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Sandia National Laboratories
Waste Isolation Pilot Plant

Analysis Report for Modifying Parameter Distributions for S_MB139:COMP_RCK and S_MB139:SAT_RGAS

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WIPP:1.4.1.2:PA:QA-L:AP-118

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1.0 Executive Summary

An error was detected in how the code LHS version 2.41 sampled truncated normal distributions (Hansen 2004). Correction of this error led to a change in the technique that LHS version 2.42 uses to sample truncated student t-distributions, and this change in sampling necessitated a change in how the parameters S_MB139:COMP_RCK and S_MB139:SAT_RGAS are modeled. Material S_MB139 represents anhydrite marker bed 139 and many material properties defined for this material are applied to the other marker bed materials represented in the BRAGFLO grid (e.g., S_MB138 and S_ANH_AB). The property COMP_RCK is the bulk compressibility of the material. The property SAT_RGAS is the residual gas saturation of the material. To test the sensitivity of the BRAGFLO model to different values of these two parameters, BRAGFLO was run for a select number of CRA vectors using selected values for these parameters. Results of this sensitivity study indicate that variations in these parameters lead to only minor variations in pressure, brine saturation, and brine outflow for individual vectors. Additionally, BRAGFLO was run for a complete set of 100 vectors in which these two parameters were held constant at the median value instead of being sampled. Analysis indicates that holding these parameters constant had no significant impact on pressure, brine saturation levels, or brine outflow results. Furthermore, DBR volumes were only slightly affected. The impact that these results could have on total releases has not been determined in the present analysis. However, the results of this analysis suggest that total releases will not be significantly affected.

2.0 Introduction and Objectives

In 1996, the U.S. Department of Energy (DOE) completed a performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP). The PA was part of the Compliance Certification Application (CCA) submitted to the Environmental Protection Agency (EPA) to demonstrate compliance with the long-term radioactive disposal standards of 40 CFR 191 (subparts B and C) (U.S. E.P.A. 1993) and the associated certification criteria of 40 CFR 194 (U.S. E.P.A. 1996). Based on the CCA and subsequent information and analyses, the EPA certified the WIPP's compliance in May 1998. As required by the WIPP Land Withdrawal Act (Public Law 102-579 [as amended by Public Law 104-201]) (U.S. Congress 1992), DOE is required to submit documentation of continued compliance to EPA for the recertification of the WIPP every five years following the first receipt of waste. In March of 2004, DOE submitted the Compliance Recertification Application (CRA) (U.S. DOE 2004), which included an updated PA done by Sandia National Laboratories.

Both stochastic and subjective uncertainties are considered by the WIPP PA. Stochastic uncertainty pertains to unknowable future events such as intrusion times and locations, while subjective uncertainty concerns parameter values that are uncertain because of a lack of knowledge about the system. WIPP PA models use approximately seventy uncertain parameters to account for these uncertainties. The WIPP PA uses Latin hypercube sampling (LHS), which minimizes correlations among sampled values and ensures that the model results include the effects of sampling from the full range of each parameter's distribution.

The 2004 WIPP PA used the code LHS version 2.41 to perform the Latin hypercube sampling (WIPP-PA 2004). Hansen (2004) identified that the code was incorrectly sampling from the truncated normal and lognormal distributions. (It should be noted that this error does not impact any CCA or CRA calculations since no sampled parameters used normal or lognormal distributions for these analyses.) Additionally, for uniformity, it was determined that student and logstudent parameters would be sampled from ranges bounded by the 1st and 99th quantiles (Vugrin 2005). These are the same quantiles used for normal and lognormal distributions.

This change in sampling methodology for parameters modeled with student and logstudent distributions can lead to some physically unrealistic sampled values. Most notably, sampled values of the parameters S_MB139:COMP_RCK (ANHCOMP) and S_MB139:SAT_RGAS (ANRGSSAT) should be restricted between 0.00 and 1.00 so that they represent physically realistic values, but when these parameters are modeled with student distributions, their first quantiles correspond to negative values. (These parameters are used by the code BRAGFLO, the WIPP PA code that simulates the flow of brine and gas in and around the repository. The model includes processes such as disposal room consolidation and closure, gas generation, and interbed and disturbed rock zone fracturing in response to elevated pressures (WIPP-PA 2003)).

The objective of this analysis is to evaluate an alternative method for modeling the parameters S_MB139:COMP_RCK and S_MB139:SAT_RGAS such that physically realistic values for these parameters will be used in the PA analysis.

3.0 Approach

The primary purpose of this analysis, referred to in this document as the new parameter analysis, was to evaluate the impact of modifying the distributions that are used to model the parameters S_MB139:COMP_RCK and S_MB139:SAT_RGAS. Two separate but related analyses were conducted. The first analysis selected several vectors from the CRA PA and tested the sensitivity of model results to changes in these two parameters. This analysis determined that the uncertainty in these parameters contributed little to the uncertainty in model results. This result supported replacing the student t distribution with a constant value for these parameters. The second analysis was designed to determine the effect on PA of treating these parameters as constants, using the median value of the former distributions. This analysis ran a full 100 vectors from the CRA in which these two parameters were held constant instead of being sampled. Both of these analyses are described in more detail in the following sections.

This work was conducted in accordance with Analysis Plan AP-118, which was written specifically to guide modification of the parameter distributions for S_MB139:COMP_RCK and S_MB139:SAT_RGAS (Vugrin and Kirchner 2005). For the sake of brevity, this document will refer to the parameters S_MB139:COMP_RCK and S_MB139:SAT_RGAS by their MATERIAL:PROPERTY name stored in the WIPP PA Parameter Database (PAPDB) and their respective CAMDAT variable names, ANHCOMP and ANRGSSAT, that are used in BRAGFLO documentation.

3.1 *New Parameter Analysis- step 1*

In the first step of this analysis, six different values of ANHCOMP were selected that encompassed the current range of values allowed by the WIPP PA Parameter Database (PAPDB). Several vectors from the 2004 CRA PA were selected to be evaluated. The majority of these vectors represent cases having high DBR or spallings releases. Each vector was run through BRAGFLO six different times, holding all input parameters constant except for ANHCOMP. Each vector calculation used a different value for ANHCOMP. This process was repeated for ANRGSSAT.

In this preliminary analysis, no changes were made to the PAPDB. Instead, all changes were implemented through manual modification of a single LHS output file (see Section 4.1.2). The output variables of interest are repository pressure, brine saturation, and cumulative brine outflow, as they affect subsequent compliance modeling analyses. Pressure is an input to the calculation of spallings releases, brine saturation and pressure are inputs to the calculation of direct brine release (DBR), and brine outflow is an input to the calculation of flow and transport through the Salado formation and Culebra dolomite.

Two scenarios were calculated: the undisturbed scenario (S1), and a disturbed scenario (S2), which models a drilling penetration through the waste panel into a pressurize brine pocket in the Castile at 350 years. Scenario S2 produced the highest brine outflows in previous analyses (Stein and Zelinski 2003). These two scenarios bound the full range of results that occur in all six scenarios that comprise the full suite of BRAGFLO analyses required for a complete performance assessment calculation.

