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Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Package for Direct Brine Releases: Panel Closure Redesign and Repository Reconfiguration Performance Assessment (PC3R PA)

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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.

In addition to its role in certification decisions for the repository, PA is used to determine the impacts of repository modifications proposed by the DOE as part of planned change requests (PCRs). Previous analyses have been performed to assess the impacts of modifications to the panel closure system implemented in the repository (Hansen 2002, Vugrin and Dunagan 2006). The 1998 rulemaking that certified WIPP to receive TRU waste had several conditions, one of which involved the design of the panel closure system. The EPA based its certification decision on the condition that the DOE implement the most robust panel closure design, referred to as the "Option D" design in the CCA (U.S. EPA 1998). 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 recertification of the facility, the DOE plans to submit two PCRs to the EPA that propose changes to the repository. The first PCR is centered on a new design of the WIPP panel closure system. The panel closure "Option D" design considered in the PABC-2009 (Clayton et al. 2010) is to be modified to a configuration consisting of 100 feet run of mine salt backfill emplaced against a substantial barrier. The second PCR proposes the relocation of future waste panels 9 and 10 to the south end of the repository, i.e. south of panels 4 and 5, where they will be denoted as panels 9a and 10a. With panels 9 and 10 relocated, the current repository configuration will be modified to one with an open central drift area with installed panel closures located only at the end of filled waste panels. The DOE has requested that SNL conduct a single PA to determine the overall impact of the repository changes proposed in the two PCRs. Impacts of these changes are determined by way of a comparison of release probabilities to those calculated in the PABC-2009. This analysis package details the analysis of direct brine releases (DBRs) performed in the panel closure redesign and repository reconfiguration performance assessment, henceforth referred to as the PC3R PA.

The work undertaken in the PC3R PA is prescribed in AP-151, *Analysis Plan for the WIPP Panel Closure Redesign and Repository Reconfiguration Performance Assessment* (Camphouse 2010), which was specifically written to determine the impact of changes proposed in the two PCRs on long-term repository performance. In order to isolate the impacts of repository changes, the PC3R PA was designed to deviate as little as possible from the PABC-2009 implementation. In particular, the PC3R PA utilizes the same waste inventory information, drilling rate and plugging pattern parameters, and radionuclide solubility parameters as were used in the PABC-2009. The PC3R PA examines all aspects of repository performance that are potentially impacted by the proposed changes to the repository.

2 BACKGROUND

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

1. Volume averaged pressure in the vicinity of the repository encountered by drilling must exceed drilling fluid hydrostatic pressure (calculated to be 8 MPa).
2. Brine saturation in the repository must exceed the residual saturation of the waste material (Sampled from a uniform distribution ranging from 0.0 to 0.552).

If both of these criteria are met, a DBR is calculated using the multi-phase flow code BRAGFLO with a two dimensional, semi-horizontally oriented grid, which represents the vicinity of the waste panels. If either of these conditions is not satisfied, no DBR is calculated.

DBRs are calculated from the following well deliverability equation in BRAGFLO (Mattax and Dalton 1990):

$$q_p(t) = J_p(P_p(t) - P_{wf}) \tag{1}$$

where $q_p(t)$ is the volumetric brine flux to the well as a function of time, J_p is the well productivity index, $P_p(t)$ is the repository pressure as a function of time, and P_{wf} is the flowing bottom-hole pressure (assumed to be constant during each drilling intrusion). The flowing bottom-hole pressure is defined as the dynamic pressure at the inlet to the wellbore adjacent to the point of entry into the repository. It is less than the static pressure due to elevation, friction and acceleration effects (Stoelzel and O'Brien 1996).

The well productivity index quantifies how readily brine can enter the well and flow to the surface. It is calculated from the following equation (Mattax and Dalton 1990; Chappelear and Williamson 1981):

$$J_p = \frac{2\pi k k_{rp} h}{\mu_p \left[\ln\left(\frac{r_e}{r_w}\right) + s - 0.5 \right]} \tag{2}$$

k Intrinsic permeability of the waste (constant: 2.4 x 10^{-13} m^2, WAS_AREA:PRMX_LOG)

k_{rp} Relative permeability of the waste assuming the modified Brooks-Corey relative permeability model: $k_{rp} = S_{e1}^{(2+3\lambda)/\lambda}$, where λ is the pore distribution parameter (WAS_AREA:PORE_DIS), S_{e1} is the effective brine saturation without correction for residual gas saturation $S_{e1} = (S_b - S_{br})/(1 - S_{br})$, S_b is the brine saturation, and S_{br} is the residual brine saturation (WAS_AREA:SAT_RBRN)

- h Crushed panel height $h = h_i(1 - \phi_i) / (1 - \phi)$, where h_i is initial panel height (3.96 m), ϕ_i is the initial room-scale porosity (0.848, WAS_AREA:POROSITY)), and ϕ is the room-scale porosity at the time of intrusion (calculated by BRAGFLO see Helton et al. 1998)
- μ Brine viscosity (0.0021 Pa-s, BRINESAL:VISCO)
- r_e External drainage radius of the grid block containing the well ($r_e = \sqrt{(\Delta x)(\Delta y)/\pi}$) where Δx and Δy are the grid cell dimensions of the grid cell containing the well.
- r_w Well radius (0.1556 m, assuming a 12.25 in. drill bit diameter, BOREHOLE:DIAMMOD divided by two)
- s Skin factor (enhanced well productivity due to the presence of a cavity at base of well)

The skin factor is calculated (Lee 1982):

$$s = \left(\frac{k}{k_s} - 1\right)\ln\left(\frac{r_s}{r_w}\right) \tag{3}$$

where k_s is the permeability of an open channel as a result of cuttings, cavings and spallings releases (assumed to be infinite) and r_s is the effective radius of the well bore with the cuttings, cavings and spallings volume (V_i) removed.

The effective radius r_s is obtained by converting the cuttings, cavings and spallings volume removed into a cylinder of equal volume with the initial height of the waste (h_i), and then computing the radius of the cylinder:

$$r_s = \sqrt{\frac{V_i}{h_i \pi}} \tag{4}$$

In general, k_s is assumed to be infinite, and Equation (3) can be simplified to:

$$s = \ln\left(\frac{r_w}{r_s}\right) \tag{5}$$

DBRs are calculated using the code BRAGFLO and a two-dimensional semi-horizontal grid that dips 1° to the south. Five scenarios were simulated and are discussed in section 4.1.

3 APPROACH

The conceptual models implemented in the PC3R PA calculations are unchanged from those used in the PABC-2009. However, several changes were included in the DBR calculations for the PC3R PA. These are discussed below.

3.1 Model Geometry

A schematic that depicts the WIPP spatial layout as it has been modeled in the 2009-PABC is shown in Figure 3-1. As seen in that figure, the waste disposal region consists of 10 waste panels. Panels 1-4 are located east of the central area with panels 5-8 located to the west. Panels 9 and 10 are located in the center area between panels 1-4 and panels 5-8. Additionally, panel closures are located at the innermost ends of panels 1-8. A set of panel closures is located between waste panels 9 and 10. Another set of closures is located between panels 1-10 and the southern end of the operations region. A final set of closures is located in the operations region south of the repository shafts. These locations of waste panels and panel closures have been implemented in the models used in performance assessments since the original CCA, including the PABC-2009. The repository configuration shown in Figure 3-1 was used to guide the development of the numerical grid used to analyze DBRs in the PABC-2009 (Clayton 2010). The PABC-2009 numerical grid used to investigate DBRs is shown in Figure 3-2.

The changes proposed to the repository configuration that are modeled in the PC3R PA are aimed at relocating panels 9 and 10, eliminating panel closures in the central area, and redesigning the panel closures that remain. Panels 9 and 10 will be moved south of panels 4 and 5 in the PC3R PA and denoted as panels 9a and 10a. In effect, the waste area is lengthened with duplicate copies of panels 4 and 5, and their corresponding panel closures, being located at the southernmost end of the repository. The resulting waste panel configuration will consist of panels 1-4, and 9a east of the central area and panels 10a, and 5-8 west of the center. Panels 1-8, 9a, and 10a will be modeled as having identical panel closures located at their innermost ends.

With the relocation of panels 9 and 10 to the southernmost end of the repository, panel closures located in the central area are proposed to be removed. Consequently, the set of panel closures located between current panels 9 and 10, between the waste disposal region and the operations area, and between the southern portion of the operations area and the repository shafts will be eliminated in the PC3R PA. With the panel closures in the center area removed, the central area in the PC3R PA will be modeled as a continuous open region and prescribed properties corresponding to material OPS_AREA in the PABC-2009. Finally, the PA representation of panel closures that remain for panels 1-8, 9a, and 10a will be modified. "Option D" panel closures were modeled in the PABC-2009, and are represented in Figure 3-1 by black segments at the ends of waste panels and at appropriate locations in the central drift area. Panel closures in the PC3R PA will be modeled to represent the new design that consists of a substantial barrier next to the waste drums, with 100 feet of run of mine salt on the other side of this bulkhead. As the impact of the substantial barrier on the long-term performance of the repository is minimal, PC3R panel closures will be modeled as consisting solely of 100 feet of run of mine salt. The reconfigured repository modeled in the PC3R PA is shown in Figure 3-3 (Camphouse 2010), where redesigned closures are depicted by oval segments at the innermost ends of waste panels.

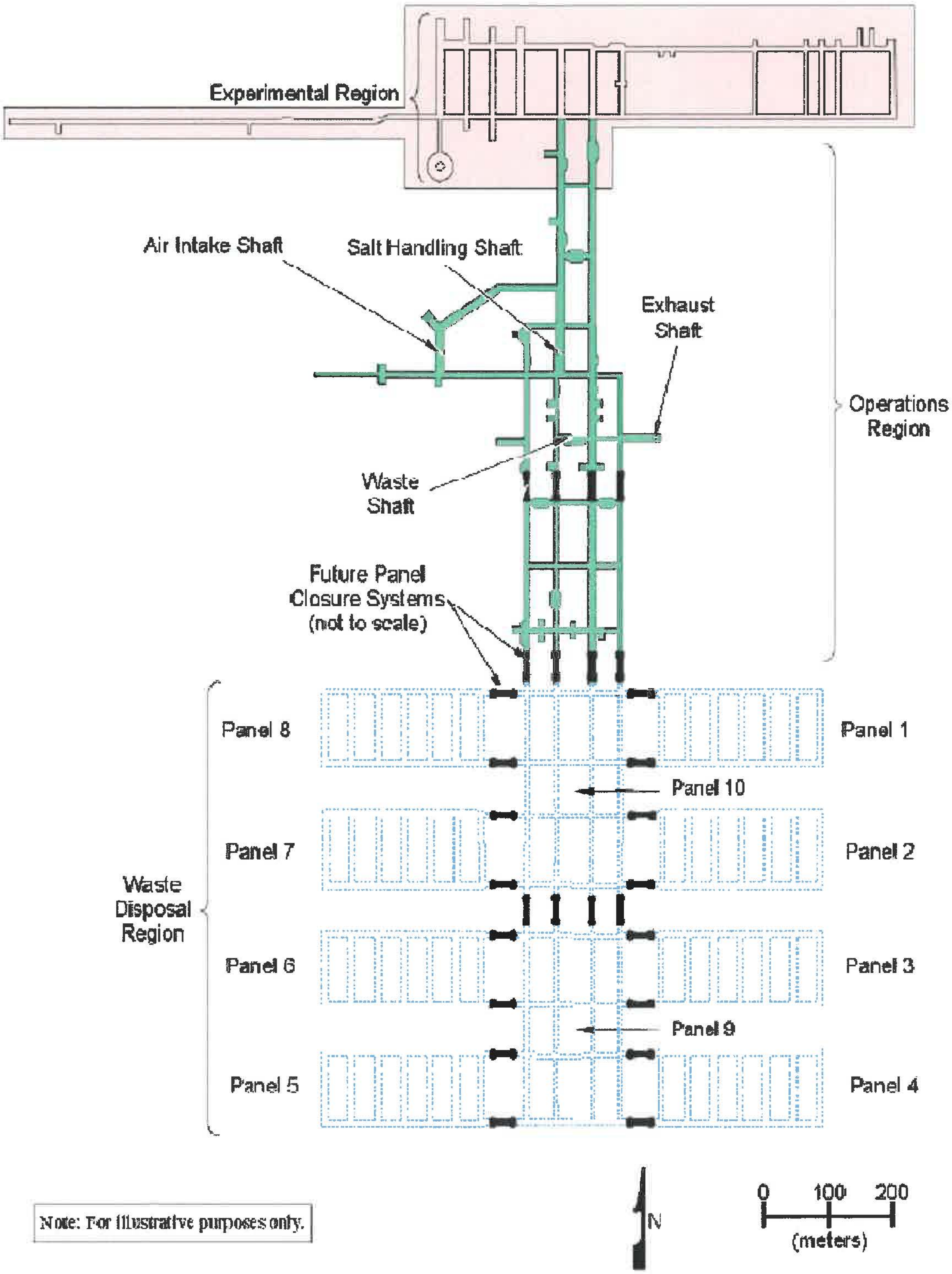
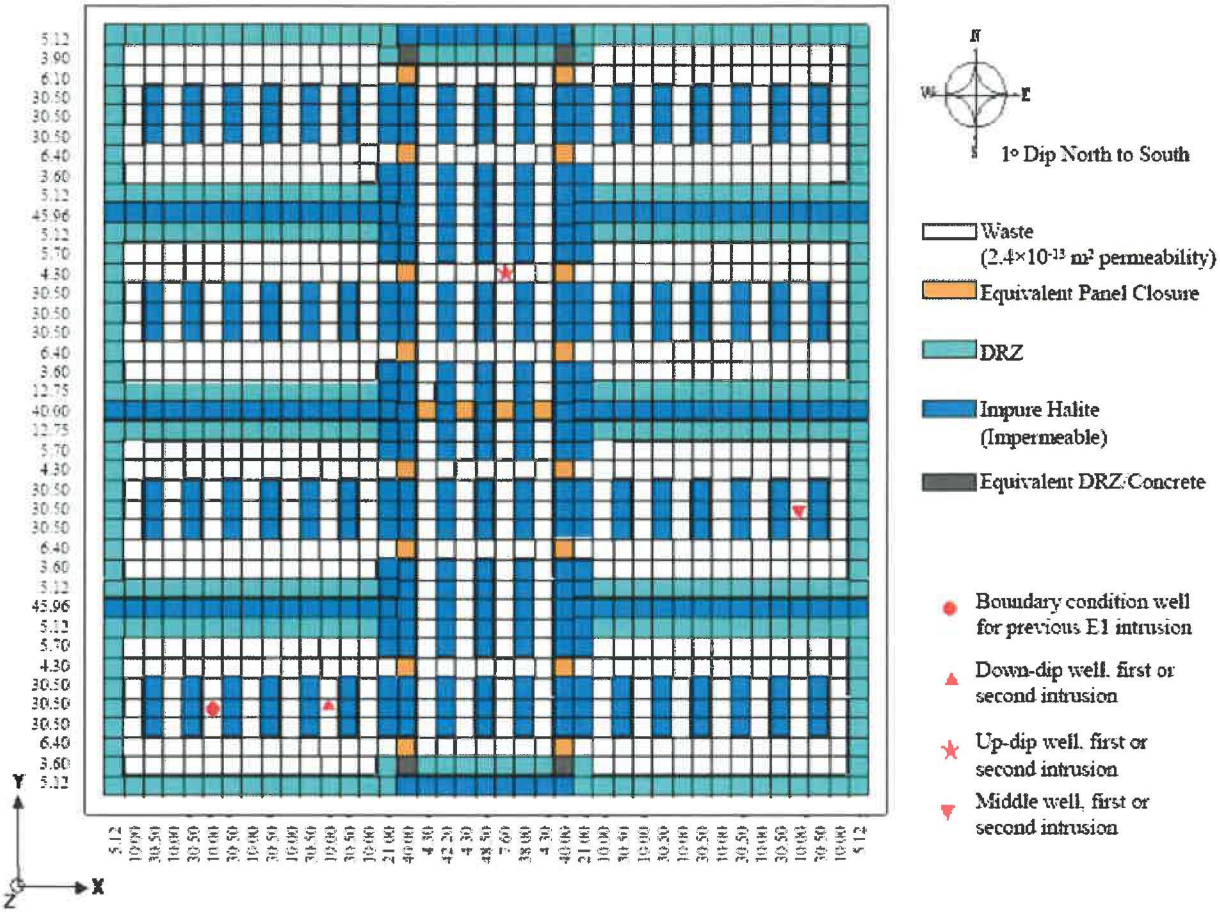


Figure 3-1: Historical WIPP Repository Layout



Note: Model cells are not to scale. The actual dimensions of the grid blocks are indicated along the edge of the diagram.

