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subject: Expected Brine volumes, Cumulative Brine Inflow, and MgO-to-Brine Solid-to-Liquid Ratio from PABC BRAGFLO Results

This memo reports the volume of brine in a Waste Panel at various times, as predicted by the Performance Assessment Baseline Calculation (PABC) (Nemer and Stein, 2005). This information may be used to determine several solid-to-liquid ratios including MgO, Iron, and Lead to brine solid-to-liquid ratios. These ratios may be important parameters to consider when writing test plans (TP) on Iron chemistry and MgO chemistry. This memo is thus programmatic and not compliance driven.

The brine volumes in the Waste Panel and cumulative brine flow into the Waste Panel were extracted from BRAGFLO simulation results obtained during the Performance Assessment Baseline Calculation (PABC) (Nemer and Stein, 2005). The brine volumes were obtained from the ALGEBRA2 output variable BRNVOL_W. The variable BRNVOL_W was extracted at all times, except t = 0, from scenarios S2, S4 and S6. Scenario S2 corresponds to a repository which is intruded at 350 years by a drilling intrusion that encounters a Castile brine pocket, Scenario S4 corresponds to a repository which is intruded at 350 years by a drilling intrusion that does not encounter a Castile brine pocket, Scenario S6 corresponds to a repository which is intruded at 1000 years by a drilling intrusion that does not encounter a Castile brine pocket, followed by a drilling intrusion at 2000 years that does encounter a Castile brine pocket (Nemer and Stein, 2005). The ALGEBRA2 variables were extracted from BRAGFLO ALG2 CDB files which are located in CMS library LIBCRA1BC_BFRrSs, where r = 1, and s = 2,4,6, class CRA1BC-0, on the PA computer cluster. More details on these files can be found in Nemer and Stein (2005).

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Brine volumes are shown in Table 1 at various percentiles, with the lowest percentile corresponding to the least brine and the highest percentile corresponding to the most brine. The percentile was determined using the Microsoft Excel function PERCENTILE; PERCENTILE takes a desired percentile (from 0 to 1) and a list of numbers as arguments. For a desired percentile, Microsoft Excel will interpolate between two values if necessary.

Table 1. Ranked Brine Volumes in the Waste Area Obtained from PABC BRAGFLO Simulations.

Percentile (0 to 1)	Scenario S2 Brine volume (m^3)	Scenario S4 Brine Volume (m^3)	Scenario S6 Brine Volume (m^3)
0.001	$8x10^1$	$5x10^{-2}$	$4x10^{-2}$
0.01	$4x10^2$	$3x10^{-1}$	$5x10^{-1}$
mean	$5x10^3$	$1x10^3$	$3x10^3$
0.99	$1x10^4$	$6x10^3$	$7x10^3$
0.999	$1x10^4$	$7x10^3$	$8x10^3$

The MgO-to-liquid ratio can be calculated given the total mass of MgO. The mass of MgO that is assumed to be emplaced in each panel is calculated by assuming one mol of MgO is emplaced per mole of organic carbon (although currently 1.6 mol of MgO is being emplaced per mole of organic carbon). Since there is at most $1.1x10^9$ mol of organic carbon due to CPR materials (Nemer and Stein, 2005) and there are 10 panels in the repository, the mass of MgO in a single panel is

$$m_{MgO} = 40.3 g/mol \times \frac{1.1\times10^{9} molC}{10 panels} = 4.43\times10^{9} g\, MgO/panel, \quad (1)$$

where 40.3 g/mol is the molecular weight of MgO. Converting the numbers in Table 1 to ml (10^6 ml/m^3) and dividing m_{MgO} by this volume yields the solid-to-liquid ratios given in Table 2, with the percentiles given from Table 1.

