546311

Sandia National Laboratories

Operated for the U.S. Department of Energy by

Sandia Corporation

Phone: (505) 234-0013 (Carlsbad)

Fax: (505) 234-0061

Internet: djclayt@sandia.gov

date: June 6, 2007

to: Eric Vugrin, Moo Lee, David Kessel

from: Daniel J. Clayton

subject: Corrections to input files for DBR PABC calculations.

Technical Review: James Garner

Direct Brine Release (DBR) calculations were performed as part of Analysis Plan AP-132 (Vugrin and Nemer, 2007). During file preparation and analysis, two inconsistencies were discovered and corrected. These corrections were made to two input files which are used by the code ALGEBRACDB as part of the DBR calculations. An impact assessment of these changes was conducted using the results from the 2004 Compliance Recertification Application (CRA-2004) Performance Assessment Baseline Calculations (PABC). All files generated, were stored in CMS as outlined in Long and Kanney (2005). To distinguish the new files from the previous files, the new files were assigned the class CRA1BC-1, while the previous files have the class CRA1BC-0. This memo summarizes these corrections and documents the impact on the CRA-2004 PABC DBR analysis. There were no significant changes in the releases due to the corrections.

The first correction is in the CRA-2004 PABC file, ALG2_DBR_CRA1BC_S3.INP, which is contained in the LIBCRA1BC_DBR library. This input file is used to set up the boundary conditions and material properties for the DBR calculations for scenario 3. On line 456, the variable PREV_TIME, which represents the time (in years) of the previous intrusion, is set. This controls the previous intrusion properties as the borehole properties are a function of time. PREV_TIME was given the value of 350 years, when it should have been 1,000 years for scenario 3. This caused the boundary condition to be mistakenly set at the 650 years later value. As time progresses, the contribution from the previous intrusion decreases, so this boundary condition inconsistency could cause the DBR releases to be smaller for the earlier times. The file ALG2_DBR_CRA1BC_S3.INP was changed so that the variable PREV_TIME was assigned the value of 1,000 years. This change only affects the results for scenario 3.

It appears that this inconsistency was introduced in the CRA-2004 calculations, and can be seen in the CRA-2004 file ALG_DBR_CRA1_PRE_DIR_REL_S3.INP, which is contained in the LIBCRA1_ALG library. Examination of line 611 in the file shows the same incorrect variable assignment. For the Compliance Certification Application (CCA) Performance Assessment Verification Test (PAVT), the file ALG_DBR_C97_PRE_DIR_REL_S3.INP, which

WIPP:1.4.1:PA:QA-L:540232

is contained in the LIBC97_ALG library, was used. Examination of line 339 shows the correct variable assignment of PREV_TIME to 1,000 years.

The second correction is in the CRA-2004 PABC file, ALG3_DBR_CRA1BC.INP, which is contained in the LIBCRA1BC_DBR library. This input file is used to post-process the DBR results and calculate the cumulative release. The DBR release is integrated from zero to at least 3 days (parameter BLOWOUT:MINFLOW) or up to 11 days (parameter BLOWOUT:MAXFLOW). This can be seen on lines 54 and 55, where the variable BRIN_REL, which represents the volume of brine released integrated based on the minimum and maximum time, is calculated. The function used to calculate BRIN_REL is IFLT0, which represents the "if less than zero" logic function. The DBR calculations are set to generate results at exactly 11 days, so when ALGEBRACDB is integrating, the results at exactly 11 days are not included in the integration, since the difference between the current time and maximum time is zero, but not "less than zero". To remedy this, a temporary variable TIMEM is used, which is assigned the value of the current time (TIME) minus one second. Using this variable, the results at 11 days are included in the integration, as the difference now is "less than zero". This change increases the calculated DBR volume and can affect the results for all the scenarios. This inconsistency has been in the calculations since the CCA.

