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subject: Estimate of volume of brine in repository that leads to a brine release

Introduction

Analysis plan AP-120 guides calculations to determine actinide (An) solubilities for use in the An source term for the U.S. Department of Energy's (DOE's) Waste Isolation Pilot Plant (WIPP) Performance Assessment Baseline Calculation (PABC). This memorandum completes part of task 7.1 described in the AP, namely, a reevaluation of the minimum volume of brine necessary to be in the repository in order that brine release from the repository can occur.

The potential concentration of organic ligands in brine present in WIPP disposal rooms is used as an input in the calculations of actinide solubilities for the WIPP Performance Assessment (PA). Since the total amount of organic ligands in the WIPP waste inventory is assumed to be known, it is necessary to determine the volume of brine into which these ligands are assumed to dissolve. To add additional conservatism to this calculation, a reasonable estimate of the minimum volume of brine required to be in the repository in order that a brine release would occur is needed. This approach is considered conservative because assuming larger volumes of brine in the repository could dilute ligand concentrations and therefore reduce actinide solubilities.

Background

Prior to the 1996 Compliance Certification Application (CCA), this estimate was provided in a memo by Kurt Larsen (Larsen, 1996). In his memo, Larsen estimated that brine saturations would have to exceed 0.75 in a waste panel for any brine to be released up a borehole. In order to estimate a minimum volume of brine in the repository he used predictions of the void volume in a disposal room with no gas generation at 2,000 years made by Stone and reported in a memo to Butcher (Stone, 1992). This memo is included in an appendix of a SAND report by Freeze and others (1995). This void volume prediction used structural calculations that predated those used in the CCA (Stone 1997a,b). From those older calculations, the consolidated void volume of a single waste room at 2,000 years with no gas generation was 343 m^3. Based on excavated volume estimates for a single room and the whole repository[1], the

[1] Larsen included a table with the following quantities: Excavated volume of a room = 3644 m^3, of a exterior panel = 46100 m^3, of the waste region (not including panel closures) = 420881 m^3. From these values he calculated room equivalents for the exterior panel (46100/3644 = 12.65) and the waste region (42088/3644 = 116).

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consolidated void volume for a single room, and the minimum brine saturation of 0.75, Larsen calculated a minimum brine volume in the repository as:

343 m^3 x 116 equivalent room volumes in repository x 0.75 = **29,841 m^3**

New Information

Since Larson's memo, new information is available and several important changes have been made to the way the repository is modeled by performance assessment (PA). Thus, an updated estimate is needed. The following new information and changes should be considered when updating the minimum brine volume estimate:

1. The structural modeling results used in Larsen's calculation preceded the final calculations that were used in the CCA PA (Stone, 1997a, b). Therefore, it is appropriate to review and update the minimum brine volume calculations so they are based on the actual structural results used by the current PA analysis.
2. Larson's approach used consolidated void volume results from structural simulations that only lasted 2,000 years and did not include any gas generation. In WIPP PA, all realizations run for 10,000 years and produce varying amounts of gas. Therefore, it is appropriate to consider these factors for the updated estimate.
3. Errors were discovered in the original excavated volume calculations made for the CCA and used to develop the BRAGFLO grid. These errors resulted in the volume of the waste filled-portion of the repository to be slightly underestimated in the CCA and PAVT (Stein, 2002). Correction of these errors resulted in a change to the parameter: REFCON:VREPOS for the 2004 Compliance Recertification Application (CRA) PA. Therefore, it is appropriate to update the minimum brine volume calculations so they are based on the current and corrected waste-filled repository volume.
4. The original estimate of a minimum brine saturation of 0.75 required for a brine release is inconsistent with the conceptual model for direct brine release (DBR), which allows the possibility of a brine release as long as both pressure is above hydrostatic (~8 MPa) and brine saturation is above the residual saturation of the waste (WAS_AREA:SAT_RBRN). Therefore, it is appropriate to update the minimum brine volume calculations so that they are consistent with the conceptual model for DBR.