3.1.1 Step 1 Deviations from AP-118

Analysis Plan AP-118 omitted the use of several intermediate processing codes. Table 1 lists all of the codes used for this analysis.

Table 1 Codes Used for Step 1 of New Parameter Analysis

Code	Version	Build Date	Executable
ALGEBRACDB	2.35	1/31/96	ALGEBRACDB_PA96.EXE
BRAGFLO	5.00	3/19/03	BRAGFLO_QA0500. EXE
GENMESH	6.08	1/31/96	GM_PA96.EXE
ICSET	2.22	2/1/96	ICSET_PA96. EXE
LHS	2.41	3/6/96	LHS_PA96.EXE
MATSET	9.10	11/29/01	MATSET_QA0910.EXE
PREBRAG	7.00	3/19/03	PREBRAG_QB0700. EXE
POSTBRAG	4.00	2/6/96	POSTBRAG_PA96.EXE
PRELHS	2.30	11/27/01	PRELHS_QA0230.EXE
POSTLHS	4.07	2/7/96	POSTLHS_PA96.EXE

3.2 *New Parameter Analysis- step 2*

The second step of this analysis is an additional deviation from AP-118. This phase of the analysis evaluated the impact on CRA results when each vector used the same constant values for ANHCOMP and ANRGSSAT.

A complete set of these 100 vectors were run in BRAGFLO. In this preliminary analysis, no changes were made to the PAPDB. Instead, all changes were implemented through manual modification of a single file LHS output file (see Section 4.1.2). The output variables of interest are repository pressure, brine saturation, cumulative brine outflow, and DBR volume released. Scenarios S1 and S2 were selected for simulation for the same reasons given in Section 3.1. Table 2 lists the codes used for step 2 of the new parameter analysis.

Table 2 Codes Used for Step 2 of New Parameter Analysis

Code	Version	Build Date	Executable
ALGEBRACDB	2.35	1/31/96	ALGEBRACDB_PA96.EXE
BRAGFLO	5.00	3/19/03	BRAGFLO_QA0500. EXE
CUTTINGS_S	5.10	10/8/03	CUTTINGS_S_QA0510.EXE
ICSET	2.22	2/1/96	ICSET_PA96. EXE
PREBRAG	7.00	3/19/03	PREBRAG_QB0700. EXE
POSTBRAG	4.00	2/6/96	POSTBRAG_PA96.EXE
POSTLHS	4.07	2/7/96	POSTLHS_PA96.EXE
RELATE	1.43	3/6/96	RELATE_PA96.EXE
SUMMARIZE	2.20	7/11/97	SUMMARIZE_QA0220.EXE

4.0 Methodology

This analysis was performed in two stages. The first stage evaluated the impact on individual vectors of varying the values of ANHCOMP and ANRGSSAT and determined the suitability of modeling these parameters as constant values instead of as random variables. The second stage involved implementation of constant values of ANHCOMP and ANRGSSAT in BRAGFLO to test the impact of these changes on repository behavior.

4.1 *Step 1 Methodology*

4.1.1 Selection of the Vectors

Table 3 shows the data points stored in the PAPDB for S_MB139:COMP_RCK and used to define the student's t distribution. Note that the median value listed in Table 3 differs from the median value listed in the PAPDB. For this analysis, the median was calculated by averaging 1.09e-11 and 3.37e-11, the second and third largest quantities in Table 3. The median value listed in the PAPDB is the median of the student's t distribution with three degrees of freedom and a mean equal to the average of the data points listed in Table 3. A similar explanation applies as well for the median value for ANRGSSAT in Table 4.

Table 3 Data Points of S_MB139:COMP_RCK Stored in PAPDB. Note that the units for these data are Pa^{-1}.

Data points	Median
1.0900000e-011	2.230e-011
1.0900000e-011	-
3.3700000e-011	-
2.7500000e-010	-

Table 4 Data Points of S_MB139:SAT_RGAS Stored in PAPDB. Note that these data points are unitless.

Data points	Median
1.3981000e-002	5.495e-002
2.5201000e-002	-
3.2177000e-002	-
7.7729000e-002	-
1.1637000e-001	-
1.9719000e-001	-

Nine vectors from replicate R1 of the CRA were selected to assess the impact of changing ANHCOMP and ANRGSSAT for individual vectors. These vectors are listed in Table 5.

Table 5 Vectors Selected for Analysis

Vector	Rank of Mean DBR (for CRA R1)	Rank of Mean Spall Release (for CRA R1)	Value of ANHCOMP (Pa^{-1}) (for CRA R1)	Value of ANRGSSAT (-) (for CRA R1)
6	20	34	2.334E-10	7.147E-02
17	49	72	1.090E-11	9.024E-02
22	1	2	8.030E-11	8.696E-02
32	10	72	1.809E-10	5.409E-02
46	2	72	8.787E-11	6.325E-02
77	6	36	1.489E-10	7.022E-02
86	3	43	7.847E-11	1.398E-02
88	28	72	2.750E-10	7.229E-02
99	93	1	4.937E-11	5.163E-02

The second and third columns of Table 5 list the ranks (largest to smallest) of mean DBRs and mean spallings releases for CRA replicate R1, respectively. The fourth column lists the value of ANHCOMP for each vector, and the fifth column lists the value of ANRGSSAT for each vector.

The majority of the vectors were selected because they exhibited large mean DBRs, the release pathway that is expected to be most affected by changes in these parameter values. Vectors 22, 32, 46, 77, and 86 had mean DBRs that were among the 10 largest for CRA replicate R1. Other vectors were selected because they had large mean spall vectors. Vectors 22 and 99 had the two largest mean spall releases for replicate R1. (Note that 57 vectors had spallings mean releases of 0.00. Thus, these vectors are assigned a rank of 72 [(44+100)/2 = 72].) The values of ANHCOMP and ANRGSSAT for these vectors encompass a broad range of values.

4.1.2 Creation of LHS and POSTLHS Files

For each vector in Table 5, 2 sets of 6 new POSTLHS output files were created (see Table 9). The first set was created by manually editing the LHS output file from the CRA (see Table 9) and setting the sampled value of ANHCOMP for the vectors in Table 5 to 2.7500E-10. All other sampled parameter values were unchanged. Figure 1 shows an excerpt of the unaltered LHS output file. Figure 2 shows the same excerpt from the modified LHS output file; in this figure the values for S_MB139:COMP_RCK have been edited.

