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SANDIA NATIONAL LABORATORIES
WASTE ISOLATION PILOT PLANT

Impact Assessment of SDI Excavation on Long-Term WIPP Performance

Revision 0

Author:	R. Chris Camphouse		7/14/2011
	Print	Signature	Date
Author:	Dwayne C. Kicker		7/14/2011
	Print	Signature	Date
Author:	Thomas B. Kirchner	Thomas B Kirchner	7/13/2011
	Print	Signature	Date
Author:	Jennifer J. Long	Jennifer J Long	7/14/11
	Print	Signature	Date
Author:	James J. Pasch	James Pasch	7/13/2011
	Print	Signature	Date
Technical Review:	Janis R. Trone		7/14/2011
	Print	Signature	Date
QA Review	Steve Davis	Steve Davis	7-13-11
	Print	Signature	Date
Management Review:	Moo Lee		7/13/2011
	Print	Signature	Date

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EXECUTIVE SUMMARY

With the recertification of the WIPP in November of 2010 (U.S. EPA 2010), a new PA baseline was established by the 2009 Performance Assessment Baseline Calculation (PABC-2009). Following this most recent recertification decision, the DOE plans to submit a planned change notice to the EPA that justifies additional excavation in the WIPP experimental area. This excavation will be done in order to support salt disposal investigations (SDI) that include field-scale heater tests at WIPP. This report summarizes the impact of the additional SDI excavation on long-term repository performance with particular emphasis on spallings and direct brine releases, two of the dominant release mechanisms.

Total normalized releases calculated in the SDI impact assessment remain below their regulatory limits. As a result, the additional excavation in the WIPP experimental area to support SDI would not result in WIPP non-compliance with the containment requirements of 40 CFR Part 191. Cuttings and cavings releases and direct brine releases are the two primary release components contributing to total releases in the SDI calculations. Cuttings and cavings releases are unchanged from those calculated in the PABC-2009. Additional excavation for SDI results in small impacts to pressures and brine saturations in repository waste-containing regions, but these changes collectively result in a negligible difference between direct brine releases seen in the SDI impact assessment and the PABC-2009. Small reductions are observed in SDI spallings releases as compared to the PABC-2009, but these differences are relatively minor and do not have a significant impact on the overall total normalized releases found in the SDI impact assessment. As a result, total normalized releases found in the SDI calculations and the PABC-2009 are indistinguishable.

An additional component of the overall SDI analysis performed is a determination of the impact that planned heater tests have on the state of the repository at the time of closure. That analysis demonstrated that the impact of heater testing on the temperature of WIPP waste-containing areas is negligible. Results from the SDI thermal analysis are presented in a separate report (Kuhlman 2011).

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 (SNL). WIPP PA calculations estimate the probability and consequence of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure. The models are maintained and updated with new information as part of a recertification process that occurs at five-year intervals following the receipt of the first waste shipment at the site in 1999.

With the recertification of the WIPP in November of 2010 (U.S. EPA 2010), a new PA baseline was established by the 2009 Performance Assessment Baseline Calculation (PABC-2009). Following this most recent recertification decision, the DOE plans to submit a planned change notice (PCN) to the EPA that justifies additional excavation in the WIPP experimental area. This excavation will be done in order to support salt disposal investigations (SDI) that include field-scale heater tests at WIPP.

The proposed expansion of the WIPP experimental area in order to facilitate SDI work requires an assessment of associated impacts on long-term repository performance. The impacts of additional volume on pressure and brine saturation in and around the waste regions of the repository must be determined as these quantities potentially impact release mechanisms such as spallings and direct brine releases (DBRs). The DOE has requested that SNL undertake calculations and analyses to determine the impacts of additional repository volume on the long-term performance of the facility (U.S. DOE 2011a, 2011b). The impacts of additional excavated volume are determined by a comparison to results obtained in the PABC-2009. This report provides a summary of calculations and analyses used to determine the impact of additional excavated volume in the WIPP experimental area on regulatory compliance.

An additional component of the overall SDI analysis performed is a determination of the impact that planned heater tests have on the state of the repository at the time of closure. That analysis demonstrated that the impact of heater testing on the temperature of WIPP waste-containing areas is negligible. Results from the SDI thermal analysis are presented in a separate report (Kuhlman 2011).

The work undertaken in the SDI impact assessment is prescribed in AP-156, *Analysis Plan for the Impact Determination of SDI Heater Testing and Associated Excavation on Long-Term WIPP Performance* (Camphouse and Kuhlman 2011). In order to isolate the impacts of additional experimental volume on regulatory compliance, the SDI impact assessment was designed to deviate as little as possible from the PABC-2009 implementation. In particular, the SDI investigation utilizes the same waste inventory information, drilling rate and plugging pattern parameters, and radionuclide solubility parameters as were used in the PABC-2009. The SDI impact assessment is essentially a focused re-run of the PABC-2009 calculation using a slightly modified numerical grid in the Salado flow calculation that accounts for additional volume in the repository experimental area.

2 SDI EXCAVATION

A schematic depicting the additional SDI excavation to the repository experimental area is included in U.S. DOE (2011b), and is shown in Figure 2-1 for convenience. From that figure, the additional volume added to the experimental area can be calculated.

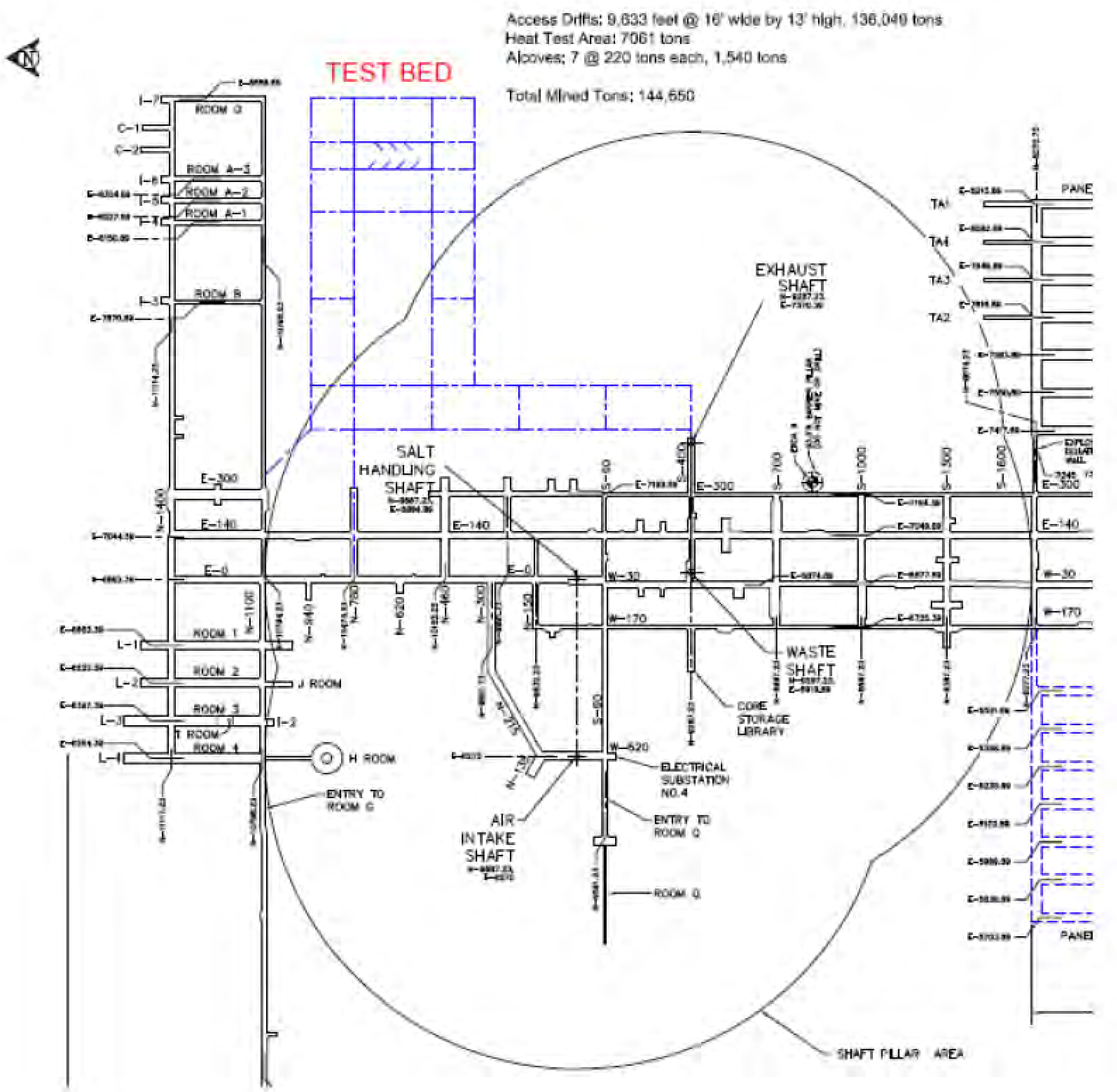

Figure 2-1: SDI Excavation Schematic

As seen in Figure 2-1, the volume of the SDI access drifts is (9,633 ft) x (16 ft) x (13 ft) = 2,003,664 ft^3. Moreover, from that figure, the tonnage of excavated salt corresponding to this volume is 136,049 tons. These quantities provide a conversion factor of tonnage to excavated volume of 1 excavated ton = 14.73 ft^3. The total mined tonnage associated with the SDI excavation is listed in Figure 2-1 as 144,650 tons because of some additional volume associated with the heater test area and alcoves. Using the conversion factor obtained above, the total volume corresponding to the additional SDI excavation is 2,130,694.5 ft^3, or 60,335 m^3 (after rounding). The SDI impact assessment includes this additional volume of 60,335 m^3 in the experimental sub-region of the numerical grid used for Salado flow modeling. Aside from this change to the Salado numerical grid, the parameters and sampled distribution values used in the SDI impact assessment are identical to those implemented in the PABC-2009.

3 FEPS RE-ASSESSMENT

An assessment of the FEPs baseline was conducted to determine if the current FEPs basis remains valid in consideration of changes introduced by the proposed SDI experimental program, and was performed according to SP 9-4, *Performing FEPs Impact Assessment for Planned or Unplanned Changes*. The FEPs analysis concludes that no additional FEPs are needed to accurately represent the changes to the repository layout resulting from additional excavation in the WIPP experimental area. Additionally, no FEPs screening arguments and associated screening decisions require modification to account for these changes (Kirkes 2011).

4 METHODOLOGY

The performance assessment 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, but the exact parameter 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 SDI impact assessment, models were executed for three replicates of 100 vectors, each vector providing model realizations resulting from a particular set of parameter values. Parameter values sampled in the PABC-2009 were also used in the SDI impact assessment, and are documented in Kirchner (2009). 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 futures.

For a random variable, the complementary cumulative distribution function (CCDF) provides the probability of the variable being greater than a particular value. By regulation, performance assessment results are presented as a distribution of CCDFs of releases (U.S. 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.

Releases are quantified in terms of “EPA units”. Each radionuclide has a release limit prescribed to it. This limit is defined as the maximum allowable release (in curies) of that radionuclide per a waste amount containing 1×10^6 curies of alpha-emitting transuranic radionuclides with half-lives greater than 20 years. 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, as specified by regulation. Mathematically, the formula used to calculate releases in terms of EPA units is of the form

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

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. Note that the definition of the release limit L_i results in a constant value of 1×10^6 curies being factored out of the summation.

The SDI impact assessment 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 impacted by additional excavated volume in the WIPP experimental area were updated, while the results from previous PAs were used for individual numerical codes not affected by these changes. The SDI impact assessment utilized the same waste inventory information, drilling rate and plugging pattern parameters, and radionuclide solubility parameters as were used in the PABC-2009.

Additional volume in the WIPP experimental area conceivably results in a pressure reduction in that region. Lower pressure in the experimental area in combination with the long WIPP regulatory time period of 10,000 years potentially results in an eventual reduction in pressure in WIPP waste-containing areas. Pressure changes in the waste panels translate directly to changes in spallings releases as reductions in pressure yield reductions in spallings volumes. Moreover, pressure reductions in waste areas potentially allow a larger influx of brine into these regions, corresponding to increases in brine saturation. Direct brine releases are a function of pressure and brine saturation at the time of intrusion. Two conditions must be met for a DBR to occur. First, the brine saturation in the intruded panel must exceed the residual brine saturation of the waste, a sampled parameter in PA. Second, the repository pressure near the drilling location must exceed the hydrostatic pressure of the drilling fluid, which is specified in PA to be 8 MPa. The combined impact of lower pressure and increased brine saturation on DBRs is nontrivial. A pressure reduction would be expected to result in a corresponding reduction in the number of vectors that satisfy the DBR pressure requirement. Increases in brine saturation would be expected to result in an increase in the number of vectors that satisfy the DBR brine saturation requirement. As a result, it is not apparent if the net impact of lower pressure and increased brine saturation results in more or fewer vectors overall that satisfy both DBR requirements. For these reasons, spallings and direct brine releases are the primary release mechanisms of interest in the SDI impact assessment. Additional volume in the experimental region has no impact on releases due to cuttings and cavings. Transport releases through the Culebra had virtually no impact on total normalized releases in the PABC-2009 (Clayton et al 2010). Additional volume in the repository experimental area will not change this result. Consequently, transport releases through the Culebra calculated in the PABC-2009 are also used in the SDI impact assessment.

5 RUN CONTROL

Run control documentation of codes executed in the SDI impact assessment is provided in 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 SDI excavation in the WIPP experimental area. Documentation of run control for results calculated in the PABC-2009 is provided in Long (2010).

6 RESULTS

Additional excavated volume in the WIPP experimental region has no impact on cuttings and cavings releases resulting from drilling intrusions in repository waste areas. Cuttings and cavings results obtained in the SDI impact assessment are identical to those found in the PABC-2009. In addition Culebra transport results calculated in the PABC-2009 were used in the SDI 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 SDI impact assessment 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 from the SDI impact assessment are broken out in sections below, and are compared to PABC-2009 results. Salado flow modeling results are presented in Section 6.1. Spallings results are presented in Section 6.2. Direct brine releases are presented in Section 6.3. The impact of proposed SDI excavation on regulatory compliance is discussed in terms of total normalized releases in Section 6.4. Files used to generate plots and summary statistics in the results that follow are included on a CD submitted with this report. As the CCDF is the regulatory metric used to demonstrate compliance, CCDFs obtained in the SDI impact assessment and the PABC-2009 are compared for each component of release in the appropriate section.

6.1 Salado Flow Results

The BRAGFLO software calculates the flow of brine and gas in the vicinity of the WIPP repository over the 10,000-year regulatory compliance period. The computational grid used in the PABC-2009 BRAGFLO calculations is shown in Figure 6-1, where the WIPP experimental area is denoted by region "Exp". As seen in that figure, the volume of the experimental region implemented in the PABC-2009 discretization is

$$2((30.61\text{m}) \times (361.65\text{m}) \times (1.32\text{m} + 1.32\text{m} + 1.32\text{m})) = 87{,}675 \text{ m}^3.$$

As developed in Section 2, the volume resulting from additional excavation in the experimental region for SDI is 60,335 m^3. As a result, the target volume of the experimental region implemented in the SDI BRAGFLO computational grid is 87,675 m^3 + 60,335 m^3 = 148,010 m^3. To achieve this value, the experimental region of the BRAGFLO grid implemented in the SDI impact assessment was modified from that used in the PABC-2009. Elements corresponding to the experimental area were lengthened in the z-direction for the SDI impact assessment. Two elements lengths of 30.61 meters in the z-direction were used in the PABC-2009. For the SDI calculations, these two lengths were increased to 51.67 meters and 51.68 meters. The resulting volume of the experimental region in the SDI BRAGFLO numerical grid is 148,011 m^3, one cubic meter greater than the target value. Changes in element sizes comprising the experimental region from the PABC-2009 to the SDI impact assessment are summarized in Figure 6-2. No other changes were made to the PABC-2009 BRAGFLO grid for the SDI impact assessment.