Figure 3-2: PABC-2009 DBR material map (logical grid).

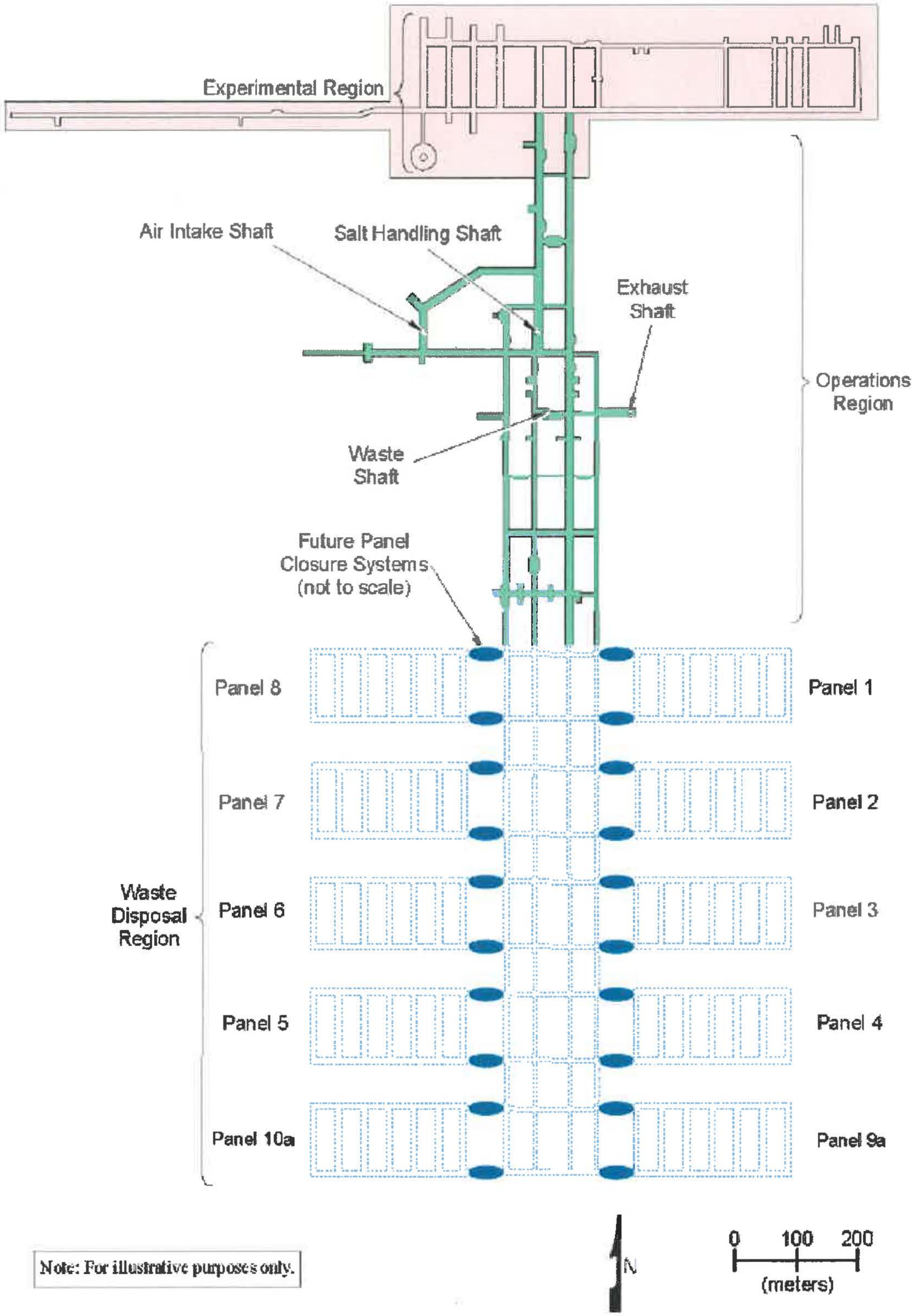


Figure 3-3: WIPP Layout Modeled in PC3R PA

The reconfigured repository seen in Figure 3-3 resulted in several changes to the numerical grid used to analyze direct brine releases. First, waste panels 9 and 10 were removed from the central drift area, relocated to the southernmost end of the repository, and denoted as panels 9a and 10a. As panels 9 and 10 have slightly less area than waste panels 1-8, panels 9a and 10a were resized to have areas equal to those of panels 1-8. Element lengths in the x-direction were kept identical to those specified in the PABC-2009 with the exception of cells corresponding to panel closures. The 100 foot salt backfill panel closures implemented in the PC3R PA resulted in a reduction in x-lengths from 40.0 meters to 30.48 meters for cells representing panel closures. In addition, cells assigned equivalent DRZ/concrete material properties due to the implementation of "Option D" panel closures were given Salado Halite properties in the PC3R PA to capture the properties of the 100 foot run of salt. Element lengths in the y-direction were similar to those used in the PABC-2009. Inspection of detailed WIPP underground maps (see Appendix A – WIPP Dimension Map) revealed that waste panel dimensions are very consistent in the y-direction for all panels. Thus, an effort was made to make element sizes more consistent across waste panels in the PC3R PA. This resulted in some of the cell lengths in the y-direction being slightly modified in the PC3R PA so that common cell lengths could be used to construct all waste panels.

In the PABC-2009, the repository was represented in a south-to-north fashion and decomposed into three regions in the BRAGFLO Salado flow modeling undertaken in that analysis. The three repository regions, namely the intruded waste panel, south rest of repository (SROR), and north rest of repository (NROR) resulted in the consideration of three drilling locations in the PABC-2009 DBR analysis. These locations can be seen in the PABC-2009 DBR computational grid of Figure 3-2. In the PC3R PA, the open central drift area between west and east waste panels results in a west-to-east orientation of the BRAGFLO grid used for Salado flow modeling. This orientation results in only two repository regions, namely the intruded waste panel and the rest of repository (ROR) (Camphouse and Clayton 2011). As a result, two drilling locations, an upper and a lower location, are implemented in the direct brine release analysis undertaken in the PC3R PA. Lower intrusions are located in panel 10a and are analogous to the panel 5 location specified in the PABC-2009. The upper location in the PABC-2009 was located in panel 10 which corresponds to the open central drift area in the PC3R PA. Therefore, the upper drilling location was moved to panel 1 in the center of room 5 in the PC3R PA. These changes result in the PC3R PA DBR numerical grid shown in Figure 3-4. With these drilling locations, the model is run for a maximum of 4.5 days and the total volume of brine that reached the well connected to the surface is used to calculate the DBR.

In the computational grid implemented in the PC3R PA Salado flow analysis, the open central region contains the open volume between west and east waste panels as well as the volumes associated with the operations and experimental regions. To achieve agreement between the three-dimensional representation of the central region in BRAGFLO and the two-dimensional representation of this region in the DBR numerical grid, a new parameter, OPS_AREA:EHEIGHT, was established for use in the PC3R PA DBR calculations. The open central drift area is assigned properties corresponding to the material OPS_AREA in the PABC-2009. Property EHEIGHT, the effective height of a given material, is calculated as the ratio of material volume implemented in the BRAGFLO computational grid to the material area prescribed in the numerical grid for DBRs. This property provides a means of matching porosity and pore compressibility across the BRAGFLO and DBR calculations for a given material. The value assigned to parameter OPS_AREA:EHEIGHT in the PC3R PA is 10.7 meters (Camphouse, 2011). The three-dimensional nature of the repository layout introduced by the 1° dip is captured in the two-dimensional DBR numerical representation by calculating the elevation of each grid cell.

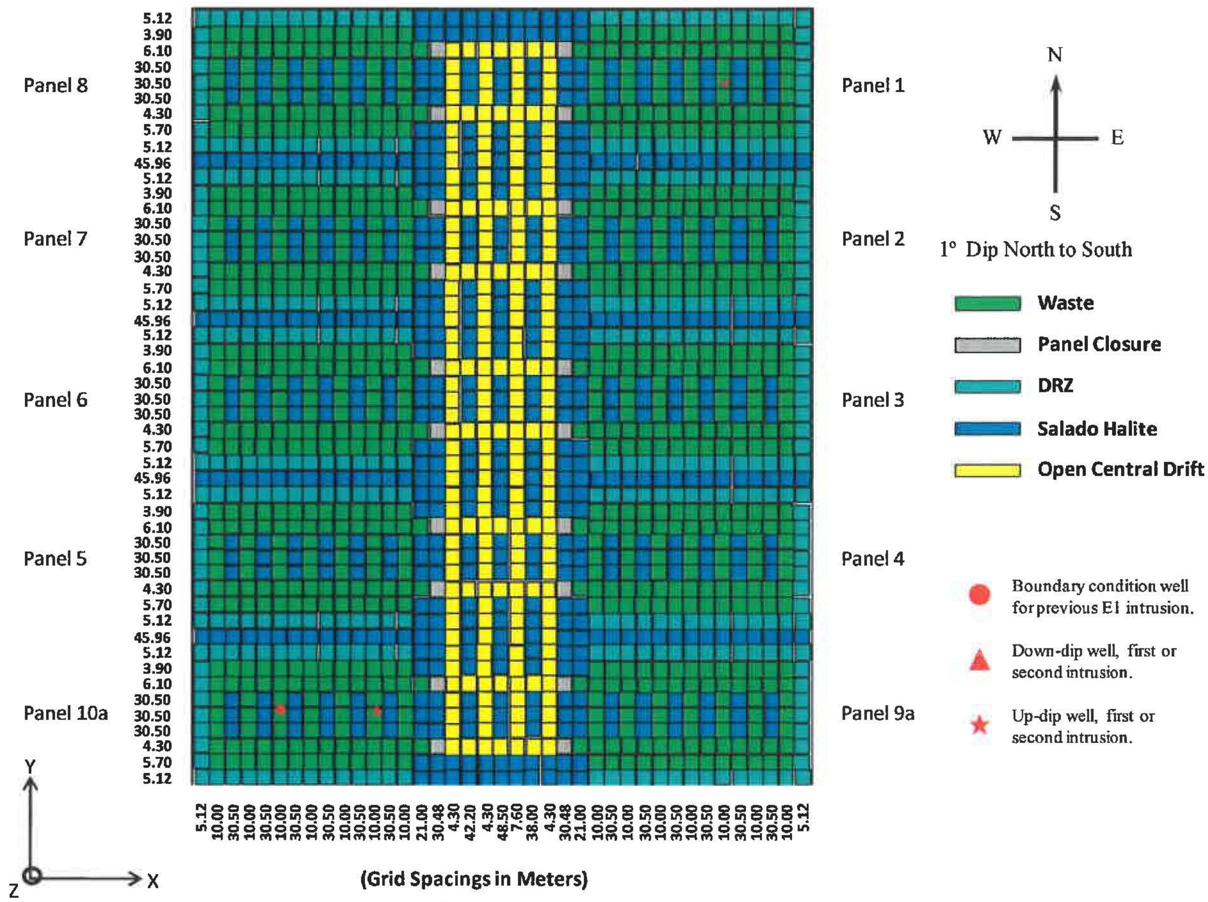


Figure 3-4: PC3R PA DBR material map (logical grid). Note that cells are not drawn to scale.

3.2 Initial Conditions

Volume averaged pressures and brine saturations are calculated from the 10,000 year BRAGFLO simulations. The BRAGFLO results, corresponding to the time of intrusion, are used in the DBR simulations as initial conditions. The waste regions in the BRAGFLO grid and the DBR grid are each divided into two regions and volume-averaged pressure and saturations were transferred from corresponding regions in the BRAGFLO grid to the DBR grid. These regions corresponded to the single waste panel in the southwest portion of the waste area (panel 10a), the rest of repository. This method ensures that the relative volumes of these regions are equal between the 10,000 year BRAGFLO runs and the DBR runs. Similar transfer of data from

BRAGFLO calculations were accomplished to establish initial pressures and saturations for the Salado, DRZ, Panel Closures, and the Operations Area.

Figure 3-5 illustrates the method used to transfer initial conditions in the waste for the PC3R PA DBR runs. This method is unchanged from the method used in the PABC-2009 PA DBR calculations. The volume averaged pressure and saturation from the two waste-filled regions in the BRAGFLO grid at the time of the intrusion are used as the initial pressure and saturation for the two waste regions in the DBR grid (Lower and Upper, respectively). The pressure and saturation can change during the DBR calculations.