RUN	NO.	X(21)	X(22)	X(23)	X(24)	X(25)
0	1	9.759E-11	4.000E+00	1.075E-01	9.597E-02	5.729E-01
0	2	3.531E-11	1.000E+00	1.088E-01	5.558E-02	6.654E-01
0	3	1.413E-10	4.000E+00	1.153E-01	1.046E-01	6.618E-01
0	4	8.132E-11	1.000E+00	1.227E-02	6.036E-02	7.428E-01
0	5	5.830E-11	4.000E+00	1.390E-01	7.068E-02	8.257E-01
0	6	**2.334E-10**	1.000E+00	9.215E-02	7.147E-02	7.312E-01
0	7	1.301E-11	4.000E+00	7.244E-02	8.478E-02	6.304E-01
......						
0	16	2.750E-10	4.000E+00	8.362E-02	1.157E-01	6.163E-01
0	17	**1.090E-11**	1.000E+00	7.834E-02	9.024E-02	5.962E-01
0	18	2.750E-10	1.000E+00	9.438E-02	1.134E-01	6.648E-01
0	19	1.291E-10	1.000E+00	1.113E-01	1.014E-01	6.381E-01
0	20	1.090E-11	1.000E+00	8.571E-02	2.298E-02	6.547E-01
0	21	7.405E-11	1.000E+00	1.010E-01	7.997E-02	5.666E-01
0	22	**8.030E-11**	4.000E+00	5.410E-02	8.696E-02	6.400E-01
0	23	1.899E-10	4.000E+00	8.816E-02	9.131E-02	6.780E-01
......						

Figure 1 Sampled Parameter Values from CRA LHS Output File.
This figure contains a subset of the sampled parameter values used in the CRA. "RUN NO." indicates the vector number, and column X(21) contains the sampled values of S_MB139:COMP_RCK for the CRA. Numbers in bold were edited to create the "modified LHS output files" discussed in this section.

RUN	NO.	X(21)	X(22)	X(23)	X(24)	X(25)
0	1	9.759E-11	4.000E+00	1.075E-01	9.597E-02	5.729E-01
0	2	3.531E-11	1.000E+00	1.088E-01	5.558E-02	6.654E-01
0	3	1.413E-10	4.000E+00	1.153E-01	1.046E-01	6.618E-01
0	4	8.132E-11	1.000E+00	1.227E-02	6.036E-02	7.428E-01
0	5	5.830E-11	4.000E+00	1.390E-01	7.068E-02	8.257E-01
0	6	**2.750000E-10**	1.000E+00	9.215E-02	7.147E-02	7.312E-01
0	7	1.301E-11	4.000E+00	7.244E-02	8.478E-02	6.304E-01
......						
0	16	2.750E-10	4.000E+00	8.362E-02	1.157E-01	6.163E-01
0	17	**2.750000E-10**	1.000E+00	7.834E-02	9.024E-02	5.962E-01
0	18	2.750E-10	1.000E+00	9.438E-02	1.134E-01	6.648E-01
0	19	1.291E-10	1.000E+00	1.113E-01	1.014E-01	6.381E-01
0	20	1.090E-11	1.000E+00	8.571E-02	2.298E-02	6.547E-01
0	21	7.405E-11	1.000E+00	1.010E-01	7.997E-02	5.666E-01
0	22	**2.750000E-10**	4.000E+00	5.410E-02	8.696E-02	6.400E-01
0	23	1.899E-10	4.000E+00	8.816E-02	9.131E-02	6.780E-01
......						

Figure 2 Subsection of the Modified LHS Output File.
"RUN NO." indicates the vector number, and column X(21) contains the sampled values of S_MB139:COMP_RCK for the CRA. The only difference between this file and the file shown in Figure 1 is that the values of S_MB139:COMP_RCK for selected vectors have been changed to 2.750000E-10. These values are indicated in bold.

The modified LHS output file was input into POSTLHS, along with the appropriate MATSET output files, and 100 POSTLHS output CAMDAT files were created. All but the files corresponding to the vectors in Table 5 were discarded. This process was repeated for the other 5 values of ANHCOMP in Table 6. Note that in Table 9, RCK1, RCK2, etc. are substituted for the "(" symbol in filenames associated with the ANHCOMP values listed in Table 6. This procedure created the first set of 6 POSTLHS output files per vector.

Table 6 S_MB139:COMP_RCK Values Used for Analysis

Label	S_MB139:COMP_RCK Values (Pa^{-1})
RCK1	2.7500E-10
RCK2	2.2218E-10
RCK3	1.6936E-10
RCK4	1.1654E-10
RCK5	6.3720E-11
RCK6	1.0900E-11

The second set of new POSTLHS output files was created, again, by modifying the LHS output file from the CRA. However, in this step, the sampled values of ANRGSSAT for the vectors in Table 5 were replaced with the values listed in Table 7 following the same procedure listed above for ANHCOMP. Note that in Table 9 and this analysis, GAS1, GAS2, etc. were substituted for the "(" symbol in filenames associated with the values listed in Table 7 for ANRGSSAT.

Table 7 S_MB139:SAT_RGAS Values Used for Analysis

Label	S_MB139:SAT_RGAS Values (-)
GAS1	1.9719E-01
GAS2	1.6055E-01
GAS3	1.2391E-01
GAS4	8.7265E-02
GAS5	5.0623E-02
GAS6	1.3981E-02

4.1.3 Execution of the PA Codes

The execution of codes for this step of the analysis is described in Section 7.0. This procedure follows the execution of codes for scenarios S1 and S2 of the 2004 CRA described in Long (2004). The only differences from the execution of the 2004 CRA PA are that POSTLHS CAMDAT files and the other files that are output by PA codes and used as input into a subsequent PA code are different. All other input files for this analysis were the same as those used in the 2004 CRA PA.

4.1.4 Evaluation of BRAGFLO Outputs

Three quantities calculated by BRAGFLO were analyzed: pressure in the waste panel, brine saturation in the waste panel, and brine outflow. In this document, these quantities are denoted by their CAMDAT variable names, WAS_SATB, WAS_SATB, and BRNREPOC, respectively. Further discussion of why these quantities were examined can be found in the following sections.

The following procedure was established to analyze the sensitivity of these quantities to ANHCOMP:

1) Let $SAT_{RCK\_j,V\_k}(t_i)$ denote that brine saturation that results from using a value of RCK_j for ANHCOMP (see Table 6) at time step t_i for vector k. For scenario S1 the maximum and minimum values of WAS_SATB for each vector were selected at each time step. That is, for each vector k analyzed in Table 5, the following quantities were calculated:
$$MXSAT_{V\_k}(t_i) = \max_{rck\_j, j=1..6} SAT_{RCK\_j,V\_k}(t_i)$$
$$MNSAT_{V\_k}(t_i) = \min_{rck\_j, j=1..6} SAT_{RCK\_j,V\_k}(t_i)$$
This gives the range of the values of WAS_SATB for each vector.
2) For each vector, the following quantity was computed:
$$D_{V\_k} = \sum_i \left(MXSAT_{V\_k}(t_i) - MNSAT_{V\_k}(t_i) \right)^2$$
where k denotes the vector number. This value gives a quantitative measure of how much the maximum and minimum saturation curves differ. For each scenario, it was determined that the vector with the highest D_{V_k} had the greatest variation of values of WAS_SATB.
3) Steps 1 and 2 were repeated for scenario 2.
4) Steps 1, 2, and 3 were repeated for WAS_PRES and BRNREPOC.

This procedure was repeated with the pressures, brine saturations, and brine outflows that resulted from changing values of ANRGSSAT. The rationale for performing this procedure is that it quantifies the maximum variability introduced into the output variables for a vector by varying ANHCOMP and ANRGSSAT. The value of D_{V_k} was used to identify the vectors whose pressures, saturation levels, and brine outflows were most affected by varying ANHCOMP and ANRGSSAT.