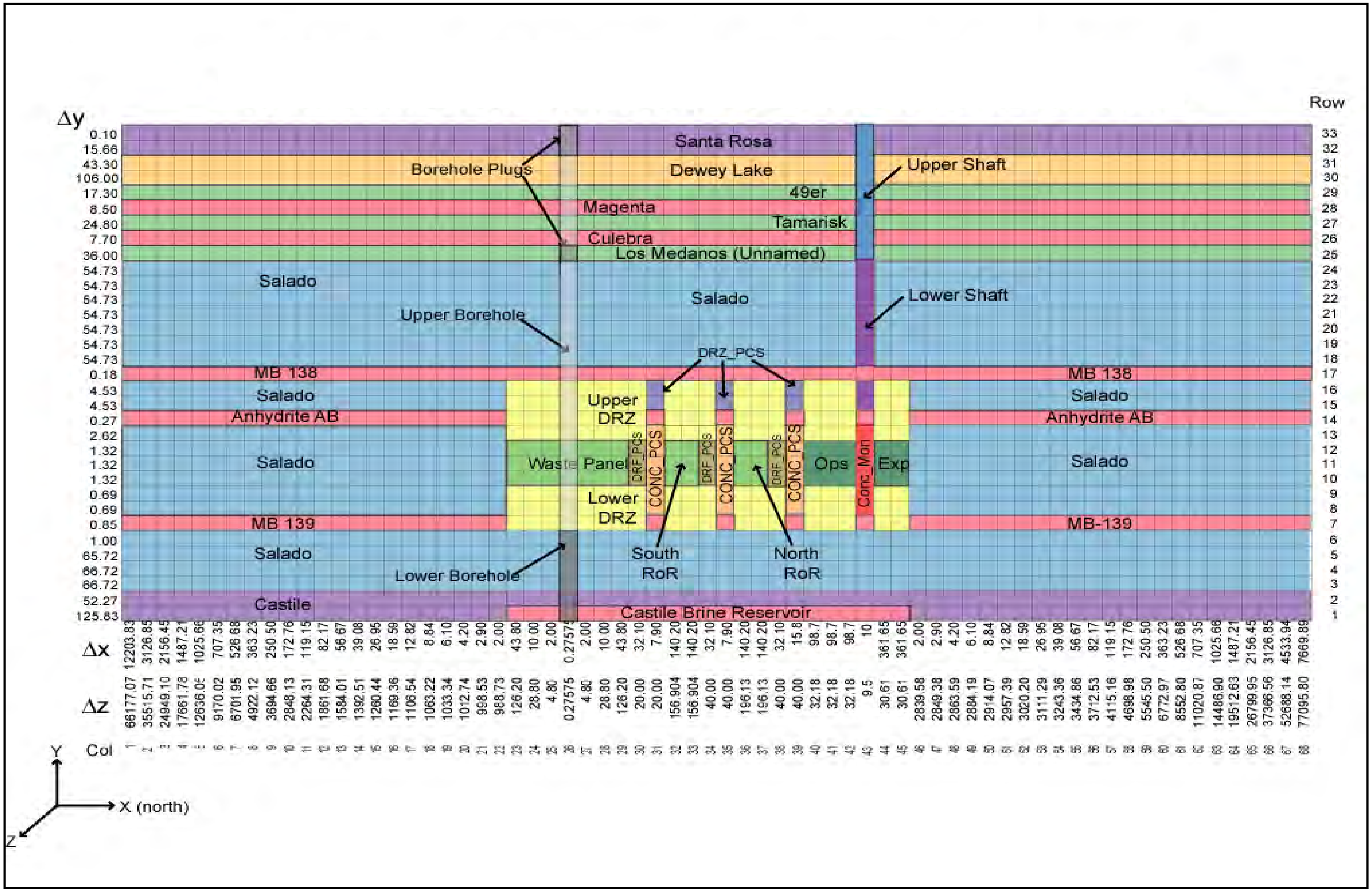

Figure 6-1: PABC-2009 BRAGFLO grid (Δx, Δy, and Δz dimensions in meters)

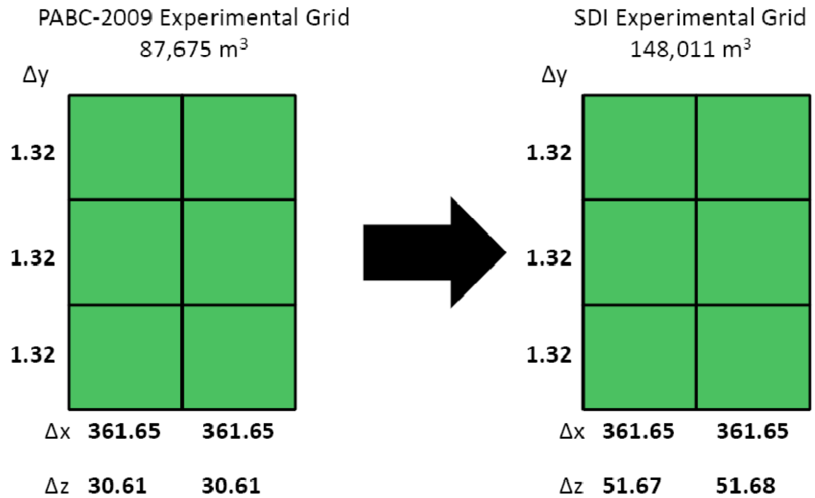

Figure 6-2: SDI BRAGFLO grid changes (Δx, Δy, and Δz dimensions in meters).

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 SDI impact assessment is 1,800 (300 vectors times 6 scenarios).

The six scenarios used in the SDI impact assessment 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. Transport releases to the Culebra are captured in Scenario S6-BF. Transport releases from the Culebra obtained in the PABC-2009 are also used in the SDI impact assessment. However, results from BRAGFLO scenario S6-BF are briefly discussed in this report for the sake of completeness. In the Salado flow results that follow, summary statistics and plots were generated with Matlab, a commercial off-the-shelf software package. Matlab files used in the SDI impact assessment are included on a cd submitted with this summary report. BRAGFLO scenarios considered in the SDI impact assessment are summarized in Table 1.

Table 1: BRAGFLO Modeling Scenarios

Scenario	Description
S1-BF	Undisturbed Repository
S2-BF	E1 intrusion at 350 years
S3-BF	E1 intrusion at 1,000 years
S4-BF	E2 intrusion at 350 years
S5-BF	E2 intrusion at 1,000 years
S6-BF	E2 intrusion at 1,000 years; E1 intrusion at 2,000 years.

BRAGFLO results are presented for the SDI impact assessment 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. Results associated with intrusions 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 BRAGFLO scenario S6-BF are also discussed.

The overall means of pressure in the experimental area, denoted by quantity EXP_PRES, are shown in Figure 6-3 for undisturbed scenario S1-BF, and Figure 6-4, Figure 6-5, Figure 6-6 for intrusion scenarios S2-BF, S4-BF, and S6-BF, respectively. As seen in those figures, the additional volume in the SDI calculations results in a reduction in the average pressure in the experimental area for all scenarios when compared to PABC-2009 results.

Reduced pressure in the experimental area combined with the long WIPP regulatory period of 10,000 years results in eventual lower average pressure in the waste panel as compared to PABC-2009 results. The reduction in average waste panel pressure, denoted by quantity WAS_PRES, for undisturbed scenario S1-BF is illustrated in Figure 6-7. Eventual pressure reductions in the waste panel are also seen for E1 intrusion scenarios (Figure 6-8), E2 intrusion scenarios (Figure 6-9), and the E2E1 intrusion scenario (Figure 6-10).

A probable consequence of lower average pressure in the waste panel is a corresponding increase in the average cumulative flow of brine into the panel, denoted by quantity BRNWASIC. As seen in Figure 6-11 through Figure 6-14, the reduction in average pressure in the waste panel does indeed yield slight increases in the total amount of brine entering the panel for both undisturbed and disturbed conditions. These slight increases of brine flow into the panel result in slight increases in the average panel brine saturation, denoted by quantity WAS_SATB. As seen for the undisturbed case shown in Figure 6-15 and the intrusion scenario results shown in Figure 6-16 through Figure 6-18, the average brine saturation in the waste panel is slightly increased for all scenarios considered in the SDI impact assessment as compared to the PABC-2009.

Summary statistics for the SDI BRAGFLO results discussed above are shown in Table 2. In that table, mean and maximum values for a given quantity are calculated over all 300 vectors. As the brine saturation in the waste panel only varies between 0 and 1, values in Table 2 for that quantity are listed to three decimal places to make differences between analyses more apparent.

Table 2: BRAGFLO SDI Summary Statistics

Quantity (units)	Scenario	Mean Value		Maximum Value	
		PABC-2009	SDI	PABC-2009	SDI
EXP_PRES (MPa)	S1-BF	4.46	4.04	15.65	15.15
	S2-BF	4.41	4.04	14.77	14.62
	S4-BF	3.70	3.36	14.70	14.56
	S6-BF	4.18	3.81	14.76	14.63
WAS_PRES (MPa)	S1-BF	6.52	6.34	16.19	16.18
	S2-BF	7.39	7.31	15.63	15.62
	S4-BF	4.64	4.56	14.92	14.68
	S6-BF	5.96	5.88	15.04	14.90
BRNWASIC (x 10^3 m^3)	S1-BF	1.78	1.80	12.46	13.24
	S2-BF	14.03	14.10	182.15	186.63
	S4-BF	2.73	2.74	23.81	24.96
	S6-BF	7.71	7.84	180.24	184.55
WAS_SATB (dimensionless)	S1-BF	0.160	0.164	0.985	0.985
	S2-BF	0.677	0.681	0.999	0.999
	S4-BF	0.283	0.285	0.995	0.995
	S6-BF	0.418	0.424	0.999	0.999

Using the BRAGFLO results presented above, the impact of SDI excavation on individual components of release can now be initially discussed. Spallings release volumes are a function of pressure. A reduction in waste panel pressure results in a corresponding reduction in spallings release volumes. Therefore, one would expect that the additional SDI excavation results in a slight decrease in spallings releases as compared to the PABC-2009 as both analyses use the same waste inventory. Impacts on spallings releases are quantified in Section 6.2.

The impact of SDI excavation on DBRs is less straightforward. Sufficient pressure and brine saturation in the panel at the time of intrusion are prerequisites for a DBR to occur. In particular, brine saturation in the panel must exceed the residual brine saturation of the waste, a sampled parameter in PA. In addition, the repository pressure near the drilling location must exceed the hydrostatic pressure of the drilling fluid, which is observed at the repository elevation and specified in PA to be 8 MPa. As seen in the SDI BRAGFLO results above, the average waste panel pressure was lowered in all scenarios as compared to the PABC-2009. Thus, one would expect a corresponding reduction in the number of vectors that satisfy the pressure criteria for a DBR. On the other hand, the average brine saturation in the waste panel increased for all scenarios in the SDI calculation. From this, one would expect to see an increase in the number of vectors that satisfy the DBR brine saturation requirement. As a result, the BRAGFLO results shown above are not sufficient to determine the impacts of SDI excavation on DBRs with certainty. Additional analysis is required to quantify these impacts and is provided in Section 6.3.

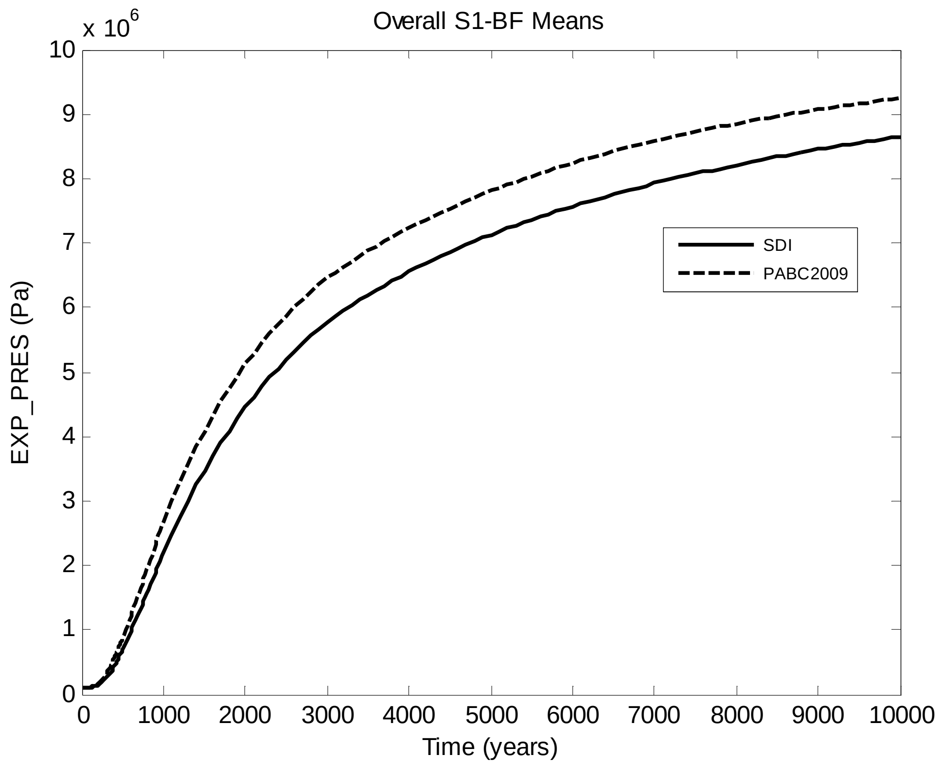

Figure 6-3: Overall Means of Volume Averaged Pressure for the Experimental Region, Scenario S1-BF.

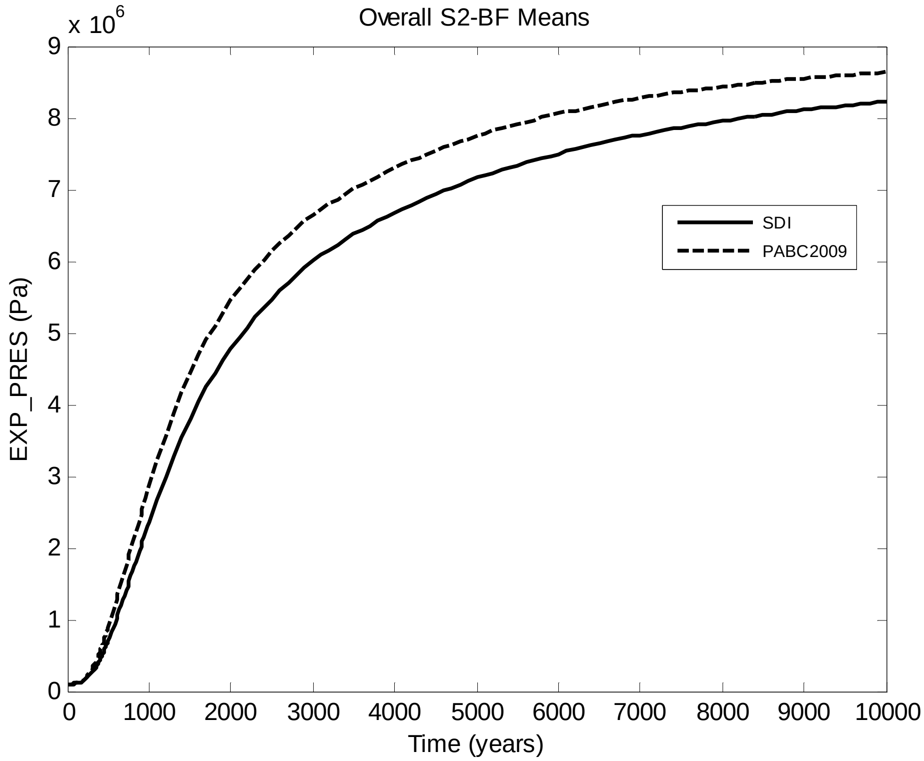

Figure 6-4: Overall Means of Volume Averaged Pressure for the Experimental Region, Scenario S2-BF.

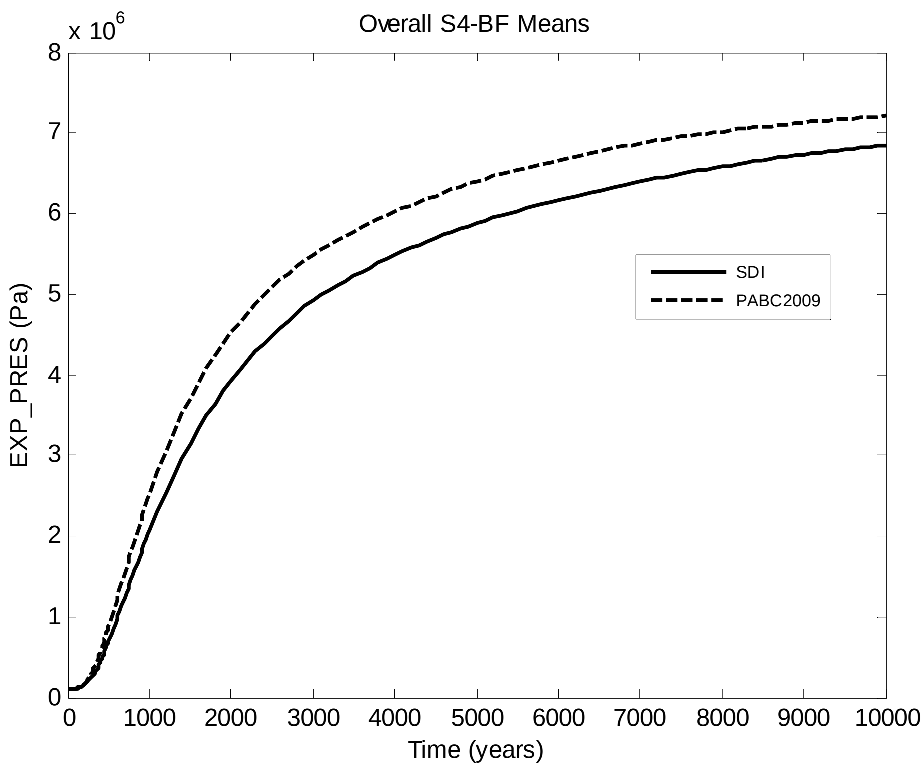

Figure 6-5: Overall Means of Volume Averaged Pressure for the Experimental Region, Scenario S4-BF.

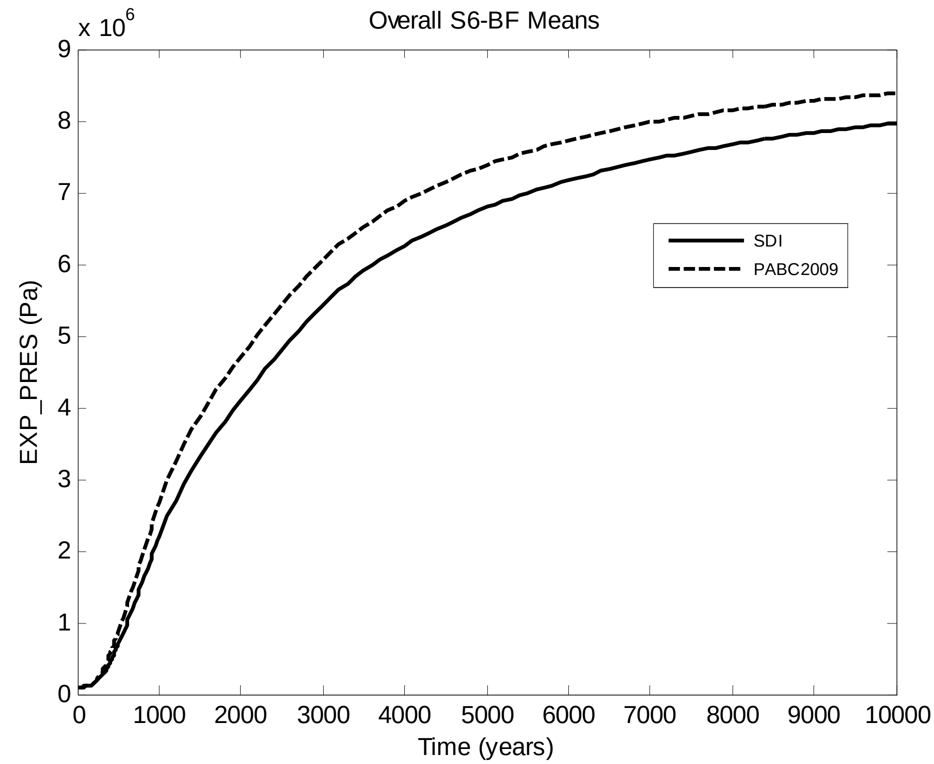

Figure 6-6: Overall Means of Volume Averaged Pressure for the Experimental Region, Scenario S6-BF.

