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to: WIPP Records Center

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subject: Update to WIPP PA parameter DBRMINBV

WIPP:4.4.1.2.1:PA:QA-L:578831

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1. Introduction

The WIPP Performance Assessment (PA) code PANEL calculates radionuclide concentrations in brine over a period of 10,000 years after repository closure. The concentrations are determined for 5 distinct volumes of brine, each an integer multiple of a minimum brine volume. With sufficient repository pressure and brine saturation, a Direct Brine Release, or DBR, may occur as the result of a borehole intrusion into a waste panel in the repository. The PA code CCDFGF uses the concentrations PANEL has determined for the 5 brine volumes to interpolate radionuclide concentrations for the volume of brine actually present in the waste panel at the time of the intrusion. The DBR is obtained as the sum of PANEL's interpolated radionuclide concentrations multiplied by the volume of brine that flows from the repository up the borehole to the ground surface.

Parameter GLOBAL:DBRMINBV, just DBRMINBV below, is described in the WIPP parameter database ParamDB as the minimum volume of brine in the repository required for a DBR to occur. DBRMINBV, after being reduced from repository scale to waste-panel scale, is used to set the minimum of the 5 brine volumes used in the PANEL concentration calculations. The remaining brine volumes in the PANEL calculations are simple multiples – 2×, 3×, 4×, and 5× – of the minimum volume. Ideally, DBRMINBV will have been determined so that the resulting 5 brine volumes span the majority of brine volumes actually encountered by a WIPP PA when DBR events occur.

This memo describes an update to the value of DBRMINBV. The update takes advantage of recent results from geomechanical modeling of a WIPP waste disposal room described by Vignes et al. (2023). The geomechanical modeling improves the treatment of waste compaction, gas pressurization, and the geomechanical model itself, producing new predictions of disposal room porosity as a function of time and pressure. Void volume estimated using the new porosity leads to an updated value for DBRMINBV. Memos by Stein (2005), Clayton (2006, 2008), and King (2021) document previous updates to DBRMINBV.

The following sections describe the formula used here to determine DBRMINBV, the choice of parameter values in the formula, the updated value of DBRMINBV, and the 5 PANEL brine volumes that result from the update to DBRMINBV. Lastly, the 5 brine volumes are compared to panel brine volumes encountered in the Replacement Panels Planned Change Request (RPPCR) PA.

2. Formula for DBRMINBV

In the report by Vignes et al. (2023), a single disposal room of a WIPP waste panel is modeled through time as the surrounding salt creeps towards and compresses the waste. Vignes et al. refer to the void volume in the room at a given time as the current gas storage volume V_g; it is obtained as the difference between the current room volume, V_r, and the solid volume, V_{sw}, of the waste inside the room[1]:

$$V_g = V_r - V_{sw} \quad . \tag{1}$$

The Vignes et al. report tabulates room pressure and two forms of room porosity for 10,000 years after closure of the repository. Porosity in the geomechanical model, denoted ϕ_E, is called the Eulerian, or true, porosity, defined as

[1] The volume of solid waste is taken to be constant. The geomechanical model has V_{sw} = 302.4 m^3.

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$$\phi_E = \frac{V_g}{V_r} \quad . \tag{2}$$

Porosity in the waste areas of the PA grid is taken to be the so-called Lagrangian porosity, ϕ_L, given by

$$\phi_L = \frac{V_g}{V_{r0}} \quad , \tag{3}$$

where V_{r0} is the initial room volume in the geomechanical model.[2] The Lagrangian porosity aims to preserve time-varying void volume, as predicted by geomechanics, in the fixed-volume grid used by PA. Vignes et al. tabulate both ϕ_E and ϕ_L, as determined by Eq. 2 and Eq. 3.

The formula used here obtains DBRMINBV as the product of Lagrangian porosity, the excavated storage volume of the repository, V_{repos}, and brine saturation, S_b:

$$\text{DBRMINBV} = \phi_L \, V_{repos} \, S_b \quad . \tag{4}$$

Stein (2005), Clayton (2006, 2008), and King (2021) use the void volume in one room multiplied by the number of rooms in the repository to get a total repository void volume; this is replaced by $\phi_L \times V_{repos}$ in Eq. 4. Note also that void volume in one room is referred to as the "consolidated void volume" in the references cited. The value of V_{repos} is given by database parameter REFCON:VREPOS; for the RPPCR it is 853,284.89 m^3. The next sections discuss the choice of suitable values for S_b and ϕ_L to use in Eq. 4.