4.2 *Step 2 Methodology*

The second portion of this analysis evaluated the impact of replacing the distributions that modeled ANHCOMP and ANRGSSAT for the CRA with constant values. A value of 2.23E-11 was selected for ANHCOMP because this quantity represents the median of the data points stored in the PAPDB for ANHCOMP. For the same reason, a value of 5.495E-2 was selected for ANRGSSAT.

The LHS output file from the CRA for replicate R1 (see Figure 1) was modified to create 1 "new LHS output file." This file that was modified is named LHS2_CRA1_TRN_A1.OUT and stored in the CMS library LIBCRA1_LHS. Table 10 contains the name of the file that resulted from the modifications. Every vector was assigned a value of 2.23E-11 for S_MB139:COMP_RCK and 5.495E-2 for S_MB139:SAT_RGAS. Figure 3 contains an excerpt of the new file. Note that the only changes to the file excerpted in Figure 1 occur in the columns corresponding to columns X(21) and X(24), the columns containing the sampled parameter values of S_MB139:COMP_RCK and S_MB139:SAT_RGAS.

RUN	NO.	X(21)	X(22)	X(23)	X(24)	X(25)
0	1	**2.230E-11**	4.000E+00	1.075E-01	**5.495E-02**	5.729E-01
0	2	**2.230E-11**	1.000E+00	1.088E-01	**5.495E-02**	6.654E-01
0	3	**2.230E-11**	4.000E+00	1.153E-01	**5.495E-02**	6.618E-01
0	4	**2.230E-11**	1.000E+00	1.227E-02	**5.495E-02**	7.428E-01
0	5	**2.230E-11**	4.000E+00	1.390E-01	**5.495E-02**	8.257E-01
0	6	**2.230E-11**	1.000E+00	9.215E-02	**5.495E-02**	7.312E-01
0	7	**2.230E-11**	4.000E+00	7.244E-02	**5.495E-02**	6.304E-01
0	8	**2.230E-11**	1.000E+00	7.248E-02	**5.495E-02**	6.831E-01

Figure 3- Modified LHS Output File.
Note that numbers in bold indicate that all vectors have the same value for S_MB139:COMP_RCK and S_MB139:SAT_RGAS.

All vectors of scenarios S1 and S2 were run using this modified LHS output file. Scenarios S1 and S2 were selected for the same reasons as discussed in Section 3.0. In addition to examining the pressures, brine saturations, and brine outflows calculated by BRAGFLO, the DBRs were analyzed as well.

5.0 Results

The plots in this section illustrate the vectors whose output variables (pressure, brine saturation, and brine outflow) demonstrated the greatest amount of variation in response to varying values of ANHCOMP and ANRGSSAT. One vector was selected for each scenario-output-parameter combination, and the vector selected had the largest value of D_{V_k} for the scenario-output-parameter combination. Thus, when it is stated in this section that a vector exhibited the greatest amount of variation from varying the value of a parameter, this statement implies that the value of D_{V_k} was larger for this vector than for all of the other vectors in this scenario-output-parameter.

5.1 *Pressure- Step 1*

Pressure is an input parameter from BRAGFLO into the DBR and spallings analyses. Pressure has to exceed the hydrostatic pressure (about 8 MPa) for there to be any release in a drilling-disturbance scenario.

For both scenarios, pressure is relatively insensitive to use of different values of both ANRGSSAT and ANHCOMP. Vector 17 showed the greatest variation in pressure that resulted by varying the values of ANHCOMP and ANRGSSAT, but these variations are not significant. Figures 4 through 7 display the resulting ranges of pressures for vector 17. As can be seen in these figures, pressure is insensitive to use of different values of both ANRGSSAT and ANHCOMP.

