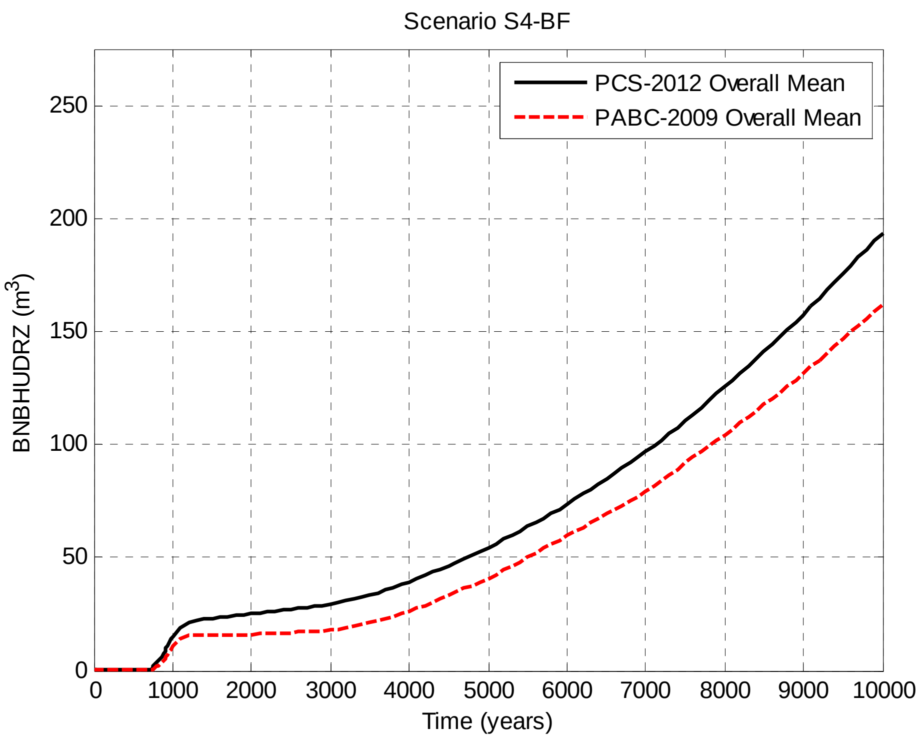


Figure 5-22: Overall Means of Brine Flow up the Borehole, Scenario S4-BF.

5.1.4 Results for an E2 Intrusion at 1000 Years Followed by a E1 Intrusion at 2000 Years (Scenario S6-BF)

BRAGFLO scenario S6-BF models an E2 intrusion occurring at 1000 years, followed by an E1 intrusion into the same panel at 2000 years. Calculated brine flows up the intrusion borehole obtained in scenario S6-BF are used in PA code PANEL to determine the radionuclide source term to the Culebra. Transport releases from the Culebra obtained in the PABC-2009 are used in the PCS-2012 PA. Results from BRAGFLO scenario S6-BF are now briefly discussed to justify the appropriateness of PABC-2009 Culebra transport calculations for the PCS-2012 PA.

The overall means obtained for quantity BNBHUDRZ in the PCS-2012 PA and the PABC-2009 are shown together in Figure 5-23. As seen in that figure, there is very close agreement between the overall means obtained in the two analyses. The replacement of the Option D panel closure with the ROMPCS design has a negligible impact on brine flow up the intrusion borehole in BRAGFLO scenario S6-BF. Actinide solubilities, the repository waste inventory, and Culebra transmissivity fields are unchanged from the PABC-2009 to the PCS-2012 PA. As the brine flows up the intrusion borehole obtained in the two analyses are virtually identical in scenario S6-BF, the radionuclide source term to the Culebra is virtually unchanged by the ROMPCS design as compared to Option D results. Consequently, transport releases from the Culebra are also virtually unchanged. Incorporating PABC-2009 Culebra transport results into the PCS-2012 PA is reasonable and appropriate.

Summary statistics for quantity BNBHUDRZ obtained in scenario S6-BF are shown in Table 5-5.

Table 5-5: Summary Statistics for Scenario S6-BF

Quantity (units)	Mean Value		Maximum Value	
	PABC-2009	PCS-2012 PA	PABC-2009	PCS-2012 PA
BNBHUDRZ ($x10^3$ m^3)	2.92	2.94	169.03	169.30

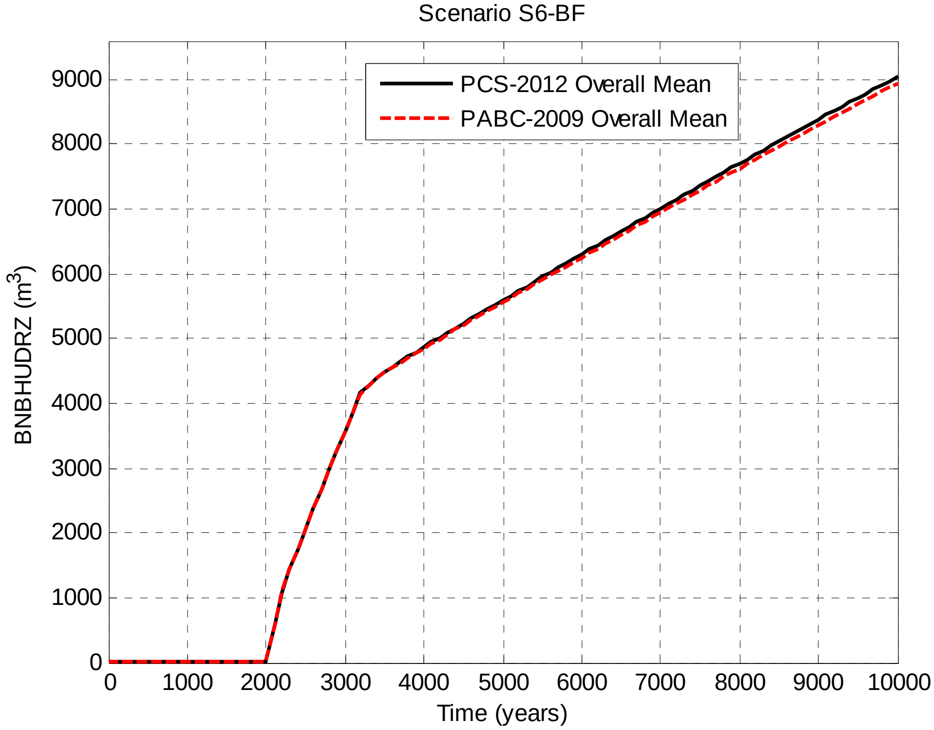


Figure 5-23: Overall Means of Brine Flow up the Borehole, Scenario S6-BF.

5.2 Spallings

The replacement of the Option D panel closure with the ROMPCS design has no impact on cuttings and cavings releases. Changes in repository pressures seen in the PCS-2012 PA BRAGFLO results potentially impact spallings releases, however. Calculation of the volume of solid waste material released to the surface from a single drilling intrusion into the repository due to spallings is a two-part procedure. First, PA code DRSPALL calculates the spallings volumes from a single drilling intrusion at four values of repository pressure (10, 12, 14, and 14.8 MPa). The second step in calculating spallings volumes from a single intrusion consists of using the code CUTTINGS_S to interpolate between DRSPALL volumes. The spallings volume for a given vector is determined in CUTTINGS_S by linearly interpolating between volumes calculated by DRSPALL based on the pressure calculated in each realization by BRAGFLO. DRSPALL volumes used in the PABC-2009 were also used in the PCS-2012 PA.

PA code CUTTINGS_S is also used as a transfer program between the BRAGFLO Salado flow calculation and the BRAGFLO DBR calculation. Results obtained by BRAGFLO for each realization in scenarios S1-BF to S5-BF are used to initialize the flow field properties necessary for the calculation of DBRs. This requires that results obtained on the BRAGFLO grid be mapped appropriately to the DBR grid. Code CUTTINGS_S is used to transfer the appropriate scenario results obtained with BRAGFLO to the DBR calculation. These transferred flow results are used as initial conditions in the calculation of DBRs. As a result, intrusion scenarios and times used in the calculation of spallings volumes correspond to those used in the calculation of DBRs. Five intrusion scenarios are considered in the DBR calculations, and are listed in Table 5-6.

Table 5-6: PA Intrusion Scenarios Used in Calculating Direct Solids Releases

Scenario	**Conditioning (or 1st) Intrusion Time (year) and Type**	**Intrusion Times – Subsequent (year)**
S1-DBR	None	100, 350, 1000, 3000, 5000, 10000
S2-DBR	350, E1	550, 750, 2000, 4000, 10000
S3-DBR	1000, E1	1200, 1400, 3000, 5000, 10000
S4-DBR	350, E2	550, 750, 2000, 4000, 10000
S5-DBR	1000, E2	1200, 1400, 3000, 5000, 10000

While CUTTINGS_S uses these standard DBR scenarios as a basis for its calculations, it does so to provide flow field results (generated with BRAGFLO) as initial conditions to the DBR calculation at each subsequent intrusion time. CUTTINGS_S does not model the intrusion scenario itself. Scenario S1-DBR corresponds to an initial intrusion into the repository, with repository flow conditions at the time of intrusion transferred from BRAGFLO scenario S1-BF results. Scenarios S2-DBR through S5-DBR are used to model an intrusion into a repository that has already been penetrated. The times at which intrusions are assumed to occur for each scenario are outlined in the last column of Table 5-6; six intrusion times are modeled for scenario S1-DBR, while five times are modeled for each of scenarios S2-DBR through S5-DBR.

Utilizing the spallings volumes calculated by DRSPALL and the PCS-2012 PA repository pressures calculated by BRAGFLO, the impact of the ROMPCS design on spallings volumes can be determined. Summary statistics of spallings volumes for the intrusion scenarios considered by CUTTINGS_S are shown in Table 5-7 for both the PCS-2012 PA and the PABC-2009. PABC-2009 results reported in that table (except for the percentage of nonzero volumes) are taken from Ismail (2010). While the results for the PABC-2009 and the PCS-2012 PA calculations are similar for some scenarios, some differences in the spallings volumes are noted. In general, the PCS-2012 results show increases in the maximum spallings volume across all three replicates. Replicate 1 showed very similar average nonzero spallings volumes in both PA calculations. In replicates 2 and 3, the average nonzero spallings volumes were higher for the PCS-2012 PA calculations compared to PABC-2009, with the most significant volume increases occurring in scenarios S2-DBR, S3-DBR, and S5-DBR. Overall, the general trend shows a slightly higher average nonzero spallings volume, a larger maximum volume, and a larger percentage of vectors with spallings considering the total from all scenarios across all three replicates (Kicker 2012).

The change in spallings volumes between the PCS-2012 PA and the PABC-2009 is the result of changing repository pressures observed in BRAGFLO calculations for the PCS-2012 PA. Because spallings volumes directly depend on repository pressure, an increase in repository pressure translates into larger spallings volumes. Since there is a minimum threshold pressure required to create spallings, an increase in repository pressure also increases the percentage of vectors with spallings.

Table 5-7: Summary of Spallings Releases by Scenario

		Scenarios					Total
		S1-DBR	S2-DBR	S3-DBR	S4-DBR	S5-DBR	
PCS-2012 PA							
R1	**Maximum [m³]**	2.34	9.35	8.69	1.67	1.67	9.35
	Average nonzero volume [m³]	0.37	0.53	0.47	0.29	0.32	0.41
	Number of nonzero volumes	157	141	138	76	104	616
	Percent of nonzero volumes	8.7%	9.4%	9.2%	5.1%	6.9%	7.9%
R2	**Maximum [m³]**	2.76	3.69	2.76	2.76	2.76	3.69
	Average nonzero volume [m³]	0.37	0.42	0.44	0.52	0.55	0.44
	Number of nonzero volumes	184	165	151	79	107	686
	Percent of nonzero volumes	10.2%	11.0%	10.1%	5.3%	7.1%	8.8%
R3	**Maximum [m³]**	6.09	7.32	3.31	2.70	3.29	7.32
	Average nonzero volume [m³]	0.54	0.48	0.38	0.32	0.33	0.43
	Number of nonzero volumes	189	134	144	72	111	650
	Percent of nonzero volumes	10.5%	8.9%	9.6%	4.8%	7.4%	8.3%
PABC-2009							
R1	**Maximum [m³]**	2.24	8.29	7.97	1.67	1.67	8.29
	Average nonzero volume [m³]	0.37	0.54	0.50	0.30	0.37	0.43
	Number of nonzero volumes	142	117	111	59	77	506
	Percent of nonzero volumes	7.9%	7.8%	7.4%	3.9%	5.1%	6.5%
R2	**Maximum [m³]**	2.36	2.76	1.86	2.26	1.93	2.76
	Average nonzero volume [m³]	0.32	0.39	0.37	0.50	0.47	0.39
	Number of nonzero volumes	168	122	122	57	84	553
	Percent of nonzero volumes	9.3%	8.1%	8.1%	3.8%	5.6%	7.1%
R3	**Maximum [m³]**	4.91	6.23	2.62	1.47	1.49	6.23
	Average nonzero volume [m³]	0.53	0.39	0.28	0.30	0.28	0.38
	Number of nonzero volumes	156	113	118	45	72	504
	Percent of nonzero volumes	8.7%	7.5%	7.9%	3.0%	4.8%	6.5%

The impacts of the changes in spallings volumes on the overall mean CCDF for normalized spallings releases obtained in the PCS-2012 PA can be seen in Figure 5-24. As seen in that figure, the CCDF of spallings releases obtained in the PCS-2012 PA is consistently higher than that found in the PABC-2009. The increases in spallings volumes and in the number of vectors that result in a nonzero spallings volume translate to an increase in spallings releases as both analyses use the same waste inventory.