3. Brine saturation, S_b

For a DBR to occur, brine saturation in the intruded waste panel must be greater than the residual brine saturation of the waste, that is, the brine must be mobile. Residual brine saturation is a sampled parameter in PA named WAS_AREA:SAT_RBRN, defined in database ParamDB by a uniform probability distribution with minimum value 0, maximum value 0.552, and both median and mean equal to 0.276. Following Stein (2005), Clayton (2006, 2008), and King (2021) the median value of WAS_AREA:SAT_RBRN is chosen as the brine saturation in the determination of DBRMINBV; that is, S_b is set to 0.276 in Eq. 4.

In the RPPCR PA, the largest fraction of non-zero DBR volumes, and the largest mean non-zero release volume, occur at the Lower, or L, intrusion location (Table 3, Docherty and King, 2023). It is also the case in the RPPCR that mean, median, and maximum release volumes are comparable across the five BRAGFLO DBR intrusion scenarios (Figure 8, Docherty and King, 2023). Figure 1 plots non-zero DBR volumes versus brine saturation for all L intrusions in the RPPCR. The red dashed vertical line in the figure indicates a panel brine saturation of 0.276. The figure supports S_b = 0.276 as a reasonable choice, since all significant brine release volumes occur for greater saturations.

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[2] While Vignes et al. do not explicitly give the value of V_{r0}, it can be determined from their Eq. D.1 and the initial porosity in either Table D-1 or Table D-2. The value so obtained is V_{r0} = 3631.56 m^3.

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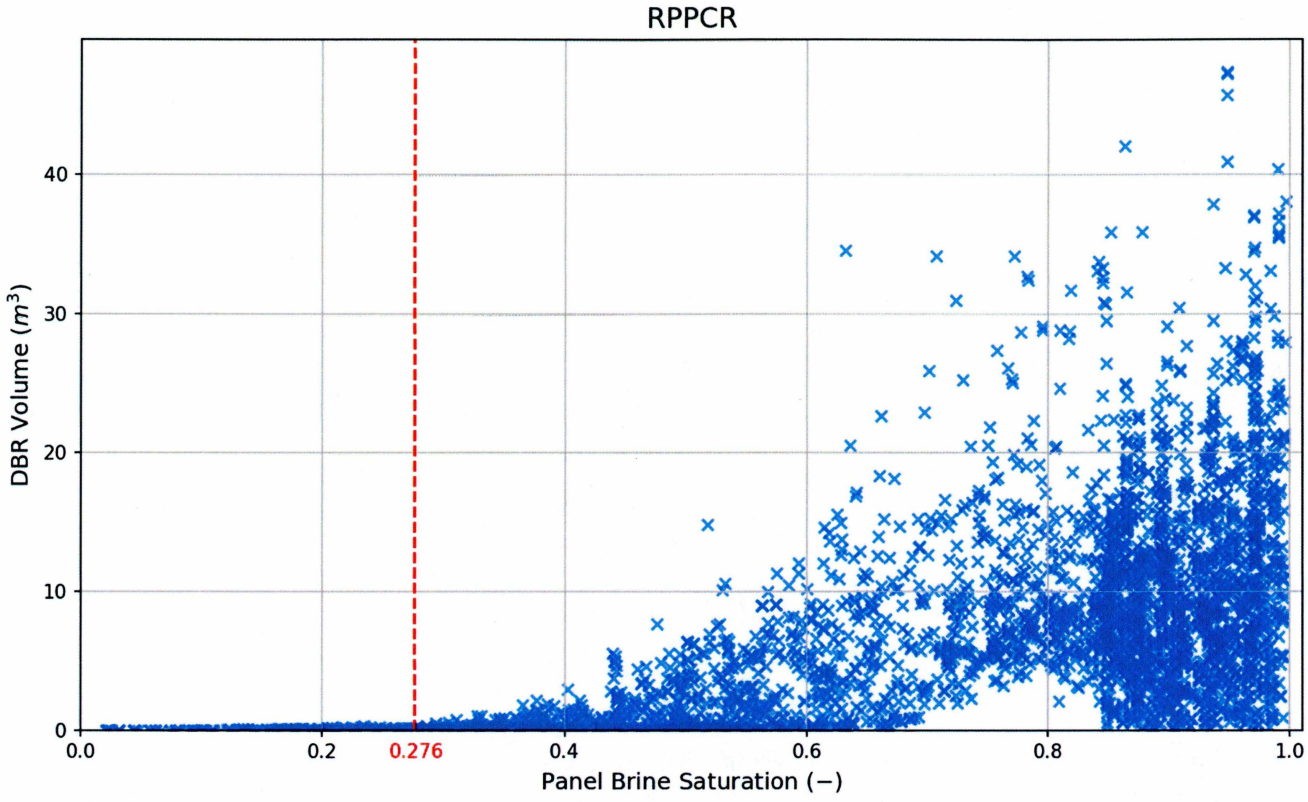

Figure 1: DBR volume versus panel brine saturation at the L intrusion location in the RPPCR. All non-zero DBRs are included for the five intrusion scenarios.