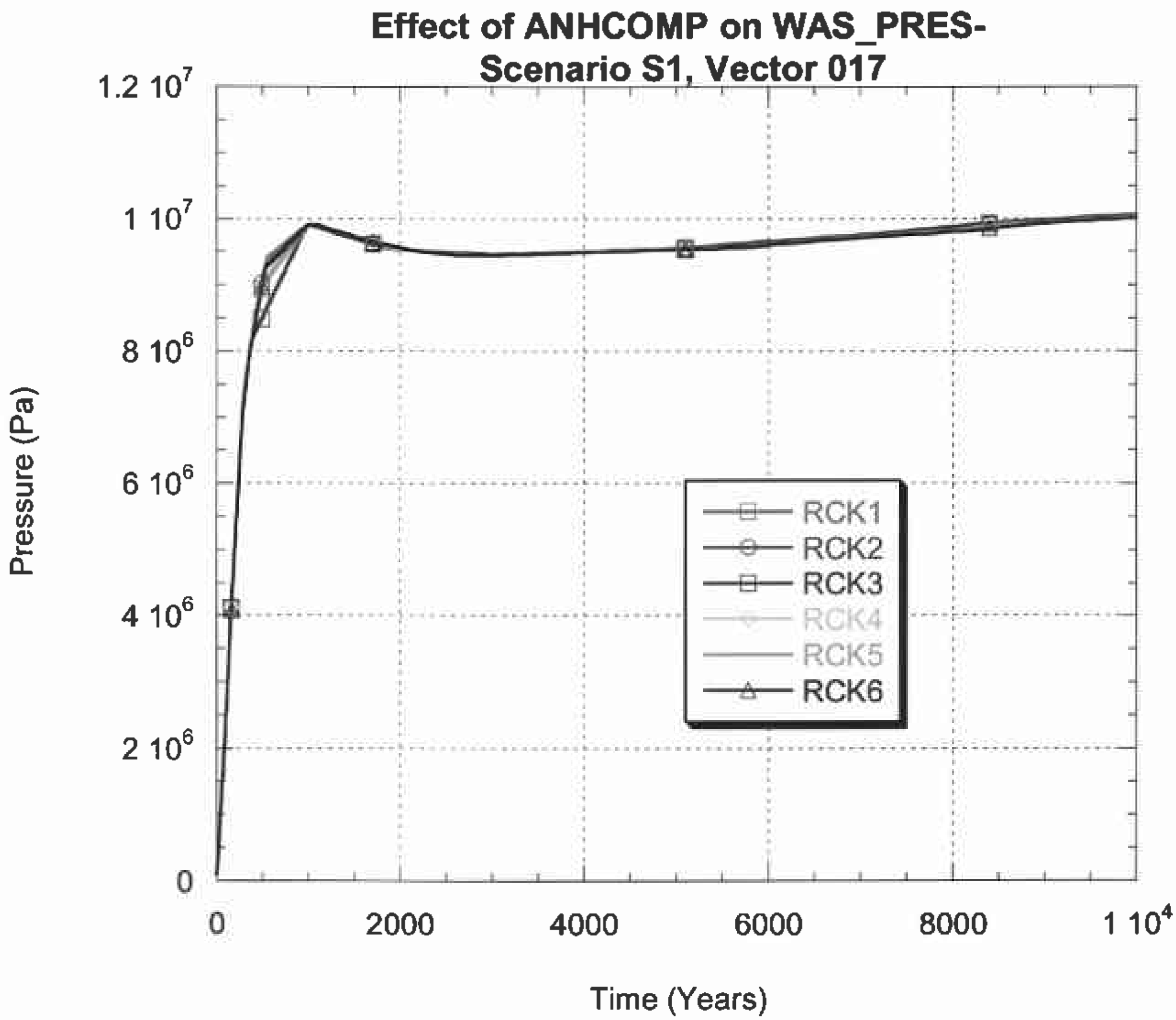

Figure 4 Pressure vs. Time for Scenario S1, Vector 017.
ANHCOMP took on 6 different values, RCK1=2.75e-10 Pa^{-1}, RCK2=2.22e-10 Pa^{-1}, RCK3=1.69e-10 Pa^{-1}, RCK4=1.17e-10 Pa^{-1} RCK5=6.37e-11 Pa^{-1}, and RCK6=1.09e-11 Pa^{-1}. All other parameters were held constant for this vector.

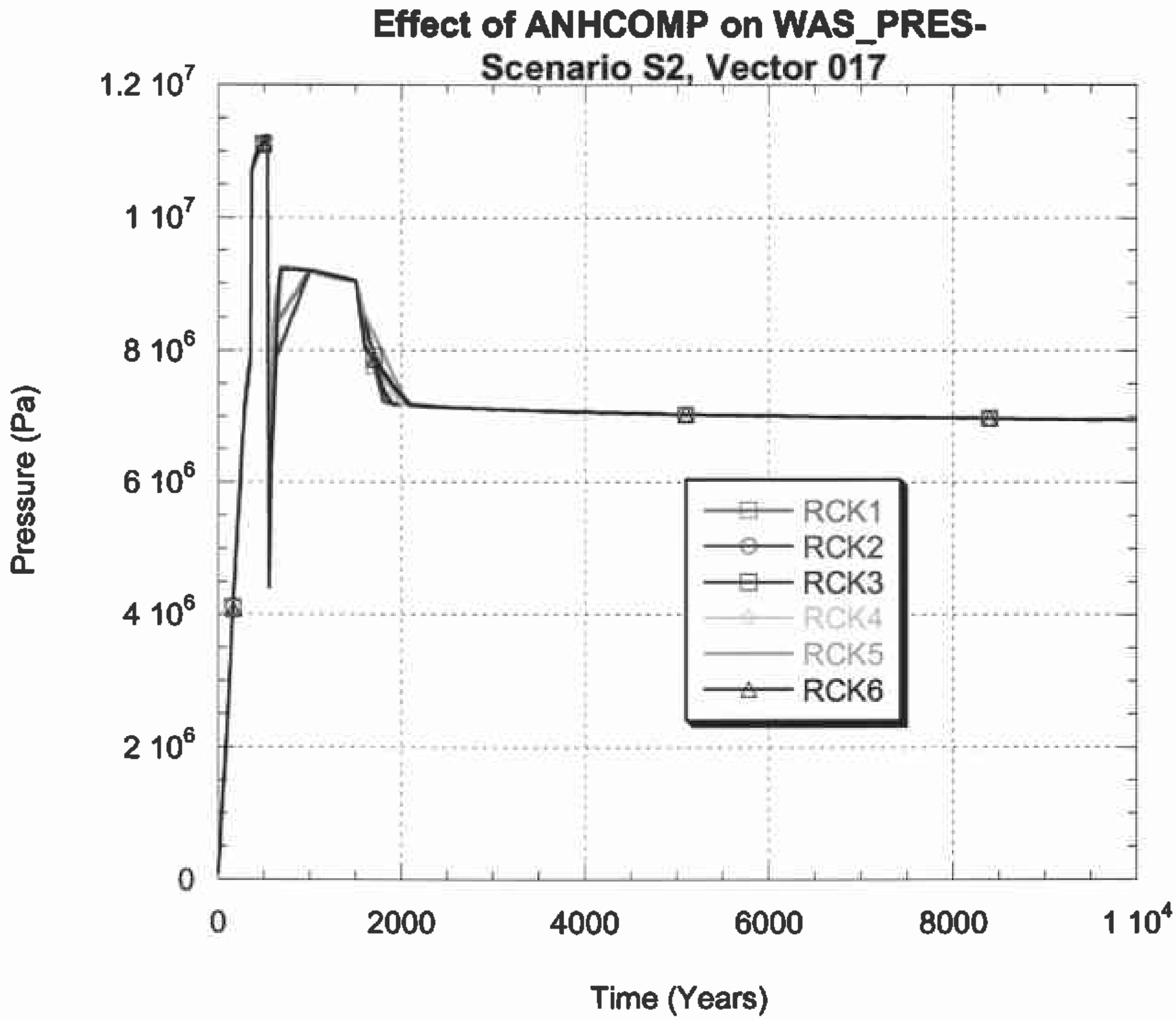

Figure 5 Pressure vs. Time for Scenario S2, Vector 017.
ANHCOMP took on 6 different values, RCK1=2.75e-10 Pa^{-1}, RCK2=2.22e-10 Pa^{-1}, RCK3=1.69e-10 Pa^{-1}, RCK4=1.17e-10 Pa^{-1} RCK5=6.37e-11 Pa^{-1}, and RCK6=1.09e-11 Pa^{-1}. All other parameters were held constant for this vector.