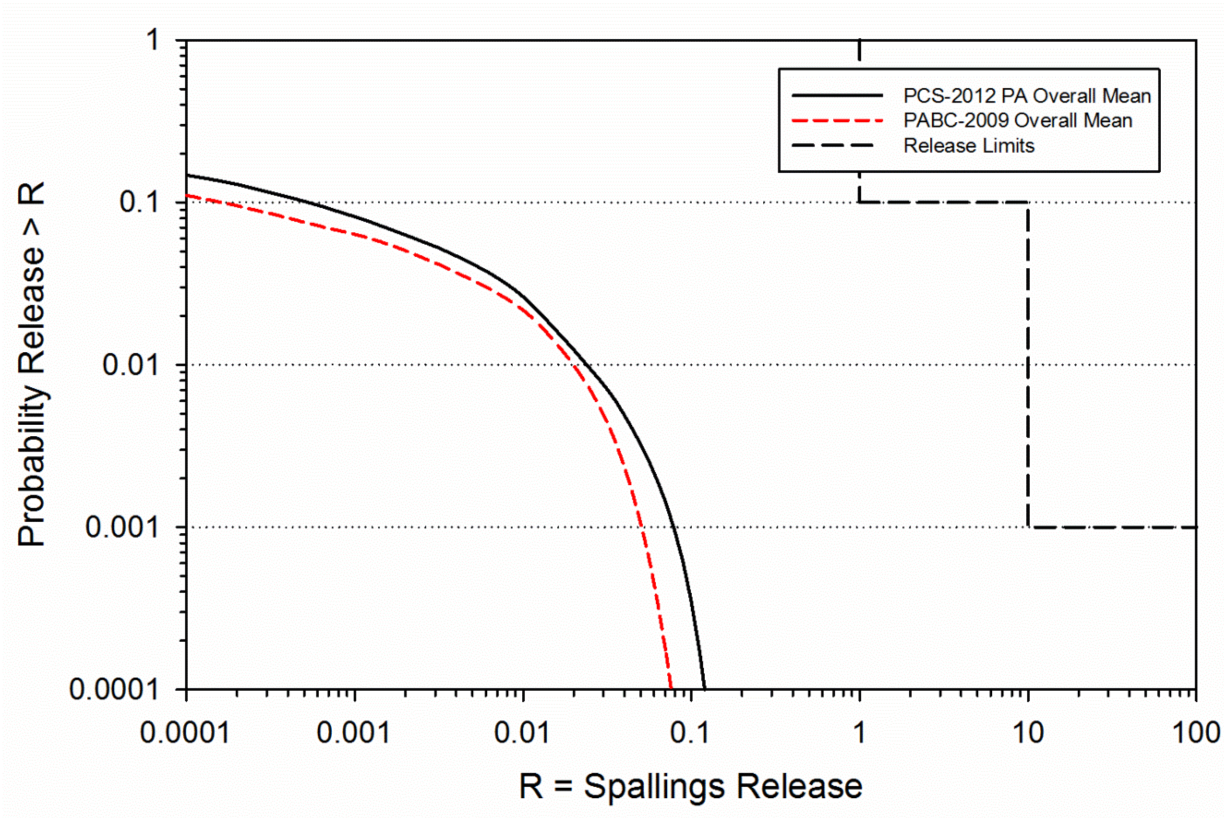


Figure 5-24: PCS-2012 PA and PABC-2009 Overall Mean CCDFs for Normalized Spallings Releases

5.3 Direct Brine Releases

PA code BRAGFLO is used in two ways in WIPP PA calculations. First, it is used to calculate the flow of brine and gas in and around the repository for undisturbed and disturbed conditions. PCS-2012 PA results from this application of BRAGFLO are shown in Section 5.1. Second, it is used for the calculation of direct brine releases. These two uses of BRAGFLO require different computational grids. Results obtained from the brine and gas flow calculation are used to initialize conditions in the DBR calculation. The representation of the waste area by three regions in the PCS-2012 PA and PABC-2009 BRAGFLO grids (see Figure 5-1 and Figure 5-2) yields initial conditions to waste regions comprising the Waste Panel (panel 5), the South Rest of Repository or SROR (panels 3,4,6, and 9), and the North Rest of Repository or NROR (panels 1,2,7,8, and 10) in the DBR calculation, with drilling intrusions considered in each of these regions. The types of intrusions considered in the DBR calculation and the times at which they occur are listed in Table 5-6. The scenarios, intrusion locations, and timings used for the PCS-2012 PA are the same as those used for the PABC-2009.

The DBR numerical grid and material map used in the PCS-2012 PA calculations are shown in Figure 5-25, and are described in Malama (2012). The color scheme in Figure 5-25 has been chosen so as to correspond to the color scheme used in the PCS-2012 PA BRAGFLO grid and material map shown in Figure 5-2. The computational grid and material map used in the PABC-2009 DBR calculations are shown in Figure 5-26.

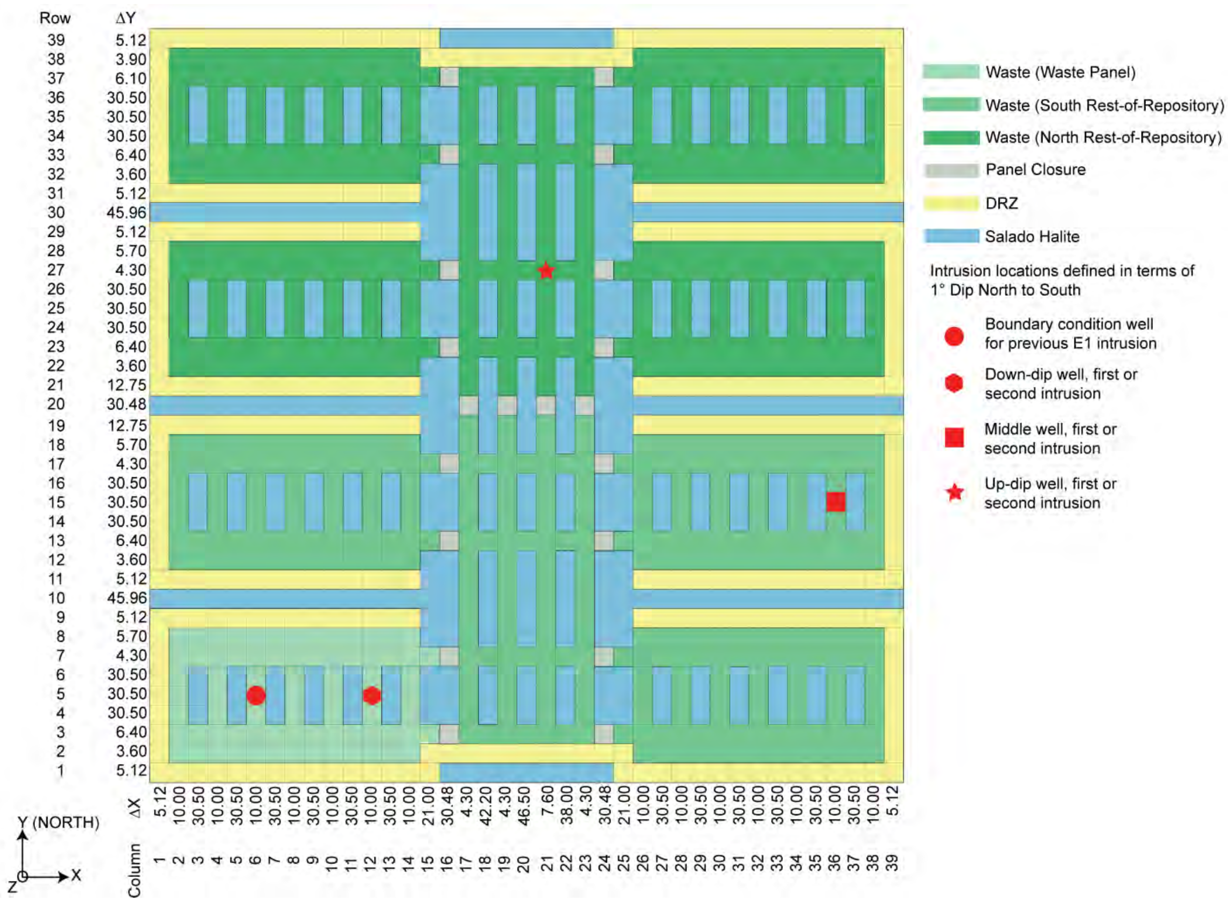


Figure 5-25: PCS-2012 PA DBR Computational Grid and Material Map (logical grid).

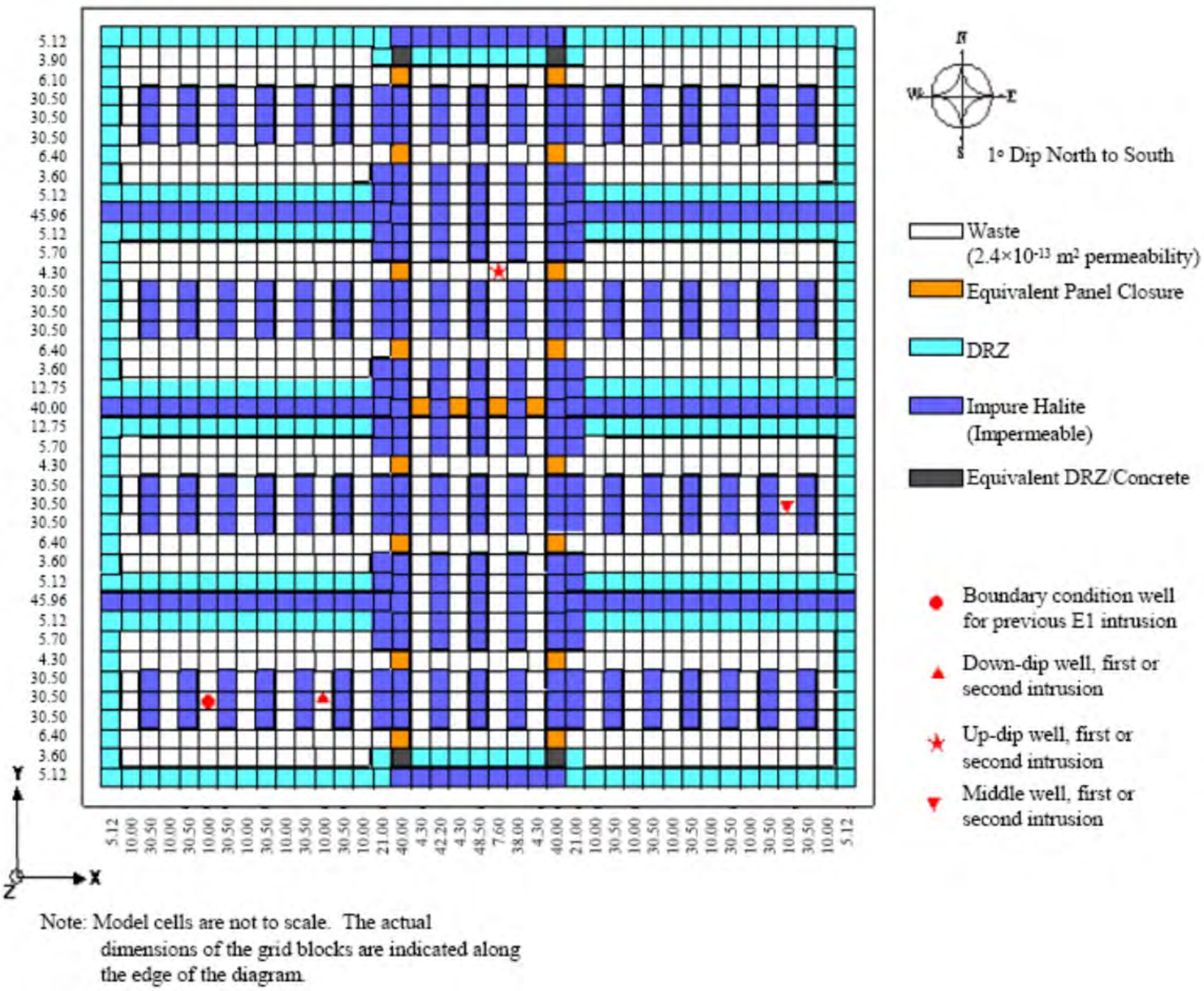


Figure 5-26: PABC-2009 DBR Computational Grid and Material Map (logical grid).