Each analysis generated 23,400 separate results for all the replicate-vector-scenario-time-location combinations. To compare the results, some basic statistics for each analysis will be compared, including the number of non-zero, maximum and average DBR volumes by replicate and scenario and are shown in Tables 1-3, respectively. For consistency with the CRA-2004 PABC analysis, non-zero DBR volumes are defined as releases that are greater than 10^{-7} m^3. As seen in Table 1, there are no differences between the number of non-zero DBR volumes between the CRA-2004 PABC and impact analysis for each replicate-scenario combination. Table 2 shows a slight increase in the maximum DBR volume from the CRA-2004 PABC for each combination, with the maximum increase of ~5%. The average DBR volume slightly increased from the CRA-2004 PABC, with a maximum increase of ~3% (Table 3).

The resulting DBR complementary cumulative distribution functions (CCDFs) generated by CCDFGF from both the CRA-2004 PABC and the impact analysis were compared and are shown in Figures 1-3 for replicates 1-3, respectively. As seen in Figures 1-3, the two set of CCDFs are indistinguishable from each other. This shows that there was no significant change in the releases due to the corrections.

Table 1. Number of non-zero DBR volumes calculated for replicates 1-3 (R1-R3) and scenarios 1-5 (S1-S5) for the CRA-2004 PABC and impact analysis.

Scenario	CRA-2004 PABC Impact			CRA-2004 PABC		
	R1	R2	R3	R1	R2	R3
S1	57	53	85	57	53	85
S2	357	343	367	357	343	367
S3	237	231	278	237	231	278
S4	27	21	34	27	21	34
S5	43	42	56	43	42	56
Total	721	690	820	721	690	820

Table 2. Maximum DBR volumes calculated for replicates 1-3 (R1-R3) and scenarios 1-5 (S1-S5) for the CRA-2004 PABC and impact analysis.

Scenario	CRA-2004 PABC Impact			CRA-2004 PABC		
	R1	R2	R3	R1	R2	R3
S1	1.80E+01	4.17E+01	1.79E+01	1.80E+01	4.02E+01	1.79E+01
S2	7.21E+01	7.17E+01	6.38E+01	6.89E+01	6.88E+01	6.09E+01
S3	6.62E+01	5.28E+01	7.11E+01	6.40E+01	5.14E+01	7.02E+01
S4	1.41E+01	2.90E+01	1.58E+01	1.41E+01	2.89E+01	1.58E+01
S5	1.41E+01	4.47E+01	1.58E+01	1.41E+01	4.46E+01	1.58E+01
Total	7.21E+01	7.17E+01	7.11E+01	6.89E+01	6.88E+01	7.02E+01

Table 3. Average DBR volumes calculated for replicates 1-3 (R1-R3) and scenarios 1-5 (S1-S5) for the CRA-2004 PABC and impact analysis.

Scenario	CRA-2004 PABC Impact			CRA-2004 PABC		
	R1	R2	R3	R1	R2	R3
S1	5.16E-01	3.47E+00	6.71E-01	5.23E-01	3.37E+00	6.60E-01
S2	1.27E+01	1.26E+01	1.13E+01	1.26E+01	1.25E+01	1.13E+01
S3	1.02E+01	9.05E+00	9.79E+00	1.01E+01	8.94E+00	9.70E+00
S4	8.05E-01	2.56E+00	6.46E-01	8.02E-01	2.55E+00	6.42E-01
S5	5.30E-01	1.96E+00	5.69E-01	5.25E-01	1.96E+00	5.64E-01