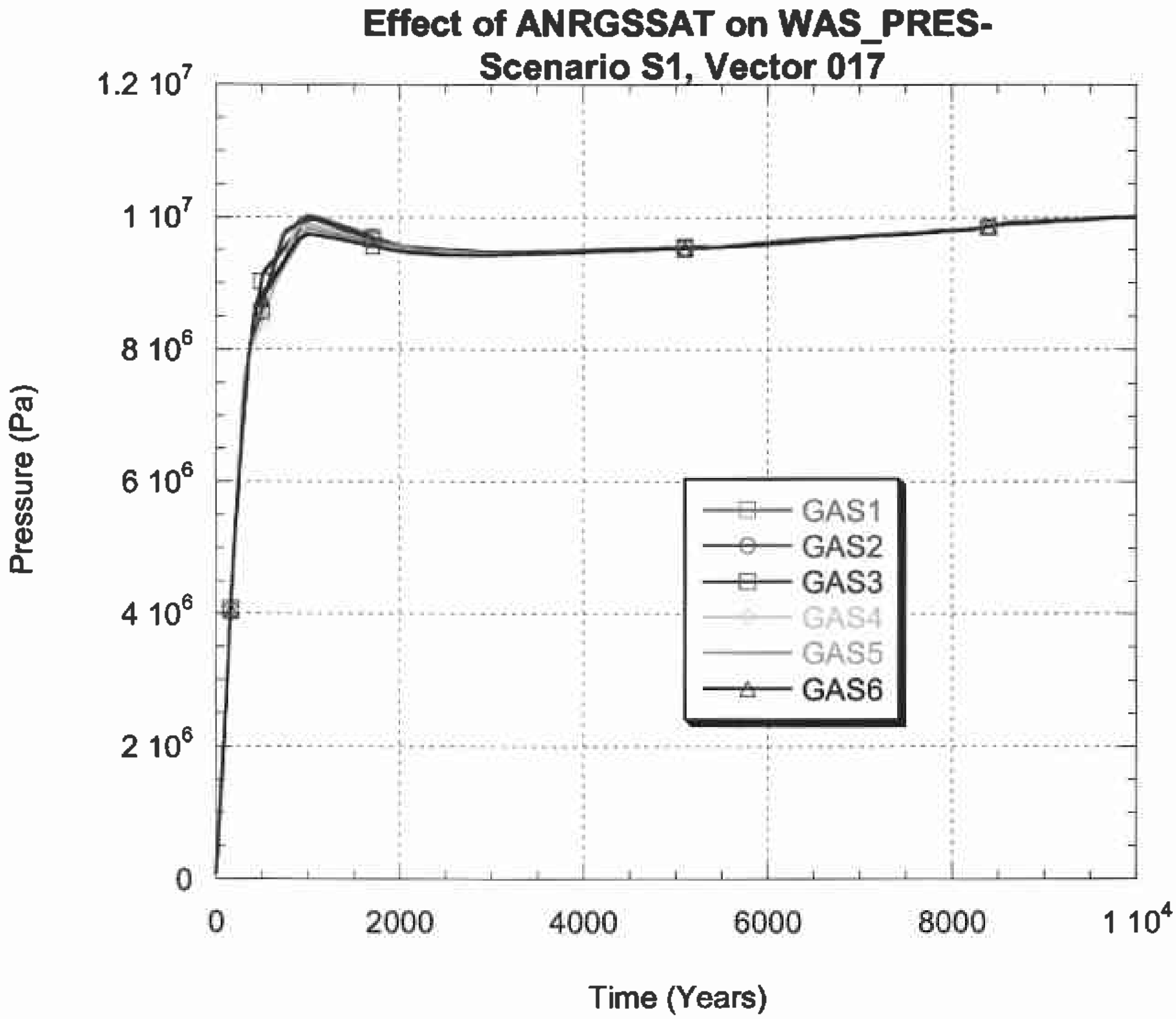

Figure 6 Pressure vs. Time for Scenario S1, Vector 017.
ANRGSSAT took on 6 different dimensionless values, GAS1=1.97e-1, GAS2=1.61e-1, GAS3=1.24e-1, GAS4=8.73e-2, GAS5=5.06e-2, and GAS6=1.40e-2. All other parameters were held constant for this vector.

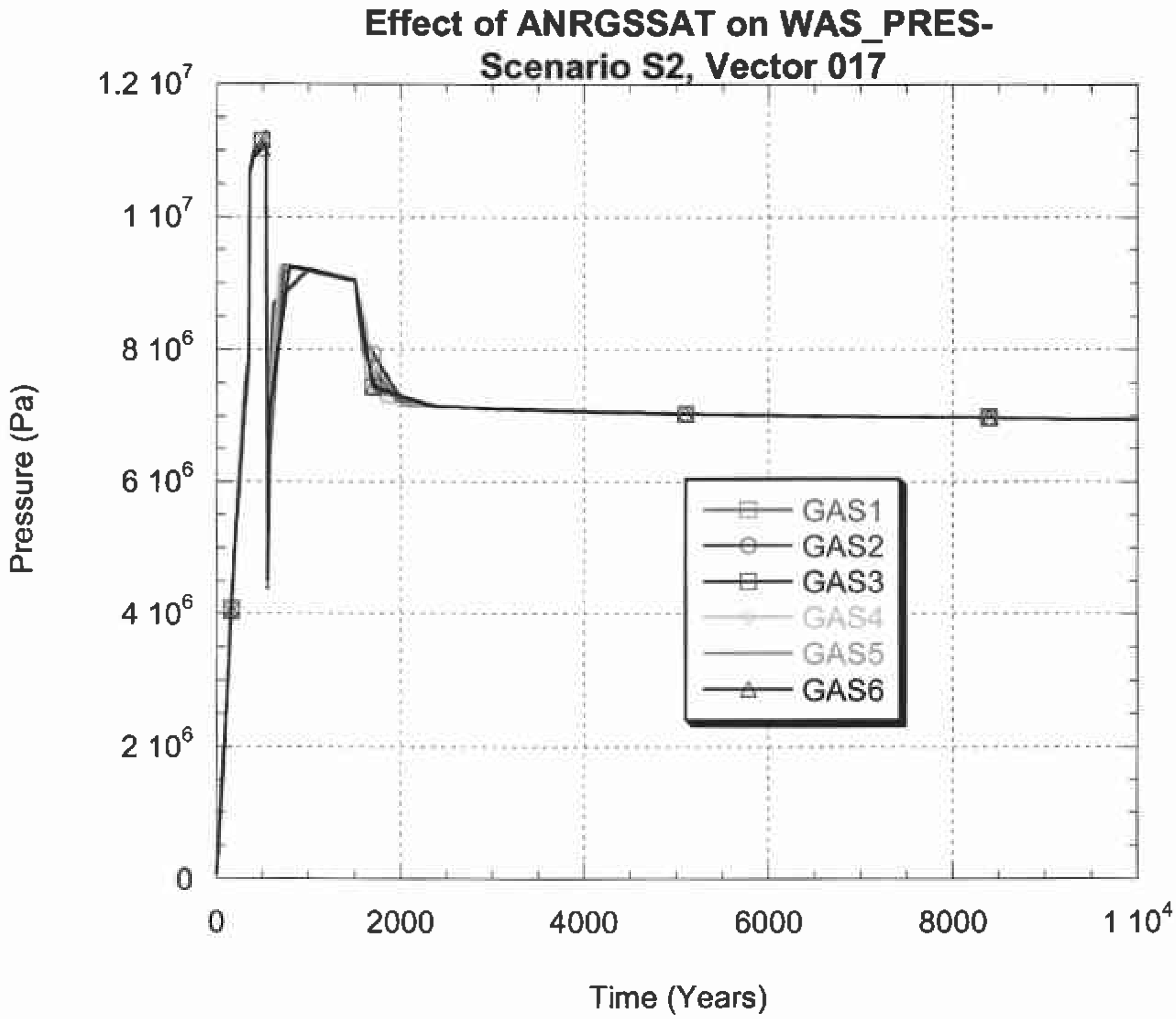

Figure 7 Pressure vs. Time for Scenario S2, Vector 017.
ANRGSSAT took on 6 different dimensionless values, GAS1=1.97e-1, GAS2=1.61e-1, GAS3=1.24e-1, GAS4=8.73e-2, GAS5=5.06e-2, and GAS6=1.40e-2. All other parameters were held constant for this vector.

5.2 *Brine Saturation- Step 1*

Brine saturation is an input parameter from BRAGFLO in the DBR analysis. DBR releases are dependent upon both pressure and brine saturation. Pressure has to exceed the hydrostatic pressure and brine saturation must exceed the residual brine saturation of waste (sampled variable) in order for there to be the possibility of a DBR release during a drilling intrusion.