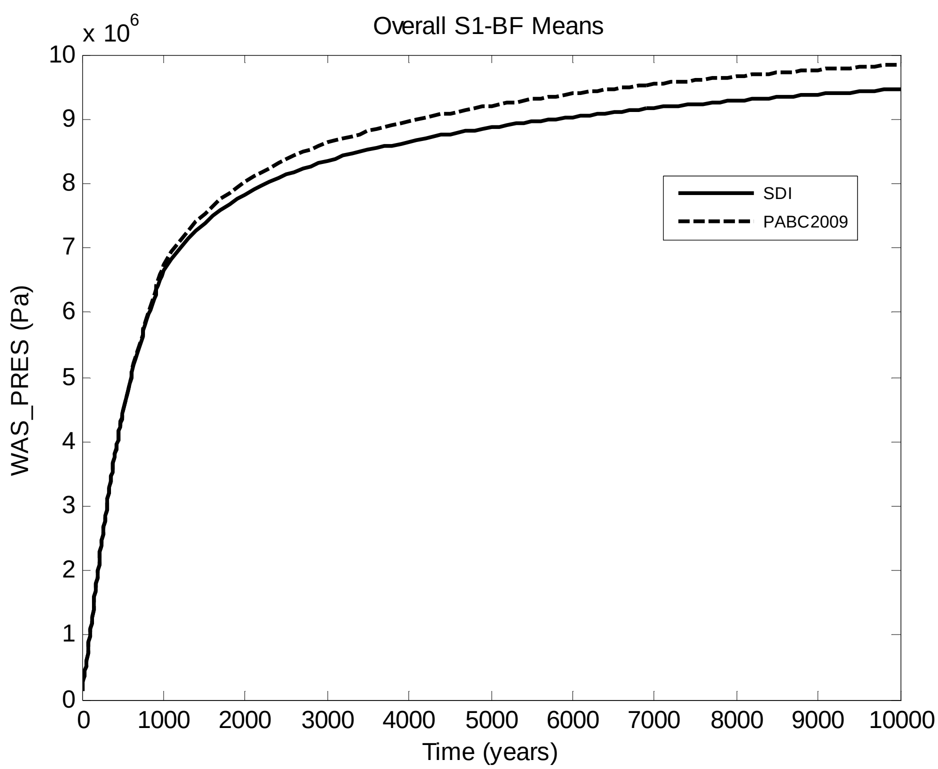

Figure 6-7: Overall Means of Volume Averaged Pressure for the Waste Panel, Scenario S1-BF.

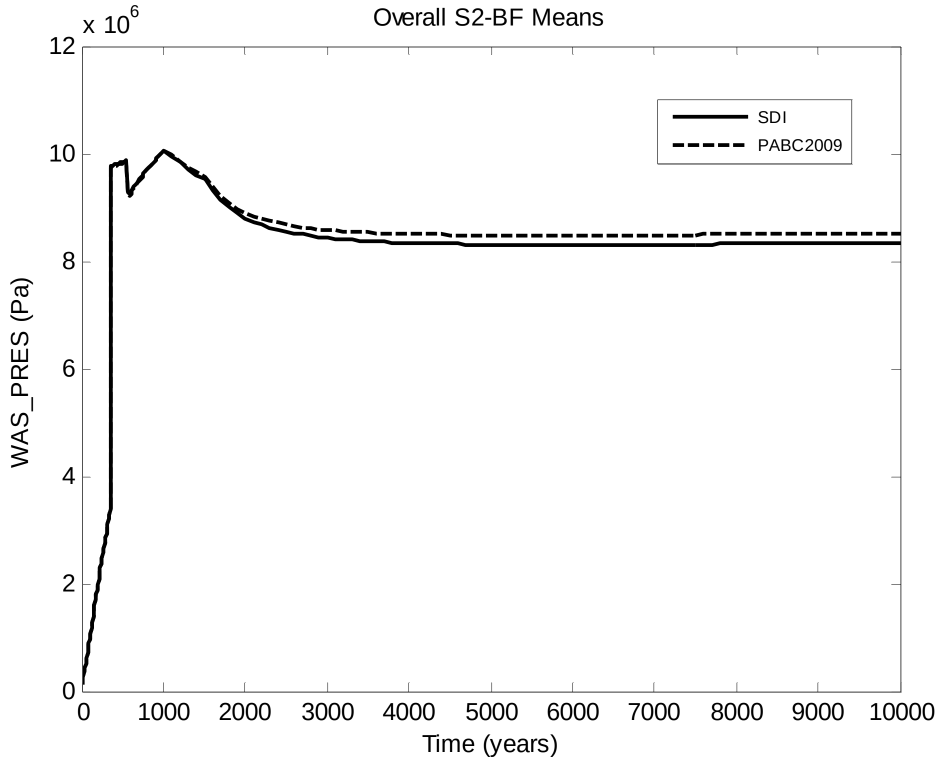

Figure 6-8: Overall Means of Volume Averaged Pressure for the Waste Panel, Scenario S2-BF.

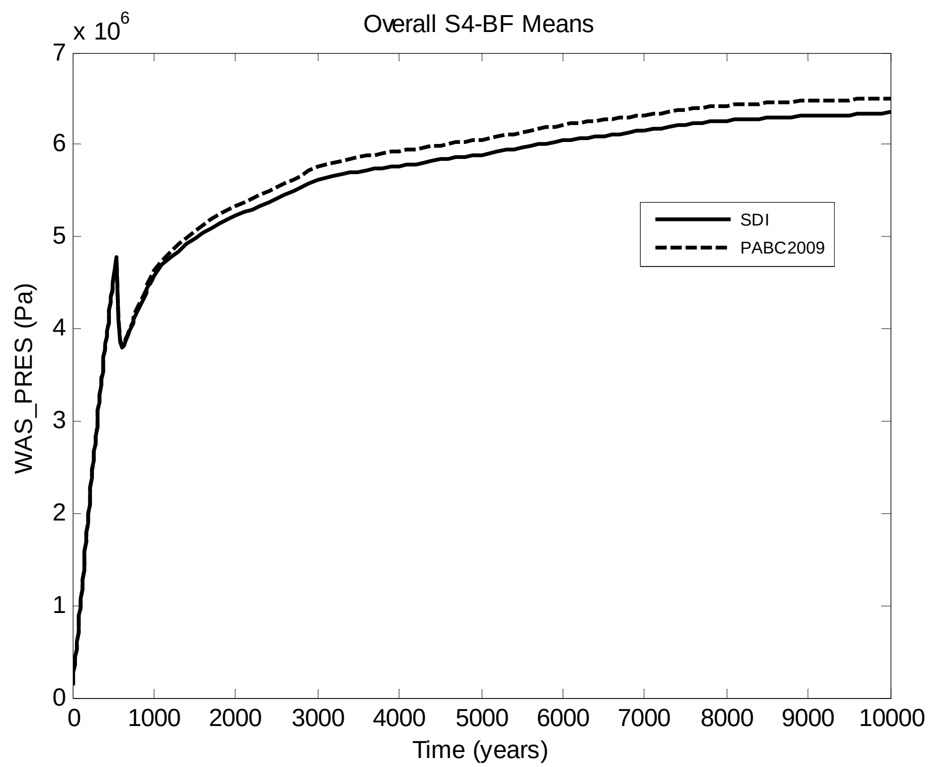

Figure 6-9: Overall Means of Volume Averaged Pressure for the Waste Panel, Scenario S4-BF.

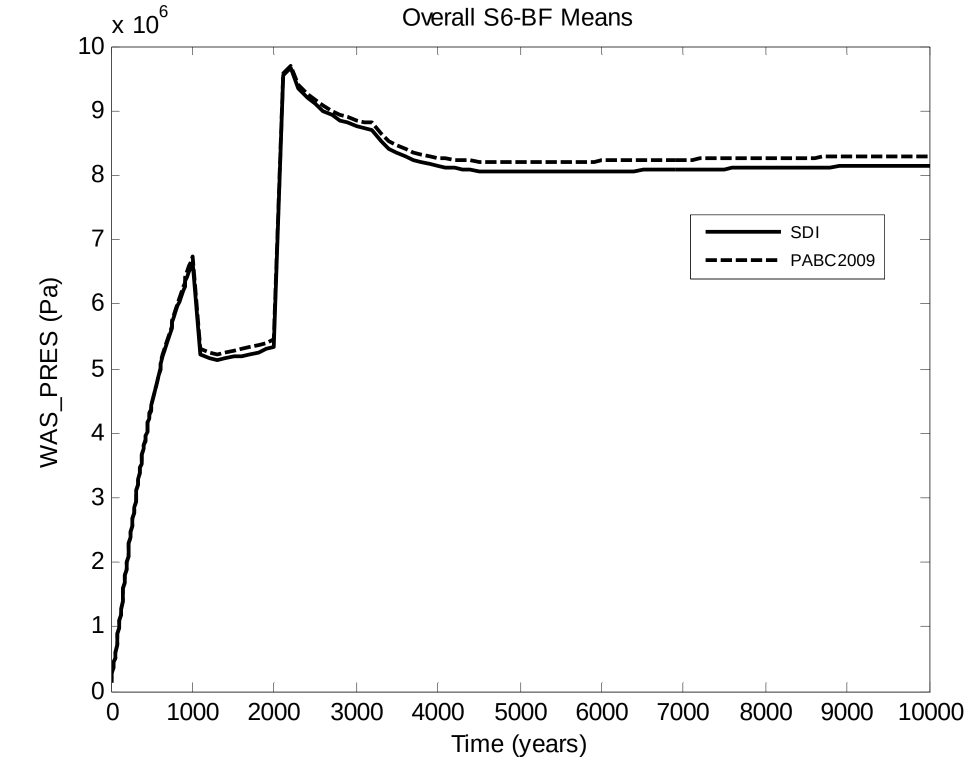

Figure 6-10: Overall Means of Volume Averaged Pressure for the Waste Panel, Scenario S6-BF.

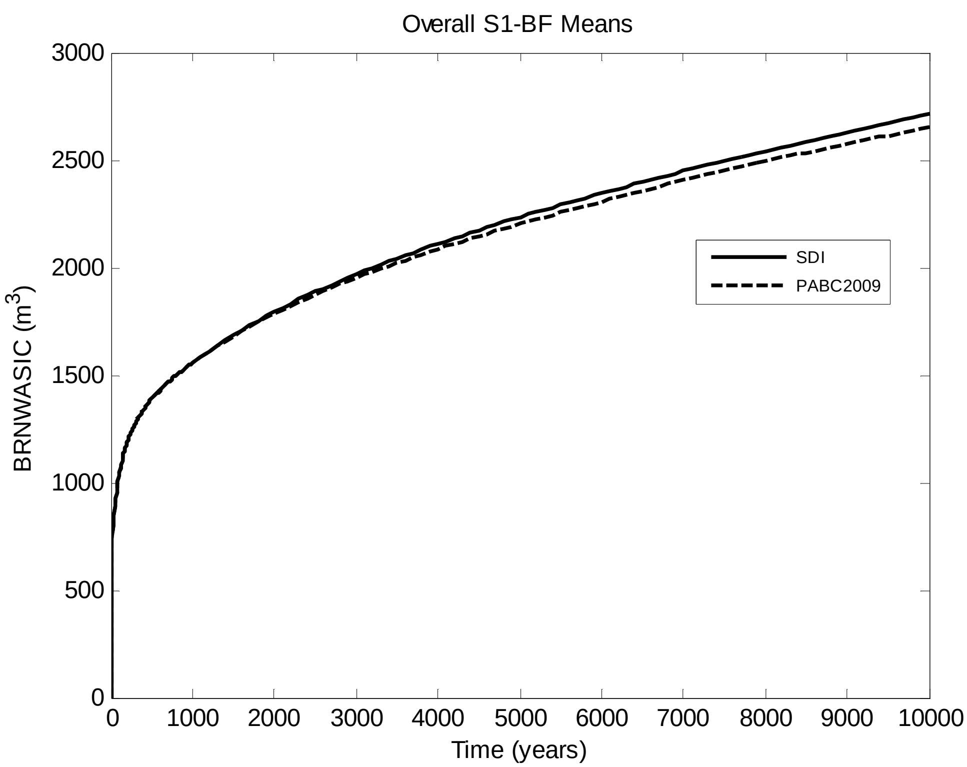

Figure 6-11: Overall Means of Total Brine Flow Into the Waste Panel, Scenario S1-BF

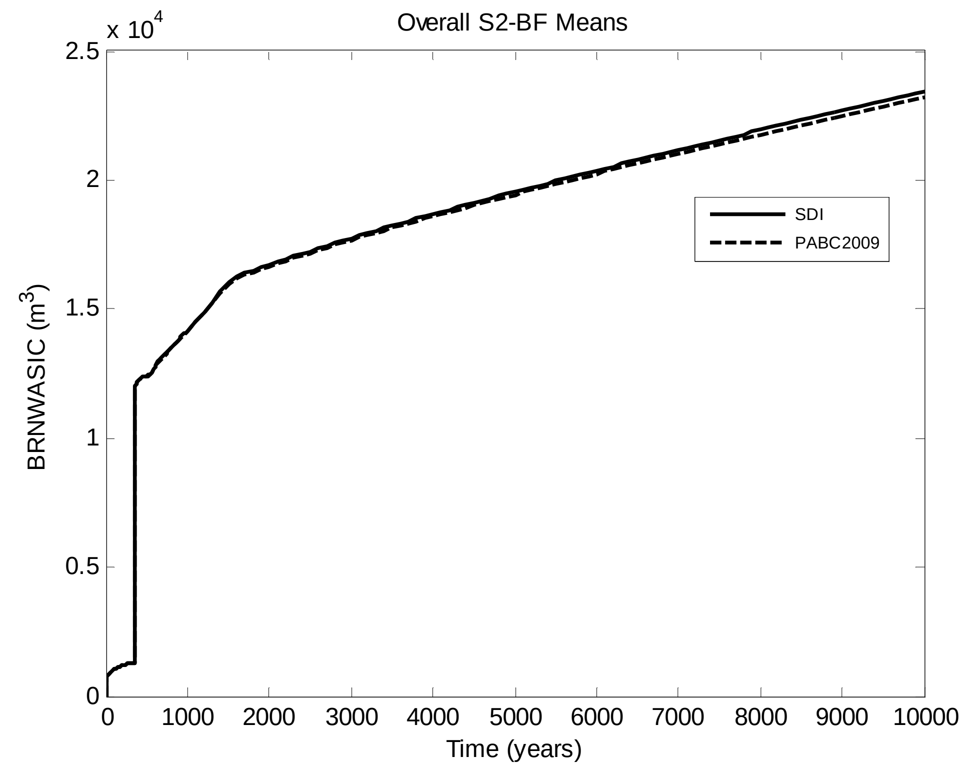

Figure 6-12: Overall Means of Total Brine Flow Into the Waste Panel, Scenario S2-BF

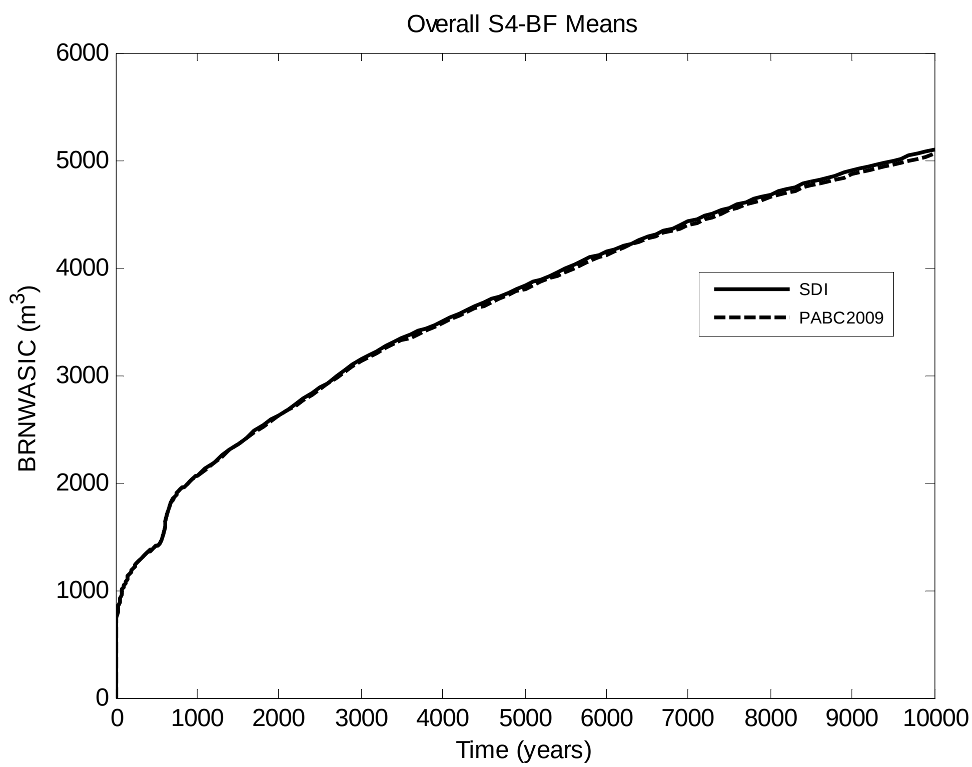

Figure 6-13: Overall Means of Total Brine Flow Into the Waste Panel, Scenario S4-BF

