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Subject: Update of the minimum brine volume for a direct brine release and new maximum Castile and Salado brine volumes in a waste panel

Executive Summary

The minimum brine volume in the repository for a direct brine release was updated to incorporate the results from the 2004 Compliance Recertification Application (CRA-2004) Performance Assessment Baseline Calculation (PABC). The calculated volume increased by ~37% to a value of 13,746 m^3. The maximum volume of brine in the intruded waste panel was determined for each scenario and replicate from the CRA-2004 PABC results. A maximum value of 13,267 m^3 was calculated for the Castile brine scenarios, while a maximum value of 7,763 m^3 was calculated for Salado brine scenarios.

Introduction

The concentration of various constituents in brine is used as an input for the actinide solubility calculation for the Waste Isolation Pilot Plant (WIPP) Performance Assessment (PA). With known quantities of the various constituents, the concentration is based on the volume of brine into which the constituents dissolve. The minimum volume of brine required to be in the repository in order for a direct brine release (DBR) to occur is a conservative estimate, since larger volumes would dilute the constituents and lower the actinide solubility. This calculation was performed using the results from the 2004 Compliance Recertification Application (CRA-2004) (Stein, 2005). As a result of technical interactions with the Environmental Protection Agency (EPA), a new BRAGFLO analysis was run, which is now the new BRAGFLO baseline following recertification (Nemer and Stein, 2005). This analysis was called the 2004 Compliance Recertification Application (CRA-2004) Performance Assessment Baseline Calculation (PABC). The purpose of this memo is to follow the same procedure used by Stein (2005) and incorporate any changes that arose from the CRA-2004 PABC. The maximum brine volume that could be present in a waste panel at any time in the repository would be used as an upper bound and a check on the sensitivity to the brine volume used in the calculations.

Consolidated Void Volume

As recommended in Stein (2005), the lowest pressure realization at 10,000 years from the WIPP PA realizations is used to determine the void volume. This is conservative, since it will result in the lowest void volume that is predicted in the PA. An examination of the CRA-2004 PABC BRAGFLO variable WAS_AREA:WAS_PRES for all three replicates (R1, R2 and R3) of the undisturbed scenario (S1), found a minimum pressure value of 6.183 MPa for vector 22 of replicate 1 at 10,000 years (Nemer and Stein, 2005). The pressure values were obtained from the ALG2_BF_CRA1BC_RxS1_Vzzz.CDB (300 files), where R is the replicate and x = 1, 2 or 3 and V is vector where zzz = 001 to 100. These files are located in CMS libraries, LIBCRA1BC_BFR1S1, LIBCRA1BC_BFR2S1 and LIBCRA1BC_BFR3S1 (Long and Kanney, 2005).

The minimum pressure of 6.183 MPa is ~48% higher than the minimum pressure from the CRA-2004 PA results (4.171 MPa). This appears to be caused by the increase in the microbial gas generation probability included in the CRA-2004 PABC. The probability of microbial gas generation was increased from 50% to 100% for the CRA-2004 PABC (Nemer and Stein, 2005). This would have a larger effect on the lower pressure realizations than on the higher pressure realizations.

Following the procedure in Stein (2005), the results from SANTOS were used to determine the void volume that is associated with the minimum pressure from the BRAGFLO results. Table 1 shows the SANTOS results at 10,000 years for the pressure and void volume versus f-Factor (SNL, 1996). These results were not changes from the CRA-2004 to the CRA-2004 PABC and are the same results that were used previously to calculate the void volume (Stein, 2005).

Table 1. SANTOS Results at 10,000 years for Pressure and Void Volume versus f-Factor (SNL, 1996).

f-Factor	Pressure (MPa)	Void Volume (m^3)
0.025	P_1=2.825	V_1=240.3
0.05	P_2=4.371	V_2=310.6
0.1	P_3=6.382	V_3=425.4
0.2	P_4=9.158	V_4=593.0

To choose an appropriate void volume (V) associated with the lowest pressure from PA (P = 6.183 MPa), the linear interpolation used is shown below:

$$V = V_2 + \frac{(P - P_2)(V_3 - V_2)}{(P_3 - P_2)} = 310.6 + \frac{(6.183 - 4.371)(425.4 - 310.6)}{(6.382 - 4.371)} = 414.0m^3.$$

This void volume is ~37% higher than the value calculated from the CRA-2004 results (301.5 m^3).

Number of Equivalent Rooms in the Repository

The volume of the waste-filled region of the repository is equivalent to a certain number of room volumes times the waste-filled region of a room. As recommended in Stein (2005), this number of equivalent rooms is determined by the total excavated volume divided by the excavated volume of a single room. The excavated volume of the waste-filled region of the repository is stored in the WIPP parameter database as REFCON:VREPOS (4.3840608×10^5). The volume of a single room is stored in the parameter database as REFCON:VROOM (3.6443780×10^3). These parameters did not change from the CRA-2004 to the CRA-2004 PABC. The number of equivalent rooms in the repository is:

$$\frac{REFCON:VREPOS}{REFCON:VROOM} = \frac{4.3840608 \times 10^5}{3.6443780 \times 10^3} = 120.3$$

which is the same value as calculated in Stein (2005).