With the DBR computational grid and intrusion locations in hand, DBR results from the PCS-2012 PA and the PABC-2009 can now be compared. Summary statistics of the calculated DBR volumes for replicates 1-3 and scenarios S1-DBR to S5-DBR are provided in Table 5-8. The maximum DBR volumes shown in that table are assessed over all three replicates, times, vectors and drilling locations. As was also the case in the PABC-2009, release volumes that are less than $1x10^{-7}$ m^3 are considered to be inconsequential and are not included in the tally of vectors that result in DBR release volumes in the PCS-2012 PA calculations.

Overall there is a consistent increase in the maximum DBR volumes from PABC-2009 to PCS-2012 PA. The largest increases were observed in scenarios S4-DBR and S5-DBR which are associated with E2 intrusions. As previously discussed in the BRAGFLO results, E2 intrusion scenarios in the PCS-2012 PA yielded waste panel pressure that is higher, on average, than that seen in the PABC-2009 at the time of intrusion and it remains higher for the duration of the 10,000 year regulatory period. Similarly, the mean waste panel brine saturation is higher at the time of intrusion in the PCS-2012 PA, resulting in higher long-term waste panel brine saturations for E2 intrusion scenarios. DBR volumes are strongly dependent on waste panel pressure and brine saturation at the time of intrusion. Hence, increases to these two quantities lead to increased maximum DBR volumes observed in scenarios S4-DBR and S5-DBR, and to the higher overall number of non-zero brine volume vectors.

Table 5-8: DBR Summary Statistics for the PCS-2012 PA and PABC-2009 DBR Calculations

Scenario	Number of Vectors		Maximum volume (m^3)		Average volume (m^3)	
	PABC-2009	PCS-2012 PA	PABC-2009	PCS-2012 PA	PABC-2009	PCS-2012 PA
S1-DBR	369	419	27.6	45.9	0.1	0.4
S2-DBR	1179	1174	48.2	52.9	2.8	2.9
S3-DBR	926	907	40.6	43.8	1.5	1.4
S4-DBR	211	281	20.4	42.5	0.1	0.2
S5-DBR	314	401	21.1	53.8	0.1	0.3
Overall	2999	3182	48.2	53.8	0.9	1.0

The moderate increases in maximum DBR volumes for scenarios S2-DBR and S3-DBR are due to the fact that the lower long-term permeability range of the ROMPCS as compared to Option D yields a period of increased waste panel pressurization following an E1 intrusion. The increased mean waste panel pressure slightly inhibits brine flow into the panel after the intrusion, resulting in a slight decrease to the mean waste panel brine saturation as compared to PABC-2009 E1 intrusion results. The effects of increased pressure and decreased brine saturation effectively cancel, resulting in only a slight increase to the maximum DBR volume seen in the PCS-2012 PA E1 results.

For undisturbed conditions, implementation of the ROMPCS yields higher long-term waste panel pressure (on average) than was seen in the PABC-2009. The increase in mean waste panel pressure is accompanied by an increase in the average waste panel brine saturation for the ROMPCS results. The ROMPCS design allows more brine inflow to the waste panel during the first 200 years when compared to Option D results. This increased brine inflow, combined with the tightness of the ROMPCS after 200 years, results in increased waste panel gas generation (on average) and a subsequent increase to waste panel mean pressure. This explains the increase in the scenario S1-DBR maximum DBR volume for the PCS-2012 PA compared to the PABC-2009.

Table 5-8 shows a modest (~6%) increase in the number of non-zero DBR volumes for the PCS-2012 PA calculations compared with the PABC-2009, and modest increases in the average DBR volumes for all scenarios. These increases are attributable to the increases in waste panel brine pressure and brine saturation discussed above and presented in the BRAGFLO results in Section 5.1.

DBR volume trends observed in the PCS-2012 PA are consistent with those found in prior analyses with regard to drilling location. DBRs are less likely to occur in intrusions situated in the upper drilling location than in the lower drilling location. Of all the intrusions that had a non-zero DBR volume for the PCS-2012 PA, 63.4% occurred during a lower drilling intrusion, a modest decrease from the value of 66.5% for PABC-2009. Furthermore, of all the intrusions that had a non-zero DBR volume and occur during a lower drilling intrusion, 78.0% are found in scenarios S2-DBR and S3-DBR, a slight decrease from 82.9% for PABC-2009 (Clayton et al. 2010). The majority of the non-zero DBR volumes occur when there is a previous E1 intrusion within the same panel. Not only are DBRs less likely to occur during upper drilling intrusions, but also the DBR volumes from such intrusions tend to be much smaller than those from lower drilling intrusions. For all three replicates of the PCS-2012 PA, the maximum DBR volume for the upper drilling location is 25.7 m^3 compared to 53.8 m^3 for the lower drilling location. These observations support the conclusion that lower drilling intrusions are the primary source for significant DBRs.

The combination of relatively high pressure and brine saturation in the intruded panel is required for direct brine release to the surface. Figure 5-27 shows a scatter plot of DBR volume versus pressure in the intruded panel at different intrusion times for scenario S2-DBR, replicate 1, lower drilling intrusion for the PCS-2012 PA. In that figure, symbols indicate the value of the mobile brine saturation, defined as brine saturation minus residual brine saturation in the waste. As prescribed by the conceptual model, there are no DBRs until pressures exceed the 8 MPa vertical line in that figure. Above 8 MPa, a significant number of vectors have zero volumes; these vectors have mobile brine saturations less than zero and thus no brine is available in a mobile form to be released. Figure 5-27 shows a high concentration of results that are near a line extending from (8 MPa, 0 m^3) to (12 MPa, 30 m^3). As mobile saturation increases, the correlation between pressure and DBR volumes also increases.

To further facilitate comparisons of DBRs calculated in the PCS-2012 PA to those obtained in the PABC-2009, the overall mean CCDFs obtained in these two analyses are plotted simultaneously in Figure 5-28. As seen in that figure, the CCDF curve obtained for direct brine releases shows greater mean probabilities in the PCS-2012 PA for the majority of release values.

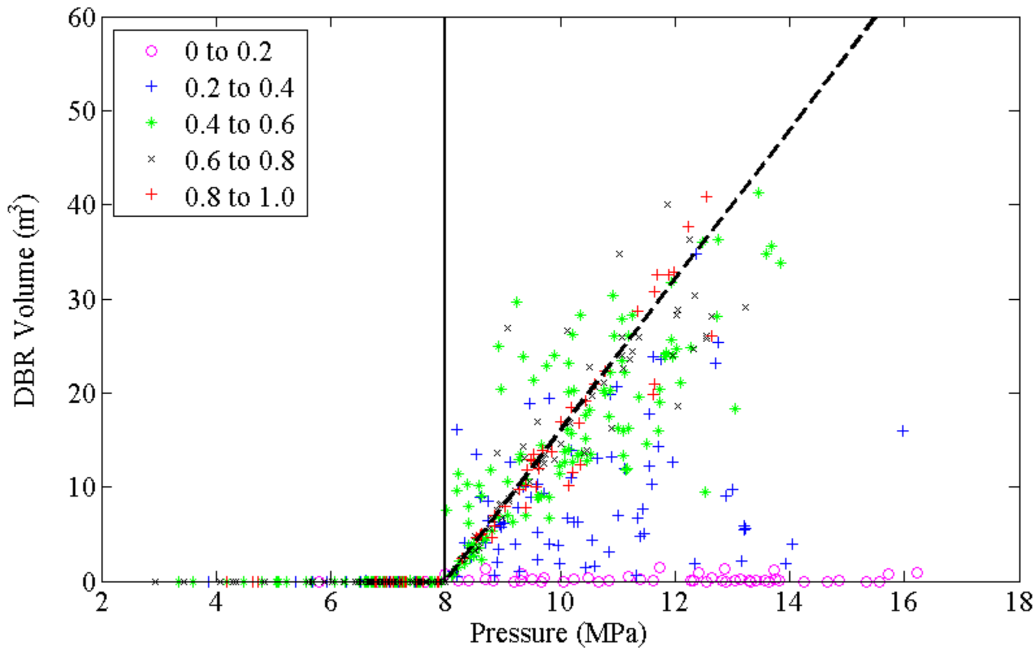


Figure 5-27: DBR Volume vs. Pressure, Scenario S2-DBR, Replicate 1, Lower Intrusion, PCS-2012 PA

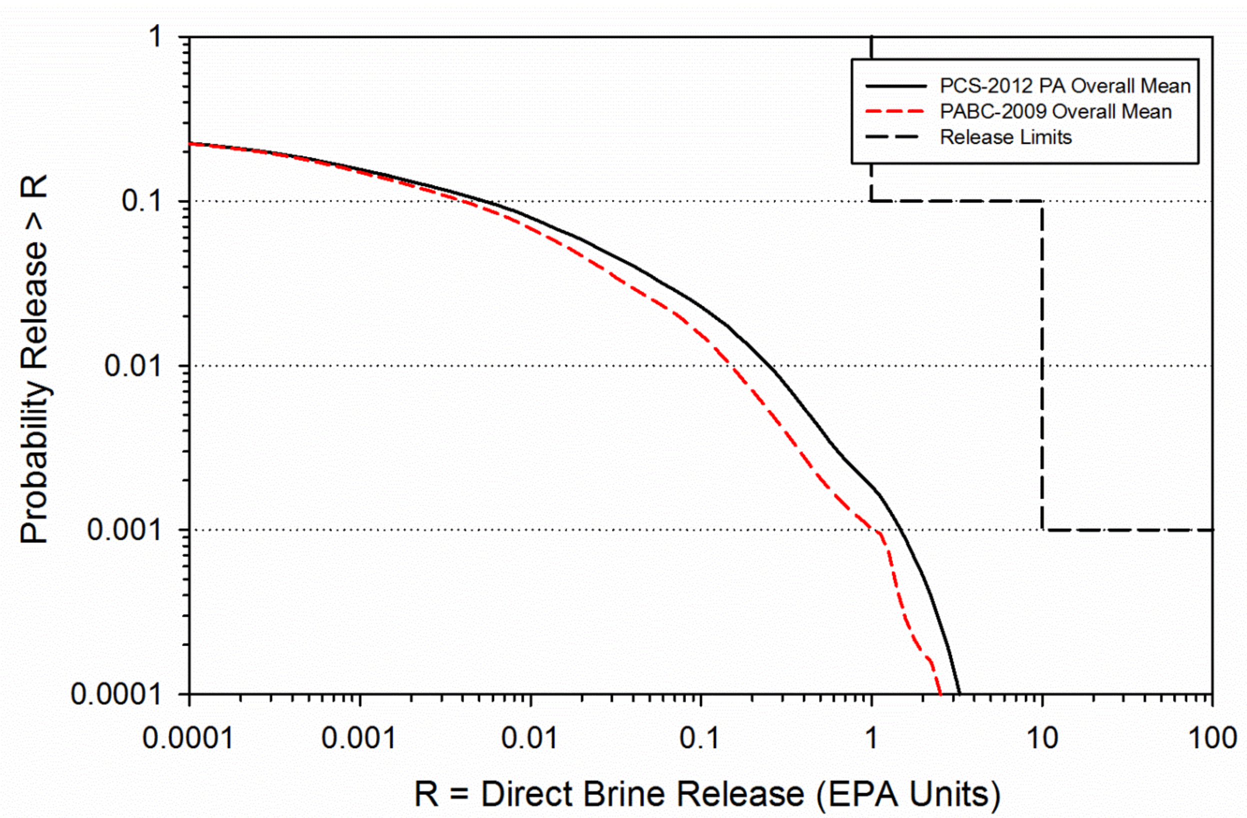


Figure 5-28: PCS-2012 PA and PABC-2009 Overall Mean CCDFs for Normalized Direct Brine Releases

5.4 Total Normalized Releases

Total normalized releases for PCS-2012 PA are presented in this section and subsequently compared to results obtained in the PABC-2009. Total releases are calculated by forming the summation of releases across each potential release pathway, namely cuttings and cavings releases, spallings releases, direct brine releases, and transport releases. PCS-2012 PA CCDFs for total releases are presented in Figure 5-29, Figure 5-30, and Figure 5-31 for replicates 1, 2, and 3, respectively. Mean and quantile CCDF distributions for the three replicates are shown together in Figure 5-32. Figure 5-33 contains the 95 percent confidence limits about the overall mean of total releases. As seen in Figure 5-33, the overall mean for normalized total releases and its lower/upper 95% confidence limits are well below acceptable release limits. As a result, the ROMPCS design investigated in the PCS-2012 PA does not result in WIPP non-compliance with the containment requirements of 40 CFR Part 191.

PCS-2012 PA and PABC-2009 overall mean CCDFs for total releases are shown together in Figure 5-34. As seen in that figure, the overall mean CCDFs obtained in the two analyses are nearly identical for release values less than approximately 0.1 EPA units. For releases greater than 0.1 EPA units, the CCDF curve obtained in the PCS-2012 PA is higher than that found in the PABC-2009. This increase corresponds primarily to the differences found for direct brine releases between the two analyses as discussed in Section 5.3 and illustrated in Figure 5-28. The differences found for spallings may slightly affect the total CCDF curve as well (Section 5.2, Figure 5-24). PCS-2012 PA cuttings and cavings results are unchanged from those found in the PABC-2009. The ROMPCS design investigated in the PCS-2012 PA has an impact on the overall mean of total releases from the PABC-2009 to the PCS-2012 PA due to the changes in direct brine releases calculated in those analyses (Figure 5-35) (Zeitler 2012).