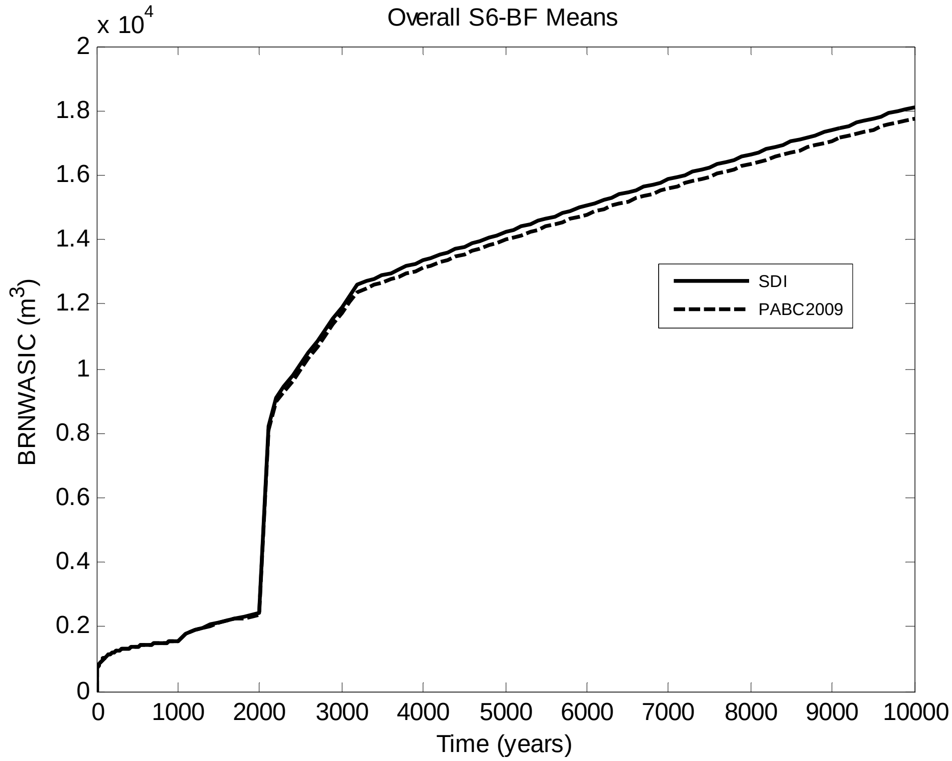

Figure 6-14: Overall Means of Total Brine Flow Into the Waste Panel, Scenario S6-BF

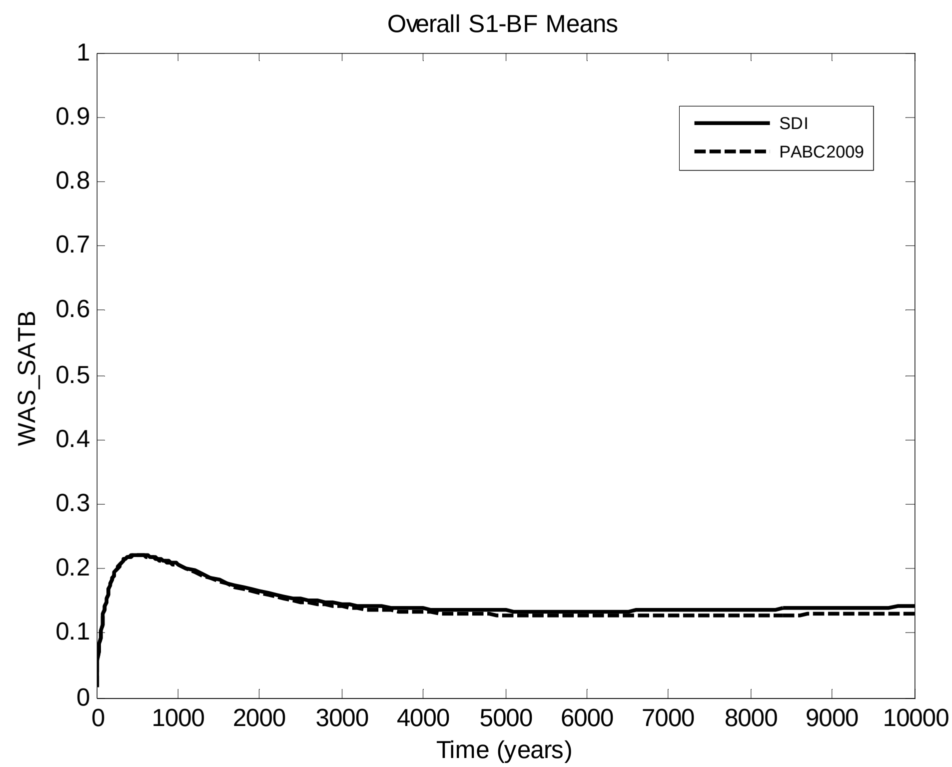

Figure 6-15: Overall Means of Brine Saturation in the Waste Panel, Scenario S1-BF

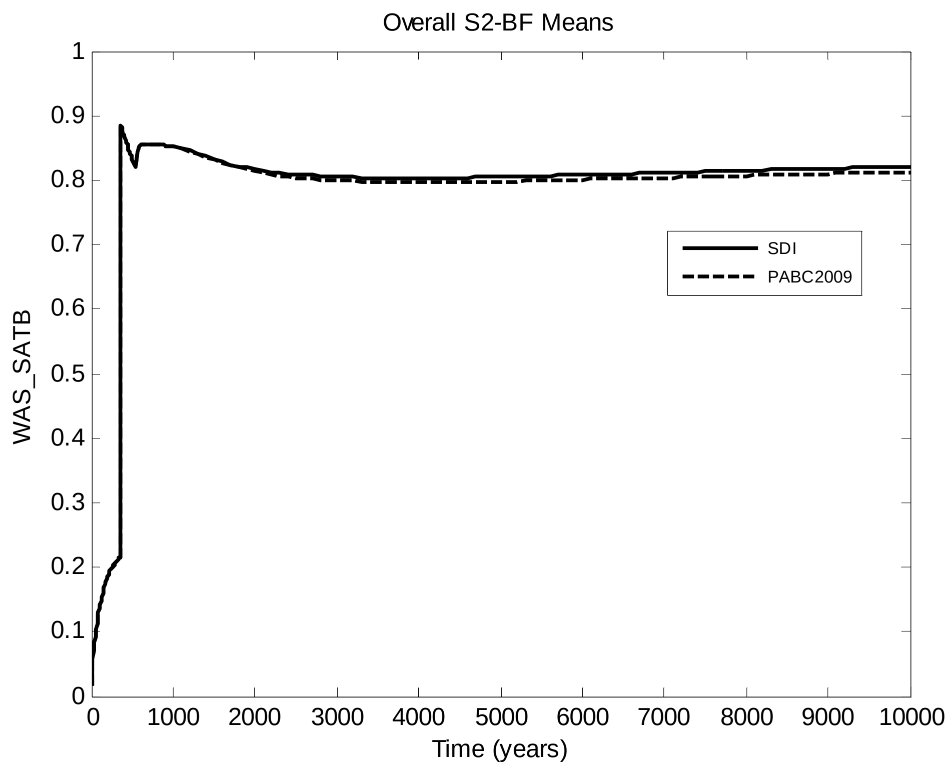

Figure 6-16: Overall Means of Brine Saturation in the Waste Panel, Scenario S2-BF

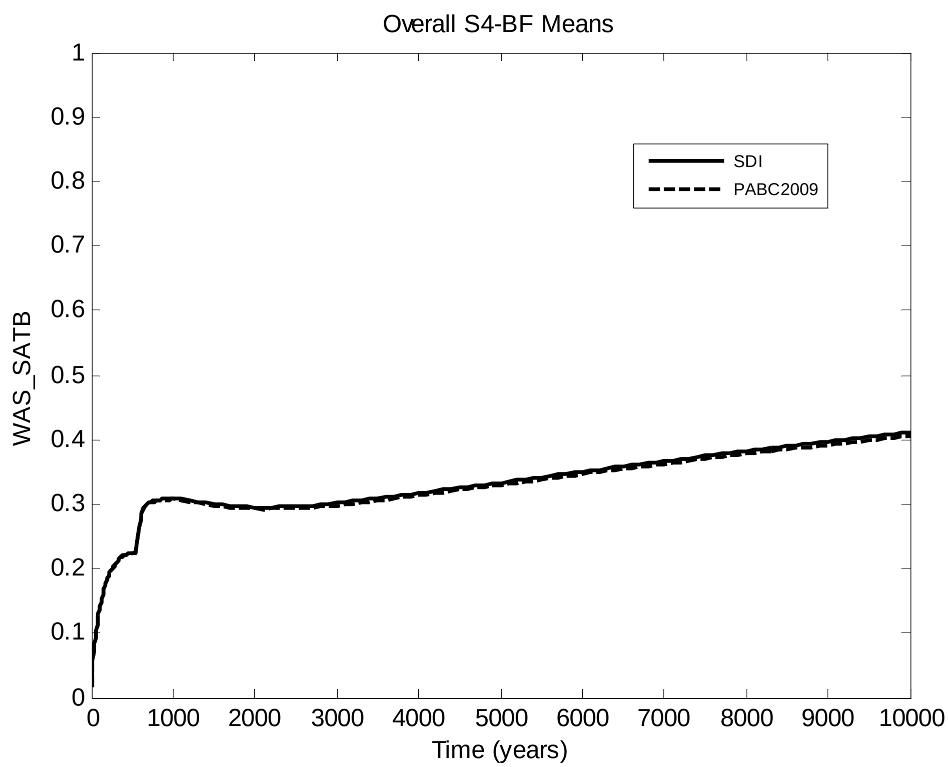

Figure 6-17: Overall Means of Brine Saturation in the Waste Panel, Scenario S4-BF

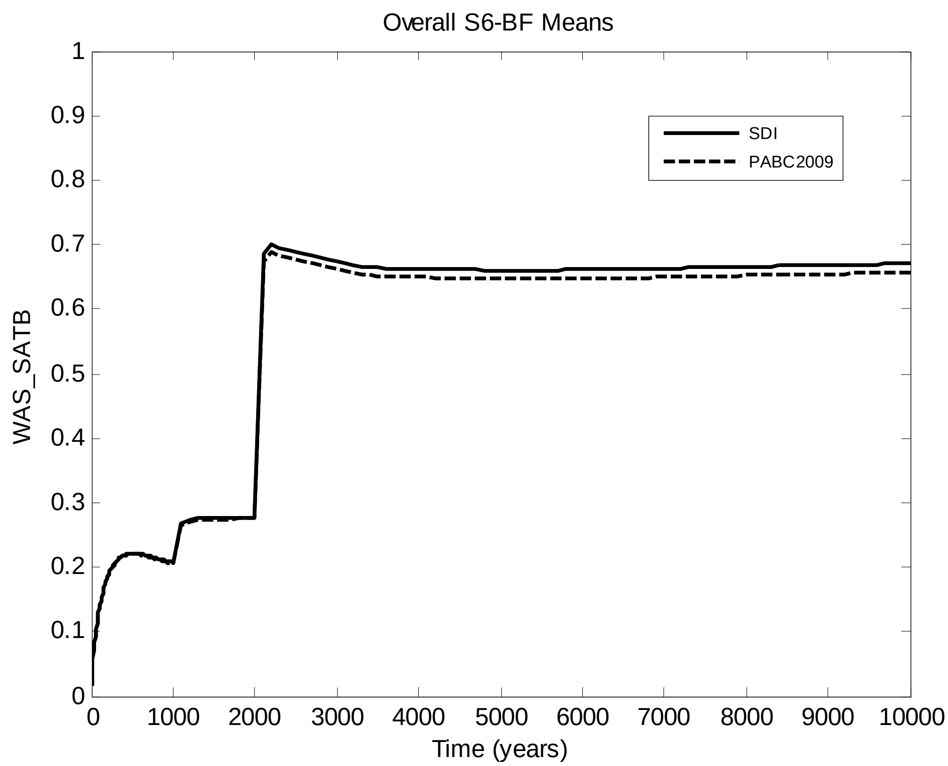

Figure 6-18: Overall Means of Brine Saturation in the Waste Panel, Scenario S6-BF

6.2 Spallings

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, the 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 SDI impact assessment.

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 3.

Table 3: 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 3; 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 SDI repository pressures calculated by BRAGFLO, the impact of SDI excavation on spallings volumes can be determined. Summary statistics of spallings volumes for the intrusion scenarios considered by CUTTINGS_S are shown in Table 4 for both the SDI impact assessment and the PABC-2009. PABC-2009 results reported in that table are taken from Ismail (2010). As seen in that table, values obtained in the SDI impact assessment are generally equal or lower overall when compared to those obtained in the PABC-2009. For scenario S1-DBR, a consistent reduction in the number of nonzero spallings volumes is seen across replicates R1 – R3 in the SDI impact assessment. Moreover, the average and maximum spallings volumes seen in that scenario are lower in all three replicates for the SDI calculation. Similar reductions are evident in scenarios S2-BF to S5-BF. Overall, the general trend is an equal or lower maximum volume, an equal or lower average volume, and a lower percentage of vectors resulting in nonzero spallings volumes in the SDI calculation than were seen in the PABC-2009.

Spallings volumes are a function of repository pressure. Previous analyses have determined that no tensile failure of repository material occurs at initial repository pressures less than 10 MPa, and that no spallings are observed at pressures less than 13 MPa (Lord et al 2003). Thus, waste failure and subsequent transport for spallings is assumed to be non-existent for repository pressures less than 10 MPa. As seen in the BRAGFLO results in Section 6.1, additional excavation in the WIPP experimental area for SDI translates to an eventual pressure reduction in waste-containing regions. As there is a minimum threshold pressure of 10 MPa required for a spallings release, a decrease in repository pressure also decreases the percentage of vectors with nonzero spallings volumes.

Table 4: Summary of Spallings Releases by Scenario

		Scenarios					Total
		S1-DBR	S2-DBR	S3-DBR	S4-DBR	S5-DBR	
SDI PA							
R1	**Maximum [m^3]**	1.67	8.29	7.98	1.67	1.67	8.29
	Average nonzero volume [m^3]	0.35	0.54	0.55	0.29	0.37	0.43
	Number of nonzero volumes	127	105	99	58	74	463
	Percent of nonzero volumes	7.1%	7.0%	6.6%	3.9%	4.9%	5.9%
R2	**Maximum [m^3]**	2.17	2.74	1.73	2.26	1.93	2.74
	Average nonzero volume [m^3]	0.28	0.35	0.34	0.42	0.40	0.34
	Number of nonzero volumes	145	100	108	54	80	487
	Percent of nonzero volumes	8.1%	6.7%	7.2%	3.6%	5.3%	6.2%
R3	**Maximum [m^3]**	3.66	6.20	2.48	0.85	1.08	6.20
	Average nonzero volume [m^3]	0.41	0.38	0.23	0.24	0.23	0.32
	Number of nonzero volumes	140	92	98	36	63	429
	Percent of nonzero volumes	7.8%	6.1%	6.5%	2.4%	4.2%	5.5%
PABC-2009							
R1	**Maximum [m^3]**	2.24	8.29	7.97	1.67	1.67	8.29
	Average nonzero volume [m^3]	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 [m^3]**	2.36	2.76	1.86	2.26	1.93	2.76
	Average nonzero volume [m^3]	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 [m^3]**	4.91	6.23	2.62	1.47	1.49	6.23
	Average nonzero volume [m^3]	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 SDI impact assessment can be seen in Figure 6-19. As seen in that figure, the CCDF of spallings releases obtained in the SDI impact assessment is consistently lower than that found in the PABC-2009. The overall reduction in spallings volumes and in the number of vectors that result in a nonzero spallings volume translate to a reduction in spallings releases as both analyses use the same waste inventory.