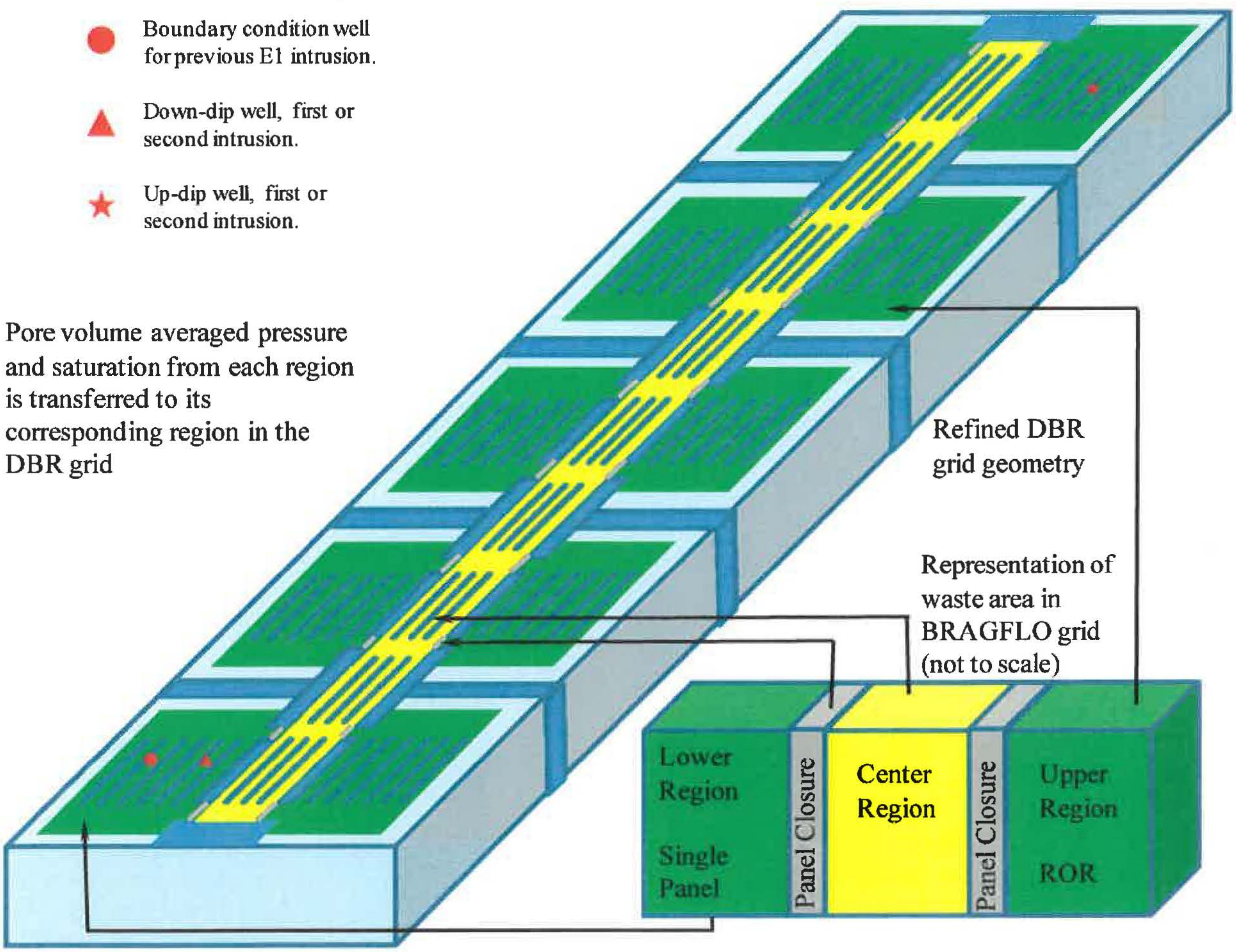


Figure 3-5: Regions to be used to transfer initial pressure and saturation between the 10,000 year BRAGFLO grid and the DBR grid for the PC3R PA.

4 CALCULATION METHODOLOGY

DBR calculations are divided into five scenarios. Each DBR scenario represents an intrusion into the repository due to a drilling event. The initial conditions for the DBR simulations are obtained from the BRAGFLO Salado Flow simulations (Camphouse and Clayton, 2011) using an appropriate scenario and at an appropriate time for the particular drilling intrusion time. An E1 intrusion scenario is defined as an intrusion into the repository, which creates a pathway to a pressurized brine pocket below the repository. An E2 intrusion scenario is defined as an intrusion into the repository that does not create a pathway to a pressurized brine pocket below the repository. The results of the DBR calculations are the volumes of brine that leave the repository and reach the surface at the time of drilling and up to 4.5 days after. These results are used by the code CCDFGF to interpolate volumes of waste for the specific conditions that arise in a given future (location and timing of future drilling intrusions).

4.1 Modeled Scenarios

Based on the features, events and processes analysis for the PC3R PA, no changes to DBR scenarios were needed to address the differences in the reconfigured repository or modified PCS (Kirkes, 2011). Below, an overview is given of the DBR calculations performed for the PC3R PA. In performing DBR calculations, the five BRAGLFO scenarios S1-DBR through S5-DBR are used as initial conditions for the DBR calculations. These initial conditions along with DBR simulations cover a range of possible numbers of intrusions, locations and timing. A summary of intrusion times and number of calculations for each scenario is given in Table 4-4-1.

Table 4-4-1: Intrusion times modeled by DBR for each scenario.

Scenario	Conditioning (or 1st) Intrusion time and type (year)	Intrusion times-Subsequent (year), all E2	No. of Calculations Per replicate
S1-DBR	None	100, 350, 1000, 3000, 5000, 10000	2 locations (U,L) 6 intrusions 100 vectors 1 replicate = 1200
S2-DBR	350 E1	550, 750, 2000, 4000, 10000	2 locations (U,L) 5 intrusions 100 vectors 1 replicate =1000
S3-DBR	1000 E1	1200, 1400, 3000, 5000, 10000	2 locations (U,L) 5 intrusions 100 vectors 1 replicate =1000
S4-DBR	350 E2	550, 750, 2000, 4000, 10000	2 locations (U,L) 5 intrusions 100 vectors 1 replicate =1000
S5-DBR	1000 E2	1200, 1400, 3000, 5000, 10000	2 locations (U,L) 5 intrusions 100 vectors 1 replicate =1000

4.1.1 Scenario 1 (S1-DBR)

The BRAGFLO Salado modeling results from the S1-DBR scenario are used as initial conditions to construct the first intrusion into the repository in which a DBR may occur. In BRAGFLO Salado modeling (Camphouse and Clayton, 2011), this scenario represents an undisturbed repository. Upper and lower drilling intrusions are modeled at 100, 350, 1,000, 3,000, 5,000, and 10,000 years (2 locations × 6 intrusion times × 100 vectors = 1,200 calculations per replicate).

4.1.2 Scenario 2 (S2-DBR)

The BRAGFLO Salado modeling results from the S2-DBR scenario are used as initial conditions to construct a second or subsequent intrusion into the repository in which a DBR may occur and in which the first intrusion had hit a Castile brine reservoir at 350 years (Camphouse and Clayton, 2011). For the second or subsequent intrusion, upper and lower drilling intrusions were modeled at 550, 750, 2,000, 4,000 and 10,000 years (2 locations × 5 intrusion times × 100 vectors = 1,000 calculations per replicate). The effect of the prior E1 intrusion is incorporated in the calculations by the specification of a boundary condition well as denoted by the red circle in Figure 3-5. The properties of the boundary condition well correspond to the properties at the time of the second intrusion.

Runs for the lower drilling location assume that the second or subsequent intrusion occurs at the location labeled in Figure 3-5 as the "down-dip well". This represents an intrusion in the same panel that was intersected by a previous intrusion (assumed to be at the location labeled "boundary condition well") and therefore the abandoned borehole still connects the panel with the brine reservoir. Runs for the upper drilling location assume that the second or subsequent intrusion occurs at the location labeled "up-dip well" in Figure 3-5; a previous intrusion is assumed to have occurred at the location labeled "boundary condition well," which is in a panel that is not adjacent to the current intrusion.

4.1.3 Scenario 3 (S3-DBR)

The BRAGFLO Salado modeling results from the S3-DBR scenario are used as initial conditions to construct a second or subsequent intrusion into the repository in which a DBR may occur and in which the first intrusion had hit a Castile brine reservoir at 1,000 years (Camphouse and Clayton, 2011). Upper and lower second or subsequent intrusions are modeled at 1,200, 1,400, 3,000, 5,000 and 10,000 years (2 locations × 5 intrusion times × 100 vectors = 1,000 calculations per replicate). The effect of the prior E1 intrusion and the lower and upper drilling locations are treated the same as for the S2-DBR scenario.

4.1.4 Scenario 4 (S4-DBR)

The BRAGFLO Salado modeling results from the S4-DBR scenario are used as initial conditions to construct a second or subsequent intrusion into the repository in which a DBR may occur and in which the first intrusion occurs at 350 years without hitting a Castile brine reservoir (Camphouse and Clayton, 2011). Upper and lower second or subsequent intrusions are modeled at 550, 750, 2,000, 4,000 and 10,000 years (2 locations × 5 intrusion times × 100 vectors = 1,000 calculations per replicate). Runs for the lower drilling location assume the second or subsequent intrusion occurs at the location labeled in Figure 3-5 as the "down-dip well". This represents an intrusion into the same panel that was intersected by a previous E2 intrusion. The borehole from the previous intrusion is not represented explicitly in the model. Runs for the upper drilling location assume that the second or subsequent intrusion occurs at the location labeled "up-dip well" in Figure 3-5.

4.1.5 Scenario 5 (S5-DBR)

The BRAGFLO Salado modeling results from the S5-DBR scenario are used as initial conditions to construct a second or subsequent intrusion into the repository in which a DBR may occur and in which the first intrusion occurs at 1,000 years without hitting a Castile brine reservoir (Camphouse and Clayton, 2011). Upper and lower second or subsequent intrusions are modeled at 1,200, 1,400, 3,000, 5,000 and 10,000 years (2 locations × 5 intrusion times × 100 vectors = 1,000 calculations per replicate). The lower and upper drilling locations are treated the same as for the S4-DBR scenario.

4.1.6 Run Control

Run control, including code versions used and descriptions of code sequencing used to obtain DBR results in the PC3R PA, is documented in Long (2011). PC3R PA results obtained from BRAGFLO DBR post-processing have file names ALG2_DBR_PC3R_Rr_Ss_Ttttt_Vvvv.CDB and ALG3_DBR_PC3R_Rr_Ss_Ttttt_ c_Vvvv.CDB, where r (the replicate number) equals 1,2, or 3, s (the scenario number) equals 1,2,3,4,5, or 6, ttttt (time in years) equals 00550, 00750, 02000, 04000, or 10000, c (drilling location) is either L or U, and vvv (the vector number) is between 001 and 100. These files are located in CMS library LIBPC3R_DBRRrSs under class PC3R-0. PABC-2009 results used for comparison purposes have equivalent file names with 'PC3R' replaced by 'PABC09', and are located in CMS library LIBPABC09_DBRRrSs under class PABC09-0.

5 RESULTS

Computed results are now presented for the PC3R PA and compared with those obtained in the PABC-2009. In the results that follow, the calculations of basic statistics were accomplished with a Fortran program (see section 9, Appendix B) and Excel, a commercial off-the-shelf application. The generation of their corresponding plots and tables were done with Excel. The DBR calculations for all three replicates of the PC3R PA are presented in this section and compared with results from the three replicates of the PABC-2009, except where noted. The analysis of the PABC-2009 results is described in an earlier report (Clayton 2010) and will only be summarized here as appropriate.

5.1 Summary

In this section, results from the PC3R PA and the PABC-2009 are compared. Table 5-1 compares some summary statistics for the calculations. The maximums shown are the maximum

DBR volumes over all replicates, times, vectors and drilling locations. Table 5-1 shows a decrease in the number of non-zero DBR volumes of 201 for the PC3R PA calculations compared with the PABC-2009 PA. The overall maximum DBR volume increased slightly from 48.2 m^3 to 52.0 m^3 for the PC3R PA.

Table 5-1: Summary statistics for the PC3R PA and PABC-2009 DBR calculations.

	PABC-2009	**PC3R PA**
Total number of model runs	15,600	15,600
Number non-zero DBR volumes	2474	2273
Maximum DBR volume for scenario S1 (m^3)	21.9	29.7
Maximum DBR volume for scenario S2 (m^3)	48.2	52.0
Maximum DBR volume for scenario S3 (m^3)	40.6	49.7
Maximum DBR volume for scenario S4 (m^3)	20.4	28.1
Maximum DBR volume for scenario S5 (m^3)	21.1	24.0

Note: The volume of direct brine released was obtained from the output variable BRIN_REL which is calculated in the ALGEBRACDB step 3 post processing step, and contained in the ALG3 CDB files.

5.2 Direct Brine Releases from the Lower Drilling Location

Table 5-2 through Table 5-6 summarize the number of vectors for the PC3R PA calculations that had a non-zero DBR volume and the maximum and average DBR volumes for the 300 vectors in each scenario-time-drilling location combination. The same data for the PABC-2009 PA is shown for comparison.

One important result that is evident from Table 5-2 through Table 5-6 is that DBRs 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 PC3R PA, 74.8% occurred during a lower drilling intrusion. Furthermore, of all the intrusions that had a non-zero DBR volume and occur during a lower drilling intrusion, 82.8% 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 from lower drilling intrusions. For all three replicates of the PC3R PA, the maximum DBR volume for the upper drilling location is 22.0 m^3 compared to 52.0 m^3 for the lower drilling location. These observations support the conclusion that lower drilling intrusions are the primary source for significant DBR's. For these reasons, this report only examines in detail the lower drilling intrusion results, and gives particular attention to scenario S2-DBR.

As seen in Table 5-3 and Table 5-4, the number of vectors with non-zero DBR volumes in lower intrusions declines with time faster for the PC3R PA than for the PABC-2009. For these important scenarios S2-DBR and S3-DBR, PABC-2009 consistently has the larger average DBR volume for lower intrusions, while PC3R PA consistently has the larger maximum DBR volume. Generally, however, the average and maximum DBR volumes for the two analyses are of similar magnitude.

Figure 5-1 to Figure 5-10 show percentile plots for the lower drilling locations, S1-DBR through S5-DBR for the PC3R and the PABC-2009 PA. For the PC3R PA, the largest DBR volume and the highest percentage of non-zero volumes both occur in the S2-DBR scenario, similar to the PABC-2009 PA. As seen in Figure 5-1 to Figure 5-10, the percentile plots are generally similar for the PC3R PA calculations compared with the PABC-2009 PA.

Figure 5-3 through Figure 5-6, for scenarios S2-DBR and S3-DBR, show that a higher percentage of vectors in the PABC-2009 PA will produce DBR's of at least 10 m^3, but the PC3R PA DBR volume curves rise more rapidly at the right, consistently producing the largest volumes. This is consistent with the previous observation that PABC-2009 vectors generate more nonzero DBR volumes, but the maximum DBR volumes are slightly larger for the PC3R PA. These observations are particularly evident in Figure 5-11, which includes all predicted DBR volumes for lower intrusions. The percentile scale in Figure 5-11 is adjusted to focus on significant volumes. It is evident from Figure 5-11 that roughly 80% of all predicted DBR volumes from lower intrusions are insignificant for both PC3R PA and PABC-2009 calculations.

Table 5-2: Summary table of number of vectors with non-zero, maximum and average DBR volumes for the S1-DBR calculations.

Time (yrs)	Drilling Location	Number of Vectors		Max volume (m^3)		Average volume (m^3)	
		PABC-2009	PC3R PA	PABC-2009	PC3R PA	PABC-2009	PC3R PA
100	L	0	0	0.0	0.0	0.0	0.0
350	L	0	0	0.0	0.0	0.0	0.0
1000	L	26	23	15.1	8.7	0.2	0.2
3000	L	37	40	5.9	9.6	0.1	0.1
5000	L	46	44	21.9	29.7	0.3	0.3
10000	L	46	46	20.3	17.0	0.4	0.3
100	U	0	0	0.0	0.0	0.0	0.0
350	U	0	0	0.0	0.0	0.0	0.0
1000	U	16	16	6.1	7.1	0.0	0.1
3000	U	29	28	1.7	4.4	0.0	0.1
5000	U	28	30	20.2	21.0	0.1	0.1
10000	U	30	30	19.1	11.0	0.1	0.1

Note: Volume releases less than 1×10^{-7} m^3 have been reduced to 0.0 for the purposes of this table. The maximum DBR volume is calculated as the maximum value of the 300 vectors for each replicate-scenario-time-drilling location combination. The average DBR volume is calculated by the total of the DBR volumes divided by the total number of vectors. The DBR volume was obtained from the output variable BRIN_REL which is calculated in the ALGEBRACDB step 3 post processing step, and contained in the ALG3 CDB files.

Table 5-3: Summary table of number of vectors with non-zero, maximum and average DBR volumes for the S2-DBR calculations.