New Method

The new information and changes listed above necessitate updating the method used to determine the minimum volume of brine required for a brine release to occur.

Consolidated Void Volume

The original estimate of the consolidated room volume of 343 m^3 was derived from structural simulations run for only 2,000 years. The structural models that support the CCA (and 2004 CRA) were run for the full compliance period of 10,000 years. Figure 1 shows the predicted value of total void volume in a waste room as a function of time for the case run with no gas generation. Note that void volume decreases more quickly than in the earlier analysis used by Larsen, falling to 216 m^3 at 2,000 years and reaching 169 m^3 by 10,000 years. However, because all WIPP PA realizations produce gas it is not

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appropriate to used structural modeling results based on no gas generation. Instead, I recommend finding the void volume which results from the lowest pressure realization at 10,000 years. This is conservative, since it will result in the lowest void volume that is predicted in PA. An examination of the BRAGFLO variable WAS_AREA:WAS_PRES for the 2004 CRA Replicate 1 undisturbed scenario (S1), found that vector 21 had the lowest pressure at 10,000 years ($P = 4.171$ MPa)[2]. In support of the CCA, SANTOS was run for thirteen separate gas generation rates (f-factors), which are then processed and interpolated on to calculate porosity in BRAGFLO. An examination of the SANTOS results (SNL, 1996) at 10,000 revealed that two of the F-factor scenarios bracket this minimum pressure, $f = 0.025$ and $f = 0.05$. Table 1 lists the pressures and void volumes for these SANTOS runs at 10,000 years.

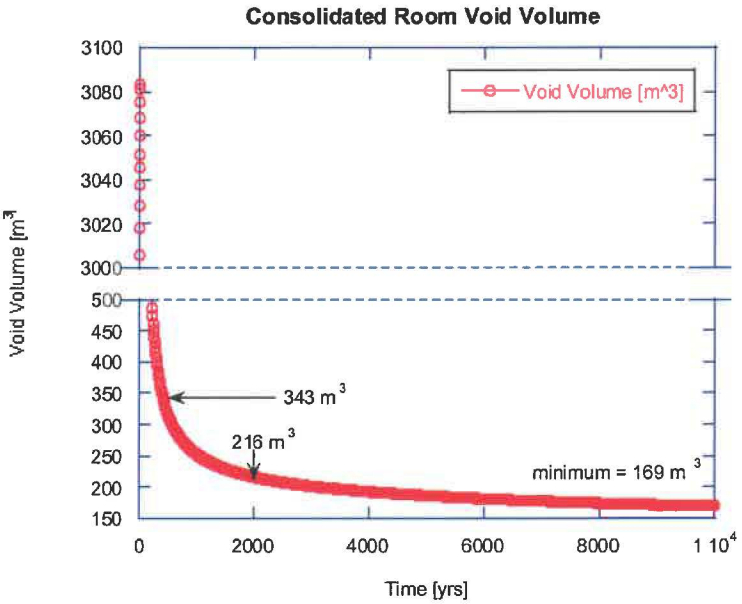


Figure 1. SANTOS predicted room void volumes assuming no gas generation ($f = 0$). This calculation is part of the suite used for the CCA and 2004 CRA (data from SNL, 1996).

Table 1. SANTOS results for pressure and void volume

f-Factor	Time [yrs]	Pressure [MPa]	Void Volume [m^3]
0.025	10,000	$P_1 = 2.825$	$V_1 = 240.6$
0.05	10,000	$P_2 = 4.371$	$V_2 = 310.6$

To choose an appropriate void volume (V) associated with the lowest pressure observed in PA (P), it is reasonable to do a linear interpolation as follows:

$$V = V_1 + \frac{(P - P_1)(V_2 - V_1)}{(P_2 - P_1)} = 301.5 \text{ m}^3$$

Equivalent Room Volume of Repository

The volume of the waste–filled region of the repository is equivalent to a certain number of room volumes. This number of equivalent rooms is determined by the total excavated repository volume divided by the excavated volume of a single room. The excavated volume of the waste filled regions of