A comparison of the statistics on the overall mean for total normalized releases obtained in the PCS-2012 PA and the PABC-2009 can be seen in Table 5-9. At a probability of 0.1, values obtained for mean total releases has increased from 0.09 to 0.10 for the PCS-2012 PA. At a probability of 0.001, the increase in DBRs seen at that probability in the PCS-2012 PA results in an increase in the mean total release by approximately 0.41 EPA units. An increase is seen in the 95% confidence limit when compared to the PABC-2009 results, while the 90th percentile remains the same.

Table 5-9: PCS-2012 PA and PABC-2009 Statistics on the Overall Mean for Total Normalized Releases in EPA Units at Probabilities of 0.1 and 0.001

Probability	Analysis	Mean Total Release	90th Percentile	Lower 95% CL	Upper 95% CL	Release Limit
0.1	PCS-2012 PA	0.10	0.17	0.10	0.10	1
	PABC-2009	0.09	0.16	0.09	0.10	1
0.001	PCS-2012 PA	1.51	1.00	0.33	2.81	10
	PABC-2009	1.10	1.00	0.37	1.77	10

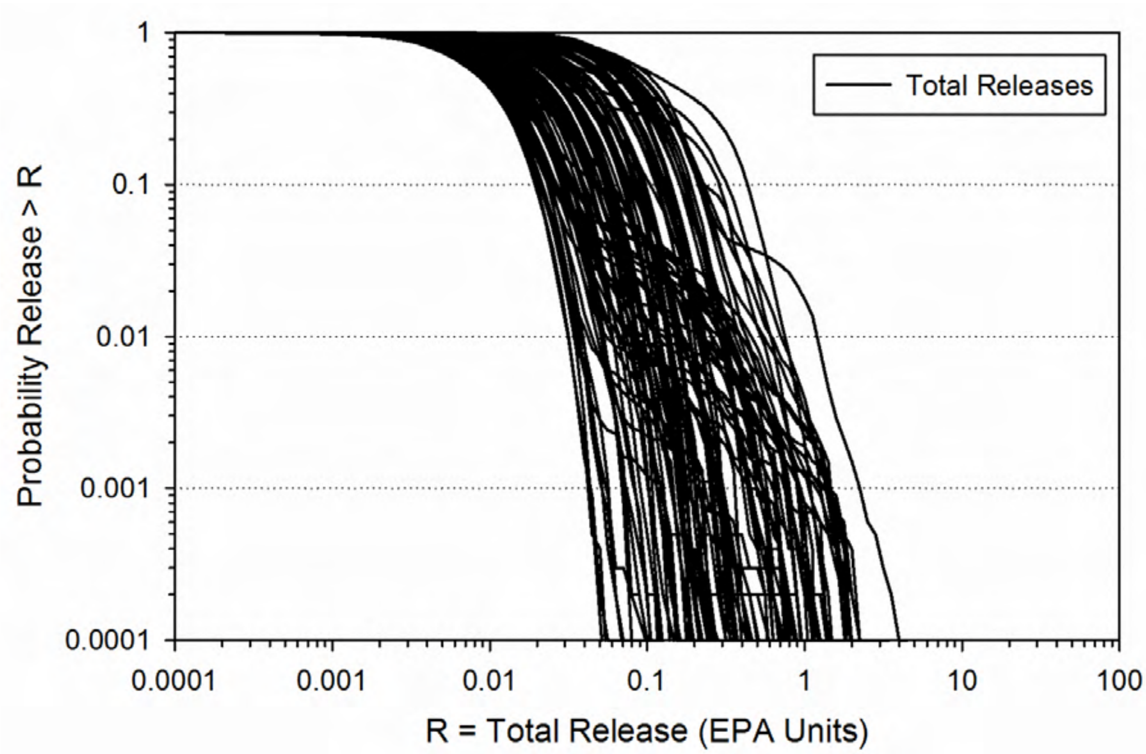


Figure 5-29: PCS-2012 PA Replicate 1 Total Normalized Releases

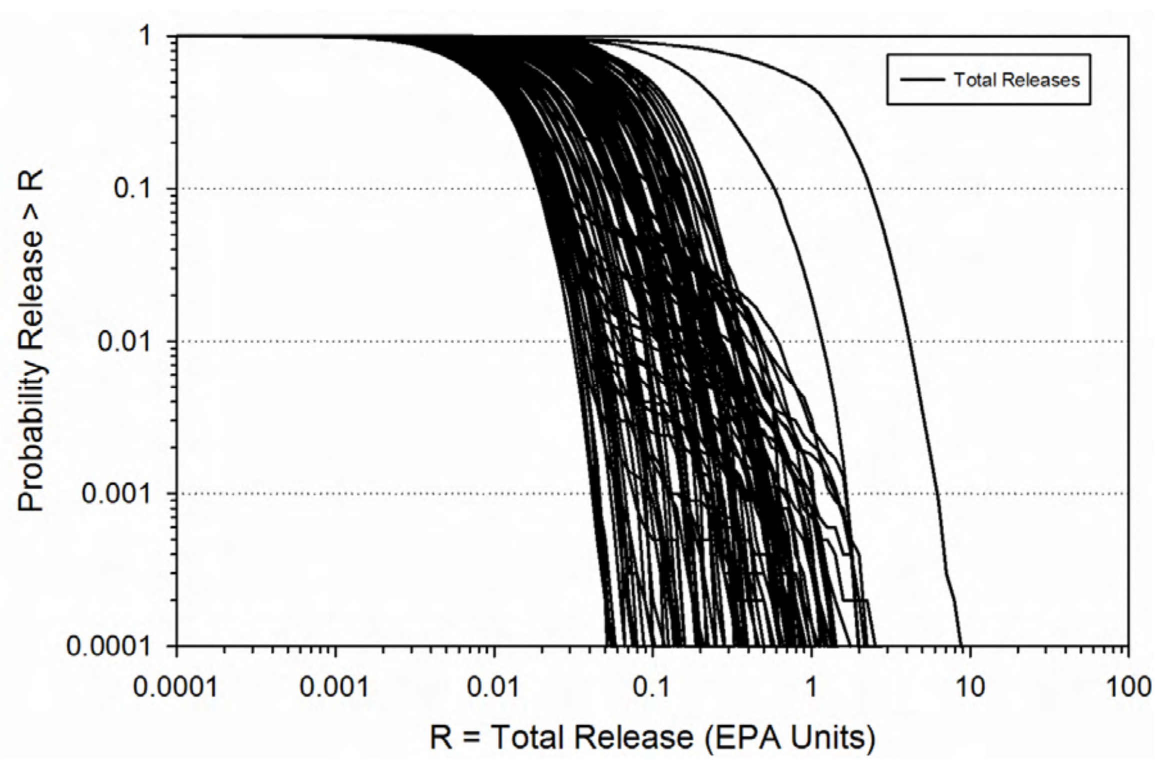


Figure 5-30: PCS-2012 PA Replicate 2 Total Normalized Releases

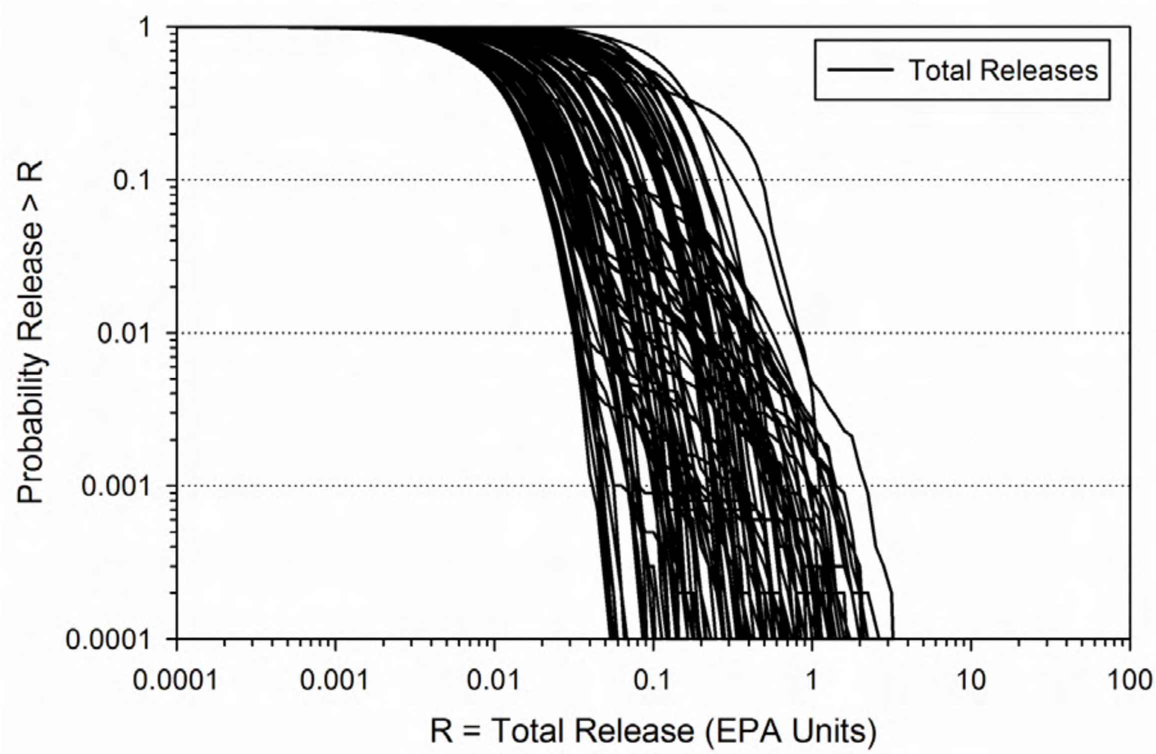


Figure 5-31: PCS-2012 PA Replicate 3 Total Normalized Releases

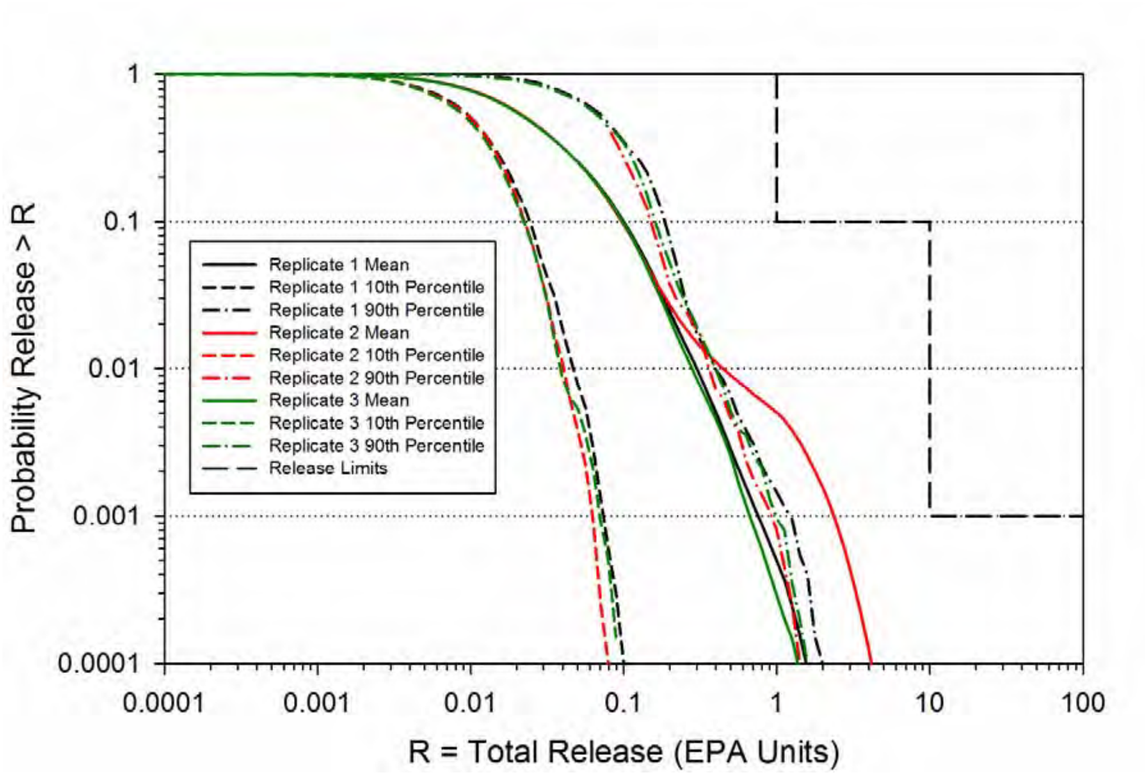


Figure 5-32: PCS-2012 PA Mean and Quantile CCDFs for Total Normalized Releases, Replicates 1-3