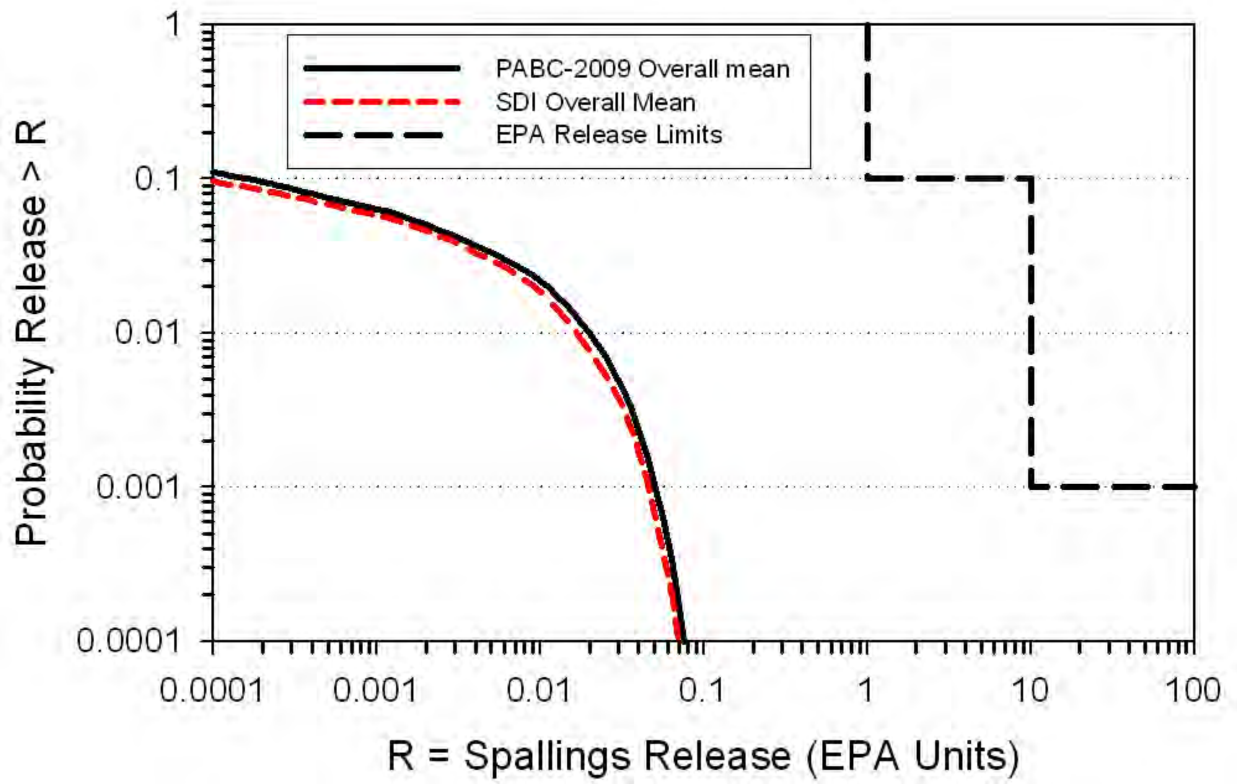

Figure 6-19: SDI and PABC-2009 Overall Mean CCDFs for Normalized Spallings Releases

6.3 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. SDI results from this application of BRAGFLO are shown in Section 6.1. Second, it is used for the calculation of direct brine releases. These two uses of BRAGFLO require different computational grids. The grid used to calculate brine and gas flow in and around the repository is different than that used to calculate DBRs. However, 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 SDI and PABC-2009 BRAGFLO grids (see Figure 6-1) 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 3. The DBR computational grid and drilling locations used for the SDI impact assessment are identical to those used in the PABC-2009, and are shown in Figure 6-20.

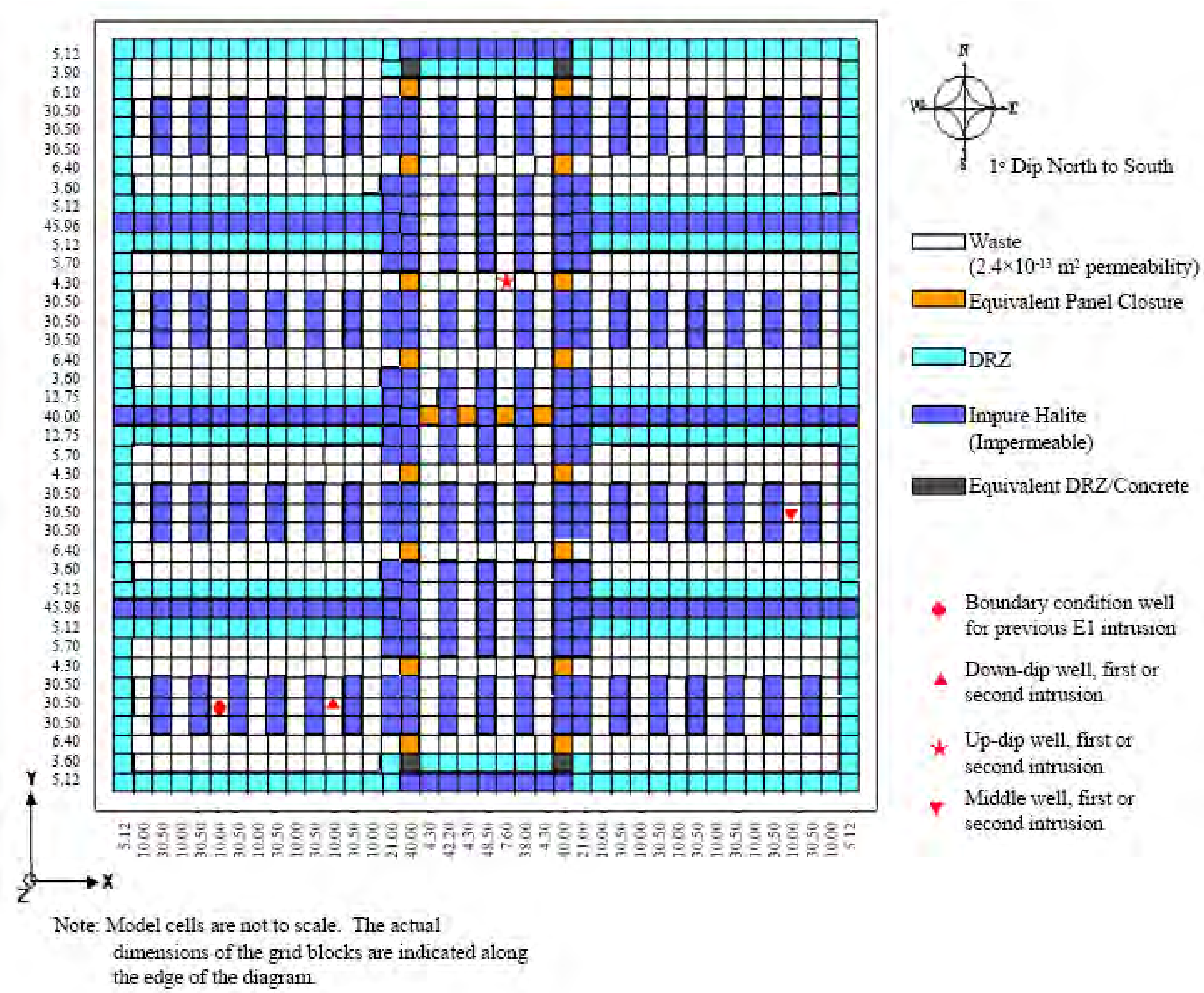

Figure 6-20: SDI and PABC-2009 DBR material map (logical grid).

With the DBR computational grid and intrusion locations in hand, DBR results from the SDI impact assessment 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. As was also the case in the PABC-2009, release volumes 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 SDI calculations. In Table 5, maximums shown are the maximum DBR volumes calculated over all replicates, times, vectors and drilling locations. As seen by the statistics for the maximum DBR volumes in Table 5, the additional excavation to the WIPP experimental area for SDI results in a decrease in the maximum DBR volume as compared to the PABC-2009. The maximum DBR volume realized in the PABC-2009 was 48.2 m^3 while that seen in the SDI impact assessment is 42.3 m^3. Additionally, the average DBR volume remained equal or decreased in the SDI impact assessment for all scenarios considered. When calculated over all intrusion scenarios and all nonzero releases, the average volumes are the same at 0.9 m^3 in the PABC-2009 and in the SDI impact assessment. As seen in the BRAGFLO results of Section 6.1, a reduction in the average pressure with a corresponding increase in average brine saturation was seen in waste-containing regions for all scenarios considered in the Salado flow calculation. These changes effectively cancel each other out in the DBR calculation, resulting in equal average DBR volumes in the SDI and PABC-2009 results. These changes have a slight impact on the number of vectors resulting in nonzero DBR volumes, however. In the PABC-2009, a total of 2,999 vectors resulted in a nonzero DBR volume realization. The number of vectors resulting in nonzero DBR volumes in the SDI impact assessment is 2,880, a reduction by 119 vectors when compared to the PABC-2009 results.

Table 5: PABC-2009 and SDI PA DBR Volume Statistics

Scenario	Maximum Volume (m^3)		Average Volume (m^3)		Number of Vectors	
	PABC-2009	SDI PA	PABC-2009	SDI PA	PABC-2009	SDI PA
S1-DBR	27.6	18.5	0.1	0.1	369	356
S2-DBR	48.2	42.3	2.8	2.7	1179	1139
S3-DBR	40.6	42.1	1.5	1.5	926	901
S4-DBR	20.4	18.9	0.1	0.0	211	198
S5-DBR	21.1	21.3	0.1	0.1	314	286
S1-DBR to S5-DBR	48.2	42.3	0.9	0.9	2999	2880

DBR releases are less likely to occur during upper drilling intrusions when compared with the lower drilling location. Of all the intrusions that had a non-zero DBR volume for the SDI impact assessment, 67.3% occurred during a lower drilling intrusion. Furthermore, of all the intrusions that had a non-zero DBR volume and occurred during a lower drilling intrusion, 83.4% are found in scenarios S2-DBR and S3-DBR. Therefore, 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 DBR volumes compared to those of lower drilling intrusions. For all three replicates of the SDI impact assessment, the maximum DBR volume for the upper drilling location is 13.4 m^3 compared to 42.3 m^3 for the lower drilling location. These observations support the conclusion that lower drilling intrusions are the primary source for significant DBRs. This trend is similarly seen in the PABC-2009 DBR results.

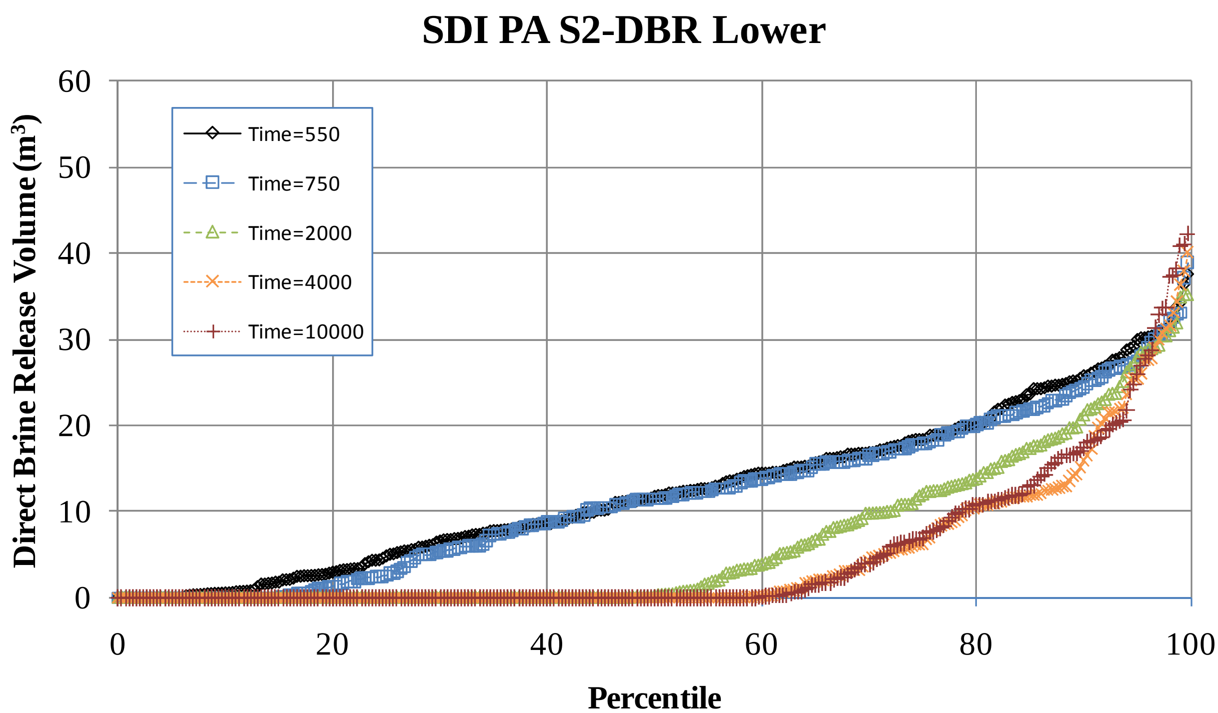

Figure 6-21: All replicates for SDI scenario S2-DBR lower intrusions.

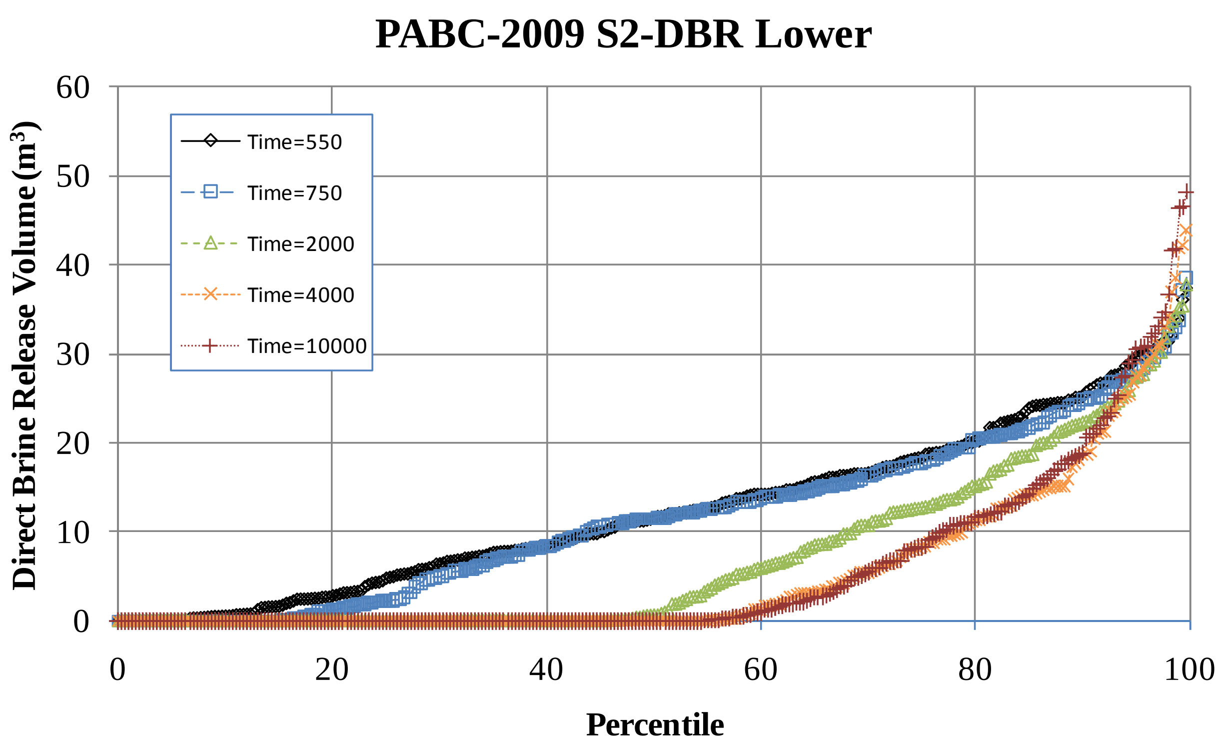

Figure 6-22, All replicates for PABC 2009 scenario S2-DBR lower intrusions

The marked similarity in DBR volumes and trends between the PABC 2009 and the SDI impact assessment is apparent by comparing S2-DBR volume percentiles. Figure 6-21 and Figure 6-22 present these results for the SDI impact assessment and the PABC-2009 across all three replicates at the five times listed in Table 3. Those figures show the percentage of vectors on the X-axis where DBR volumes are less than the value on the Y-axis. As is evident, all significant aspects of these curves are almost identical, with the exception of the maximum DBR volume attained. SDI impact assessment maximum volumes are slightly lower than for the PABC 2009 results.

Figure 6-23 presents DBR volumes versus intruded panel pressure for all replicate 1, scenario S2-DBR lower intrusions. For a nonzero DBR volume to be realized, the repository pressure near the drilling location must exceed the hydrostatic pressure of the drilling fluid, which is specified in PA to be 8 MPa. As a result, there are no releases at panel pressures less than 8 MPa in Figure 6-23. The data in that figure are segregated into mobile brine saturation fractions, for which higher numbers indicate more mobile brine available to flow up an intrusion borehole. It is noted in this figure that low mobile brine values lead to low DBR releases, as expected.

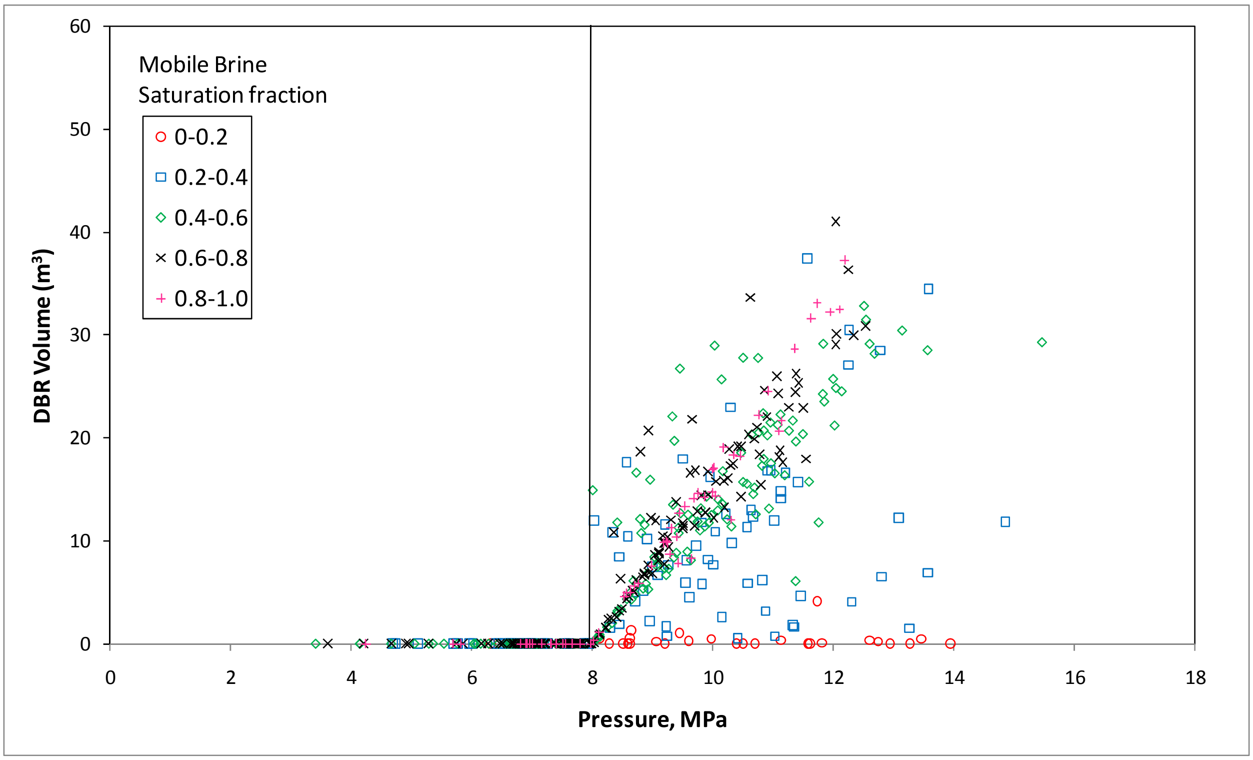

Figure 6-23: SDI DBR Volume vs. Pressure, Scenario S2-DBR, Replicate 1, Lower Intrusion

To further facilitate comparisons of DBRs calculated in the SDI impact assessment to those obtained in the PABC-2009, the overall mean CCDFs obtained in these two analyses are plotted simultaneously in Figure 6-24. As seen in that figure, the CCDF curves obtained for direct brine releases in the PABC-2009 and the SDI impact assessment are virtually identical. Additional excavation in the WIPP experimental area for SDI has slight impacts on pressures and brine saturations in waste-containing regions. These slight changes impact the number of vectors that result in nonzero DBR volumes, with slight reductions seen in the SDI impact assessment. Taken collectively, however, these slight changes result in negligible differences between the DBR CCDF curve obtained in the SDI impact assessment and that found in the PABC-2009.