[2] Data obtained from CMS library:LIBCRA1_BFR1S1

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the repository is stored in the WIPP parameter database as REFCON:VREPOS. The current value for this parameter is 4.3840608 x 10^5 m^3. This volume does not include the panel closures and is therefore appropriate to use in the present calculation of equivalent number of rooms present in the repository. The volume of a single room is stored in the parameter database as REFCON:VROOM, which has a value of 3.6443780 x 10^3 m^3. Therefore the number of equivalent rooms in the repository is:

$$\frac{4.3840608\times10^{5}}{3.6443780\times10^{3}}=120.3$$

Minimum Brine Saturation

In order that a DBR release can occur, the brine saturation in the repository must be above the sampled residual brine saturation for the waste (WAS_AREA:SAT_RBRN). This parameter is sampled from a uniform distribution between 0.0 and 0.552. The median value of this distribution (0.276) is a reasonable lower end saturation for the purposes of the present estimate. This choice is reasonable and appropriate for several reasons. First, an examination of DBR releases as a function of brine saturation (Figure 2) shows that although non-zero volume releases can occur at saturations below this median value, the volume released does not become significant until brine saturation exceeds approximately 0.3. The S2 lower intrusion scenario results in the greatest frequency of DBR releases and is therefore a scenario for comparison. Other scenarios would have far fewer releases. It would be unreasonable to use the minimum of the SAT_RBRN distribution because no PA realizations sample this value, this value is not representative of any natural porous materials, and would falsely seem to suggest that brine release is possible at any brine saturation within the waste, which is simply not true. Selecting the median of the distribution for SAT_RBRN is appropriate for the reasons given above and is conservative relative to the values used since the CCA.

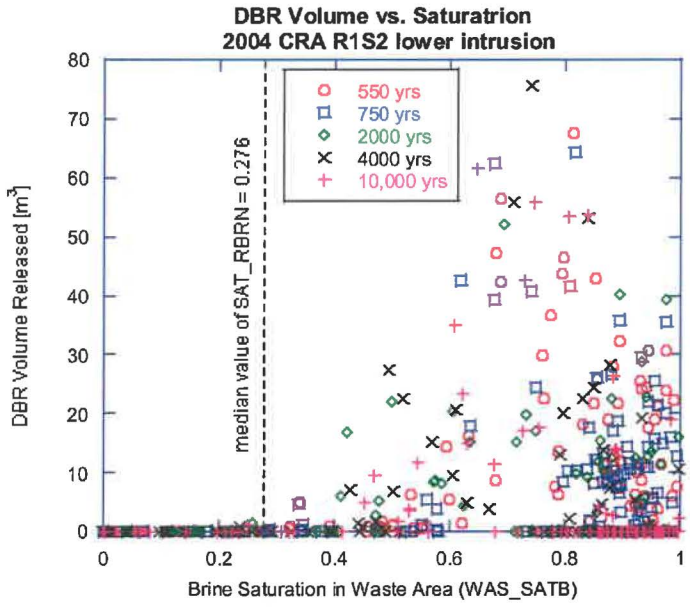


Figure 2. Scatter plot of DBR volume released vs. brine saturation in the waste panel. Significant brine volumes released occur at saturations above median value for parameter SAT_RBRN.

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Results

If we assume appropriate values detailed above for consolidated void volume, equivalent room volume of repository, and minimum brine saturation, we calculate a reasonable minimum volume of brine in the repository required for a brine release to be:

$$301.5\ m^3 \times 120.3 \text{ equivalent room volumes in repository} \times 0.276 = \mathbf{10{,}011\ m^3}$$

Compared with Larson's estimate of 29,841 this value is approximately a factor of three less and therefore is likely to result in higher actinide solubilities compared with the CCA and 2004 CRA. Therefore, compared with the volume used for the CCA and 2004 CRA, this updated value is more conservative in terms of repository performance.

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