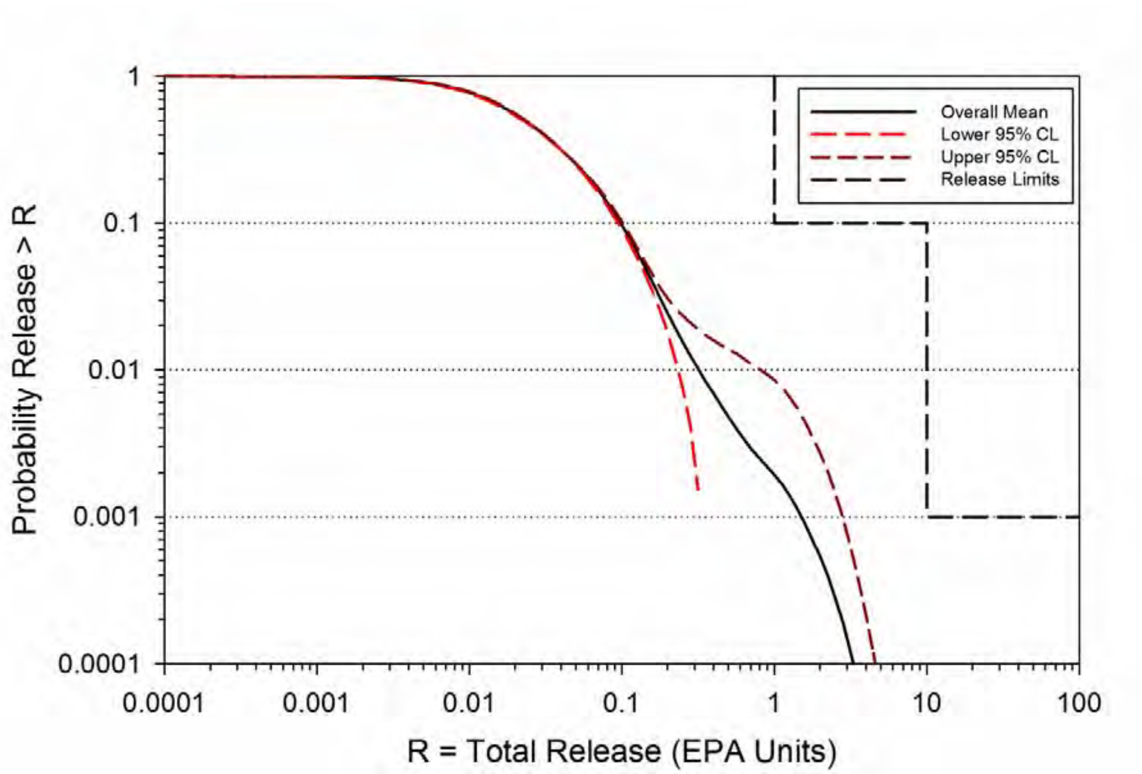


Figure 5-33: PCS-2012 PA Confidence Limits on Overall Mean for Total Normalized Releases

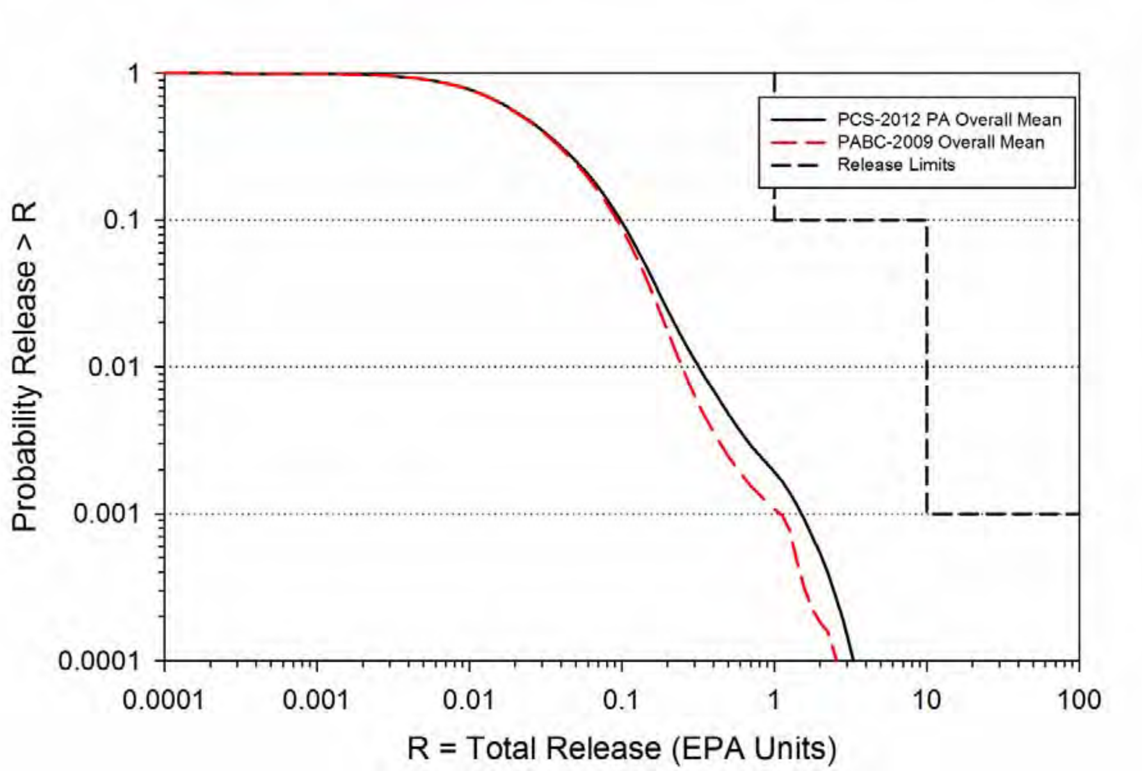


Figure 5-34: PCS-2012 PA and PABC-2009 Overall Mean CCDFs for Total Normalized Releases

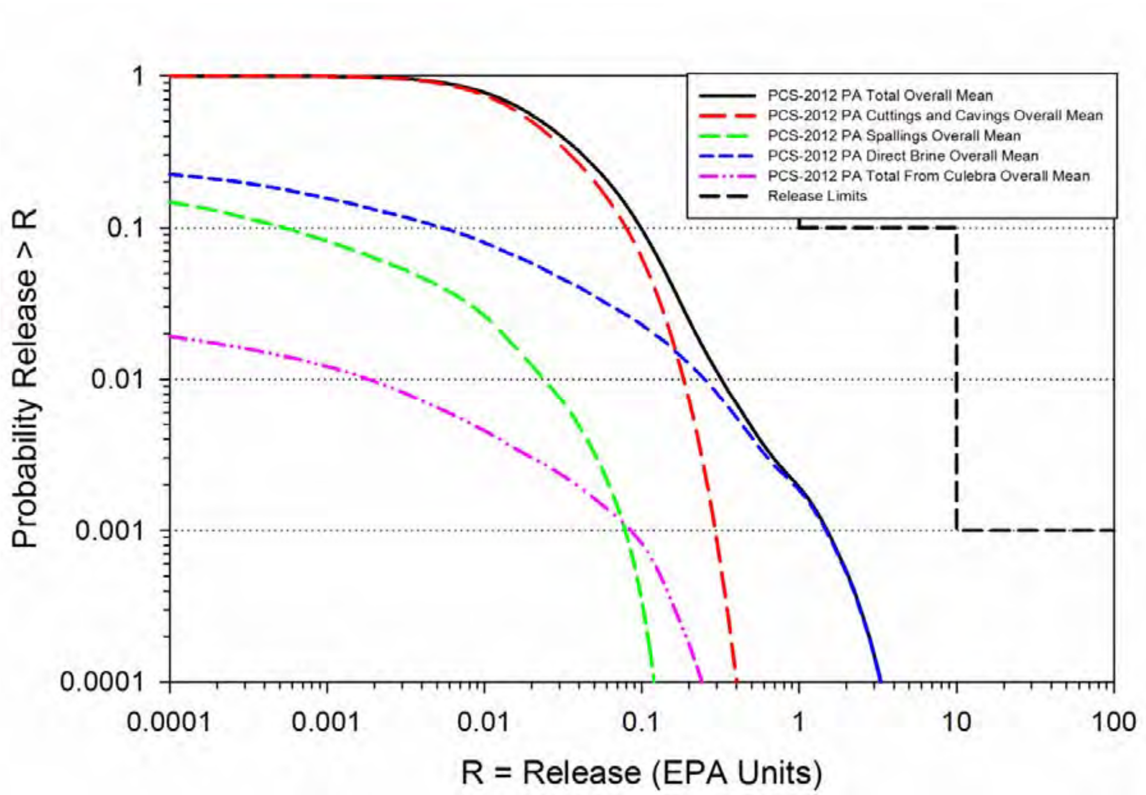


Figure 5-35: PCS-2012 PA Primary Components Contributing to Total Releases

6 SUMMARY

Waste panel closures comprise a repository feature that has been represented in WIPP PA since the original CCA of 1996. The 1998 rulemaking that certified WIPP to receive transuranic waste placed conditions on the panel closure design to be implemented in the repository. The mandated "Option D" design consists of a concrete block wall, an open drift section, and a concrete monolith. The engineering of the panel closure has been re-assessed, and a revised design is proposed that is simpler, cheaper, and easier to construct. The revised panel closure design, termed the ROMPCS, is comprised of 100 feet of ROM salt with barriers at each end. The PCS-2012 PA quantifies WIPP repository performance impacts associated with the replacement of the currently approved Option D panel closure design with the ROMPCS. Impacts are assessed via a direct comparison of results obtained in the PABC-2009 (where Option D was used) to those calculated in the PCS-2012 PA with the ROMPCS.

Total normalized releases calculated in the PCS-2012 PA are greater than those found in the PABC-2009, but continue to remain below their regulatory limits. As a result, replacement of the Option D panel closure with the ROMPCS design would not result in WIPP non-compliance with the containment requirements of 40 CFR Part 191. Cuttings and cavings releases and DBRs were the two primary release components contributing to total releases in the PABC-2009, and continue to be so in the PCS-2012 PA. Cuttings and cavings releases are not impacted by the change in panel closure design, and so remain unchanged from those calculated in the PABC-2009.

For both undisturbed and intruded repository conditions, implementation of the ROMPCS yields higher long-term waste panel pressure (on average) than was seen in the PABC-2009. Pressure increases translate to increases in spallings volumes and their frequency. As a result, increased spallings releases are seen in the PCS-2012 PA results when compared to the PABC-2009. These increases do not have a significant impact on total normalized releases found in the PCS-2012 PA.

Increased DBRs are also seen in the PCS-2012 PA results. DBRs depend on waste panel pressure and brine saturation at the time of intrusion. In addition to increases in waste panel pressure, implementation of the ROMPCS design results in increased mean waste panel brine saturation for undisturbed conditions as well as intrusion scenarios that do not intersect a Castile brine pocket. For intrusion scenarios that intersect a region of pressurized Castile brine, increases in pressure are accompanied by only slight reductions in the mean waste panel brine saturation in the PCS-2012 PA. The combined effect of these impacts is an increase to DBRs in the PCS-2012 PA. The increase in total normalized releases seen in the PCS-2012 PA as compared to the PABC-2009 is primarily due to the increase in DBRs calculated in the PCS-2012 PA.

7 REFERENCES

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APPENDIX A PCS-2012 PA Code Execution

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 A-1.

Table A-1: WIPP PA Alpha Cluster Nodes Used in PCS-2012

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

A.1 WIPP PA Codes

The major WIPP PA codes used for the AP161 PCS-2012 PA on the Alpha Cluster are shown in Table A-2. The library and class associated with each code on the Content Management System (CMS) are also shown. These codes have been qualified under Nuclear Waste Management Procedure NP 19-1: Software Requirements (Long 2012).

A.1.1 Deviation

AP-161 (Camphouse 2012a) listed PRELHS Version 2.30 and Matset Version 9.10 as codes to be used in the PCS-2012 PA. The versions of these codes as listed in AP-161 are incorrect. PRELHS Version 2.40 and MATSET Version 9.20 were used in the PCS-2012 PA, and are correctly shown in Table A-2. This comprises a deviation from AP-161.

Table A-2: WIPP PA VMS Software Used for the AP161 Panel Closure PA

Code	Version	Executable	Build Date	CMS Library	CMS Class
ALGEBRACDB	2.35	ALGEBRACDB_PA96.EXE	31-01-96	LIBALG	PA96
BRAGFLO	6.0	BRAGFLO_QB0600.EXE	12-02-07	LIBBF	QB0600
PREBRAG	8.00	PREBRAG_QA0800.EXE	08-03-07	LIBBF	QA0800
POSTBRAG	4.00A	POSTBRAG_QA0400A.EXE	28-03-07	LIBBF	QA0400A
CCDFGF	5.02	CCDFGF_QB0502.EXE	13-12-04	LIBCCGF	QB0502
PRECCDFGF	1.01	PRECCDFGF_QA0101.EXE	07-07-05	LIBCCGF	QA0101
CUTTINGS_S	6.02	CUTTINGS_S_QA0602.EXE	09-06-05	LIBCUSP	QA0602
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
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 A-2, a utility code was qualified and used under Nuclear Waste Management Procedure NP 9-1: Analyses (Chavez 2006a). The VMS utility code used on the WIPP PA Alpha Cluster is listed in Table A-3, along with references to the storage location and to the appropriate section of this document.