Time (yrs)	Drilling Location	Number of Vectors		Max volume (m^3)		Average volume (m^3)	
		PABC-2009	PC3R PA	PABC-2009	PC3R PA	PABC-2009	PC3R PA
550	L	285	283	37.4	52.0	12.3	11.3
750	L	255	242	38.6	45.8	11.6	10.4
2000	L	164	149	37.8	51.6	7.1	7.0
4000	L	140	104	43.9	51.3	5.4	4.3
10000	L	137	83	48.2	48.9	5.6	3.4
550	U	5	5	0.4	0.6	0.0	0.0
750	U	9	10	2.4	9.6	0.0	0.1
2000	U	27	27	9.7	17.8	0.1	0.2
4000	U	27	29	1.2	2.0	0.0	0.0
10000	U	22	30	12.4	8.9	0.1	0.1

Note: Volume releases less than 1×10^{-7} m^3 have been reduced to 0.0 for the purposes of this table. The maximum DBR volume is calculated as the maximum value of the 300 vectors for each replicate-scenario-time-drilling location combination. The average DBR volume is calculated by the total of the DBR volumes divided by the total number of vectors. The DBR volume was obtained from the output variable BRIN_REL which is calculated in the ALGEBRACDB step 3 post processing step, and contained in the ALG3 CDB files.

Table 5-4: Summary table of number of vectors with non-zero, maximum and average DBR volumes for the S3-DBR calculations.

Time (yrs)	Drilling Location	Number of Vectors		Max volume (m^3)		Average volume (m^3)	
		PABC-2009	PC3R PA	PABC-2009	PC3R PA	PABC-2009	PC3R PA
1200	L	231	225	36.8	40.3	8.8	6.5
1400	L	166	147	32.5	35.5	5.4	4.3
3000	L	96	67	26.8	41.3	2.5	1.7
5000	L	90	59	37.6	46.8	2.7	1.5
10000	L	90	48	40.6	49.7	2.8	1.5
1200	U	23	22	4.4	9.6	0.0	0.1
1400	U	23	27	2.6	16.3	0.0	0.2
3000	U	29	28	2.0	4.4	0.0	0.1
5000	U	24	29	19.6	22.0	0.1	0.1
10000	U	19	30	12.2	8.9	0.1	0.1

Note: Volume releases less than 1×10^{-7} m^3 have been reduced to 0.0 for the purposes of this table. The maximum DBR volume is calculated as the maximum value of the 300 vectors for each replicate-scenario-time-drilling location combination. The average DBR volume is calculated by the total of the DBR volumes divided by the total number of vectors. The DBR volume was obtained from the output variable BRIN_REL which is calculated in the ALGEBRACDB step 3 post processing step, and contained in the ALG3 CDB files.

Table 5-5: Summary table of number of vectors with non-zero, maximum and average DBR volumes for the S4-DBR calculations.

Time (yrs)	Drilling Location	Number of Vectors		Max volume (m^3)		Average volume (m^3)	
		PABC-2009	PC3R PA	PABC-2009	PC3R PA	PABC-2009	PC3R PA
550	L	6	5	1.0	0.9	0.0	0.0
750	L	5	3	19.3	12.7	0.1	0.0
2000	L	17	9	16.0	28.1	0.1	0.2
4000	L	22	16	19.2	9.1	0.1	0.1
10000	L	24	17	20.4	24.2	0.2	0.3
550	U	5	5	0.4	0.6	0.0	0.0
750	U	8	10	2.1	7.5	0.0	0.1
2000	U	22	26	9.6	15.7	0.1	0.1
4000	U	21	27	1.2	2.0	0.0	0.0
10000	U	15	30	11.1	8.8	0.1	0.1

Note: Volume releases less than 1×10^{-7} m^3 have been reduced to 0.0 for the purposes of this table. The maximum DBR volume is calculated as the maximum value of the 300 vectors for each replicate-scenario-time-drilling location combination. The average DBR volume is calculated by the total of the DBR volumes divided by the total number of vectors. The DBR volume was obtained from the output variable BRIN_REL which is calculated in the ALGEBRACDB step 3 post processing step, and contained in the ALG3 CDB files.

Table 5-6: Summary table of number of vectors with non-zero, maximum and average DBR volumes for the S5-DBR calculations.

Time (yrs)	Drilling Location	Number of Vectors		Max volume (m^3)		Average volume (m^3)	
		PABC-2009	PC3R PA	PABC-2009	PC3R PA	PABC-2009	PC3R PA
1200	L	31	27	19.7	9.1	0.3	0.2
1400	L	15	10	21.1	22.9	0.2	0.2
3000	L	18	13	6.0	10.0	0.1	0.1
5000	L	23	23	9.2	20.1	0.1	0.1
10000	L	24	17	20.3	24.0	0.2	0.3
1200	U	21	22	4.3	9.4	0.0	0.1
1400	U	20	26	2.7	15.2	0.0	0.2
3000	U	23	26	2.0	4.4	0.0	0.1
5000	U	19	29	1.1	11.9	0.0	0.1
10000	U	15	31	11.1	8.8	0.1	0.1

Note: Volume releases less than 1×10^{-7} m^3 have been reduced to 0.0 for the purposes of this table. The maximum DBR volume is calculated as the maximum value of the 300 vectors for each replicate-scenario-time-drilling location combination. The average DBR volume is calculated by the total of the DBR volumes divided by the total number of vectors. The DBR volume was obtained from the output variable BRIN_REL which is calculated in the ALGEBRACDB step 3 post processing step, and contained in the ALG3 CDB files.

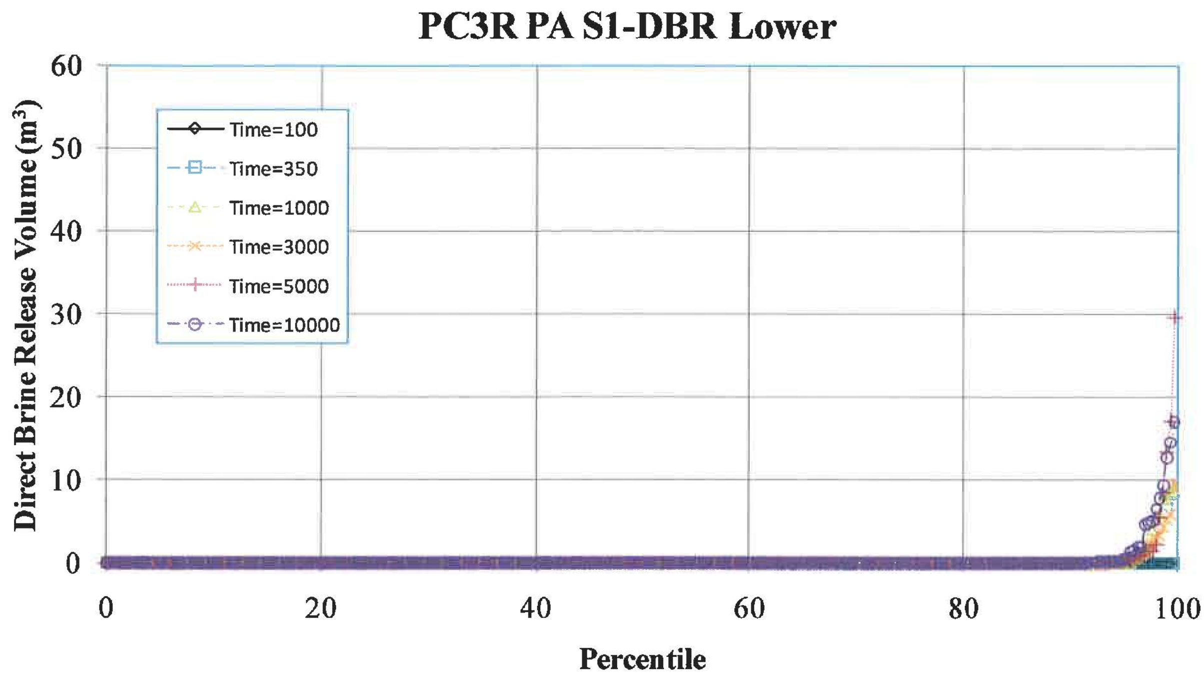


Figure 5-1: PC3R PA lower intrusion DBR volume percentile rankings for all replicates and vectors of the scenario S1-DBR.

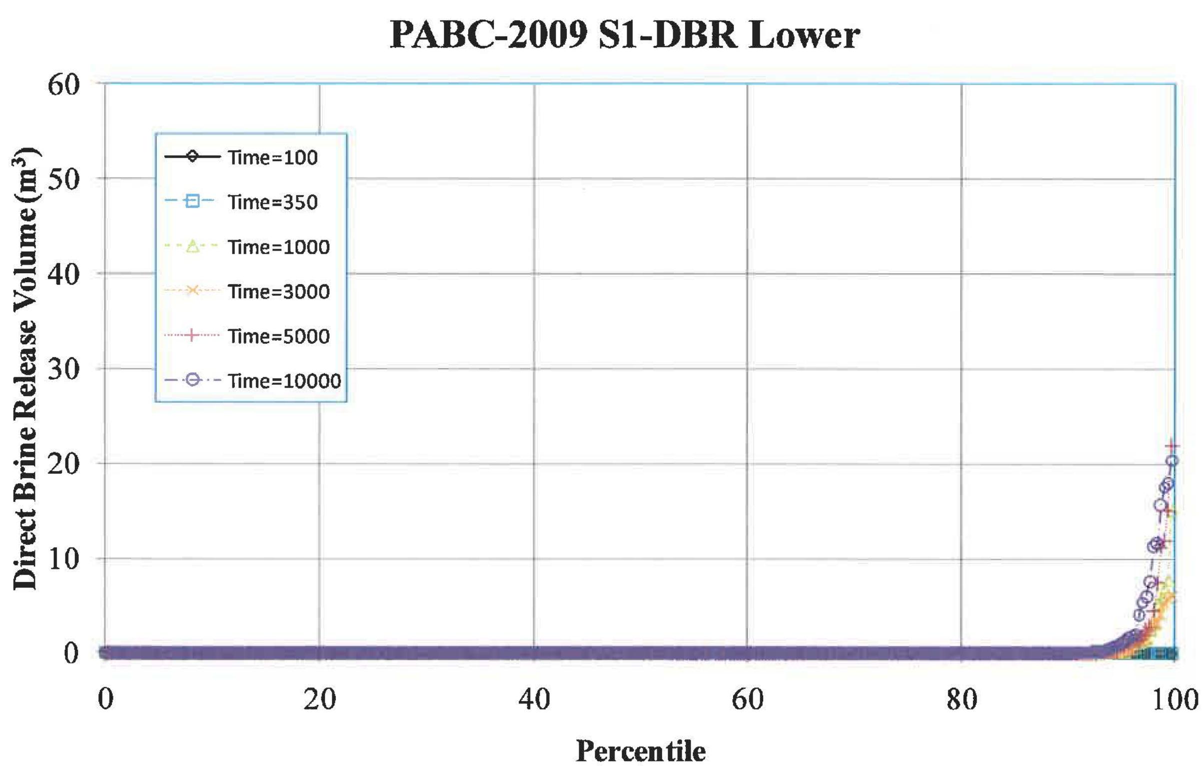


Figure 5-2: PABC-2009 lower intrusion DBR volume percentile rankings for all replicates and vectors of the scenario S1-DBR.

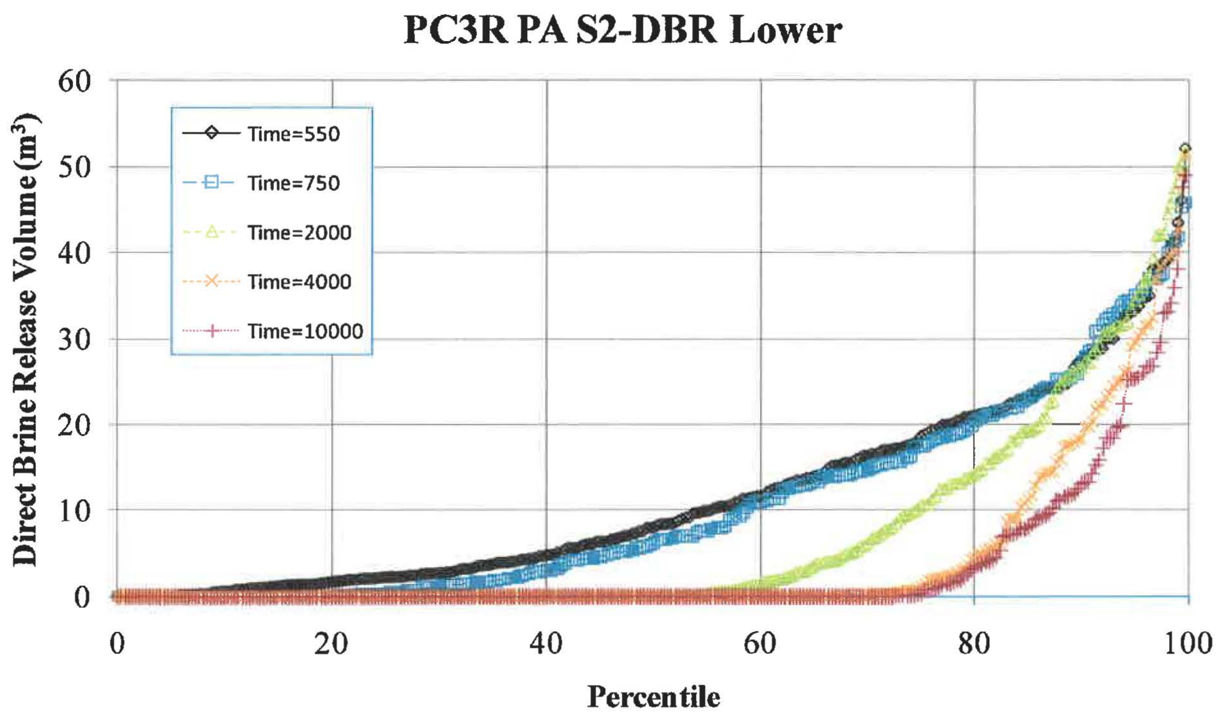


Figure 5-3: PC3R PA lower intrusion DBR volume percentile rankings for all replicates and vectors of the scenario S2-DBR.

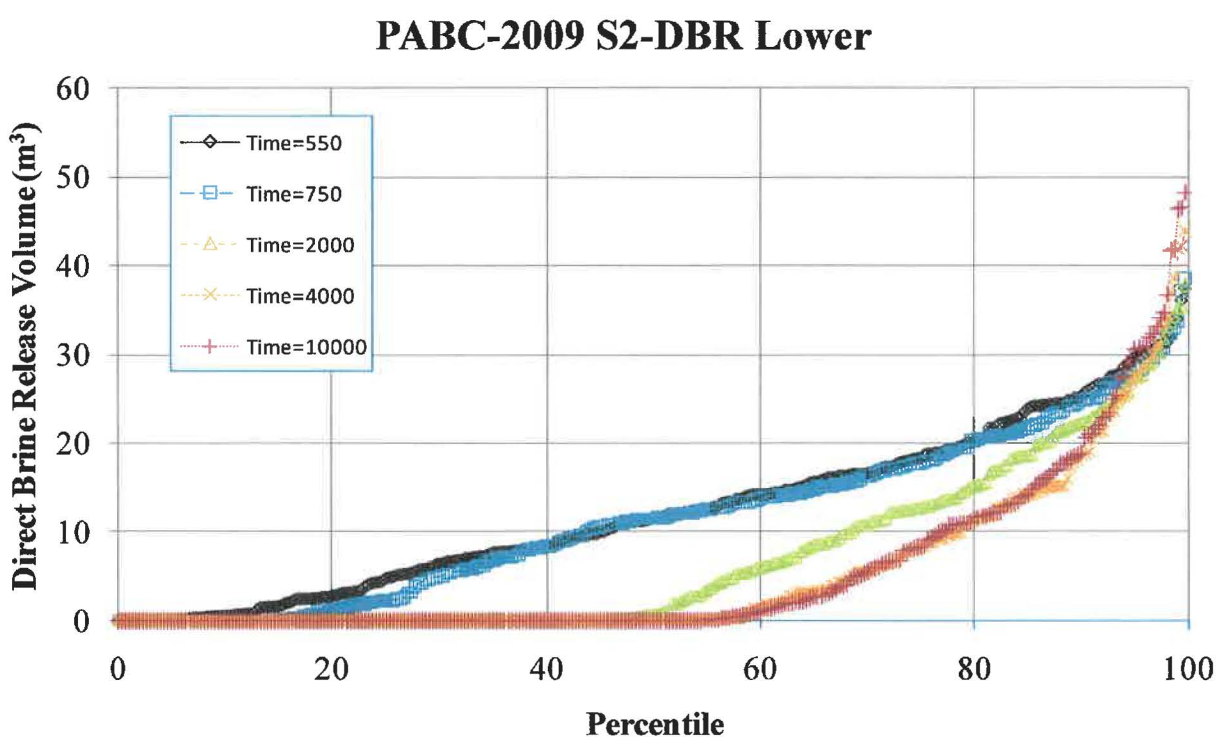


Figure 5-4: PABC-2009 lower intrusion DBR volume percentile rankings for all replicates and vectors of the scenario S2-DBR.