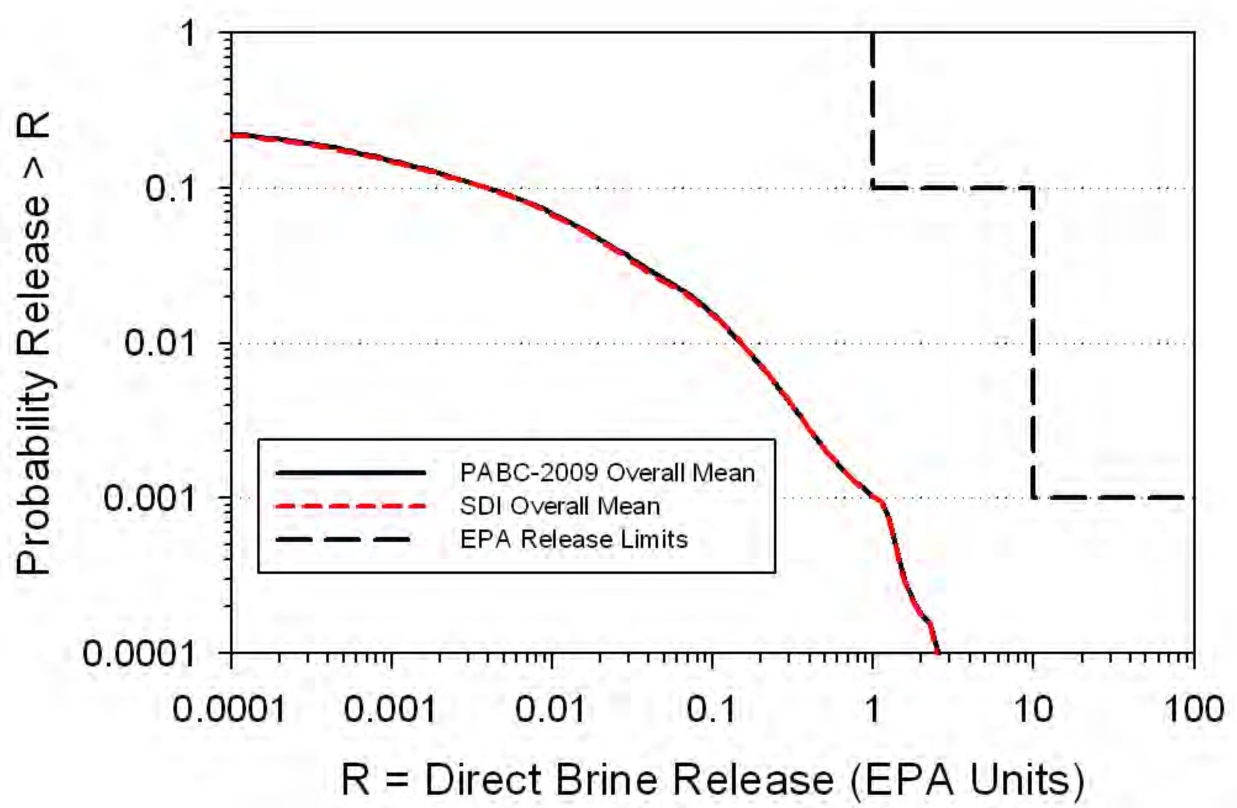

Figure 6-24: SDI and PABC-2009 Overall Mean CCDFs for Normalized Direct Brine Releases

6.4 Total Normalized Releases

Total normalized releases for the SDI impact assessment 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. As prescribed in AP-156 (Camphouse & Kuhlman 2011), transport results obtained in the PABC-2009 are also used in the SDI calculations. SDI CCDFs for total releases are presented in Figure 6-25, Figure 6-26, and Figure 6-27 for replicates 1, 2, and 3, respectively. These curves are virtually unchanged from those found in the PABC-2009. Mean and quantile CCDF distributions for the three replicates are shown together in Figure 6-28. Figure 6-29 contains the 95 percent confidence limits about the overall mean of total releases. As seen in Figure 6-29, the overall mean for normalized total releases and its lower/upper 95% confidence limits are well below acceptable release limits. As a result, the additional SDI excavation in the WIPP experimental area does not result in WIPP non-compliance with the containment requirements of 40 CFR Part 191.

The SDI impact assessment and PABC-2009 overall mean CCDFs for total releases are virtually identical (Figure 6-30). Cuttings and cavings releases and direct brine releases are the two primary release components contributing to total releases found in the SDI calculations (Figure 6-31). Additional excavation in the WIPP experimental area for SDI has no impact on cuttings and cavings releases. Consequently, SDI cuttings and cavings results are unchanged from those found in the PABC-2009. As discussed in Section 6.3, the excavation envisioned for SDI has a negligible impact on direct brine releases.

A comparison of the statistics on the overall mean for total normalized releases obtained in the SDI calculations and the PABC-2009 can be seen in Table 6. In that table, PABC-2009 values are taken from Camphouse (2010). At probabilities of 0.1 and 0.001, values obtained for mean total releases are nearly identical in both analyses and are indistinguishable statistically.

Table 6: SDI 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	90^{th} Percentile	Lower 95% CL	Upper 95% CL	Release Limit
0.1	SDI PA	0.093	0.15	0.090	0.095	1
	PABC-2009	0.094	0.16	0.091	0.096	1
0.001	SDI PA	1.1	1.0	0.38	1.8	10
	PABC-2009	1.1	1.0	0.37	1.8	10

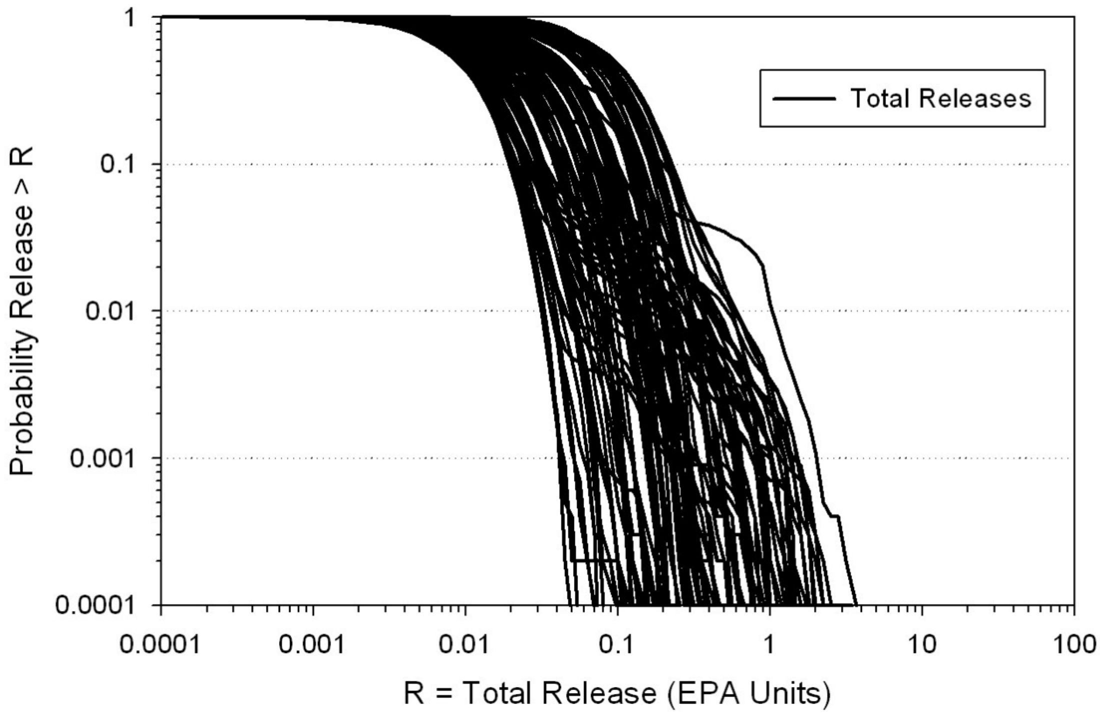

Figure 6-25: SDI Replicate 1 Total Normalized Releases

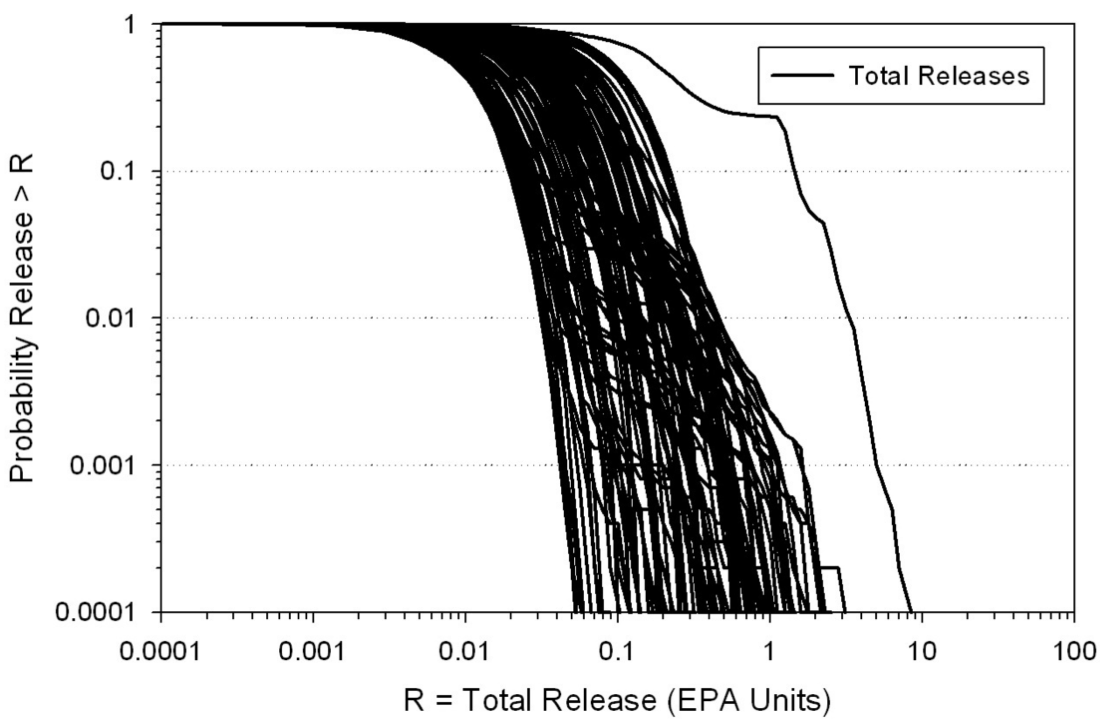

Figure 6-26: SDI Replicate 2 Total Normalized Releases

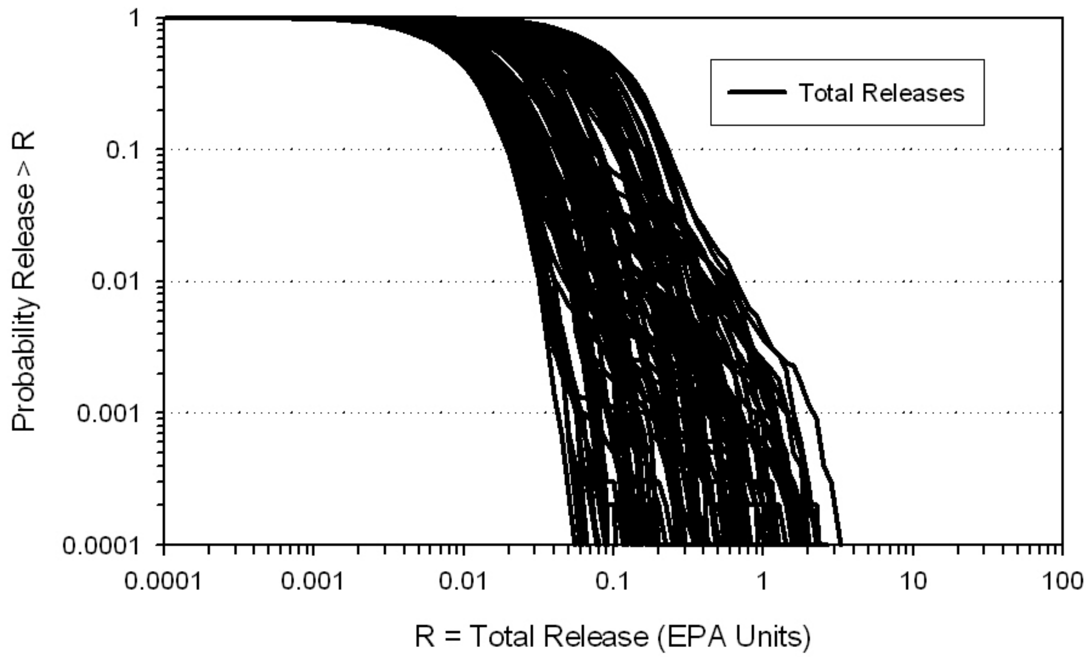

Figure 6-27: SDI Replicate 3 Total Normalized Releases

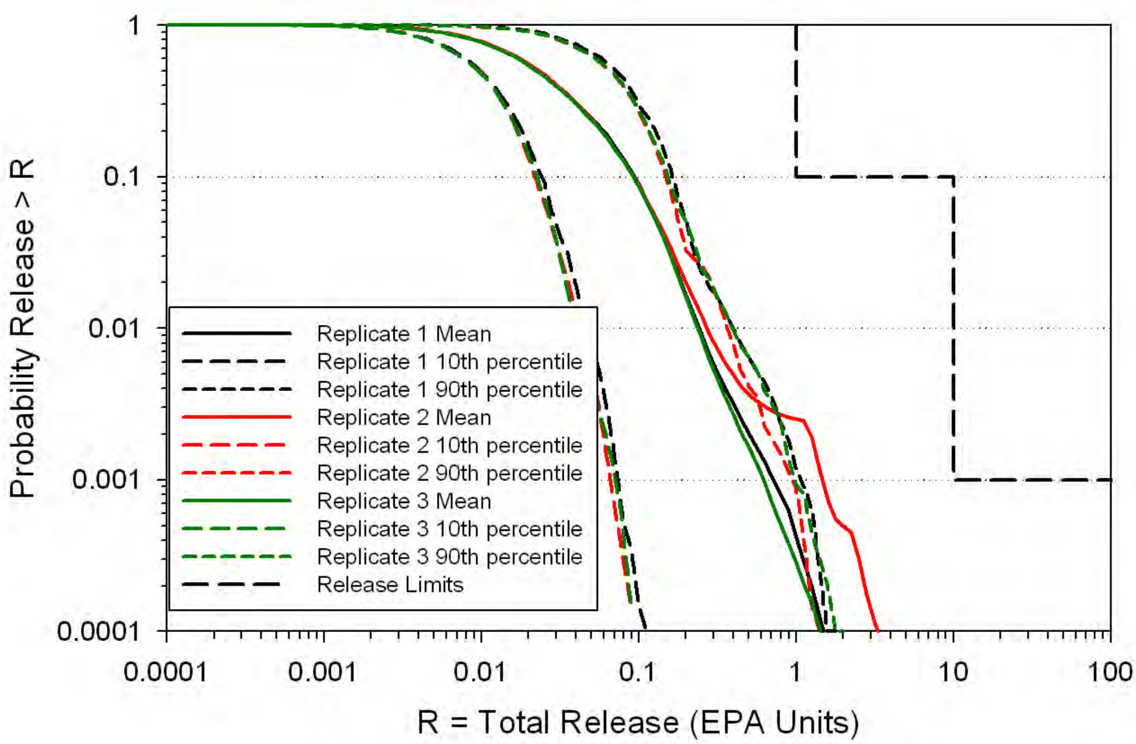

Figure 6-28: SDI Mean and Quantile CCDFs for Total Normalized Releases, Replicates 1-3