Table A-3: VMS Utility Codes Used in the PCS-2012

Utility	Executable	CMS Library	CMS Class	Section
LHS_EDIT	LHS_EDIT.EXE	LIBCRA09_LHS	LHS_EDIT_V1.0	A.2.1

A.2 Calculation Flow

The following sections describe the calculation flow for the PCS-2012 PA. The code names, 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.

A.2.1 Sampling of Uncertain Parameters (LHS)

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

PRELHS and LHS are executed in sequence by the DCL script EVAL_LHS.COM shown in Table A-4. The input and output files for PRELHS and LHS, as well as the input and log files for the script are shown in Table A-5.

Table A-4: Parameter Sampling Run Control Script

Codes	Script	CMS Library	CMS Class
PRELHS, LHS	EVAL_LHS.COM	LIBAP161_EVAL	AP161-0

Table A-5: Parameter Sampling Input and Output Files

	File Names[1]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_LHS_AP161_R*r*.INP	LIBAP161_EVAL	AP161-0
Log	EVAL_LHS_AP161_R*r*.LOG	LIBAP161_LHS	AP161-0
PRELHS			
Input	LHS1_AP161_R*r*.INP	LIBAP161_LHS	AP161-0
Output	LHS1_AP161_R*r*.TRN	LIBAP161_LHS	AP161-0
Output	LHS1_AP161_R*r*.DBG	LIBAP161_LHS	AP161-0
LHS			
Input	LHS1_AP161_R*r*.TRN	LIBAP161_LHS	AP161-0
Output	LHS2_AP161_R*r*.TRN	LIBAP161_LHS	AP161-0
Output	LHS2_AP161_R*r*.DBG	LIBAP161_LHS	AP161-0
LHS Edit			
Input	LHS_CONTROL_R*r*.INP	NOT KEPT	NOT KEPT
Input	LHS2_AP161_R*r*.TRN	LIBAP161_LHS	AP161-0
Output	LHS2_AP161_R*r* _CON.TRN	LIBAP161_LHS	AP161-0

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

A.2.2 Salado Flow Calculations (BRAGFLO)

Brine and gas flow in and around the repository and in overlying formations is calculated using the BRAGFLO suite of codes (PREBRAG, BRAGFLO, and POSTBRAG) in conjunction with several utility codes. The entire set of calculations is performed for three replicates. Each replicate includes six scenarios (S1-BF to S6-BF) designed to cover a range of drilling intrusion types and times, as shown in Table A-6. For each replicate/scenario combination, calculations are performed for 100 vectors of uncertain model input parameters.

Table A-6: BRAGFLO Scenarios

BRAGFLO Scenario	Description[1,2]
S1-BF	Undisturbed
S2-BF	E1 intrusion at 350 years
S3-BF	E1 intrusion at 1000 years
S4-BF	E2 intrusion at 350 years
S5-BF	E2 intrusion at 1000 years
S6-BF	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 A-7.

Table A-7: Salado Flow Run Control Scripts

Step	Codes in Step	Script(s)	CMS Library	CMS Class
1	GENMESH MATSET	EVAL_GENERIC_STEP1.COM	LIBAP161_EVAL	AP161-0
2	POSTLHS	EVAL_GENERIC_STEP2.COM	LIBAP161_EVAL	AP161-0
3	ICSET ALGEBRACDB	EVAL_BF_STEP3.COM	LIBAP161_EVAL	AP161-0
4	PREBRAG	EVAL_BF_STEP4.COM	LIBAP161_EVAL	AP161-0
5	BRAGFLO POSTBRAG ALGEBRACDB	EVAL_BF_STEP5_MASTER.COM EVAL_BF_STEP5_SLAVE.COM	LIBAP161_EVAL LIBAP161_EVAL	AP161-0 AP161-0

A.2.2.1 Salado Flow Step 1

Step 1 uses GENMESH and MATSET to generate the computational grid and assign material properties to element blocks. Step 1 is run once. The input and log files for the Step 1 script as well as the input and output files for GENMESH and MATSET are shown in Table A-8.

Table A-8: Salado Flow Step 1 Input and Output Files

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_BF_AP161_STEP1.INP	LIBAP161_EVAL	AP161-0
Log	EVAL_BF_AP161_STEP1.LOG	LIBAP161_BF	AP161-0
GENMESH			
Input	GM_BF_AP161.INP	LIBAP161_BF	AP161-0
Output	GM_BF_AP161.CDB	LIBAP161_BF	AP161-0
Output	GM_BF_AP161.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_BF_AP161.INP	LIBAP161_BF	AP161-0
Input	GM_BF_AP161.CDB	LIBAP161_BF	AP161-0
Output	MS_BF_AP161.CDB	LIBAP161_BF	AP161-0
Output	MS_BF_AP161.DBG	NOT KEPT	NOT KEPT

A.2.2.2 Salado Flow Step 2

Step 2 uses POSTLHS to assign the sampled parameter values used by BRAGFLO (generated by LHS) 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 A-9.

Table A-9: Salado Flow Step 2 Input and Output Files

	File Names[1,2]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_BF_AP161_STEP2_R*r*.INP	LIBAP161_EVAL	AP161-0
Log	EVAL_BF_AP161_STEP2_R*r*.LOG	LIBAP161_BF	AP161-0
POSTLHS			
Input	LHS3_DUMMY.INP	LIBAP161_LHS	AP161-0
Input	LHS2_AP161_R*r*_CON.TRN	LIBAP161_LHS	AP161-0
Input	MS_BF_AP161.CDB	LIBAP161_BF	AP161-0
Output	LHS3_BF_AP161_R*r*_V*vvv*.CDB	LIBAP161_BF	AP161-0
Output	LHS3_BF_AP161_R*r*.DBG	LIBAP161_BF	AP161-0

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

A.2.2.3 Salado Flow Step 3

Step 3 assigns initial conditions with ICSET and performs some pre-processing of input data with ALGEBRACDB. Since ALGEBRACDB is used in multiple BRAGFLO steps, this use is referred to as ALG1. Step 3 is run once for each replicate. The script loops over all 100 vectors in the replicate. The input and log files for the Step 3 script as well as the input and output files for ICSET and ALGEBRACDB are shown in Table A-10.

Table A-10: Salado Flow Step 3 Input and Output Files

	File Names[1,2]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_BF_AP161_STEP3_R*r*.INP	LIBAP161_EVAL	AP161-0
Log	EVAL_BF_AP161_STEP3_R*r*.LOG	LIBAP161_BF	AP161-0
ICSET			
Input	IC_BF_AP161.INP	LIBAP161_BF	AP161-0
Input	LHS3_BF_AP161_R*r*_V*vvv*.CDB	LIBAP161_BF	AP161-0
Output	IC_BF_AP161_R*r*_V*vvv*.CDB	LIBAP161_BF	AP161-0
Output	IC_BF_AP161_R*r*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG1_BF_AP161.INP	LIBAP161_BF	AP161-0
Input	IC_BF_AP161_R*r*_V*vvv*.CDB	LIBAP161_BF	AP161-0
Output	ALG1_BF_AP161_R*r*_V*vvv*.CDB	LIBAP161_BF	AP161-0
Output	ALG1_BF_AP161_R*r*_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

A.2.2.4 Salado Flow Step 4

Step 4 consists of running the pre-processing code PREBRAG. Step 4 is repeated for each replicate/scenario combination. The script loops over all 100 vectors in the replicate/scenario combination. The input and log files for the Step 4 script as well as the input and output files for PREBRAG are shown in Table A-11.

Table A-11: Salado Flow Step 4 Input and Output Files

	File Names[1,2,3]	CMS Library[1,2]	CMS Class
SCRIPT			
Script Input	EVAL_BF_AP161_STEP4_R*r*_S*s*.INP	LIBAP161_EVAL	AP161-0
Script Log	EVAL_BF_AP161_STEP4_R*r*_S*s*.LOG	LIBAP161_BFR*r*S*s*	AP161-0
PREBRAG			
Input	BF1_AP161_S*s*.INP	LIBAP161_BF	AP161-0
Input	ALG1_BF_AP161_R*r*_V*vvv*.CDB	LIBAP161_BF	AP161-0
Output	BF2_AP161_R*r*_S*s*_V*vvv*.INP	LIBAP161_BFR*r*S*s*	AP161-0
Output	BF1_AP161_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

A.2.2.5 Salado Flow Step 5

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

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

<u>*General Case*</u>

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 A-12.

Table A-12: Salado Flow Step 5 Input and Output Files (Generic Case)

	File Names[1,2,3,4]	CMS Library[1,2]	CMS Class
MASTER SCRIPT			
Input	EVAL_BF_AP161_STEP5_R*r*_S*s*.INP	LIBAP161_EVAL	AP161-0
Log	EVAL_BF_AP161_STEP5_R*r*_S*s*.LOG	LIBAP161_BFR*r*S*s*	AP161-0
SLAVE SCRIPT			
Log[4]	EVAL_BF_AP161_STEP5_R*r*_S*s*_V*vvv*.LOG	LIBAP161_BFR*r*S*s*	AP161-0
BRAGFLO			
Input	BF2_AP161_R*r*_S*s*_V*vvv*.INP	LIBAP161_BFR*r*S*s*	AP161-0
Input	BF2_PABC09_CLOSURE.DAT	LIBPABC09_BF	AP161-0
Output	BF2_AP161_R*r*_S*s*_V*vvv*.OUT	NOT KEPT	NOT KEPT
Output	BF2_AP161_R*r*_S*s*_V*vvv*.SUM	LIBAP161_BFR*r*S*s*	AP161-0
Output	BF2_AP161_R*r*_S*s*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Output	BF2_AP161_R*r*_S*s*_V*vvv*.ROT	NOT KEPT	NOT KEPT
Output	BF2_AP161_R*r*_S*s*_V*vvv*.RIN	NOT KEPT	NOT KEPT
POSTBRAG			
Input	BF2_AP161_R*r*_S*s*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Input	ALG1_BF_AP161_R*r*_V*vvv*.CDB	LIBAP161_BF	AP161-0
Output	BF3_AP161_R*r*_S*s*_V*vvv*.CDB	LIBAP161_BFR*r*S*s*	AP161-0
Output	BF3_AP161_R*r*_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG2_BF_AP161.INP	LIBAP161_BF	AP161-0
Input	BF3_AP161_R*r*_S*s*_V*vvv*.CDB	LIBAP161_BFR*r*S*s*	AP161-0
Output	ALG2_BF_AP161_R*r*_S*s*_V*vvv*.CDB	LIBAP161_BFR*r*S*s*	AP161-0
Output	ALG2_BF_AP161_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

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 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 A-13. In that table, vector numbers with a (*) superscript correspond to vectors where quantity

FTOL_SAT was changed from 1e-2 to 1e-1 in the BRAGFLO input file. Vector numbers with a (#) superscript correspond to vectors where quantity FTOL_SAT was changed from 1e-2 to 1e-1 and Convergence Test Flag was changed from 1 to 0 in the BRAGFLO input file. The modified file names are shown in Table A-14. 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 A-13: Salado Flow Step 5 Modified Input Runs

Replicate	Scenario	Vectors
R1	S1	29*, 51#
	S2	51#
	S3	51#
	S4	29*, 51#
	S5	51#
	S6	51#
R2	S1	99*
	S4	99*
	S5	99*
R3	S1	35*
	S2	35*
	S3	35*
	S5	35*
	S6	35*

Table A-14: Salado Flow Step 5 Modified Input Runs File Names

	File Names[1,2,3]	CMS Library[1,2]	CMS Class
MASTER SCRIPT			
Input	EVAL_BF_AP161_STEP5_R*r*_S*s*_V*vvv*_MOD.INP	LIBAP161_EVAL	AP161-0
Log	EVAL_BF_AP161_STEP5_R*r*_S*s*_V*vvv*_MOD.LOG	LIBAP161_BFR*r*S*s*	AP161-0
BRAGFLO			
Input	BF2_AP161_R*r*_S*s*_V*vvv*_MOD.INP	LIBAP161_BFR*r*S*s*	AP161-0

1. $r \in \{1, 2, 3\}$ as shown in Table A-13
2. $s \in \{1, 2, 3, 4, 5, 6\}$ as shown in Table A-13
3. vectors as shown in Table A-13

A.2.3 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 A-15. Step 3 also includes a small utility used to submit the script to a batch queue.