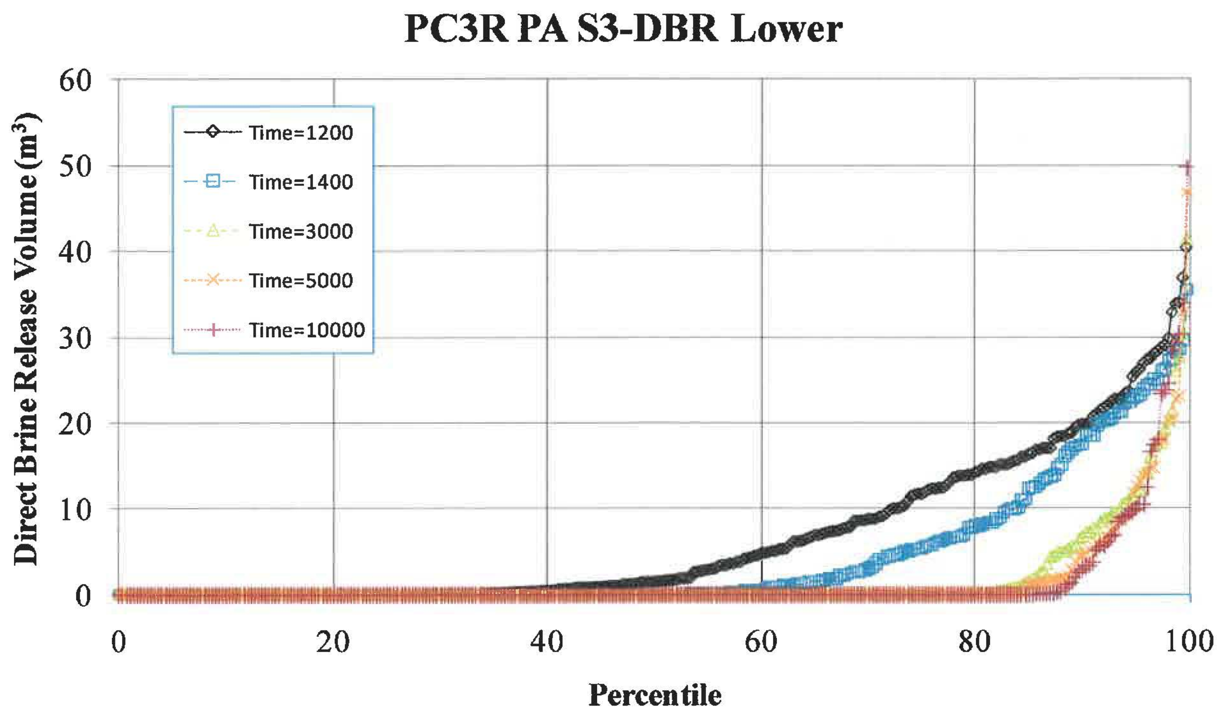


Figure 5-5: PC3R PA lower intrusion DBR volume percentile rankings for all replicates and vectors of the scenario S3-DBR.

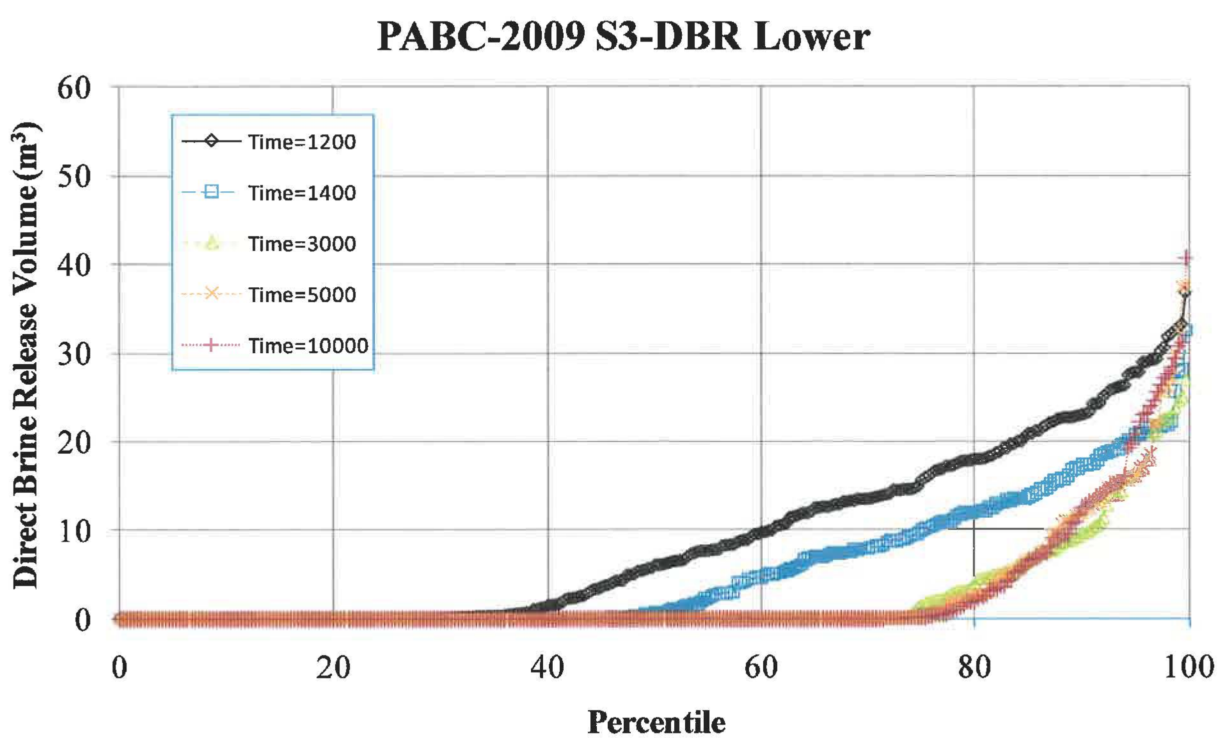


Figure 5-6: PABC-2009 lower intrusion DBR volume percentile rankings for all replicates and vectors of the scenario S3-DBR.

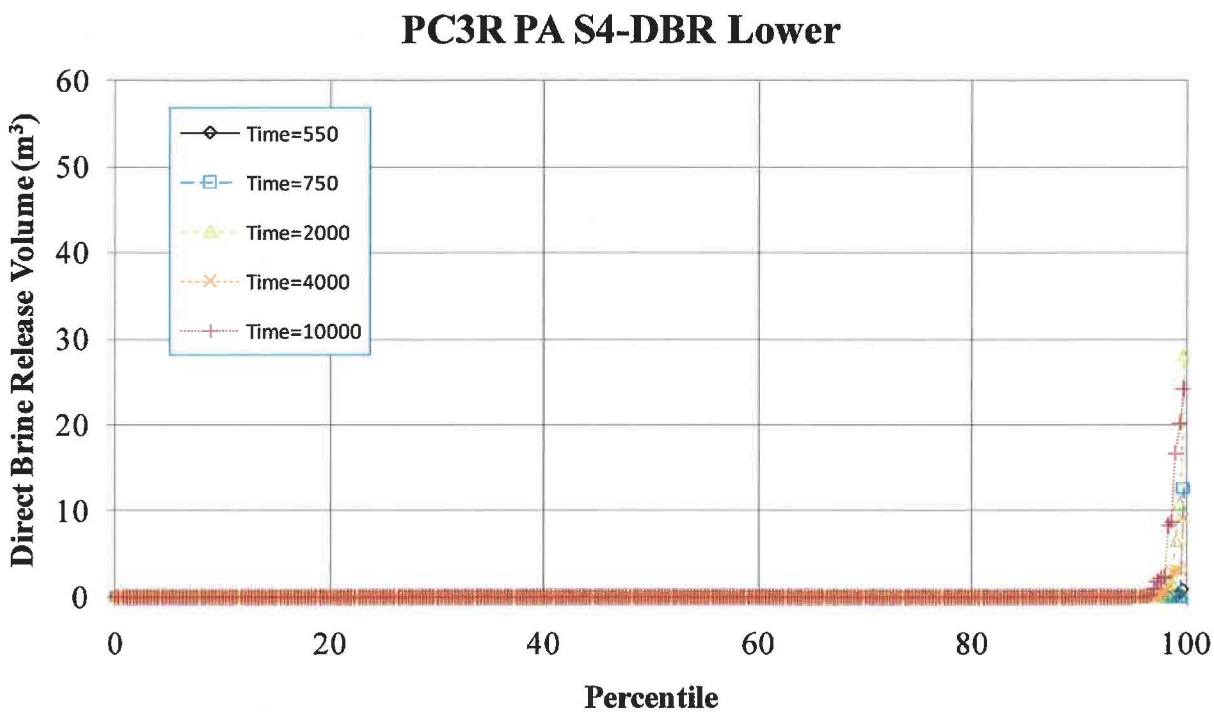


Figure 5-7: PC3R PA lower intrusion DBR volume percentile rankings for all replicates and vectors of the scenario S4-DBR.

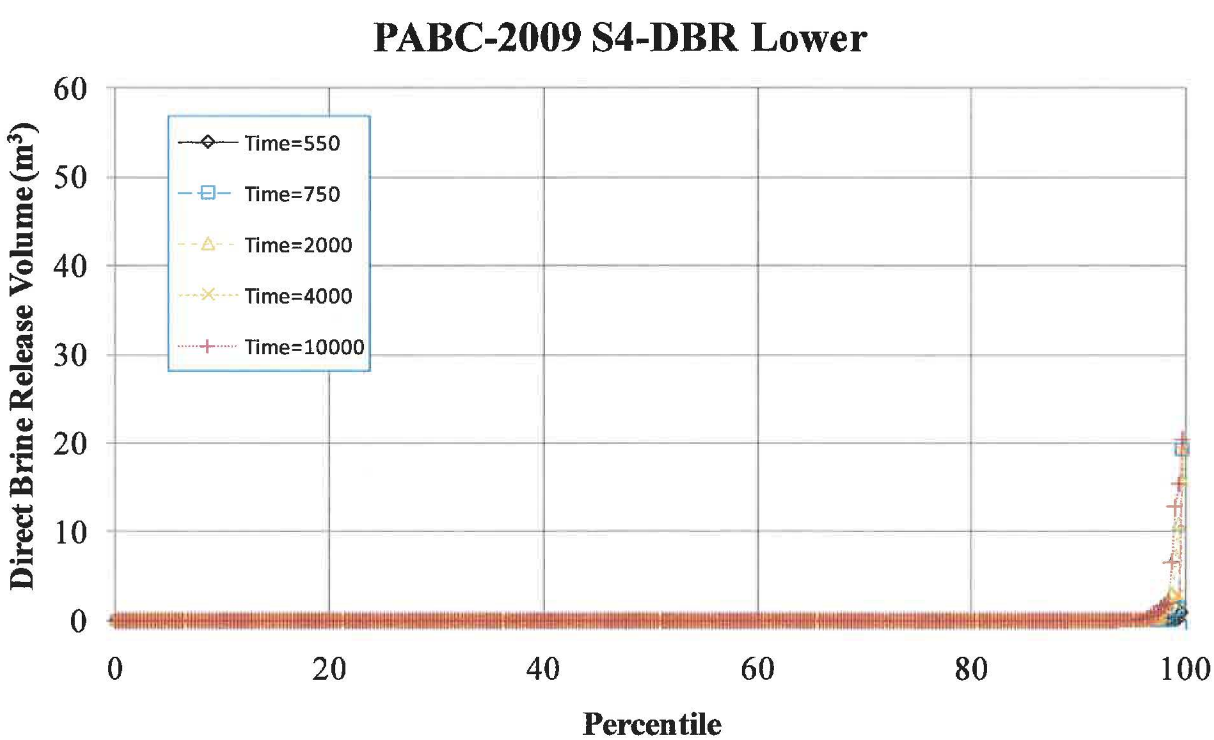


Figure 5-8: PABC-2009 lower intrusion DBR volume percentile rankings for all replicates and vectors of the scenario S4-DBR.

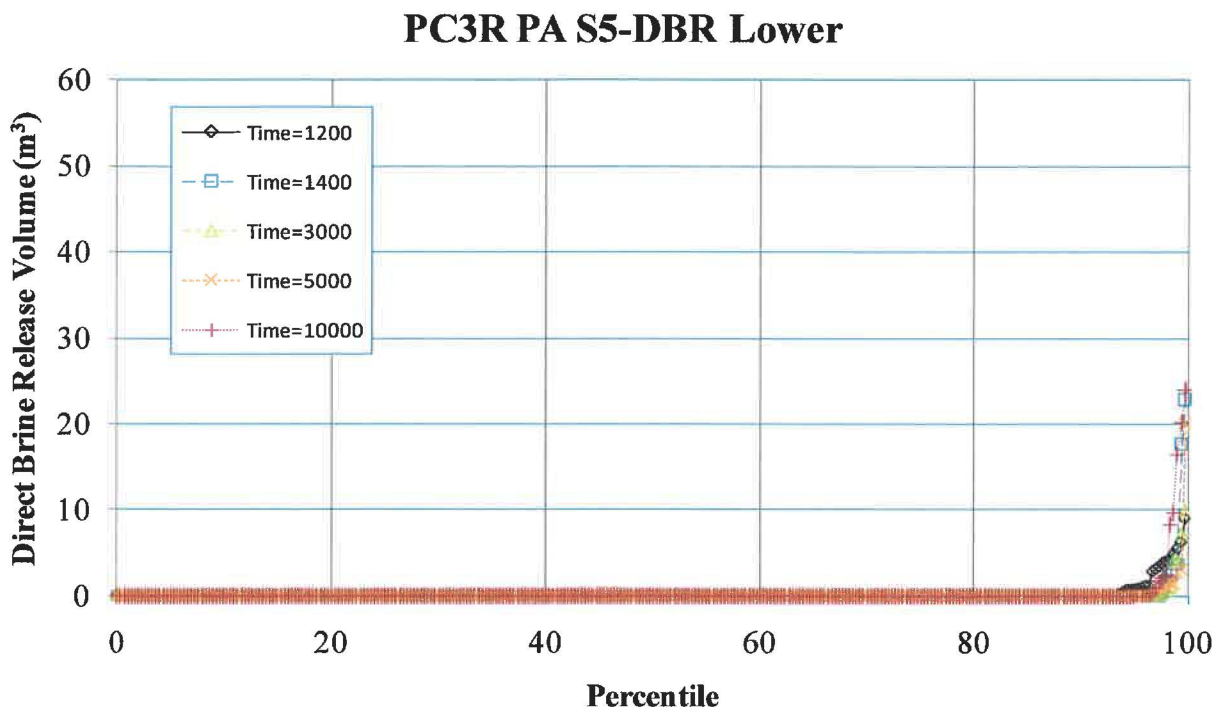


Figure 5-9: PC3R PA lower intrusion DBR volume percentile rankings for all replicates and vectors of the scenario S5-DBR.