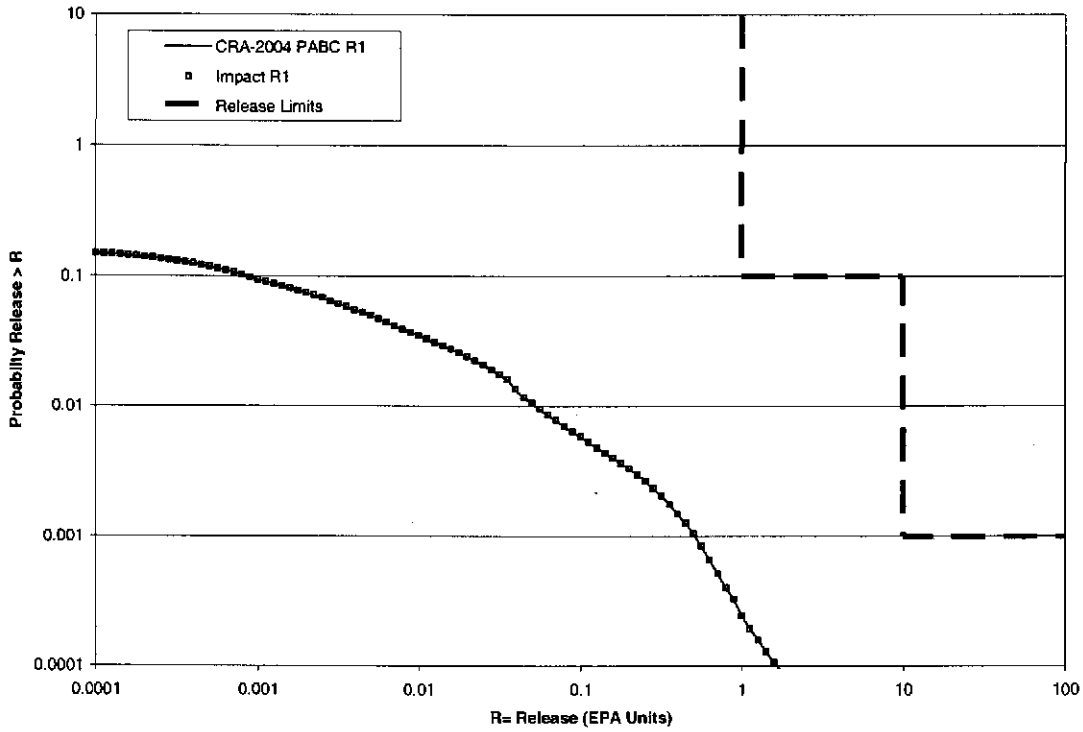

Figure 1. CCDFs of DBR releases for the CRA-2004 PABC and impact analysis, for replicate 1.