For scenario S1, brine saturation in vector 17 showed the greatest variability in response to varying ANHCOMP. Figure 8 shows that over most time ranges, all saturation levels remained within approximately 10% of each other.

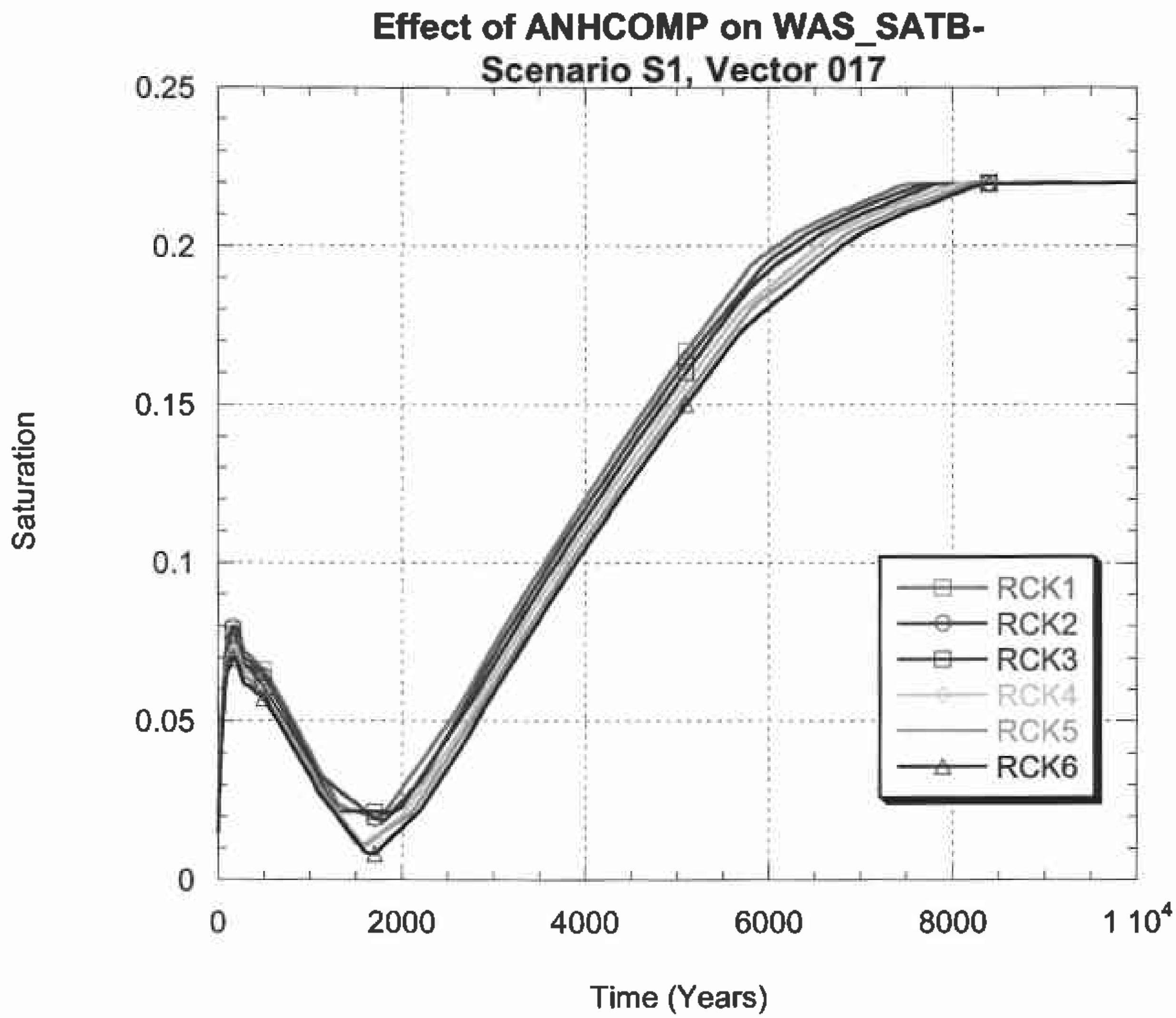

Figure 8 Brine Saturation vs. Time for Scenario S1, Vector 017.
ANHCOMP took on 6 different values, RCK1=2.75e-10 Pa^{-1}, RCK2=2.22e-10 Pa^{-1}, RCK3=1.69e-10 Pa^{-1}, RCK4=1.17e-10 Pa^{-1} RCK5=6.37e-11 Pa^{-1}, and RCK6=1.09e-11 Pa^{-1}. All other parameters were held constant for this vector.

For scenario S2, brine saturation in vector 22 exhibited the most significant variability as a result of varying ANHCOMP. Figure 9 shows that saturation levels remain within about 20% of the other saturation levels for most times in this vector. For this vector it appears that larger values of ANHCOMP tend to result in slightly higher saturation levels. The pressures for vector 22 of scenario 2 are unusually high when compared with other vectors from the CRA (see Figure 10). These higher pressures result in fracturing, which is implemented in the BRAGFLO model by elevating rock compressibility which results in higher permeability and porosity (WIPP PA 2003). The higher compressibilities allow storage of greater quantities of brine, and the higher permeabilities allow brine to flow more freely. The combination of higher compressibility and permeability values can allow faster and larger responses to changes in the system and higher brine saturation levels. It should be noted that this explanation is specific only to vectors in which fracturing has occured. Figure 11 is more typical of the variability in brine saturation levels that is observed when ANHCOMP is varied for vectors with more moderate pressures.