While Table 2 gives the range of possible solid-to-brine ratios, for repository performance a more applicable solid-to-liquid ratio is given by the total mass of MgO to be emplaced in the repository divided by the minimum brine volume needed for an actual release of brine to the surface. Stein (2005) has shown that the minimum brine volume needed for a Direct Brine Release is 10,011 m^3 for the entire repository. Since a single waste panel corresponds to approximately 1/10 the volume of the entire repository, we estimate the minimum brine volume needed for a Direct Brine Release to be 1,001 m^3 for a single waste panel. Given the mass of MgO from equation (1), and 1,001 m^3 of brine per panel, yields a solid-to-liquid ratio of $4x10^0$ g/ml.

The solid-to-liquid ratios can be converted into mole ratios for the purpose of determining whether any liquid water remains after MgO is converted to brucite $Mg(OH)_2$,

$$MgO(s) + H_2O(l,gas) \rightarrow Mg(OH)_2(s). \quad (2)$$

To determine the mass of water per cubic meter of brine we use the average brine density given in the WIPP parameter database (BRINESAL:DNSFLUID) $\rho_{brine} = 1.22\times10^3 kg/m^3$, and the mass of salt per cubic meter in Castile brine (ERDA-6) 305.32 kg/m^3, and Salado brine (GWB) 466.75 kg/m^3. The mass of salts in these two brines can be found in Snider et al., (2004). It follows then that the densities of water in the two brines are

$$\rho_{H2O,ERDA-6} = 915\ kg/m^3, \qquad \rho_{H20,GWB} = 753 kg/m^3. \quad (3)$$

The molar ratio is calculated by

$$x = \left(\frac{1.1\times10^{9} mol\, MgO}{10 panels}\right) \Big/ \left(\frac{\text{Brine Volume}\times\rho_{H2O,BRINE}}{18\times10^{-3}\ kg/mol}\right), \quad (4)$$

where as above we assume one mol of MgO for every mol of organic carbon, $\rho_{H2O,BRINE}$ is equal to $\rho_{H2O,ERDA-6}$ for Scenarios S2 and S6, and is equal to $\rho_{H20,GWB}$ for Scenario S4, and the molecular weight of water is $18x10^{-3}$ kg/mol. The results of this conversion are shown in Table 3. For Stein's minimum brine volume needed for a Direct Brine release (1,001 m^3), the molar ratio using equation (4) is $3x10^0$.

Table 2. Ranked Solid-to-Liquid Ratios in the Waste Area Obtained from PABC BRAGFLO Simulations.

Percentile[1] (0 to 1)	Scenario S2 Solid-to-Liquid Ratio (g/ml)	Scenario S4 Solid-to-Liquid Ratio (g/ml)	Scenario S6 Solid-to-Liquid Ratio (g/ml)
0.001	$6x10^{1}$	$9x10^{4}$	$1x10^{5}$
0.01	$1x10^{1}$	$1x10^{4}$	$9x10^{3}$
mean	$9x10^{-1}$	$4x10^{0}$	$1x10^{0}$
0.99	$4x10^{-1}$	$7x10^{-1}$	$6x10^{-1}$
0.999	$4x10^{-1}$	$6x10^{-1}$	$6x10^{-1}$

1. Percentiles are the carried from Table 1.

Table 3. Ranked Moles of MgO-to-Moles of H_2O Ratios in the Waste Area Obtained from PABC BRAGFLO Simulations.

Percentile[1] (0 to 1)	Scenario S2 Mol MgO-to-Mol H_2O Ratio (mol/mol)	Scenario S4 Mol MgO-to-Mol H_2O Ratio (mol/mol)	Scenario S6 Mol MgO-to-Mol H_2O Ratio (mol/mol)
0.001	$3x10^{1}$	$5x10^{4}$	$5x10^{4}$
0.01	$5x10^{0}$	$9x10^{3}$	$4x10^{4}$
mean	$4x10^{-1}$	$3x10^{0}$	$7x10^{-1}$
0.99	$2x10^{-1}$	$4x10^{-1}$	$3x10^{-1}$
0.999	$2x10^{-1}$	$4x10^{-1}$	$3x10^{-1}$

1. Percentiles are the carried from Table 1.

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