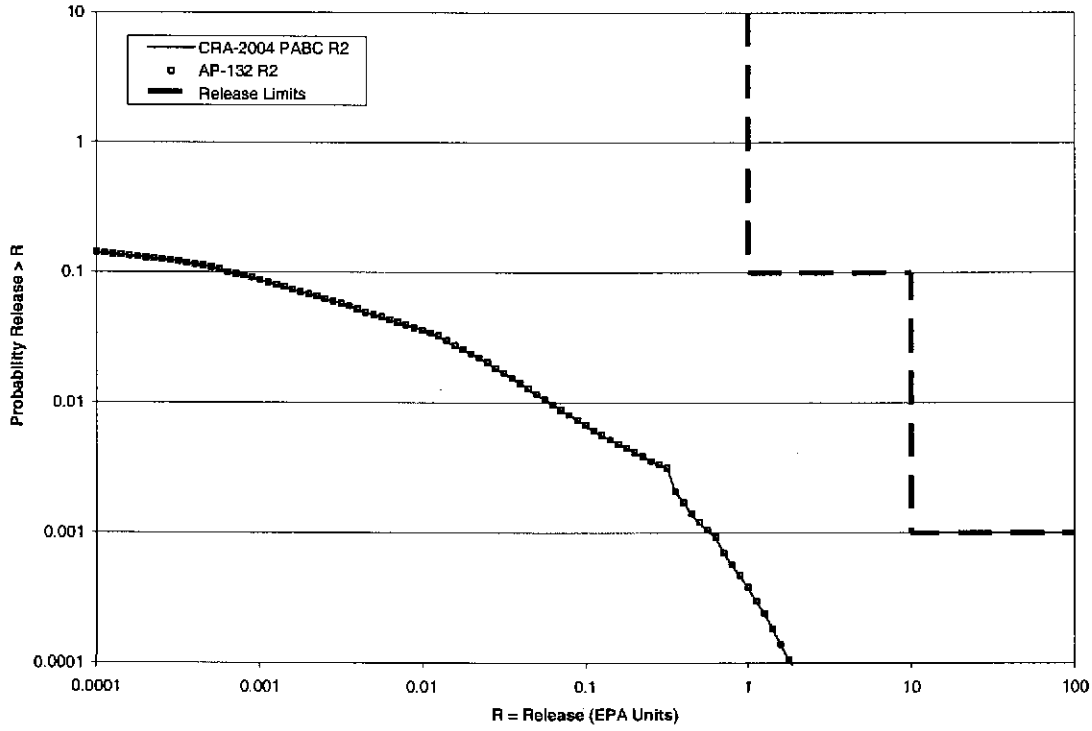

Figure 2. CCDFs of DBR releases for the CRA-2004 PABC and impact analysis, for replicate 2.

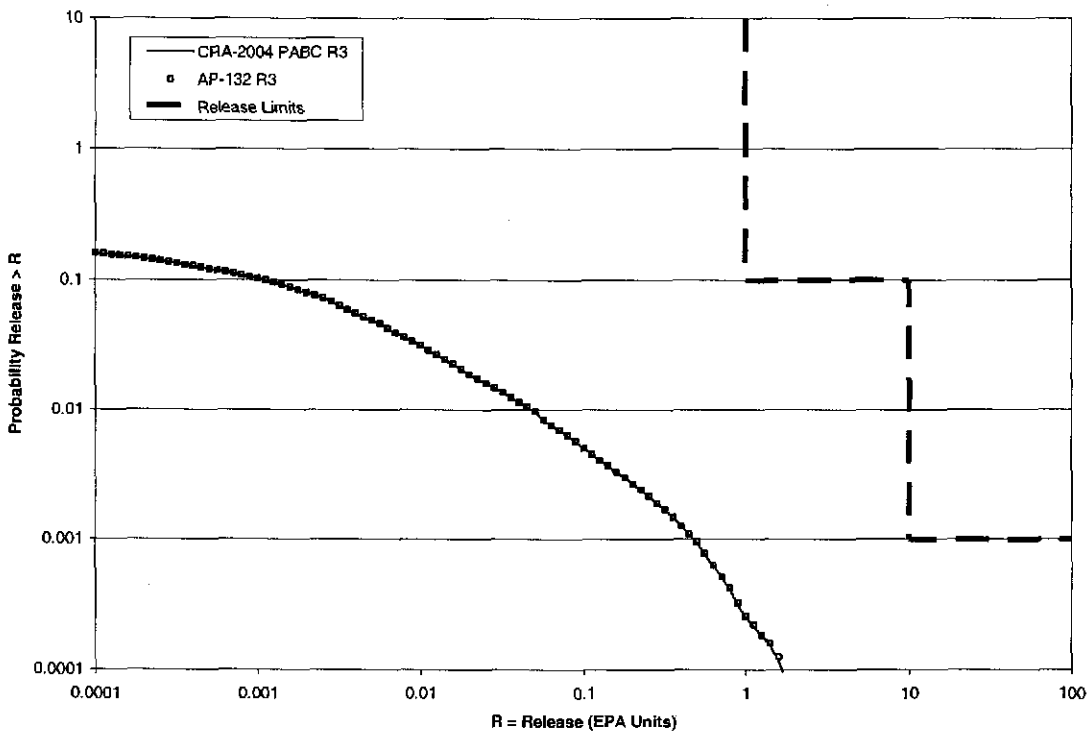

Figure 3. CCDFs of DBR releases for the CRA-2004 PABC and impact analysis, for replicate 3.

References

Long, J.J. and J.F. Kanney. 2005. "Execution of Performance Assessment Codes for the CRA-2004 Performance Assessment Baseline Calculation." Carlsbad, NM. Sandia National Laboratories. ERMS 541394.

Vugrin, E.D. and M.B. Nemer. 2007. "Analysis Plan for the 2009 Compliance Recertification Application Performance Assessment. AP-132, Revision 0." Carlsbad, SM. Sandia National Laboratories. ERMS 545496.