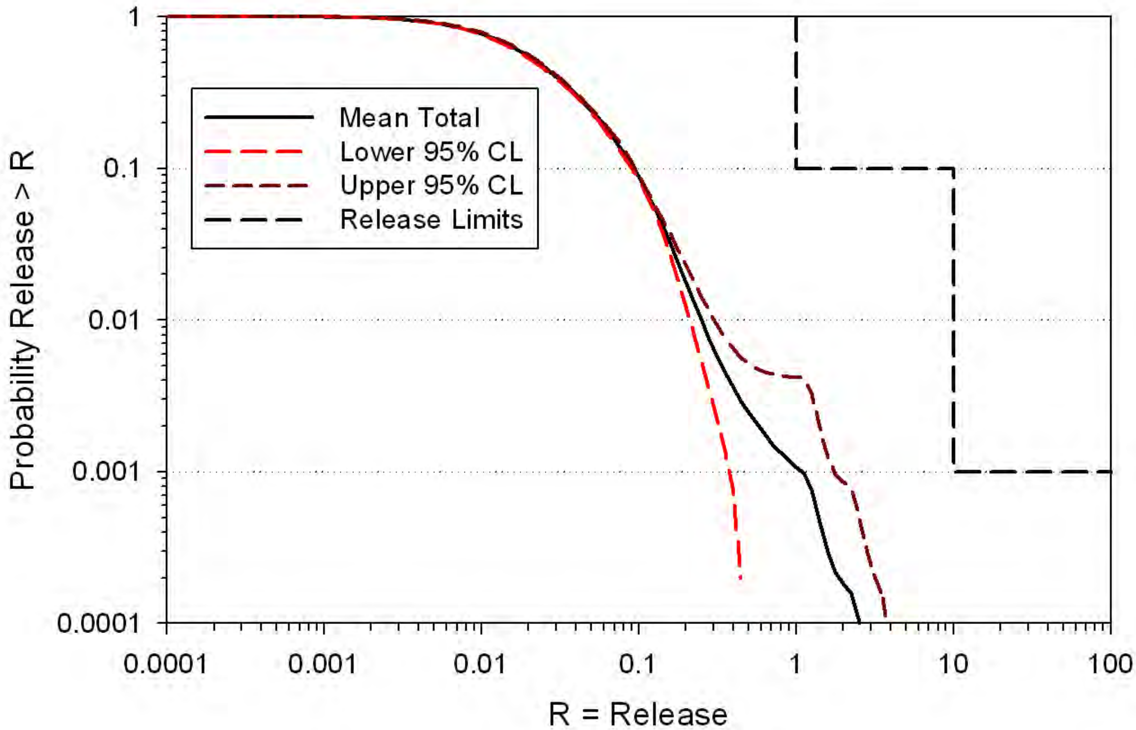

Figure 6-29: SDI Confidence Limits on Overall Mean for Total Normalized Releases

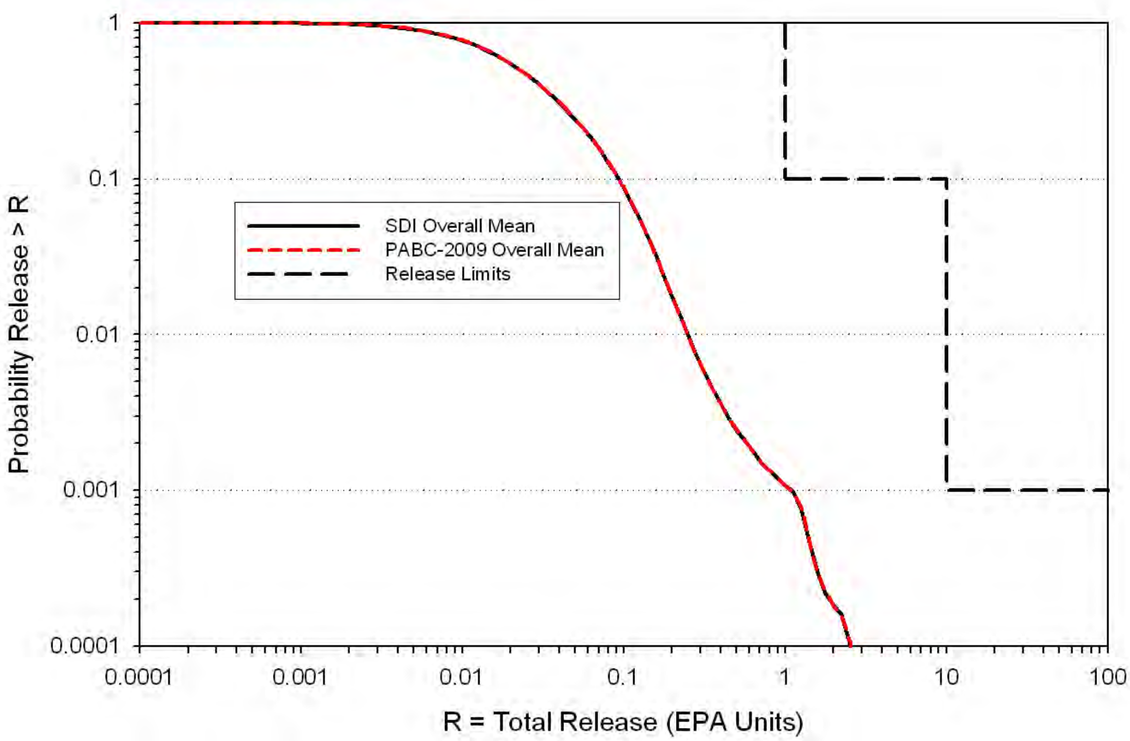

Figure 6-30: SDI and PABC-2009 Overall Mean CCDFs for Total Normalized Releases

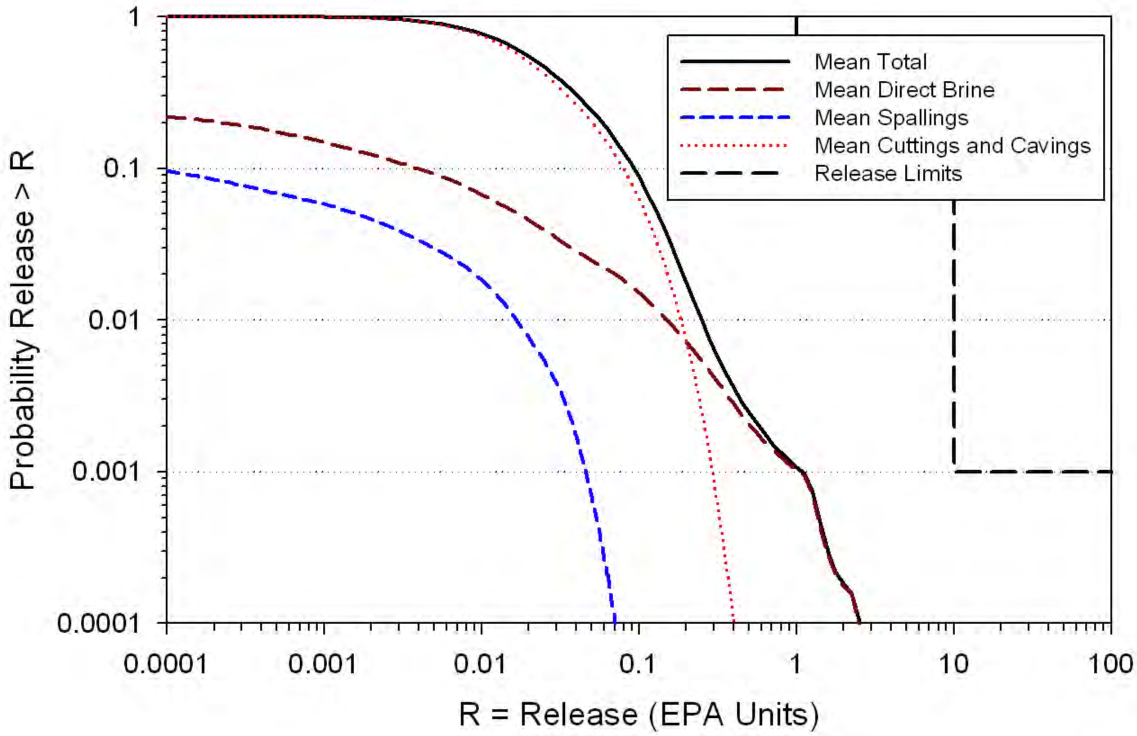

Figure 6-31: SDI Primary Components Contributing to Total Releases

7 SUMMARY

Total normalized releases calculated in the SDI impact assessment remain below their regulatory limits. As a result, the additional excavation in the WIPP experimental area to support SDI would not result in WIPP non-compliance with the containment requirements of 40 CFR Part 191. Cuttings and cavings releases and direct brine releases are the two primary release components contributing to total releases in the SDI calculations. Cuttings and cavings releases are unchanged from those calculated in the PABC-2009. Additional excavation for SDI results in small changes to pressures and brine saturations in repository waste-containing regions, but these collectively result in a negligible difference between direct brine releases seen in the SDI impact assessment and the PABC-2009. Small reductions are observed in SDI spallings releases as compared to the PABC-2009, but these differences are relatively minor and do not have a significant impact on the overall total normalized releases found in the SDI impact assessment. Total normalized releases found in the SDI calculations and the PABC-2009 are indistinguishable.

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APPENDIX A SDI Code Execution

As mentioned in Section 1 and outlined in AP-156 (Camphouse and Kuhlman 2011), the SDI impact assessment is essentially a focused re-run of the PABC-2009 calculation using a slightly modified numerical grid in the Salado flow calculation. Execution and run control for the PABC-2009 are documented in Long (2010). The hardware and operating system used in the SDI impact assessment are identical to those used in the PABC-2009, and are shown in Table 7.

Table 7: WIPP PA Alpha Cluster Nodes Used in SDI Calculations

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

Determining the impact of additional SDI excavation on spallings and DBRs as compared to the PABC-2009 is the primary focus of the SDI impact assessment. Quantifying these impacts requires an execution of the Salado flow, spallings, DBR, and CCDFGF PA code chains. The necessary suite of codes that were executed in the SDI impact assessment is listed in Table 8, and has been qualified under Nuclear Waste Management Procedure NP 19-1: Software Requirements (Chavez 2006).

Table 8: WIPP PA VMS Software Used in the SDI Calculations

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
POSTLHS	4.07A	POSTLHS_QA0407A.EXE	25-04-05	LIBLHS	QA0407A
MATSET	9.10	MATSET_QA0910.EXE	29-11-01	LIBMS	QA0910
RELATE	1.43	RELATE_PA96.EXE	06-03-96	LIBREL	PA96
SUMMARIZE	3.01	SUMMARIZE_QB0301.EXE	21-12-05	LIBSUM	QB0301

Discussion of run control is limited to the execution of codes done for the SDI impact assessment. Discussion of run control for PABC-2009 results used in the SDI calculation can be found in Long (2010).

A.1 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 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 9.

Table 9: Salado Flow Run Control Scripts

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

A.1.1 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 10.

Table 10: Salado Flow Step 1 Input and Output Files

	File Names	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_BF_SDI_STEP1.INP	LIBSDI_EVAL	SDI-0
Log	EVAL_BF_SDI_STEP1.LOG	LIBSDI_BF	SDI-0
GENMESH			
Input	GM_BF_SDI.INP	LIBSDI_BF	SDI-0
Output	GM_BF_SDI.CDB	LIBSDI_BF	SDI-0
Output	GM_BF_SDI.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_BF_SDI.INP	LIBSDI_BF	SDI-0
Input	GM_BF_SDI.CDB	LIBSDI_BF	SDI-0
Output	MS_BF_SDI.CDB	LIBSDI_BF	SDI-0
Output	MS_BF_SDI.DBG	NOT KEPT	NOT KEPT

A.1.2 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 11.

Table 11: Salado Flow Step 2 Input and Output Files

	File Names[1,2]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_BF_SDI_STEP2_R*r*.INP	LIBSDI_EVAL	SDI-0
Log	EVAL_BF_SDI_STEP2_R*r*.LOG	LIBSDI_BF	SDI-0
POSTLHS			
Input	LHS3_DUMMY.INP	LIBPABC09_LHS	SDI-0
Input	LHS2_PABC09_R*r*_CON.TRN	LIBPABC09_LHS	SDI-0
Input	MS_BF_SDI.CDB	LIBSDI_BF	SDI-0
Output	LHS3_BF_SDI_R*r*_V*vvv*.CDB	LIBSDI_BF	SDI-0
Output	LHS3_BF_SDI_R*r*.DBG	LIBSDI_BF	SDI-0

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

A.1.3 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 12.

Table 12: Salado Flow Step 3 Input and Output Files

	File Names[1,2]	**CMS Library**	**CMS Class**
SCRIPT			
Input	EVAL_BF_SDI_STEP3_R*r*.INP	LIBSDI_EVAL	SDI-0
Log	EVAL_BF_SDI_STEP3_R*r*.LOG	LIBSDI_BF	SDI-0
ICSET			
Input	IC_BF_SDI.INP	LIBSDI_BF	SDI-0
Input	LHS3_BF_SDI_R*r*_V*vvv*.CDB	LIBSDI_BF	SDI-0
Output	IC_BF_SDI_R*r*_V*vvv*.CDB	LIBSDI_BF	SDI-0
Output	IC_BF_SDI_R*r*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG1_BF_SDI.INP	LIBSDI_BF	SDI-0
Input	IC_BF_SDI_R*r*_V*vvv*.CDB	LIBSDI_BF	SDI-0
Output	ALG1_BF_SDI_R*r*_V*vvv*.CDB	LIBSDI_BF	SDI-0
Output	ALG1_BF_SDI_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.1.4 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 13.

Table 13: Salado Flow Step 4 Input and Output Files

	File Names[1,2,3]	CMS Library[1,2]	CMS Class
SCRIPT			
Script Input	EVAL_BF_SDI_STEP4_R*r*_S*s*.INP	LIBSDI_EVAL	SDI-0
Script Log	EVAL_BF_SDI_STEP4_R*r*_S*s*.LOG	LIBSDI_BFR*r*S*s*	SDI-0
PREBRAG			
Input	BF1_SDI_S*s*.INP	LIBSDI_BF	SDI-0
Input	ALG1_BF_SDI_R*r*_V*vvv*.CDB	LIBSDI_BF	SDI-0
Output	BF2_SDI_R*r*_S*s*_V*vvv*.INP	LIBSDI_BFR*r*S*s*	SDI-0
Output	BF1_SDI_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.1.5 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 lack of or unreasonably slow convergence.

A.1.5.1 General Case

Two DCL run control scripts are used in Step 5. The master script is invoked once for each replicate/scenario combination. The master script loops over all 100 vectors in the replicate/scenario combination. For each vector, the master script writes an input file for the slave script, and then calls the slave script with that input file to run BRAGFLO, POSTBRAG, and ALGEBRACDB. The input and log files for the Step 5 script as well as the input and output files for BRAGFLO, POSTBRAG, and ALGEBRACDB are shown in Table 14.

Table 14: Salado Flow Step 5 Input and Output Files (Generic Case)

	File Names[1,2,3,4]	CMS Library[1,2,5]	CMS Class
MASTER SCRIPT			
Input	EVAL_BF_SDI_STEP5_R*r*_S*s*.INP	LIBSDI_EVAL	SDI-0
Log	EVAL_BF_SDI_STEP5_R*r*_S*s*.LOG	LIBSDI_BFR*r*S*s*	SDI-0
SLAVE SCRIPT			
Log[4]	EVAL_BF_SDI_STEP5_R*r*_S*s*_V*vvv*.LOG	LIBSDI_BFR*r*S*s*	SDI-0
BRAGFLO			
Input	BF2_SDI_R*r*_S*s*_V*vvv*.INP	LIBSDI_BFR*r*S*s*	SDI-0
Input	BF2_SDI_CLOSURE.DAT	LIBSDI_BF	SDI-0
Output	BF2_SDI_R*r*_S*s*_V*vvv*.OUT	NOT KEPT	NOT KEPT
Output	BF2_SDI_R*r*_S*s*_V*vvv*.SUM[5]	LIBSDI_BF	SDI-0
Output	BF2_SDI_R*r*_S*s*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Output	BF2_SDI_R*r*_S*s*_V*vvv*.ROT	NOT KEPT	NOT KEPT
Output	BF2_SDI_R*r*_S*s*_V*vvv*.RIN	NOT KEPT	NOT KEPT
POSTBRAG			
Input	BF2_SDI_R*r*_S*s*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Input	ALG1_BF_SDI_R*r*_V*vvv*.CDB	LIBSDI_BF	SDI-0
Output	BF3_SDI_R*r*_S*s*_V*vvv*.CDB	LIBSDI_BFR*r*S*s*	SDI-0
Output	BF3_SDI_R*r*_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG2_BF_SDI.INP	LIBSDI_BF	SDI-0
Input	BF3_SDI_R*r*_S*s*_V*vvv*.CDB	LIBSDI_BFR*r*S*s*	SDI-0
Output	ALG2_BF_SDI_R*r*_S*s*_V*vvv*.CDB	LIBSDI_BFR*r*S*s*	SDI-0
Output	ALG2_BF_SDI_R*r*_S*s*_V*vvv*.DBG	NOT KEPT	NOT KEPT

1. $r \in \{1, 2, 3\}$
2. $s \in \{1, 2, 3, 4, 5, 6\}$ for each r
3. $vvv \in \{001, 002, ..., 100\}$ for each s
4. The script inputs are echoed into the log file, so the input file is not kept
5. Due to an error in the master script input file, the *.SUM output files were placed in CMS library LIBSDI_BF instead of the library for the replicate/scenario combination. Note that output files for simulations reported in Table 15 (modified input runs) were archived in the correct libraries (LIBSDI_BFR*r*S*s*).

A.1.5.2 Modified BRAGFLO Input Case

In the few instances when BRAGFLO failed to converge using the generic numerical control parameters, a new BRAGFLO input file was submitted by the analysts and the case was re-run in a manner similar to that described above in Section A.1.5.1 In order to track these cases a special tag ("MOD") was inserted into the BRAGFLO input file name, as well as the master script input file and log file names.