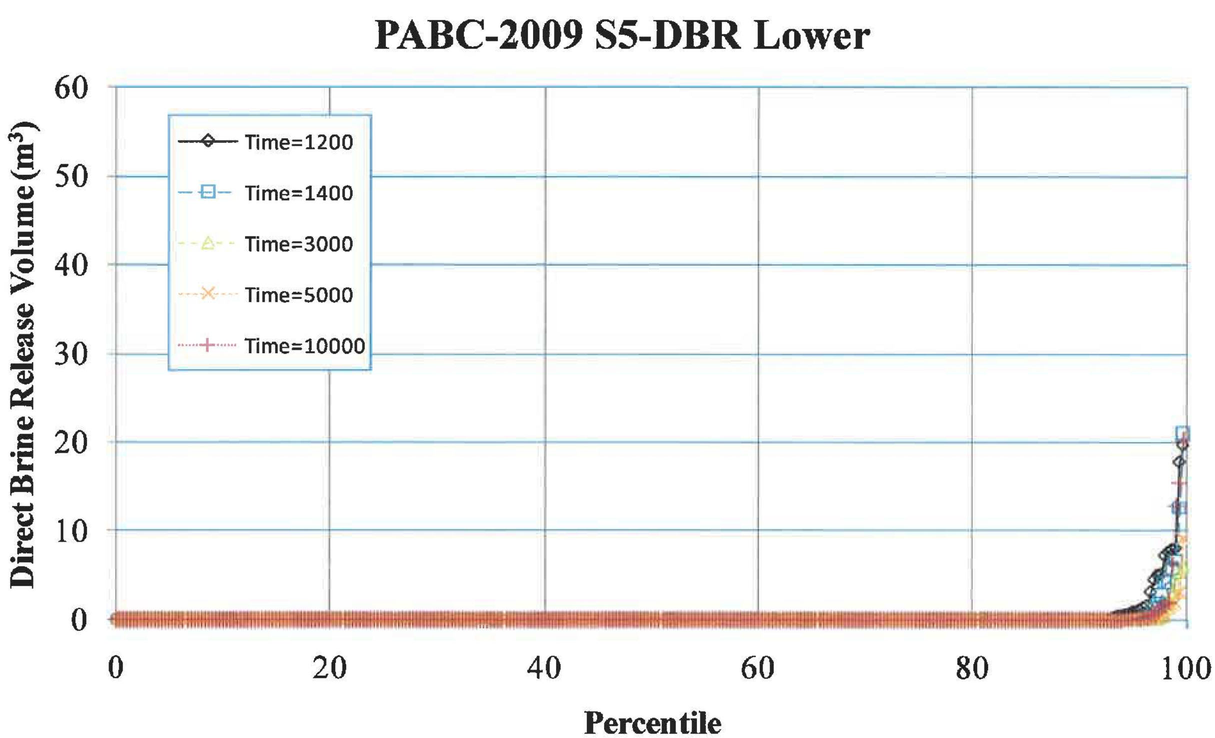


Figure 5-10: PABC-2009 lower intrusion DBR volume percentile rankings for all replicates and vectors of the scenario S5-DBR.

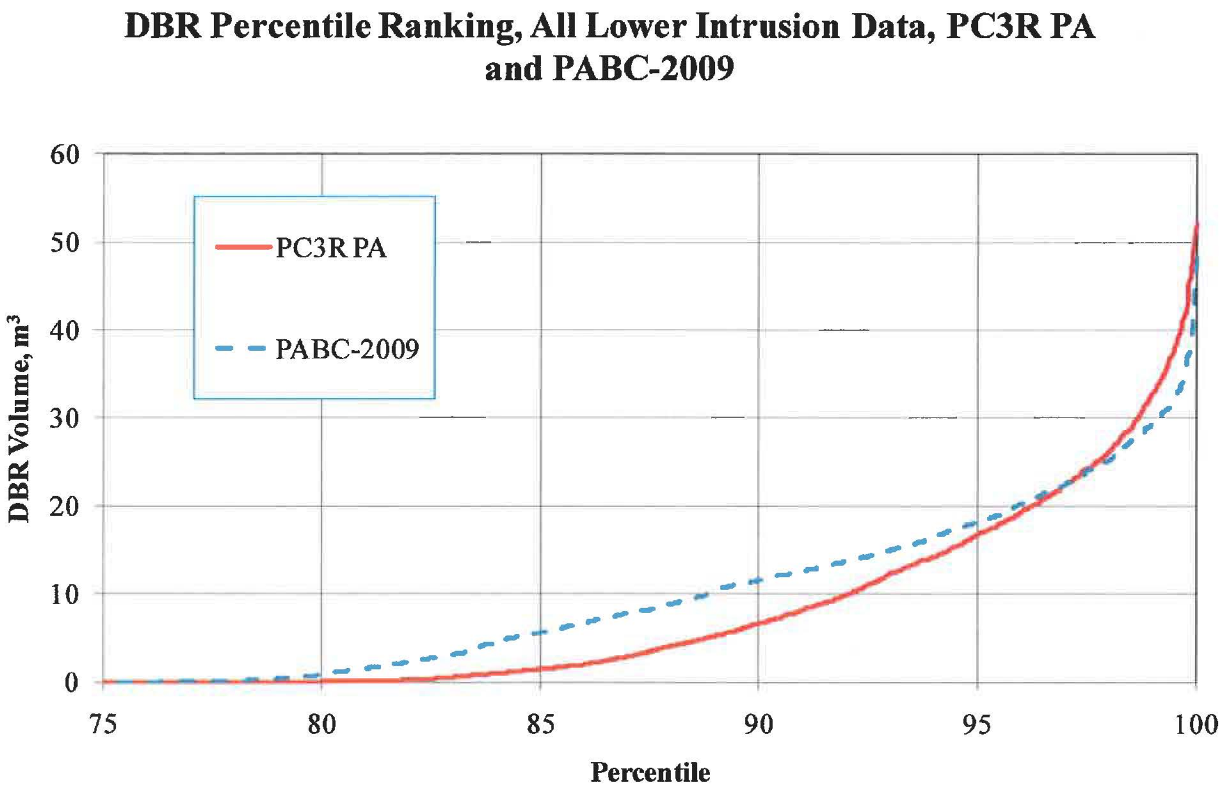


Figure 5-11: Comparison of PC3R PA and PABC-2009 lower intrusion DBR volume percentile rankings for all replicates, scenarios, times, and vectors.

5.3 Sensitivity of Direct Brine Releases to Input Parameters

In recent PAs, sensitivity analyses determined that the pressure and brine saturation in the intruded panel were the two most important variables that controlled DBR volumes (Clayton 2008). These two parameters are shown below for the PC3R PA along with the PABC-2009 for comparison. For the plots given below, the values of these parameters were extracted from the ALG2 files from the DBR calculations.

Scenarios S2-DBR and S3-DBR have significant DBR volumes because of the presence of a previous borehole connecting the repository with the Castile brine reservoir, which generally increases the waste panel pressure. The sensitivity analysis will focus on the S2-DBR and S3-DBR scenarios because these scenarios have the greatest number of significant DBR volumes. Scenarios S1-DBR, S4-DBR, and S5-DBR have so few runs with non-zero DBR volumes that these scenarios are excluded from the sensitivity analysis. As scenarios S2-DBR and S3-DBR are similar, only scenario S2-DBR is discussed in the sensitivity analysis.

Pressure in the intruded panel at the time of the intrusion is an important factor for many vectors. Figure 5-12 and Figure 5-13 show scatter plots of DBR volume versus pressure in the intruded panel at different intrusion times for the S2-DBR scenario, lower drilling intrusion for the PC3R and the PABC-2009 PA's, respectively. As prescribed by the conceptual model, there are no DBRs until pressures exceed 8 MPa as indicated by the vertical line in the figures. 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 5-14 and Figure 5-15 show scatter plots of DBR volume versus pressure in the intruded panel at different mobile brine saturations for the S2-DBR scenario, lower drilling intrusion for the PC3R and the PABC-2009 PA's, respectively, which show that DBR volumes tend to increase with increasing pressure and increasing mobile brine saturation.

Figure 5-13 and Figure 5-15 show a high concentration of results that are near a line extending from (8 MPa, 0 m^3) to (12 MPa, 30 m^3). Increased deviation from this line is evident in Figure 5-12 and Figure 5-14. Figure 5-15 shows that as mobile saturation increases, the correlation between pressure and DBR volumes also increases. This trend is less evident in Figure 5-14. In general, these figures show more variability in DBR volumes as a function of the parameters to which they are historically sensitive. Figure 5-16 presents the percentage differences between PC3R PA and PABC-2009 standard deviations for the intruded panel parameters that affect DBR volumes. These data are restricted to nonzero DBR's in replicate 1, scenario S2-DBR. Figure 5-16 shows larger variations in the parameters that control DBR volumes from the PC3R PA, thus leading to generally larger variations in DBR volumes. One point to note is that the highest mobile saturations do not correspond to the highest DBR volumes in either calculation. This is because pressure and saturation tend to be inversely correlated for high pressures in the 10,000 year BRAGFLO results (Nemer 2010).

Figure 5-17 and Figure 5-18 plot mobile brine saturation versus pressure for the S2-DBR scenario for all intrusion times with symbols indicating the range of DBR volumes, for the PC3R PA and the PABC-2009, respectively. These figures show the general increase in DBR volume with both brine saturation and pressure.

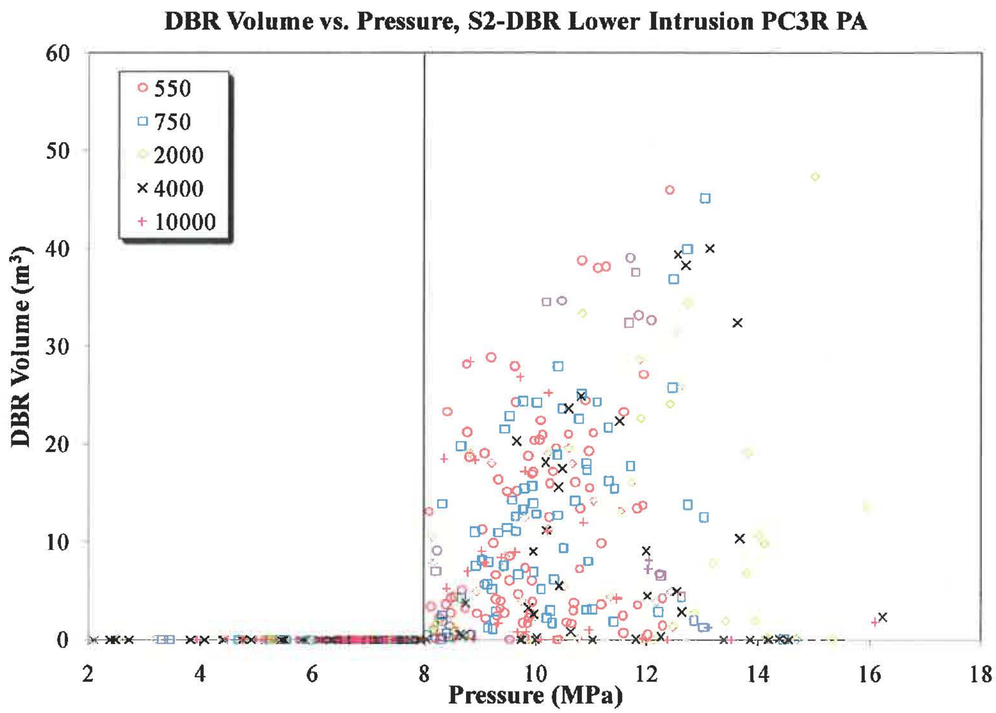


Figure 5-12: Scatter plot of DBR volume versus pressure in the intruded panel for replicate 1, S2-DBR scenario, lower drilling intrusion, PC3R PA. Symbols indicate intrusion times in years.

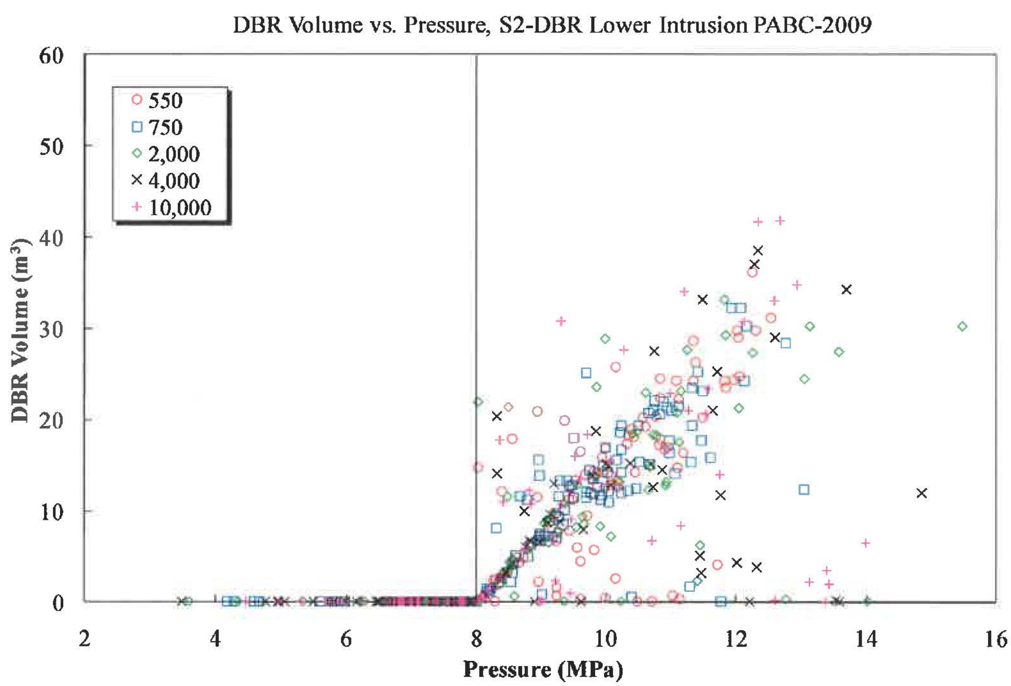


Figure 5-13: Scatter plot of. DBR volume versus pressure in the intruded panel for replicate 1, S2-DBR scenario, lower drilling intrusion, PABC-2009. Symbols indicate intrusion times in years.