Table A-15: Solids Volume (CUTTINGS_S) Run Control Scripts

Step	Codes in Step	Scripts	Script CMS Library	Script CMS Class
1	GENMESH MATSET	EVAL_CUSP_STEP1.COM	LIBAP161_EVAL	AP161-0
2	POSTLHS	EVAL_CUSP_STEP2.COM	LIBAP161_EVAL	AP161-0
3	CUTTINGS_S	EVAL_CUSP_STEP3.COM SUB_CUSP_STEP3.COM	LIBAP161_EVAL	AP161-0

Three replicate calculations are performed. Five scenarios, S1-DBR to S5-DBR are included in each replicate. The cuttings calculation extracts volume-averaged brine pressure and brine saturation from Salado flow BRAGFLO results. These extracted quantities are then used downstream in the calculation of direct brine releases. As a result, the intrusion times and locations considered during the cuttings calculation are identical to those used in the DBR calculation. Cuttings scenarios indicate which BRAGFLO scenario provides the input conditions for the simulation (CUTTINGS_S scenario S1-DBR means that CUTTINGS_S uses BRAGFLO scenario S1-BF results as the inputs for the solids release calculations, CUTTINGS_S scenario S2-DBR means that CUTTINGS_S uses BRAGFLO scenario S2-BF 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-DBR 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-DBR calculates the volume of solids released by an intrusion 200 years after the E1 intrusion at 350 years modeled in BRAGFLO scenario S2-BF. An intrusion time of 1200 years in CUTTINGS_S scenario S3-DBR calculates the volume of solids released by an intrusion 200 years after the E1 intrusion at 1000 years modeled in BRAGFLO scenario S3-BF.

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.

A.2.3.1 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 A-16.

Table A-16: Solids Volume Step 1 Input and Output Files

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_CUSP_AP161_STEP1.INP	LIBAP161_EVAL	AP161-0
Log	EVAL_CUSP_AP161_STEP1.LOG	LIBAP161_CUSP	AP161-0
GENMESH			
Input	GM_CUSP_AP161.INP	LIBAP161_CUSP	AP161-0
Output	GM_CUSP_AP161.CDB	LIBAP161_CUSP	AP161-0
Output	GM_CUSP_AP161.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_CUSP_AP161.INP	LIBAP161_CUSP	AP161-0
Input	GM_CUSP_AP161.CDB	LIBAP161_CUSP	AP161-0
Output	MS_CUSP_AP161.CDB	LIBAP161_CUSP	AP161-0
Output	MS_CUSP_AP161.DBG	NOT KEPT	NOT KEPT

A.2.3.2 Solids Volume Step 2

Step 2 uses POSTLHS to assign the sampled parameter values (generated by LHS) used by CUTTINGS_S 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 A-17.

Table A-17: Solids Volume Step 2 Input and Output Files

	File Names[1,2]	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CUSP_AP161_STEP2_R*r*.INP	LIBAP161_EVAL	AP161-0
Script Log	EVAL_CUSP_AP161_STEP2_R*r*.LOG	LIBAP161_CUSP	AP161-0
POSTLHS			
Input	LHS3_DUMMY.INP	LIBAP161_LHS	AP161-0
Input	LHS2_AP161_R*r*_CON.TRN	LIBAP161_LHS	AP161-0
Input	MS_CUSP_AP161.CDB	LIBAP161_CUSP	AP161-0
Output	LHS3_CUSP_AP161_R*r*_V*vvv*.CDB	LIBAP161_CUSP	AP161-0
Output	LHS3_CUSP_AP161_R*r*.DBG	LIBAP161_CUSP	AP161-0

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

A.2.3.3 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 A-18.

Table A-18: Solids Volume Step 3 Input and Output Files

	File Names[1,2,3,4,5]	CMS Library[1,2]	CMS Class
SCRIPT			
Input	EVAL_CUSP_AP161_STEP3_R*r*.INP	LIBAP161_EVAL	AP161-0
Output	CUSP_AP161_MASTER_R*r*.INP	LIBAP161_CUSP	AP161-0
Log	EVAL_CUSP_AP161_STEP3_R*r*.LOG	LIBAP161_CUSP	AP161-0
CUTTINGS_S			
Input	CUSP_AP161_MASTER_R*r*.INP	LIBAP161_CUSP	AP161-0
Input	CUSP_AP161.INP	LIBAP161_CUSP	AP161-0
Input	LHS3_CUSP_AP161_R*r*_V*vvv*.CDB	LIBAP161_CUSP	AP161-0
Input	BF3_AP161_R*r*_S*s*_V*vvv*.CDB	LIBAP161_BFR*r*S*s*	AP161-0
Input	MSPALL_DRS_CRA1BC_R*r*.OUT	LIBCRA1BC_DRS	AP161-0
Output	CUSP_AP161_R*r*.TBL	LIBAP161_CUSP	AP161-0
Output	CUSP_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBAP161_CUSPR*r*S*s*	AP161-0
Output	CUSP_AP161_R*r*.DBG	LIBAP161_CUSP	AP161-0

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. $c \in \{\text{L, U, M}\}$ for each intrusion time
5. $vvv \in \{001, 002, ..., 100\}$ for each c

A.2.4 Single-Intrusion Direct Brine Release Calculations (BRAGFLO_DBR)

Single-intrusion direct brine release volumes are calculated using the BRAGFLO suite of codes (PREBRAG, BRAGFLO, POSTBRAG), in conjunction with several utility codes. The steps, the codes run in each step, and the DCL script(s) used to perform the step are shown in Table A-19.

Three replicates are performed. Each replicate includes five scenarios (S1-DBR to S5-DBR). 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 A-19: 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	LIBAP161_EVAL	AP161-0
2	ALGEBRACDB RELATE ICSET	EVAL_DBR_STEP2.COM SUB_DBR_STEP2.COM	LIBAP161_EVAL	AP161-0
3	PREBRAG BRAGFLO POSTBRAG ALGEBRACDB	EVAL_DBR_STEP3.COM SUB_DBR_STEP3.COM	LIBAP161_EVAL	AP161-0

A.2.4.1 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 A-20.

Table A-20: Direct Brine Release Step 1 Input and Output Files

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_DBR_AP161_STEP1.INP	LIBAP161_EVAL	AP161-0
Log	EVAL_DBR_AP161_STEP1.LOG	LIBAP161_DBR	AP161-0
GENMESH			
Input	GM_DBR_AP161.INP	LIBAP161_DBR	AP161-0
Output	GM_DBR_AP161.CDB	LIBAP161_DBR	AP161-0
Output	GM_DBR_AP161.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_DBR_AP161.INP	LIBAP161_DBR	AP161-0
Input	GM_DBR_AP161.CDB	LIBAP161_DBR	AP161-0
Output	MS_DBR_AP161.CDB	LIBAP161_DBR	AP161-0
Output	MS_DBR_AP161.DBG	NOT KEPT	NOT KEPT

A.2.4.2 Direct Brine Release Step 2

Step 2 performs pre-processing of input data with ALGEBRACDB. ALGEBRACDB is run twice (ALG1 and ALG2). 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 A-21.

Table A-21: Direct Brine Release Step 2 Input and Output Files

	File Names[1,2,3,4]	**CMS Library[1,2]**	**CMS Class**
SCRIPT			
Input	EVAL_DBR_AP161_STEP2_R*r*_S*s*.INP	LIBAP161_EVAL	AP161-0
Log	EVAL_DBR_AP161_STEP2_R*r*_S*s*.LOG	LIBAP161_DBRR*r*S*s*	AP161-0
ALGEBRACDB			
Input	ALG1_DBR_AP161.INP	LIBAP161_DBR	AP161-0
Input	CUSP_AP161_R*r*_S*s*_T*ttttt*_L_V*vvv*.CDB[5]	LIBAP161_CUSPR*r*S*s*	AP161-0
Output	ALG1_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	ALG1_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
RELATE_1			
Input	REL1_DBR_AP161.INP	LIBAP161_DBR	AP161-0
Input	MS_DBR_AP161.CDB	LIBAP161_DBR	AP161-0
Input	ALG1_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	REL1_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	REL1_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
RELATE_2			
Input	REL2_DBR_AP161_S*s*.INP	LIBAP161_DBR	AP161-0
Input	REL1_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Input	BF3_AP161_R*r*_S*s*_V*vvv*.CDB	LIBAP161_BFR*r*S*s*	AP161-0
Output	REL2_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	REL2_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ICSET			
Input	IC_DBR_AP161_S*s*.INP	LIBAP161_DBR	AP161-0
Input	REL2_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	IC_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	IC_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG2_DBR_AP161_S*s*.INP	LIBAP161_DBR	AP161-0
Input	IC_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	ALG2_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	ALG2_DBR_AP161_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_AP161_R*r*_S*s*_T*ttttt*_L_V*vvv*.CDB do not have leading zeros in front of the intrusion time *ttttt*.

A.2.4.3 Direct Brine Release Step 3

Step 3 runs PREBRAG, BRAGFLO, POSTBRAG, and ALGEBRACDB (ALG3). 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 A-22.

Table A-22: Direct Brine Release Step 3 Input and Output Files

	File Names[1,2,3,4,5,6]	**CMS Library[1,2]**	**CMS Class**
SCRIPT			
Input	EVAL_DBR_AP161_STEP3_R*r*_S*s*.INP	LIBAP161_EVAL	AP161-0
Input	EVAL_DBR_AP161_STEP3_R1_S1_T100.INP[6]	LIBAP161_EVAL	AP161-0
Log	EVAL_DBR_AP161_STEP3_R*r*_S*s*.LOG	LIBAP161_DBRR*r*S*s*	AP161-0
PREBRAG			
Input	BF1_DBR_AP161_*c*.INP	LIBAP161_DBR	AP161-0
Input	BF1_DBR_AP161_S1_100_*c*.INP[6]	LIBAP161_DBR	AP161-0
Input	ALG2_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	BF2_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.INP	LIBAP161_DBRR*r*S*s*	AP161-0
Output	BF1_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.DBG	NOT KEPT	NOT KEPT
BRAGFLO			
Input	BF2_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.INP	LIBAP161_DBRR*r*S*s*	AP161-0
Output	BF2_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.OUT	NOT KEPT	NOT KEPT
Output	BF2_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.SUM	NOT KEPT	NOT KEPT
Output	BF2_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Output	BF2_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.ROT	NOT KEPT	NOT KEPT
Output	BF2_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.RIN	NOT KEPT	NOT KEPT
POSTBRAG			
Input	ALG2_DBR_AP161_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Input	BF2_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Output	BF3_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	BF3_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG3_DBR_AP161.INP	LIBAP161_DBR	AP161-0
Input	BF3_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	ALG3_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	ALG3_DBR_AP161_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. $tttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} & \text{for S1} \\ \{00550, 00750, 02000, 04000, 10000\} & \text{for S2, S4} \\ \{01200, 01400, 03000, 05000, 10000\} & \text{for S3, S5} \end{cases}$
4. $c \in \{L, M, U\}$ for each intrusion
5. $vvv \in \{001, 002, ..., 100\}$ for each c
6. Files used for R1_S1_T00100 only.

A.2.5 CCDF Input Tabulation (SUMMARIZE)

The output CDB files from the various process model codes are combined into text tables by the SUMMARIZE code, for subsequent use in calculating releases to the accessible environment. The type of data extracted from each process model is described in the PRECCDFGF Design Document (WIPP PA 2005) and in Kanney and Kirchner (2005). The run control scripts used to process the CDB data for the various process models are shown in Table A-23. A single run control script is used to extract data from CDB files for all process model codes. The script performs the following steps:

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

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

Table A-23: CCDF Input Tabulation Run Control Scripts

Code	Script	Script CMS Library	Script CMS Class
SUMMARIZE	EVAL_SUM.COM SUB_SUM.COM	LIBAP161_EVAL	AP161-0

A.2.5.1 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. The run control script is invoked for scenarios S1-DBR through S5-DBR 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 A-24.

Table A-24: CCDF Input Tabulation Input and Output Files (Direct Brine Release)

	File Names[1,2,3,4,5]	**CMS Library[1,2]**	**CMS Class**
SCRIPT			
Input	EVAL_SUM_DBR_AP161_R*r*_S*s*.INP	LIBAP161_EVAL	AP161-0
Input	SUM_DBR_AP161.TMPL	LIBAP161_SUM	AP161-0
Output	SUM_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*.INP	LIBAP161_SUM	AP161-0
Log	EVAL_SUM_DBR_AP161_R*r*_S*s*.LOG	LIBAP161_SUM	AP161-0
SUMMARIZE			
Input	SUM_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*.INP	LIBAP161_SUM	AP161-0
Input	ALG3_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBAP161_DBRR*r*S*s*	AP161-0
Output	SUM_DBR_AP161_R*r*_S*s*_Tttttt_*c*.TBL	LIBAP161_SUM	AP161-0
Output	SUM_DBR_AP161_R*r*_S*s*_Tttttt_*c*.DBG	NOT KEPT	NOT KEPT

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

A.2.6 CCDF Construction (PRECCDFGF, CCDFGF)

The complimentary cumulative distribution functions (CCDFs) for radionuclide releases to the accessible environment are constructed using the PRECCDFGF/CCDFGF code suite. The calculations are separated into several steps according to the number of times a particular code is run and to allow for timely inspection of intermediate results. The steps, the codes run in each step, and the DCL script(s) used to perform the steps are shown in Table A-25.

Table A-25: CCDF Construction Run Control Scripts

Step	**Codes in Step**	**Scripts**	**CMS Library**	**CMS Class**
1	GENMESH MATSET	EVAL_CCGF_STEP1.COM	LIBAP161_EVAL	AP161-0
2	POSTLHS	EVAL_CCGF_STEP2.COM	LIBAP161_EVAL	AP161-0
3	PRECCDFGF CCDFGF	EVAL_CCGF_STEP3.COM SUB_CCGF_STEP3.COM	LIBAP161_EVAL	AP161-0

A.2.6.1 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 A-26.