4. Lagrangian Porosity, ϕ_L

For a DBR to occur, a minimum pressure of 8 MPa is required in the repository. Referring to Vignes et al. (2023), their Figure 3-7 and Table D-3 give pressure versus time for a sequence of gas generation factors, f, while their Figure 3-5b and Table D-2 give Lagrangian porosity versus time for the same gas generation factors. Note that Lagrangian porosity is lowest for small gas generation factors, varying little beyond about time 500 years (Figure 3-5b); and that the smallest gas generation factor for which pressure exceeds 8 MPa is $f = 0.025$ near time 10,000 years (Figure 3-7). Pressures from Table D-3 and Lagrangian porosities from Table D-2 for the three smallest gas generation factors, at time 10,000 years, are reproduced below in Table 1:

Gas generation factor f	Pressure (MPa)	Porosity ϕ_L
0	0	0.037745
0.025	8.0364	0.040812
0.05	15.057	0.043572

Table 1: Pressure and Lagrangian porosity at time 10,000 years for gas generation factors 0, 0.025 and 0.05.

Values for $f = 0$ and $f = 0.025$ in Table 1 can be linearly interpolated to obtain the Lagrangian porosity at 8 MPa pressure. The approach is conservative in the determination of DBRMINBV as it produces the lowest Lagrangian porosity at any time for which pressure reaches 8 MPa. (Gas generation factors greater

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than 0.025 cause 8 MPa to be realized at earlier times in the geomechanical model, but with greater values of porosity. See Vignes et al.'s Tables D-3 and D-2.) From Table 1, the interpolated Lagrangian porosity at time 10,000 years is

$$\phi_L = 0.037745 + \frac{(0.040812-0.037745)}{(8.0364-0)} \times 8.0 = 0.040798 \quad . \tag{5}$$

5. New values for DBRMINBV and PANEL's 5 brine volumes

With S_b and ϕ_L chosen as described above, Eq. 4 is evaluated to give the new value of DBRMINBV:

$$\text{DBRMINBV} = 0.040798 \times 853{,}284.89 \times 0.276 = 9{,}608 \ [\text{m}^3] \quad . \tag{6}$$

The new value of DBRMINBV is less than a third of the value, 33,804 m^3, used in the RPPCR. The cause of the change is reduced disposal room porosity in the geomechanical model of Vignes et al. (2023). Previous determinations of DBRMINBV used results from the program SANTOS (Stone 1997) to determine void volume. Most recently, Clayton (2008) and King (2021) used SANTOS results to obtain a room void volume of 523.1 m^3 at 8 MPa pressure; dividing by the excavated volume of a room[3], this is equivalent to a Lagrangian porosity of 0.1435 – about 3.5 times the Lagrangian porosity from the Vignes et al. model.

DBRMINBV is reduced from repository scale to waste-panel scale to set the minimum, b_1, of the 5 brine volumes used in the PANEL radionuclide concentration calculations:

$$b_1 = \text{DBRMINBV} \times \frac{V_{panlex}}{V_{repos}} = 519 \ [\text{m}^3] \quad , \tag{7}$$

where V_{panlex} is the excavated volume of one panel, given by parameter REFCON:VPANLEX as 46097.65 m^3. The remaining brine volumes are obtained as $b_i = i \times b_1$, $2 \le i \le 5$. The 5 brine volumes are: 519, 1038, 1557, 2076, and 2595, all in m^3.

The box plot in Figure 2 shows the volumes of brine actually encountered in the waste panels for all intrusions that led to a non-zero DBR in the RPPCR BRAGFLO DBR simulations. Also plotted, in blue, are PANEL's 5 brine volumes determined as described above. Note that releases occur for panel brine volumes less than b_1, which is a consequence of the probability distribution for parameter WAS_AREA_SAT_RBRN. These releases are, however, small in volume, having a mean of only 0.03 m^3. Figure 2 also shows releases occurring at panel brine volumes greater than volume b_5. Here PANEL will use b_5 rather than the actual panel brine volume in its calculations; the result, if not limited by solubility, will be larger, and thus conservative, estimates of radionuclide concentration.

[3] The volume of one disposal room in the repository is given by parameter REFCON:VROOM as 3644.378 m^3.