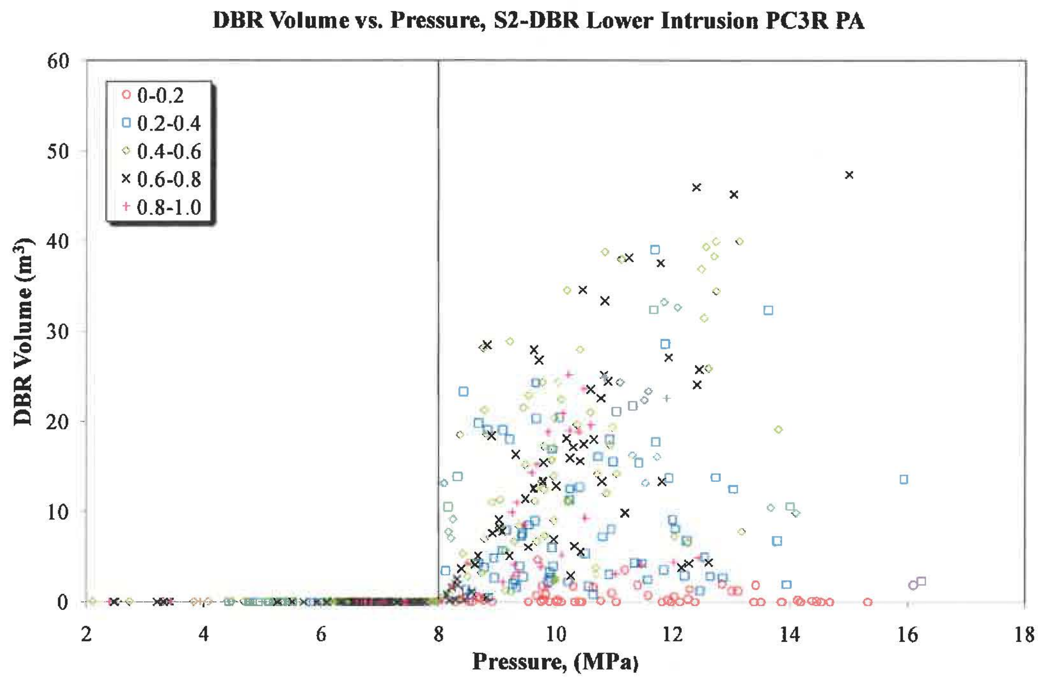


Figure 5-14: Scatter plot of DBR volume versus pressure in the intruded panel for replicate 1, S2-DBR scenario, lower drilling intrusion, PC3R PA. Symbols indicate the range of mobile brine saturation (dimensionless).

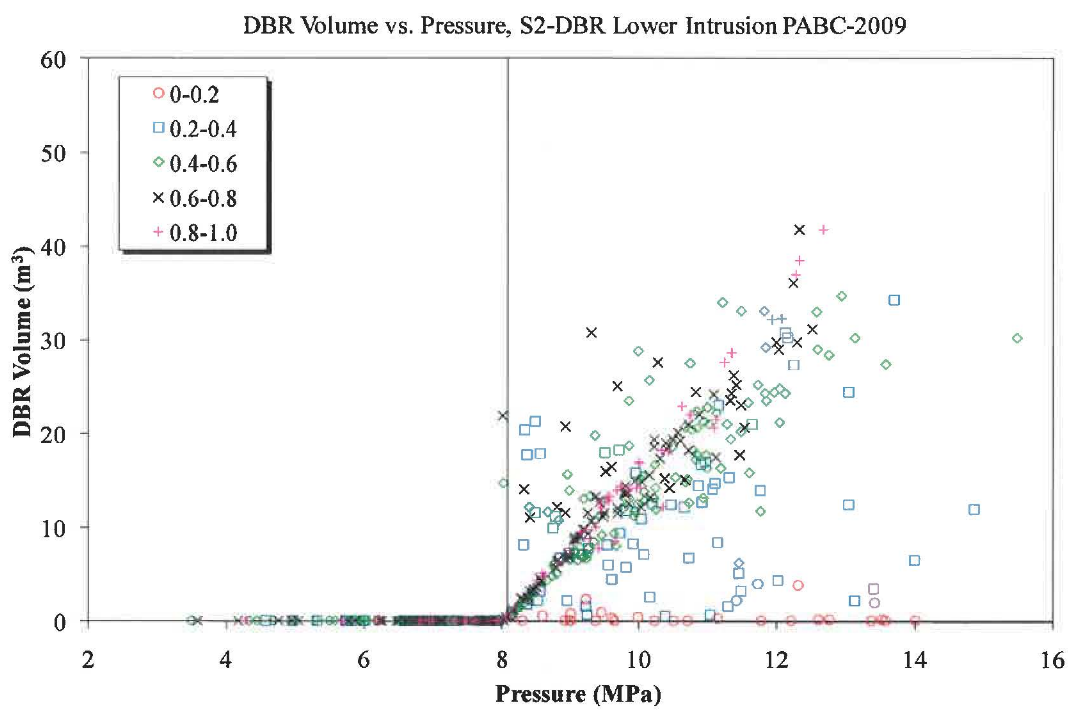


Figure 5-15: Scatter plot of DBR volume versus pressure in the intruded panel for replicate 1, S2-DBR scenario, lower drilling intrusion, PABC-2009. Symbols indicate the range of mobile brine saturation (dimensionless).

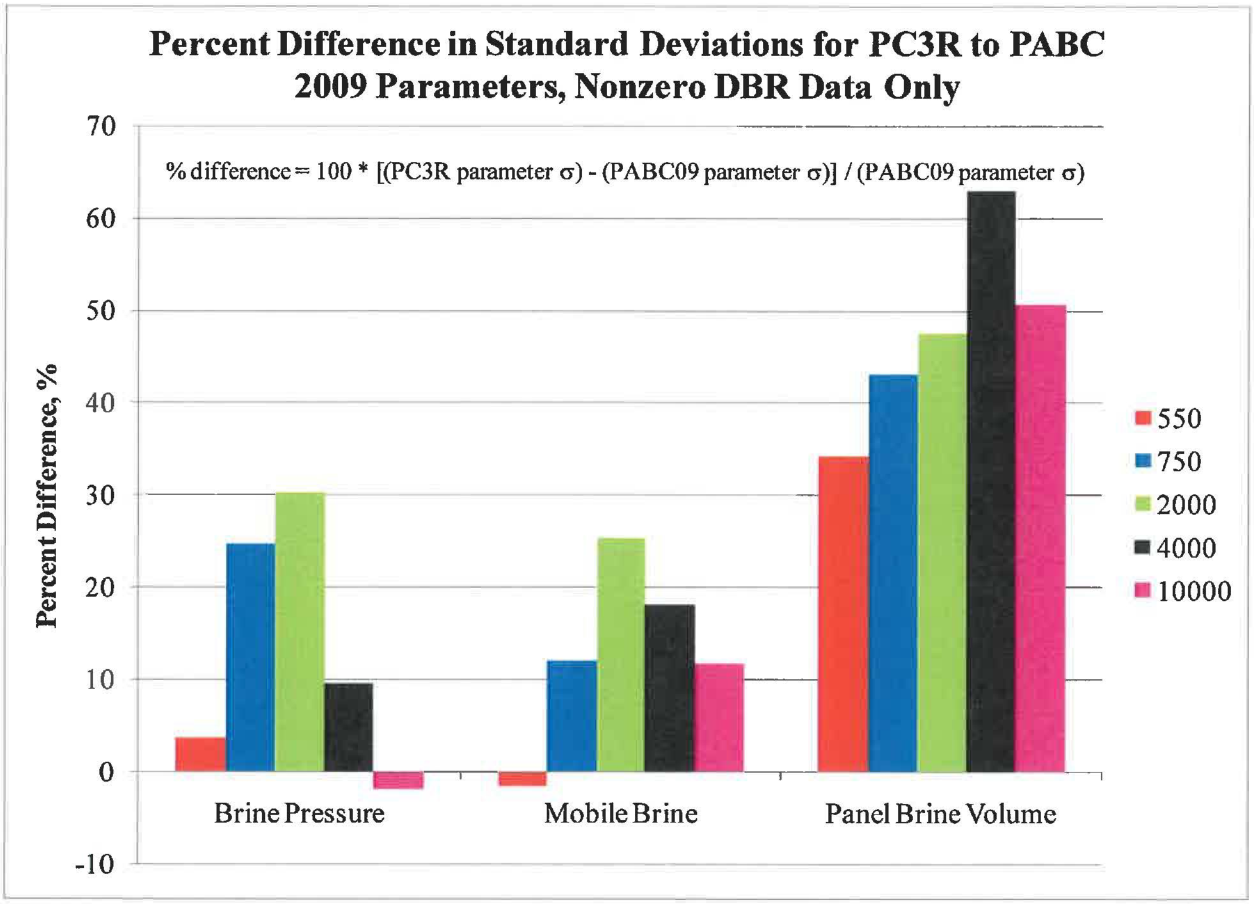


Figure 5-16: Percent difference in PC3R PA and PABC-2009 standard deviations for parameters that control DBR volumes, normalized to PABC-2009 values. Only results from nonzero DBR volumes from replicate 1, S2-DBR, and specified times are used.

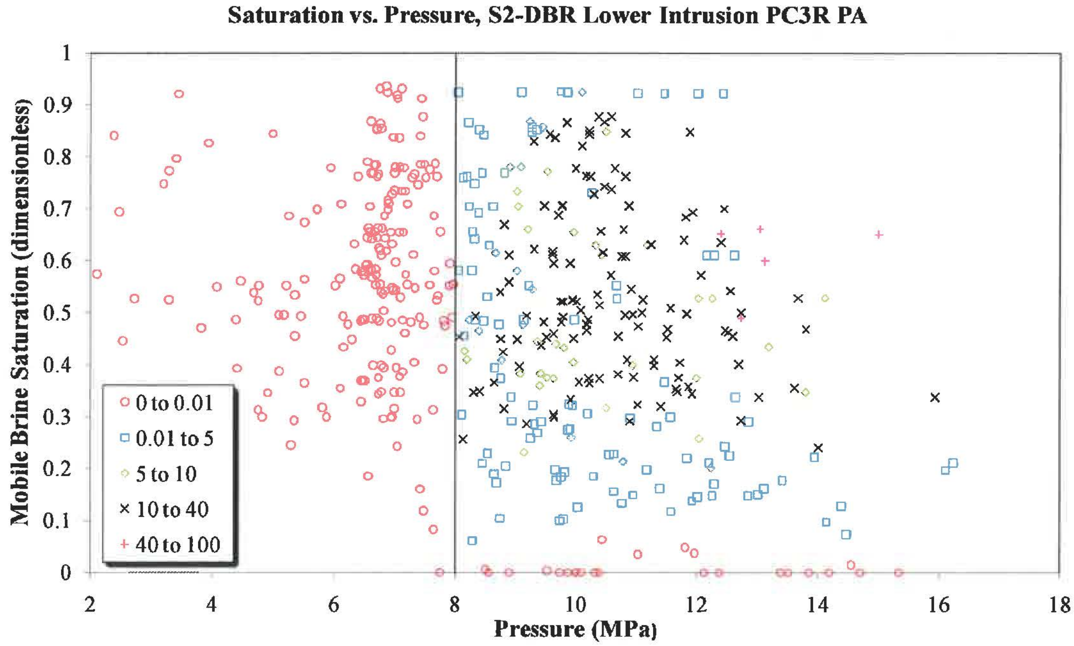


Figure 5-17: Scatter plot of mobile brine saturation versus pressure for replicate 1, S2-DBR scenario, lower drilling intrusion, all intrusion times, PC3R PA. Symbols indicate the range of DBR volumes in m^3.

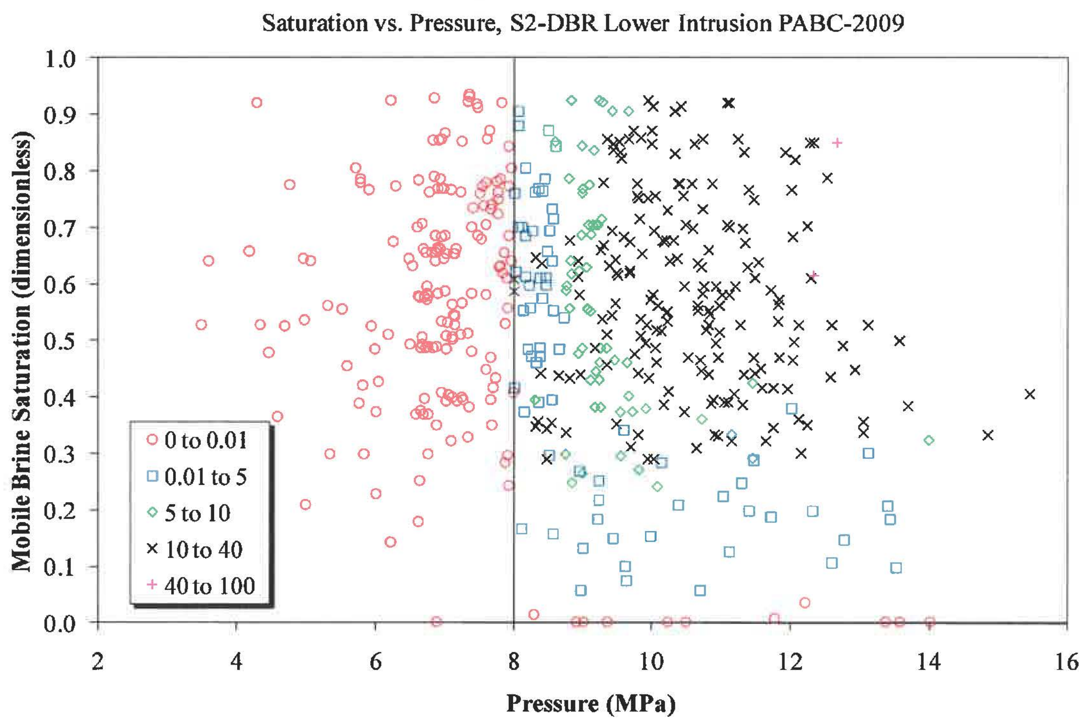


Figure 5-18: Scatter plot of mobile brine saturation versus pressure for replicate 1, S2-DBR scenario, lower drilling intrusion, all intrusion times, PABC-2009. Symbols indicate the range of DBR volumes in m^3.

6 CONCLUSIONS

The DBR results from all three replicates of the PC3R PA and PABC-2009 show that DBR's to the surface are very unlikely for most intrusions into the repository and in most cases result in inconsequential DBR volumes. The exception to this statement is for intrusions into a panel that had previously experienced a brine reservoir intrusion. Such intrusions are represented in PA by the lower drilling intrusions in the S2-DBR and S3-DBR scenarios. Assessing results from the PC3R PA in terms of those from the PABC-2009 PA, it is concluded that the PC3R PA DBR magnitudes are slightly higher for each scenario, the frequency of DBR releases is somewhat lower, and the variability in DBR volumes is higher. These results have been explained in terms of the parameters that affect DBR volumes.

7 REFERENCES

Camphouse, R.C. 2010. Analysis Plan for the WIPP Panel Closure Redesign and Repository Reconfiguration. Sandia National Laboratories, Carlsbad, NM. ERMS 554595.

Camphouse, R.C. 2011. Value Recommendation and Justification for Parameters DRZ_1:EHEIGHT and OPS_AREA:EHEIGHT needed during calculation of direct brine releases in the PC3R PA. Memo to Records Center, January 5, 2011. Sandia National Laboratories, Carlsbad, NM. ERMS 554694.

Camphouse, R.C. and Clayton, D.J. Analysis Package for Salado Flow Modeling Done in the AP-151 (PC3R) Performance Assessment. Sandia National Laboratories, Carlsbad, NM. (In preparation.)

Chappelear, J.E. and A.S. Williamson. 1981. Representing Wells in Numerical Reservoir Simulation. ERMS 249488.