Table A-26: CCDF Construction Step 1 Input and Output Files

	File Names	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CCGF_AP161_STEP1.INP	LIBAP161_EVAL	AP161-0
Script Log	EVAL_CCGF_AP161_STEP1.LOG	LIBAP161_CCGF	AP161-0
GENMESH			
Input	GM_CCGF_AP161.INP	LIBAP161_CCGF	AP161-0
Output	GM_CCGF_AP161.CDB	LIBAP161_CCGF	AP161-0
Output	GM_CCGF_AP161.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_CCGF_AP161.INP	LIBAP161_CCGF	AP161-0
Input	GM_CCGF_AP161.CDB	LIBAP161_CCGF	AP161-0
Output	MS_CCGF_AP161.CDB	LIBAP161_CCGF	AP161-0
Output	MS_CCGF_AP161.DBG	NOT KEPT	NOT KEPT

A.2.6.2 CCDF Construction Step 2

Step 2 uses POSTLHS to assign the sampled parameter values (generated by LHS) used by CCDFGF 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 A-27.

Table A-27: CCDF Construction Step 2 Input and Output Files

	File Names[1,2]	CMS Library	CMS Class
STEP 2			
Script Input	EVAL_CCGF_AP161_STEP2_R*r*.INP	LIBAP161_EVAL	AP161-0
Script Log	EVAL_CCGF_AP161_STEP2_R*r*.LOG	LIBAP161_CCGF	AP161-0
POSTLHS			
Input	LHS3_DUMMY.INP	LIBAP161_LHS	AP161-0
Input	LHS2_AP161_R*r*_CON.TRN	LIBAP161_LHS	AP161-0
Input	MS_CCGF_AP161.CDB	LIBAP161_CCGF	AP161-0
Output	LHS3_CCGF_AP161_R*r*_V*vvv*.CDB	LIBAP161_CCGF	AP161-0
Output	LHS3_CCGF_AP161_R*r*.DBG	LIBAP161_CCGF	AP161-0

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

A.2.6.3 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 A-28.

Table A-28: CCDF Construction Step 3 Input and Output Files

	File Names[1-7]	**CMS Library**	**CMS Class**
SCRIPT			
Script Input	EVAL_CCGF_STEP3_AP161_R*r*.INP	LIBAP161_EVAL	AP161-0
Script Log	EVAL_CCGF_STEP3_AP161_R*r*.LOG	LIBAP161_CCGF	AP161-0
PRECCDFGF			
Input	INTRUSIONTIMES.IN	LIBAP161_CCGF	AP161-0
Input	MS_CCGF_AP161.CDB	LIBAP161_CCGF	AP161-0
Input	LHS3_CCGF_AP161_R*r*_V*vvv*.CDB	LIBAP161_CCGF	AP161-0
Input	SUM_DBR_AP161_R*r*_S*s*_T*ttttt*_*c*.TBL	LIBAP161_SUM	AP161-0
Input	CUSP_AP161_R*r*.TBL	LIBAP161_CUSP	AP161-0
Input	SUM_NUT_PABC09_R*r*_S1.TBL	LIBPABC09_SUM	AP161-0
Input	SUM_NUT_PABC09_R*r*_S*s*_T*ttttt*.TBL	LIBPABC09_SUM	AP161-0
Input	SUM_PANEL_INT_PABC09_R*r*_S6_T*ttttt*.TBL	LIBPABC09_SUM	AP161-0
Input	SUM_ST2D_PABC09_R*r*_M*m*.TBL	LIBPABC09_SUM	AP161-0
Input	EPU_PABC09_*h*H.DAT	LIBPABC09_EPU	AP161-0
Input	SUM_PANEL_CON_PABC09_R*r*_S*s*.TBL	LIBPABC09_SUM	AP161-0
Input	SUM_PANEL_ST_PABC09_R*r*_S*s*.TBL	LIBPABC09_SUM	AP161-0
Output	CCGF_AP161_RELTAB_R*r*.DAT	LIBAP161_CCGF	AP161-0
CCDFGF			
Input	CCGF_AP161_CONTROL_R*r*.INP	LIBAP161_CCGF	AP161-0
Input	CCGF_AP161_RELTAB_R*r*.DAT	LIBAP161_CCGF	AP161-0
Output	CCGF_AP161_R*r*.OUT	LIBAP161_CCGF	AP161-0
Output	CCGF_AP161_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. $ttttt \in \begin{cases} \{00100, 00350, 01000, 03000, 05000, 10000\} \text{ for S1 for each } r \text{ for SUM\_DBR} \\ \{00550, 07500, 02000, 04000, 10000\} \text{ for S2, S4 for each } r \text{ for SUM\_DBR} \\ \{01200, 01400, 03000, 05000, 10000\} \text{ for S3, S5 for each } r \text{ for SUM\_DBR} \\ \{00100, 00350\} \text{ for S2, S4 for each } r \text{ for SUM\_NUT} \\ \{01000, 03000, 05000, 07000, 09000\} \text{ for S3, S5 each } r \text{ for SUM\_NUT} \\ \{00100, 00350, 01000, 02000, 04000, 06000, 09000\} \text{ for each } r \text{ for SUM\_PANEL\_INT} \end{cases}$
5. $c \in \{L, M, U\}$ for each intrusion for SUM_DBR
6. $m \in \{F, P\}$
7. $h \in \{C, H\}$

A.2.7 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 A-29. The input and output files for STEPWISE, as well as the input and log files for the script are shown in Table A-30.

Table A-29: Sensitivity Analysis Run Control Scripts

Code	Script	Script CMS Library	Script CMS Class
STEPWISE	EVAL_STP.COM	LIBAP161_EVAL	AP161-0

Table A-30: Sensitivity Analysis Input and Output Files

	File Names[1,2]	CMS Library	CMS Class
SCRIPT			
Input	EVAL_STP_AP161_*_ALL_R*r*.INP	LIBAP161_EVAL	AP161-0
Log	EVAL_STP_AP161_*_ALL_R*r*.LOG	LIBAP161_STPW	AP161-0
STEPWISE			
Input	STP_AP161_*_ALL_R*r*.INP	LIBAP161_STPW	AP161-0
Input	STP_AP161_LHS_R*r*.TRN	LIBAP161_STPW	AP161-0
Input	STP_AP161_MEANS_R*r*.TRN	LIBAP161_STPW	AP161-0
Output	STP_AP161_*_R*r*.TXT	LIBAP161_STPW	AP161-0
Output	STP_AP161_*_R*r*.SP	LIBAP161_STPW	AP161-0

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

APPENDIX B Addendum

Following the completion of the PCS-2012 PA calculations, but prior to the completion of the summary report, an error was discovered in the ALG1 input file for BRAGFLO. The error is associated with the calculation of permeability for ROMPCS materials PCS_T2 and PCS_T3. As seen in Camphouse et al. (2012), sampled porosity values for these materials are used to calculate their respective permeabilities according to

$$k = 10^{-21.187(1 - \Phi) + 1.5353 + \alpha},$$

where k is the calculated permeability, Φ is the sampled porosity value, and α is the sampled value from a normal distribution with a mean of 0, a standard deviation of 0.86, and truncated at ±2 standard deviations. Upon closer inspection, the leading-term constant of -21.187 in the equation above was incorrectly transcribed to the ALG1 input file as -21.87 for both materials PCS_T2 and PCS_T3. This error leads to calculated permeabilities for materials PCS_T2 and PCS_T3 that are lower than the minimum listed in Camphouse et al. (2012) for some vectors.

This transcription error has a negligible impact on the PCS-2012 PA results presented and discussed in this report. Indeed, for the first 200 years post-closure, gas and brine flows toward or away from a waste panel in the PCS-2012 PA are through the upper and lower DRZ before the DRZ material about the ROMPCS is modeled as having healed (e.g., see Figure 6-8 in Camphouse 2012d). Slightly lower calculated permeabilites for the ROMPCS in some vectors will not appreciably impact these flow behaviors as the DRZ about the panel closure is more permeable (on average) than the ROMPCS before the DRZ heals at 200 years, with or without the transcription error. After 200 years, the DRZ above and below the ROMPCS is modeled as having healed, and is represented by material DRZ_PCS. Material DRZ_PCS is unchanged from the PABC-2009 to the PCS-2012 PA. After 200 years, the calculated ROMPCS permeability range presented in Camphouse et al. (2012) results in a panel closure that is “tighter” (on average) than the Option D closure. Permeabilities that are lower than intended for material PCS_T3, due to the transcription error, do not alter this comparison between the ROMPCS and Option D after 200 years.

To fully quantify the impact of the transcription error, the ALG1 input file to BRAGFLO was corrected, and replicate 1 of the PCS-2012 PA was re-run starting at the ALG1 BRAGFLO step through to CCDFGF. Files associated with this re-run are located in class CALC_MODS, and having the same library and naming conventions as listed in Appendix A. The results of the re-run are shown in Figure B-1, and are compared to the original PCS-2012 PA results with the transcription error. As is evident in that figure, the transcription error has essentially no impact on the replicate 1 mean for total normalized releases. The same is also true of the 10th and 90th percentiles obtained in the original and corrected cases. The transcription error in the ALG1 input file to BRAGFLO has a negligible impact on the PCS-2012 PA results presented and discussed in this report.

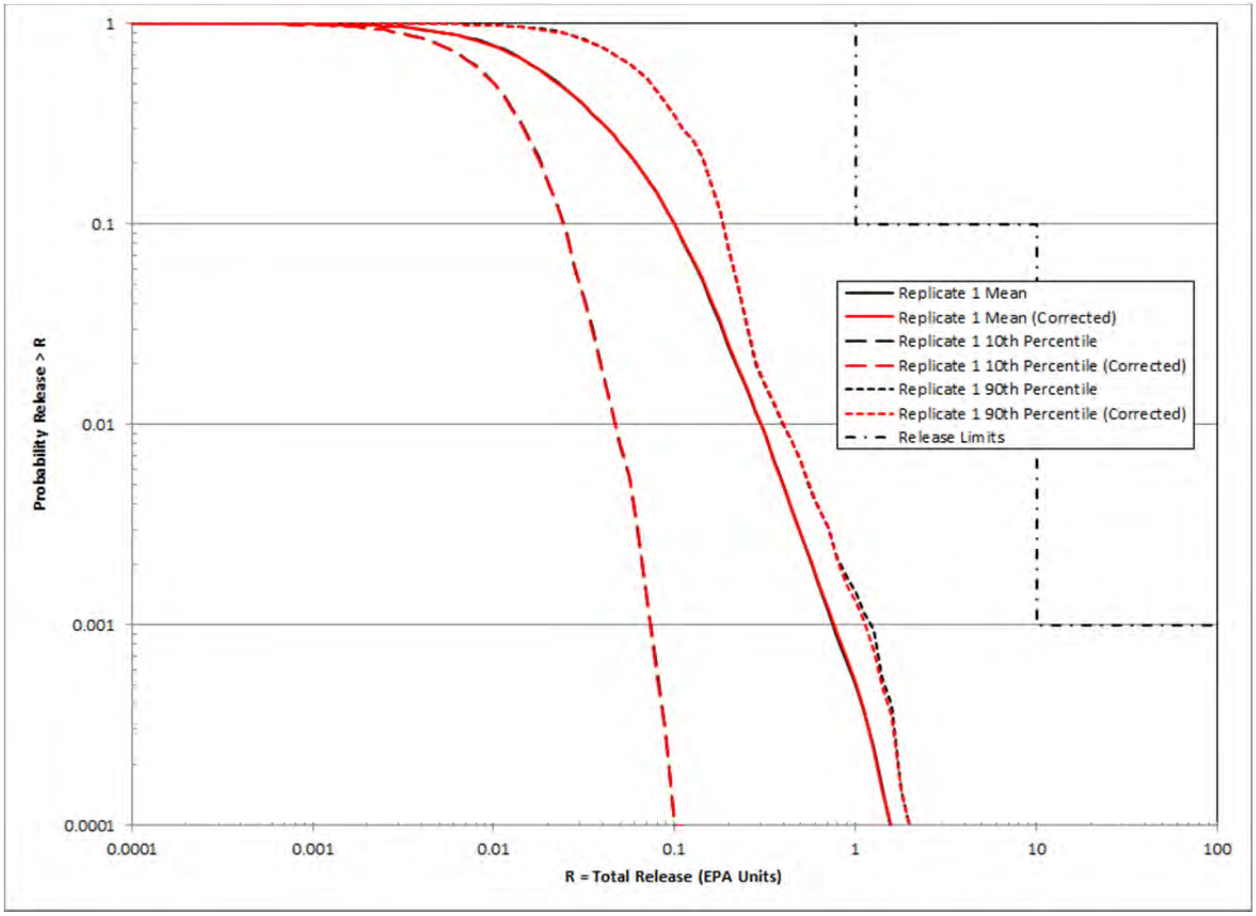

Figure B-1: Comparison of PCS-2012 PA Mean and Quantile CCDFs for Total Normalized Releases, Replicate 1