Minimum Brine Saturation

In order for a DBR release to occur, the brine saturation in the repository must be above the sampled residual brine saturation for the waste (WAS_AREA:SAT_RBRN). As recommended in Stein (2005), the median value of the WAS_AREA:SAT_RBRN parameter (0.276) is a reasonable lower end estimate. This parameter did not change from the CRA-2004 to the CRA-2004 PABC.

Minimum Brine Volume

Using the parameter values discussed above for consolidated void volume, number of equivalent rooms in the repository and minimum brine saturation, a reasonable minimum volume of brine in the repository required for a DBR is:

$$414.0 \times 120.3 \times 0.276 = 13{,}746 \text{ m}^3$$

A comparison of the parameters from the CRA-2004 results versus the CRA-2004 PABC is shown in Table 2, with the differences italicized.

Table 2. Comparison of the parameters from the CRA-2004 results versus the CRA-2004 PABC.

Parameter	CRA-2004	CRA-2004 PABC
Minimum BRAGFLO Pressure	4.171 (MPa)	*6.183 (MPa)*
Void Volume	301.5 (m^3)	*414.0 (m^3)*
REFCON:VREPOS	4.3840608×10^5 (m^3)	4.3840608×10^5 (m^3)
REFCON:VROOM	3.6443780×10^3 (m^3)	3.6443780×10^3 (m^3)
# of Rooms in Repository	120.3	120.3
Minimum Brine Saturation	0.276	0.276
Minimum DBR Volume	10,011 (m^3)	*13,746 (m^3)*

As seen in Table 2, the minimum brine volume for a DBR is ~37% higher compared with the value from the CRA-2004 (10,011 m^3), which arose from the higher void volume. The higher minimum pressure from the CRA-2004 PABC results versus the CRA-2004 results produced the higher calculated void volume. The higher minimum brine volume for a DBR is likely to result in lower actinide solubilities.

Maximum Brine Volume in a Panel

Brine may enter the repository from three sources. Under all scenarios, Salado brine may flow from the surrounding Salado into the repository. In scenarios with a borehole, brine may flow down from the Rustler and Dewey Lake formations. In scenarios when the Castile brine reservoir is hit, brine from the Castile may flow up the borehole into the repository. The composition of the brines changes as they react with the surrounding Salado minerals and approach the composition of the Salado brine with more time and mixing. Given the uncertainties in composition, scenarios in which a borehole penetrates the Castile brine reservoir use the properties of the Castile brine and the properties of the Salado brine are used where it does not (see Appendix SOTERM 7.1.2, U.S. DOE, 1996). Intrusions where the Castile brine reservoir is hit are labeled E1, while intrusions that do not are labeled E2. The time and type of the intrusion in the six BRAGFLO scenarios are shown in Table 3. Scenarios S2, S3 and S6 have an E1 intrusion and so, the properties of the Castile brine are used. The scenarios S1, S4 and S5 do not have an E1 intrusion and therefore, the properties of the Salado brine are used for these scenarios. Hence, to establish the maximum Castile brine volume in a panel, the maximum value at any time for the S2, S3 and S6 scenarios was used and the maximum value at any time for the S1, S4 and S5 scenarios was used to ascertain the maximum Salado brine volume in a panel.

To determine the maximum brine volume in a panel, the BRAGFLO variable BRVOL_W of the CRA-2004 PABC was examined at each year, for all three replicates (R1, R2 and R3) and all six scenarios (S1-S6). Table 3 is a summary of the maximum for each scenario. The values were obtained from ALG2_BF_CRA1BC_RxSy_Vzzz.CDB (1800 files), where R is the replicate and x = 1, 2 or 3, S is the scenario where y = 1 to 6, and V is vector where zzz = 001 to 100. These files are located in CMS libraries, LIBCRA1BC_BFRxSy (Long and Kanney, 2005).

As seen in Table 3, for the S2, S3 and S6 scenarios the maximum value for each replicate is reached in the given vector shortly after the E1 intrusions, except for the replicate 3 of the S6 scenario, where in vector 15, the maximum was reached 6,197 years (4,197 years after the E1 intrusion). The maximum volume of Castile brine present in a panel at any time is 13,267 m^3. The maximum brine volume in the intruded panel is the highest at 10,000 years for the S1, S4, and S5 scenarios in the given vectors for each replicate. The maximum volume of Salado brine present in a panel at any time would be 7,763 m^3.

Table 3. Maximum Brine Volume in the Intruded Panel for each Scenario and Replicate from the CRA-2004 PABC.

Scenario	Intrusion Type, Time	Maximum Brine Volume (m^3)	Replicate	Vector	Time (year)
1	None	7,746	1	16	10,000
		7,413	2	53	10,000
		6,763	3	35	10,000
2	E1 @ 350 years	13,267	1	93	354
		13,264	2	35	353
		12,882	3	77	352
3	E1 @ 1,000 years	8,856	1	93	1,002
		8,648	2	35	1,002
		8,881	3	68	1,200
4	E2 @ 350 years	7,522	1	16	10,000
		7,723	2	53	10,000
		6,699	3	35	10,000
5	E2 @ 1,000 years	7,521	1	16	10,000
		7,763	2	53	10,000
		6,700	3	35	10,000
6	E2 @ 1,000 years followed by an E1 @ 2000 years	8,744	1	93	2,003
		8,765	2	74	2,041
		8,772	3	15	6,197

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