The replicate/scenario/vectors requiring modified BRAGFLO input files are shown in Table 15. For all vectors listed in that table, simulation control parameter FTOL_SAT was increased from the default value of 1e-2 to a value of 1e-1. With that modification, vectors listed in Table 15 were successfully run to the final time of 10,000 years. The modified file names are shown in Table 16. 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 15: Salado Flow Step 5 Modified Input Runs

Replicate	Scenario	Vectors
R1	S1	29
R2	S1	99
	S4	95, 99
	S5	99
R3	S3	35

Table 16: 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_SDI_STEP5_R*r*_S*s*_V*vvv*_MOD.INP	LIBSDI_EVAL	SDI-0
Log	EVAL_BF_SDI_STEP5_R*r*_S*s*_V*vvv*_MOD.LOG	LIBSDI_BFR*r*S*s*	SDI-0
BRAGFLO			
Input	BF2_SDI_R*r*_S*s*_V*vvv*_MOD.INP	LIBSDI_BFR*r*S*s*	SDI-0

1. $r \in \{1, 2, 3\}$ as shown in Table 15
2. $s \in \{1, 2, 3, 4, 5, 6\}$ as shown in Table 15
3. vectors as shown in Table 15

A.2 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 17. Step 3 also includes a small utility used to submit the script to a batch queue.

Table 17: 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	LIBSDI_EVAL	SDI-0
2	POSTLHS	EVAL_CUSP_STEP2.COM	LIBSDI_EVAL	SDI-0
3	CUTTINGS_S	EVAL_CUSP_STEP3.COM SUB_CUSP_STEP3.COM	LIBSDI_EVAL	SDI-0

A.2.1 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 18.

Table 18: Solids Volume Step 1 Input and Output Files

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_CUSP_SDI_STEP1.INP	LIBSDI_EVAL	SDI-0
Log	EVAL_CUSP_SDI_STEP1.LOG	LIBSDI_CUSP	SDI-0
GENMESH			
Input	GM_CUSP_SDI.INP	LIBSDI_CUSP	SDI-0
Output	GM_CUSP_SDI.CDB	LIBSDI_CUSP	SDI-0
Output	GM_CUSP_SDI.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_CUSP_SDI.INP	LIBSDI_CUSP	SDI-0
Input	GM_CUSP_SDI.CDB	LIBSDI_CUSP	SDI-0
Output	MS_CUSP_SDI.CDB	LIBSDI_CUSP	SDI-0
Output	MS_CUSP_SDI.DBG	NOT KEPT	NOT KEPT

A.2.2 Solids Volume Step 2

Step 2 uses POSTLHS to assign the sampled parameter values used by CUTTINGS_S (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 script as well as the input and output files for POSTLHS are shown in Table 19.

Table 19: Solids Volume Step 2 Input and Output Files

	File Names[1,2]	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CUSP_SDI_STEP2_R*r*.INP	LIBSDI_EVAL	SDI-0
Script Log	EVAL_CUSP_SDI_STEP2_R*r*.LOG	LIBSDI_CUSP	SDI-0
POSTLHS			
Input	LHS3_DUMMY.INP	LIBPABC09_LHS	SDI-0
Input	LHS2_PABC09_R*r*_CON.TRN	LIBPABC09_LHS	SDI-0
Input	MS_CUSP_SDI.CDB	LIBSDI_CUSP	SDI-0
Output	LHS3_CUSP_SDI_R*r*_V*vvv*.CDB	LIBSDI_CUSP	SDI-0
Output	LHS3_CUSP_SDI_R*r*.DBG	LIBSDI_CUSP	SDI-0

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

A.2.3 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 20.

Table 20: 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_SDI_STEP3_R*r*.INP	LIBSDI_EVAL	SDI-0
Output	CUSP_SDI_MASTER_R*r*.INP	LIBSDI_CUSP	SDI-0
Log	EVAL_CUSP_SDI_STEP3_R*r*.LOG	LIBSDI_CUSP	SDI-0
CUTTINGS_S			
Input	CUSP_SDI_MASTER_R*r*.INP	LIBSDI_CUSP	SDI-0
Input	CUSP_SDI.INP	LIBSDI_CUSP	SDI-0
Input	LHS3_CUSP_SDI_R*r*_V*vvv*.CDB	LIBSDI_CUSP	SDI-0
Input	BF3_SDI_R*r*_S*s*_V*vvv*.CDB	LIBSDI_BFR*r*S*s*	SDI-0
Input	MSPALL_DRS_CRA1BC_R*r*.OUT	LIBCRA1BC_DRS	SDI-0
Output	CUSP_SDI_R*r*.TBL	LIBSDI_CUSP	SDI-0
Output	CUSP_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBSDI_CUSPR*r*S*s*	SDI-0
Output	CUSP_SDI_R*r*.DBG	LIBSDI_CUSP	SDI-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.3 Single-Intrusion Direct Brine Release Calculations (BRAGFLO)

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 21.

Table 21: 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	LIBSDI_EVAL	SDI-0
2	ALGEBRACDB RELATE ICSET	EVAL_DBR_STEP2.COM SUB_DBR_STEP2.COM	LIBSDI_EVAL	SDI-0
3	PREBRAG BRAGFLO POSTBRAG ALGEBRACDB	EVAL_DBR_STEP3.COM SUB_DBR_STEP3.COM	LIBSDI_EVAL	SDI-0

A.3.1 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 22.

Table 22: Direct Brine Release Step 1 Input and Output Files

	File Names	CMS Library	CMS Class
SCRIPT			
Input	EVAL_DBR_SDI_STEP1.INP	LIBSDI_EVAL	SDI-0
Log	EVAL_DBR_SDI_STEP1.LOG	LIBSDI_DBR	SDI-0
GENMESH			
Input	GM_DBR_SDI.INP	LIBSDI_DBR	SDI-0
Output	GM_DBR_SDI.CDB	LIBSDI_DBR	SDI-0
Output	GM_DBR_SDI.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_DBR_SDI.INP	LIBSDI_DBR	SDI-0
Input	GM_DBR_SDI.CDB	LIBSDI_DBR	SDI-0
Output	MS_DBR_SDI.CDB	LIBSDI_DBR	SDI-0
Output	MS_DBR_SDI.DBG	NOT KEPT	NOT KEPT

A.3.2 Direct Brine Release Step 2

Step 2 performs pre-processing of input data with ALGEBRACDB (because ALGEBRACDB is used in multiple steps, this use is referred to as ALG1). The RELATE code is used to assign material properties to element blocks. RELATE is run twice (RELATE_1 and RELATE_2). Finally, ICSET is used to assign initial conditions. The Step 2 script is run for each replicate/scenario combination. The script loops over the appropriate intrusion times for the scenario. For each intrusion time, the script loops over all 100 vectors. The input and log files for the Step 2 script as well as the input and output files for ALGEBRACDB, RELATE, and ICSET are shown in Table 23.

Table 23: 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_SDI_STEP2_Rr_Ss.INP	LIBSDI_EVAL	SDI-0
Log	EVAL_DBR_SDI_STEP2_Rr_Ss.LOG	LIBSDI_DBRRrSs	SDI-0
ALGEBRACDB			
Input	ALG1_DBR_SDI.INP	LIBSDI_DBR	SDI-0
Input	CUSP_SDI_Rr_Ss_Tttttt_L_Vvvv.CDB[5]	LIBSDI_CUSPRrSs	SDI-0
Output	ALG1_DBR_SDI_Rr_Ss_Tttttt_Vvvv.CDB	LIBSDI_DBRRrSs	SDI-0
Output	ALG1_DBR_SDI_Rr_Ss_Tttttt_Vvvv.DBG	NOT KEPT	NOT KEPT
RELATE_1			
Input	REL1_DBR_SDI.INP	LIBSDI_DBR	SDI-0
Input	MS_DBR_SDI.CDB	LIBSDI_DBR	SDI-0
Input	ALG1_DBR_SDI_Rr_Ss_Tttttt_Vvvv.CDB	LIBSDI_DBRRrSs	SDI-0
Output	REL1_DBR_SDI_Rr_Ss_Tttttt_Vvvv.CDB	LIBSDI_DBRRrSs	SDI-0
Output	REL1_DBR_SDI_Rr_Ss_Tttttt_Vvvv.DBG	NOT KEPT	NOT KEPT
RELATE_2			
Input	REL2_DBR_SDI_Ss.INP	LIBSDI_DBR	SDI-0
Input	REL1_DBR_SDI_Rr_Ss_Tttttt_Vvvv.CDB	LIBSDI_DBRRrSs	SDI-0
Input	BF3_SDI_Rr_Ss_Vvvv.CDB	LIBSDI_BFRrSs	SDI-0
Output	REL2_DBR_SDI_Rr_Ss_Tttttt_Vvvv.CDB	LIBSDI_DBRRrSs	SDI-0
Output	REL2_DBR_SDI_Rr_Ss_Tttttt_Vvvv.DBG	NOT KEPT	NOT KEPT
ICSET			
Input	IC_DBR_SDI_Ss.INP	LIBSDI_DBR	SDI-0
Input	REL2_DBR_SDI_Rr_Ss_Tttttt_Vvvv.CDB	LIBSDI_DBRRrSs	SDI-0
Output	IC_DBR_SDI_Rr_Ss_Tttttt_Vvvv.CDB	LIBSDI_DBRRrSs	SDI-0
Output	IC_DBR_SDI_Rr_Ss_Tttttt_Vvvv.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG2_DBR_SDI_Ss.INP	LIBSDI_DBR	SDI-0
Input	IC_DBR_SDI_Rr_Ss_Tttttt_Vvvv.CDB	LIBSDI_DBRRrSs	SDI-0
Output	ALG2_DBR_SDI_Rr_Ss_Tttttt_Vvvv.CDB	LIBSDI_DBRRrSs	SDI-0
Output	ALG2_DBR_SDI_Rr_Ss_Tttttt_Vvvv.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_SDI_Rr_Ss_Tttttt_L_Vvvv.CDB do not have leading zeros in front of the intrusion time *ttttt*.

A.3.3 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 24.

Table 24: Direct Brine Release Step 3 Input and Output Files

	File Names[1,2,3,4,5]	**CMS Library**[1,2]	**CMS Class**
SCRIPT			
Input	EVAL_DBR_SDI_STEP3_R*r*_S*s*.INP	LIBSDI_EVAL	SDI-0
Log	EVAL_DBR_SDI_STEP3_R*r*_S*s*.LOG	LIBSDI_DBRR*r*S*s*	SDI-0
PREBRAG			
Input	BF1_DBR_SDI_*c*.INP	LIBSDI_DBR	SDI-0
Input	ALG2_DBR_SDI_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBSDI_DBRR*r*S*s*	SDI-0
Output	BF2_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.INP	LIBSDI_DBRR*r*S*s*	SDI-0
Output	BF1_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.DBG	NOT KEPT	NOT KEPT
BRAGFLO			
Input	BF2_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.INP	LIBSDI_DBRR*r*S*s*	SDI-0
Output	BF2_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.OUT	NOT KEPT	NOT KEPT
Output	BF2_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.SUM	NOT KEPT	NOT KEPT
Output	BF2_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Output	BF2_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.ROT	NOT KEPT	NOT KEPT
Output	BF2_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.RIN	NOT KEPT	NOT KEPT
POSTBRAG			
Input	ALG2_DBR_SDI_R*r*_S*s*_T*ttttt*_V*vvv*.CDB	LIBSDI_DBRR*r*S*s*	SDI-0
Input	BF2_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.BIN	NOT KEPT	NOT KEPT
Output	BF3_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBSDI_DBRR*r*S*s*	SDI-0
Output	BF3_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.DBG	NOT KEPT	NOT KEPT
ALGEBRACDB			
Input	ALG3_DBR_SDI.INP	LIBSDI_DBR	SDI-0
Input	BF3_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBSDI_DBRR*r*S*s*	SDI-0
Output	ALG3_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBSDI_DBRR*r*S*s*	SDI-0
Output	ALG3_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.DBG	NOT KEPT	NOT KEPT

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

A.4 CCDF Input Tabulations (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 run control scripts used to process the CDB data for the various process models are shown in Table 25. 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 25: CCDF Input Tabulation Run Control Scripts

Code	Script	Script CMS Library	Script CMS Class
SUMMARIZE	EVAL_SUM.COM SUB_SUM.COM	LIBSDI_EVAL	SDI-0

A.4.1 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 (see Section A.3). 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 26.

Table 26: 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_SDI_R*r*_S*s*.INP	LIBSDI_EVAL	SDI-0
Input	SUM_DBR_SDI.TMPL	LIBSDI_SUM	SDI-0
Output	SUM_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*.INP	LIBSDI_SUM	SDI-0
Log	EVAL_SUM_DBR_SDI_R*r*_S*s*.LOG	LIBSDI_SUM	SDI-0
SUMMARIZE			
Input	SUM_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*.INP	LIBSDI_SUM	SDI-0
Input	ALG3_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*_V*vvv*.CDB	LIBSDI_DBRR*r*S*s*	SDI-0
Output	SUM_DBR_SDI_R*r*_S*s*_Tttttt_*c*.TBL	LIBSDI_SUM	SDI-0
Output	SUM_DBR_SDI_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. $c \in \{L, M, U\}$ for each intrusion time
5. $vvv \in \{001, 002, ..., 100\}$ for each c

A.5 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 27.

Table 27: CCDF Construction Run Control Scripts

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

A.5.1 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 28.

Table 28: CCDF Construction Step 1 Input and Output Files

	File Names	CMS Library	CMS Class
SCRIPT			
Script Input	EVAL_CCGF_SDI_STEP1.INP	LIBSDI_EVAL	SDI-0
Script Log	EVAL_CCGF_SDI_STEP1.LOG	LIBSDI_CCGF	SDI-0
GENMESH			
Input	GM_CCGF_SDI.INP	LIBSDI_CCGF	SDI-0
Output	GM_CCGF_SDI.CDB	LIBSDI_CCGF	SDI-0
Output	GM_CCGF_SDI.DBG	NOT KEPT	NOT KEPT
MATSET			
Input	MS_CCGF_SDI.INP	LIBSDI_CCGF	SDI-0
Input	GM_CCGF_SDI.CDB	LIBSDI_CCGF	SDI-0
Output	MS_CCGF_SDI.CDB	LIBSDI_CCGF	SDI-0
Output	MS_CCGF_SDI.DBG	NOT KEPT	NOT KEPT

A.5.2 CCDF Construction Step 2

Step 2 uses POSTLHS to assign the sampled parameter values used by CCDFGF (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 script as well as the input and output files for POSTLHS are shown in Table 29.

Table 29: CCDF Construction Step 2 Input and Output Files

	File Names[1,2]	**CMS Library**	**CMS Class**
STEP 2			
Script Input	EVAL_CCGF_SDI_STEP2_R*r*.INP	LIBSDI_EVAL	SDI-0
Script Log	EVAL_CCGF_SDI_STEP2_R*r*.LOG	LIBSDI_CCGF	SDI-0
POSTLHS			
Input	LHS3_DUMMY.INP	LIBPABC09_LHS	SDI-0
Input	LHS2_PABC09_R*r*_CON.TRN	LIBPABC09_LHS	SDI-0
Input	MS_CCGF_SDI.CDB	LIBSDI_CCGF	SDI-0
Output	LHS3_CCGF_SDI_R*r*_V*vvv*.CDB	LIBSDI_CCGF	SDI-0
Output	LHS3_CCGF_SDI_R*r*.DBG	LIBSDI_CCGF	SDI-0

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

A.5.3 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 30.

Table 30: CCDF Construction Step 3 Input and Output Files

	File Names[1-7]	**CMS Library**	**CMS Class**
SCRIPT			
Script Input	EVAL_CCGF_STEP3_SDI_R*r*.INP	LIBSDI_EVAL	SDI-0
Script Log	EVAL_CCGF_STEP3_SDI_R*r*.LOG	LIBSDI_CCGF	SDI-0
PRECCDFGF			
Input	INTRUSIONTIMES.IN	LIBPABC09_CCGF	SDI-0
Input	MS_CCGF_SDI.CDB	LIBSDI_CCGF	SDI-0
Input	LHS3_CCGF_SDI_R*r*_V*vvv*.CDB	LIBSDI_CCGF	SDI-0
Input	SUM_DBR_SDI_R*r*_S*s*_T*ttttt*_*c*.TBL	LIBSDI_SUM	SDI-0
Input	CUSP_SDI_R*r*.TBL	LIBSDI_CUSP	SDI-0
Input	SUM_NUT_PABC09_R*r*_S1.TBL	LIBPABC09_SUM	SDI-0
Input	SUM_NUT_PABC09_R*r*_S*s*_T*ttttt*.TBL	LIBPABC09_SUM	SDI-0
Input	SUM_PANEL_INT_PABC09_R*r*_S6_T*ttttt*.TBL	LIBPABC09_SUM	SDI-0
Input	SUM_ST2D_PABC09_R*r*_M*m*.TBL	LIBPABC09_SUM	SDI-0
Input	EPU_PABC09_*h*H.DAT	LIBPABC09_EPU	SDI-0
Input	SUM_PANEL_CON_PABC09_R*r*_S*s*.TBL	LIBPABC09_SUM	SDI-0
Input	SUM_PANEL_ST_PABC09_R*r*_S*s*.TBL	LIBPABC09_SUM	SDI-0
Output	CCGF_SDI_RELTAB_R*r*.DAT	LIBSDI_CCGF	SDI-0
CCDFGF			
Input	CCGF_SDI_CONTROL_R*r*.INP	LIBSDI_CCGF	SDI-0
Input	CCGF_SDI_RELTAB_R*r*.DAT	LIBSDI_CCGF	SDI-0
Output	CCGF_SDI_R*r*.OUT	LIBSDI_CCGF	SDI-0
Output	CCGF_SDI_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. $h \in \{C, R\}$