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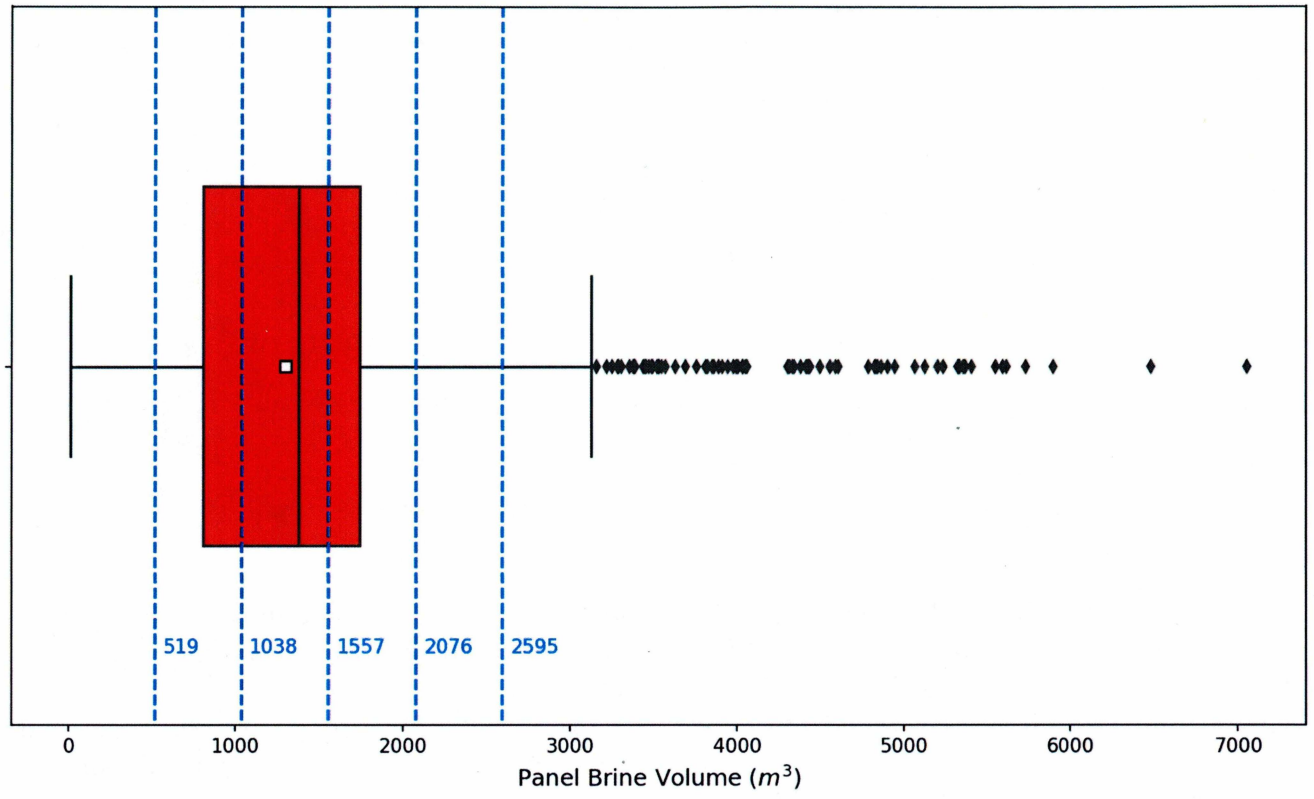

Figure 2: Box plot of panel brine volumes in the RPPCR BRAGFLO DBR simulations. Data are for non-zero DBRs only; all scenarios are included. Shown in blue are the 5 PANEL brine volumes determined from the new value of DBRMINBV. The red box is drawn around the 25th (Q_{25}) and 75th (Q_{75}) percentiles with a bisecting line at the median. The box whiskers extend out from the box to either an additional 1.5(Q_{75} - Q_{25}) or to the full range of the data, whichever is closer to the median. Datapoints outside of the whisker range are marked on the plot with black diamonds. The mean value is marked with a white square on top of the box and whisker plot.*

6. Summary

Recent results from geomechanical modeling give new predictions of porosity in the repository as the surrounding salt encroaches on and compresses the waste over time. The new porosity predictions reduce the void volume used in the calculation of DBRMINBV to about one third of its previous value. The effect on the value of DBRMINBV is to reduce it from 33,804 m^3 to a new value of 9,608 m^3, as indicated in Table 2. Brine volumes used by code PANEL in its concentration calculations, which depend on the value of DBRMINBV, are similarly reduced.

Material	Property	Description	Units	RPPCR Value	New Value
GLOBAL	DBRMINBV	Minimum volume of brine in the repository required for a direct brine release.	m^3	33,804	9,608

Table 2: Updated Value of DBRMINBV.

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7. References

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