Clayton, D.J. 2008. Analysis Package for Direct Brine Releases: Compliance Recertification Application – 2009. Sandia National Laboratories, Carlsbad, NM. ERMS 548571.

Clayton, D.J. 2010. Analysis Package for Direct Brine Releases: CRA-2009 Performance Assessment Baseline Calculation, Revision 0. Sandia National Laboratories. Carlsbad, NM. ERMS 552829.

Clayton, D.J., R.C. Camphouse, J.W. Garner, A.E. Ismail, T.B. Kirchner, K.L. Kuhlman, M.B. Nemer. 2010. Summary Report of the CRA-2009 Performance Assessment Baseline Calculation. Sandia National Laboratories, Carlsbad, NM. ERMS 553039.

Hansen, C. W. 2002. Analysis Report for the Panel Closure Impact Assessment. Sandia National Laboratories, Carlsbad, NM. ERMS 523935.

Helton, J.C, J.E. Bean, F.W. Berglund, F.J. Davis, K. Economy, J.W. Garner, J.D. Johnson, R.J. MacKinnon, J. Miller, D.G. O'Brien, J.L. Ramsey, J.D. Schreiber, A. Shinta, L.N. Smith, D.M. Stoelzel, C. Stockman and P. Vaughn. 1998. Uncertainty and Sensitivity Analysis Results Obtained in the 1996 Performance Assessment for the Waste Isolation Pilot Plant. Sandia National Laboratories, Albuquerque, NM. SAND98-0365, ERMS 252619.

Kirkes, G.R. 2011. Features, Events and Processes Assessment for Changes Described in Analysis Plan – 151, Revision 0. Sandia National Laboratories, Carlsbad, NM. (In Preparation.)

Lee, J. 1982. Well Testing. SPE Textbook Series Vol. 1. New York, NY: Society of Petroleum Engineers of AIME.

Long, J.J. 2011. Execution of Performance Assessment Codes for the WIPP Panel Closure Redesign and Repository Reconfiguration. Sandia National Laboratories, Carlsbad, NM. (In Preparation.)

Mattax, C.C. and R.L. Dalton. 1990. Reservoir Simulation. Henery L. Doherty Memorial Fund Society of Petroleum Engineers Inc., Richardson, TX.

Nemer, M.B. 2010. Analysis Package for Salado Flow Modeling: CRA-2009 Performance Assessment Baseline Calculation. Sandia National Laboratories. Carlsbad, NM. ERMS 552956

Stoelzel, D.M. and D.G. O'Brien. 1996. Conceptual Model Description of BRAGFLO Direct Brine Release Calculations to Support the Compliance Certification Application (CCA MASS Attachment 16-2). U.S. Department of Energy, Carlsbad, NM. ERMS 239090.

U.S. Environmental Protection Agency (EPA). 1998. 40 CFR 194, Criteria for the Certification and Recertification of the Waste Isolation Pilot Plant's Compliance with the Disposal Regulations: Certification Decision: Final Rule. Federal Register, Vol. 63, 27354-27406. ERMS 251924.

U.S. Environmental Protection Agency (EPA). 2010. 40 CFR Part 194 Criteria for the Certification and Recertification of the Waste Isolation Pilot Plant's Compliance With the Disposal Regulations: Recertification Decision, Federal Register No. 222, Vol. 75, pp. 70584-70595, November 18, 2010.

Vugrin, E.D., S.C. Dunagan. 2006. Analysis Package for the Impact Assessment of the Redesigned WIPP Panel Closure. Sandia National Laboratories, Carlsbad, NM. ERMS 543865.

8 APPENDIX A – WIPP DIMENSION MAP

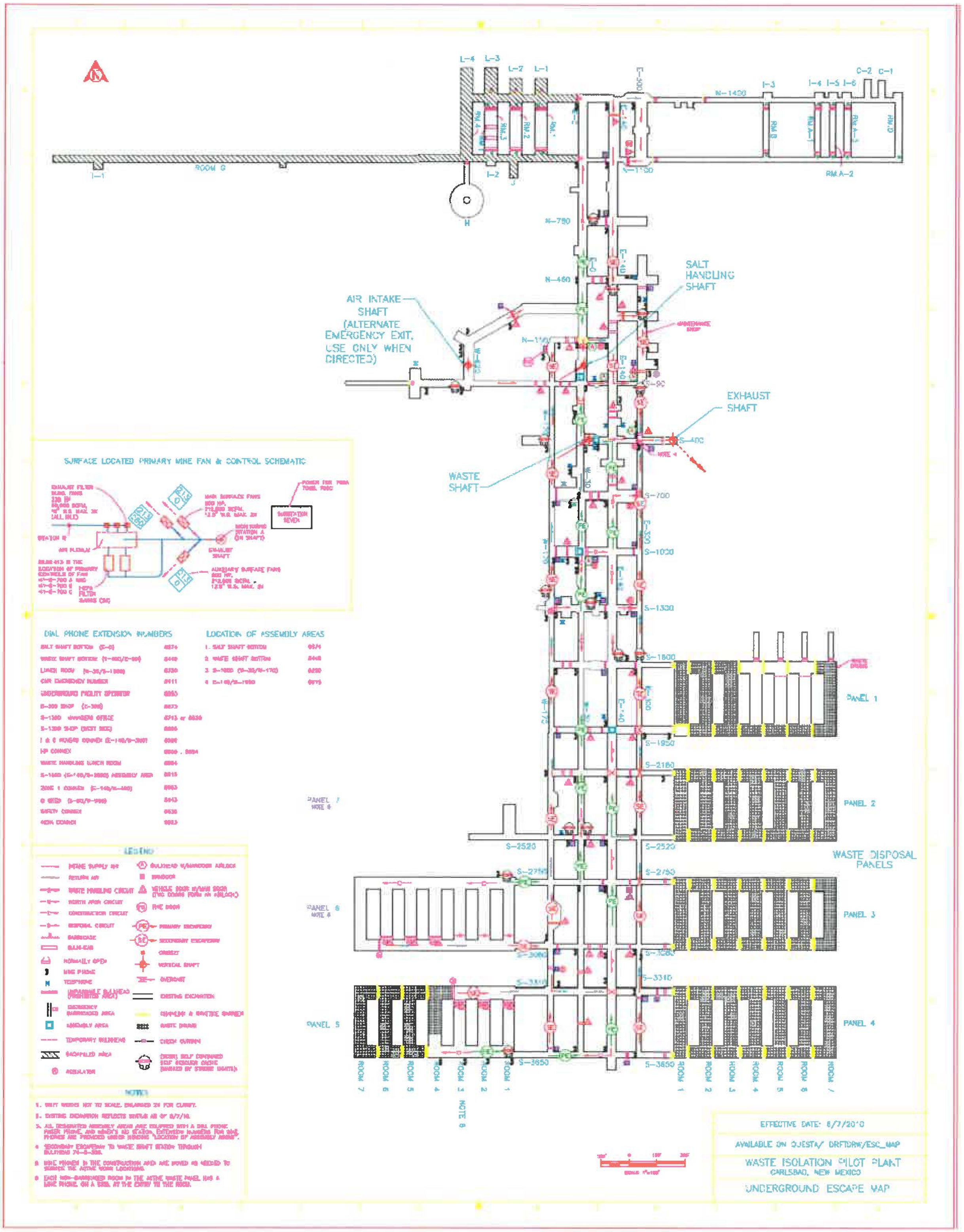


Figure 8-1: WIPP Map with Dimensions

9 APPENDIX B – FORTRAN PROGRAMMING DEVELOPED TO PROCESS DBR CALCULATION RESULTS

The following programs access data files that contain predicted DBR volumes that are output from the DBR BRAGFLO calculation process. The statistical calculations performed are a count of the number of DBR volumes that are greater than 1.0E-7, the maximum, and average DBR volumes for each scenario-time-location combination. The Fortran was validated by selecting the S2-DBR scenario, lower intrusion, at 10,000 years and manually cutting a pasting results from all 3 replicates into Excel. The count, maximum, and average values calculated using Excel tools exactly matched those calculated by the Fortran program. Table 9-1 below presents the comparison.

Table 9-1: Comparison of statistics from Excel calculation and Fortran calculation.

	Statistics for all 3 replicates of scenario S2-DBR, lower intrustion, at 10,000 years	
	values generated with Excel	**values calculated from Fortran code**
maximum	48.21548	48.21548
average	5.6387628	5.63876
#>1.0E-7	137	137

Another subroutine orders the DBR volumes from smallest to largest and saves the table of ordered volumes. This was validated by noting that the values were the same for the ordered and unordered numbers, the total number of values were the same, and the values were correctly ordered.

```
      PROGRAM TEST2
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      parameter (nruns=234)
      double precision max,avg
      DIMENSION DBRVOL(nruns,300)
      INTEGER REPLI, SCENARIO, TIME, CAVITY, COUNT,nznum,nruns,jlim,j
      CHARACTER INFILE1*48, INFILE*69, OUTFILE*49,
     1      REP*1, SCEN*1, TIM*5, CAV*1,
     2      TIME1(6)*5, TIME2(5)*5, TIME3(5)*5,CAVI(3)*1,
     3      LABEL(nruns)*11

      DATA TIME1 /'00100','00350','01000','03000','05000','10000'/
      DATA TIME2 /'00550','00750','02000','04000','10000'/
      DATA TIME3 /'01200','01400','03000','05000','10000'/
      DATA CAVI /'L','M','U'/

c     call filefix
c     stop
```

```
      jlim = 100
      REP  = '0'
      SCEN = '0'
      TIM  = '00000'
      CAV  = '0'
      COUNT  = 0
      INFILE1 = '../../../../pabc2009/sum/sumtbl/SUM_DBR_pabc09_R'
      OUTFILE = '../../../../pabc2009/sum/out/DBR_SUM_pabc09.OUT'
      OPEN (UNIT=21,FILE=OUTFILE,STATUS='unknown',RECL=8000)
      open (unit = 23,file='../../../../pabc2009/sum/out/stats.txt',
     $ status='unknown')
      write(23,*)'scenario time cavity num>0 max avg'
      REPLI = 1
c 10   REPLI = REPLI + 1
c      IF (REPLI .Ge. 4) GOTO 70
      WRITE (REP,'(I1)') REPLI
      SCENARIO = 0
20    SCENARIO = SCENARIO + 1
c      IF (SCENARIO .GT. 5) GOTO 10
      if(scenario .gt. 5) goto 70
      WRITE (SCEN,'(I1)') SCENARIO
      TIME = 0
30    TIME = TIME + 1
      IF (SCENARIO .EQ. 1) THEN
        IF (TIME .GT. 6) GOTO 20
        TIM = TIME1(TIME)
      END IF
      IF (SCENARIO .EQ. 2) THEN
        IF (TIME .GT. 5) GOTO 20
        TIM = TIME2(TIME)
      END IF
      IF (SCENARIO .EQ. 3) THEN
        IF (TIME .GT. 5) GOTO 20
        TIM = TIME3(TIME)
      END IF
      IF (SCENARIO .EQ. 4) THEN
        IF (TIME .GT. 5) GOTO 20
        TIM = TIME2(TIME)
      END IF
      IF (SCENARIO .EQ. 5) THEN
        IF (TIME .GT. 5) GOTO 20
        TIM = TIME3(TIME)
      END IF
      CAVITY = 0
40    CAVITY = CAVITY + 1
      IF (CAVITY .GT. 3) GOTO 30
```

```
      CAV = CAVI(CAVITY)
      COUNT  = COUNT + 1
      LABEL(COUNT) = 'R'//REP//'S'//SCEN//'T'//TIM//CAV
      J = 1
      jlim = 100
      repli = 1
      WRITE (REP,'(I1)') REPLI          !
 41   INFILE = INFILE1//REP//'_S'//SCEN//'_T'//TIM//'_'//CAV//'.TBL.1'
      WRITE (*,*) INFILE
      OPEN (UNIT=20,FILE=INFILE,STATUS='OLD',READONLY)
      READ(20,*)
      READ(20,*)
      READ(20,*)
      READ(20,*)
50    IF (J .LE. jlim) THEN
        READ (20,*) I,T,DBRVOL(COUNT,J)
        J = J + 1
        GOTO 50
      END IF
      CLOSE (20)
      if(repli .eq. 3) goto 42
      repli = repli + 1                 !
      jlim = repli * 100
      WRITE (REP,'(I1)') REPLI          !
      goto 41
 42   call stats(count,nznum,max,avg,dbrvol)
      write(23,'(3a7,i6,2f10.5)')scen,tim,cav,nznum,max,avg
      GOTO 40

70    WRITE (21,'(78(A13))')  (LABEL(I), I=1,COUNT)
      J = 1
60    IF (J .LE. 300) THEN
        WRITE (21,'(78(E13.3))')  (DBRVOL(I,J), I=1,COUNT)
        J = J + 1
        GOTO 60
      END IF
      CLOSE (21)
      close(23)
      END

      subroutine stats(count,nznum,max,avg,dbrvol)
      parameter (nruns=234)
      parameter (nvectors=300)
      double precision dbrvol(nruns,nvectors),vol,sum,max,avg,
     $ darray(nvectors)
      integer i,j,count,nznum,nruns,nvectors
```

```
      integer COUNTS,NCOMP,NSWAP
c initialize
      nznum = 0
      sum = 0.0d0
      max = 0.0d0
      do j=1,nvectors
        darray(j)=dbrvol(count,j)
      enddo
      call SORT1(darray,nvectors,COUNTS,NCOMP,NSWAP)
      max = darray(nvectors)
      do j=1,nvectors
        dbrvol(count,j) = darray(j)
        vol=dbrvol(count,j)
c         write(*,*)j,vol
        if(vol .gt. 1.d-7) then  ! 1.d-7 comes from PABC09 DBR analysis report tables
          nznum = nznum + 1
          sum = sum + vol
        endif
      end do
      avg = sum / dble(nvectors)
c       write(*,'(3a7,i6,2f10.5)')scen,tim,cav,nznum,max,avg
      return
      end

      SUBROUTINE SORT1(LIST,N,COUNTS,NCOMP,NSWAP)
      IMPLICIT NONE
      double precision  LIST(300),m
      INTEGER N,COUNTS,NCOMP,NSWAP
      INTEGER :: I,J,K
c       PRINT 18
c  18  FORMAT(' SORTING'/)
      NCOMP=0
      NSWAP=0
      DO I=1,N-1
        DO J=I+1,N
          NCOMP=NCOMP+1
          IF(LIST(I).GT.LIST(J)) THEN
            M=LIST(i)
            LIST(i)=LIST(j)
            LIST(j)=M
            NSWAP=NSWAP+1
          ENDIF
        END DO
c         PRINT 16,(LIST(K),K=1,N)
c  16     FORMAT(20I5)
      END DO
```

```
RETURN
END SUBROUTINE SORT1
```

Following subroutine reformats data to facilitate data processing.

```
subroutine filefix
real a2,a3,a4,a5,a6
character*120 cline
integer a1,i,iv
open(unit=1,file='../../../brnvol/input_pc3r_r1_s2_t00550.tbl.1
$',status='old')
open(unit=2,file='../../../brnvol/input_pc3r_r1_s2_t00550.txt',
$ status='unknown')
read(1,'(a120)')cline
write(2,'(a120)')cline
read(1,'(a120)')cline
write(2,'(a120)')cline
do i=1,100
 read(1,*)
 read(1,*)a1,a2,a3,a4,a5,a6
 write(2,'(i15,5e15.7)')a1,a2,a3,a4,a5,a6
enddo
close(1)
close(2)
return
end
```