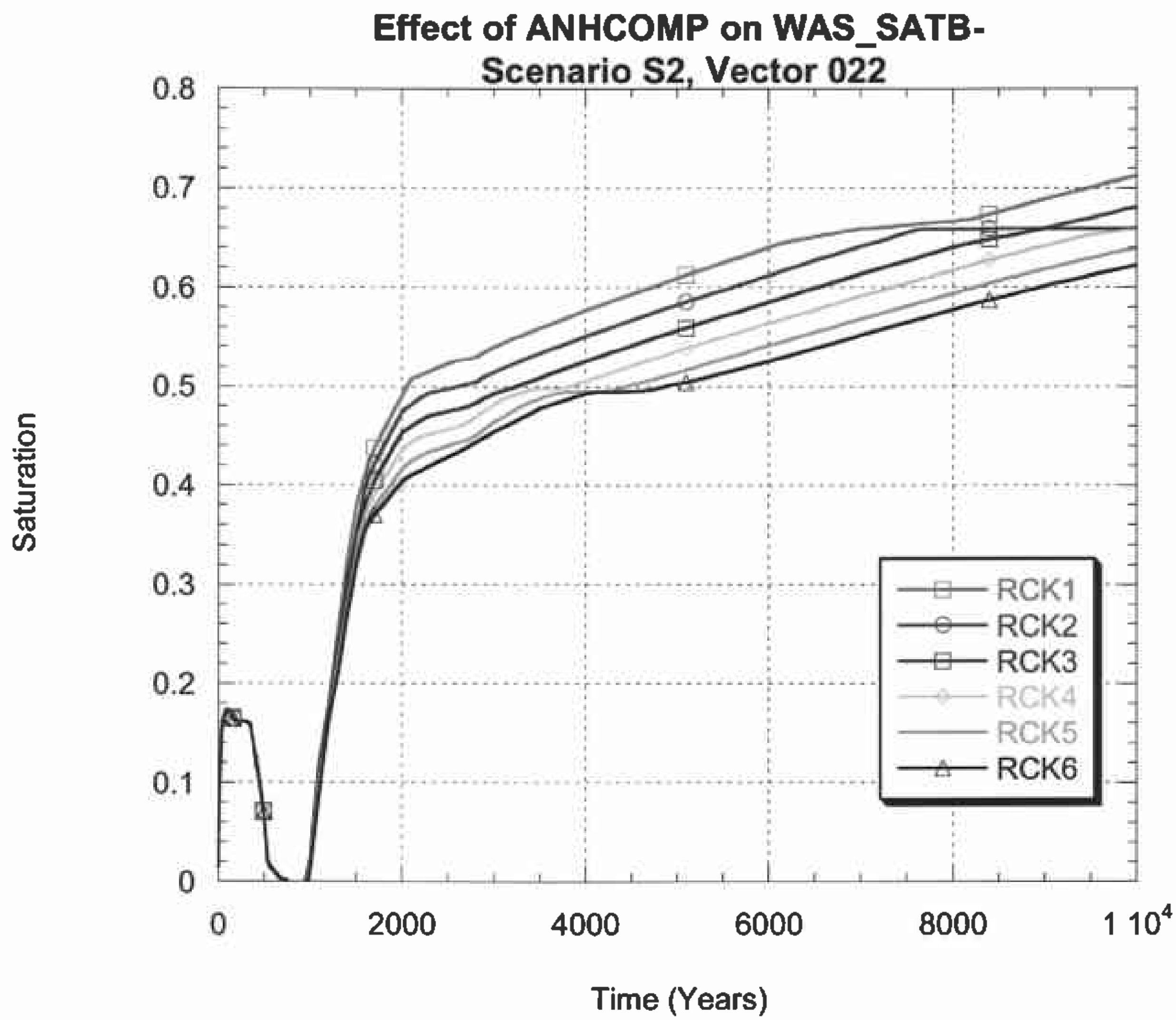

Figure 9 Brine Saturation vs. Time for Scenario S2, Vector 022.
ANHCOMP took on 6 different values, RCK1=2.75e-10 Pa^{-1}, RCK2=2.22e-10 Pa^{-1}, RCK3=1.69e-10 Pa^{-1}, RCK4=1.17e-10 Pa^{-1} RCK5=6.37e-11 Pa^{-1}, and RCK6=1.09e-11 Pa^{-1}. All other parameters were held constant for this vector.

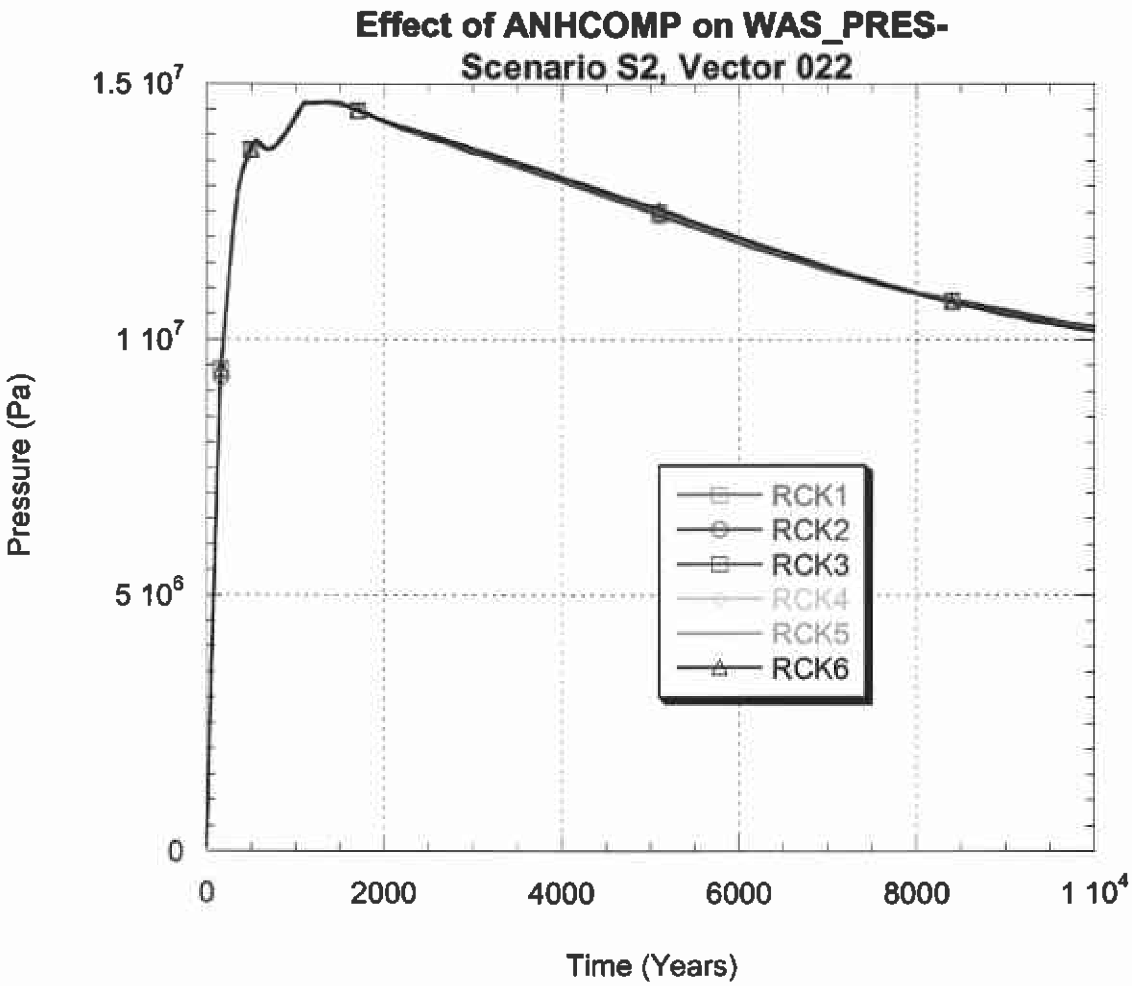

Figure 10 Pressure vs. Time for Scenario S2, Vector 022.
ANHCOMP took on 6 different values, RCK1=2.75e-10 Pa^{-1}, RCK2=2.22e-10 Pa^{-1}, RCK3=1.69e-10 Pa^{-1}, RCK4=1.17e-10 Pa^{-1} RCK5=6.37e-11 Pa^{-1}, and RCK6=1.09e-11 Pa^{-1}. All other parameters were held constant for this vector. This figures displays the unusually high pressures observed in vector 22.

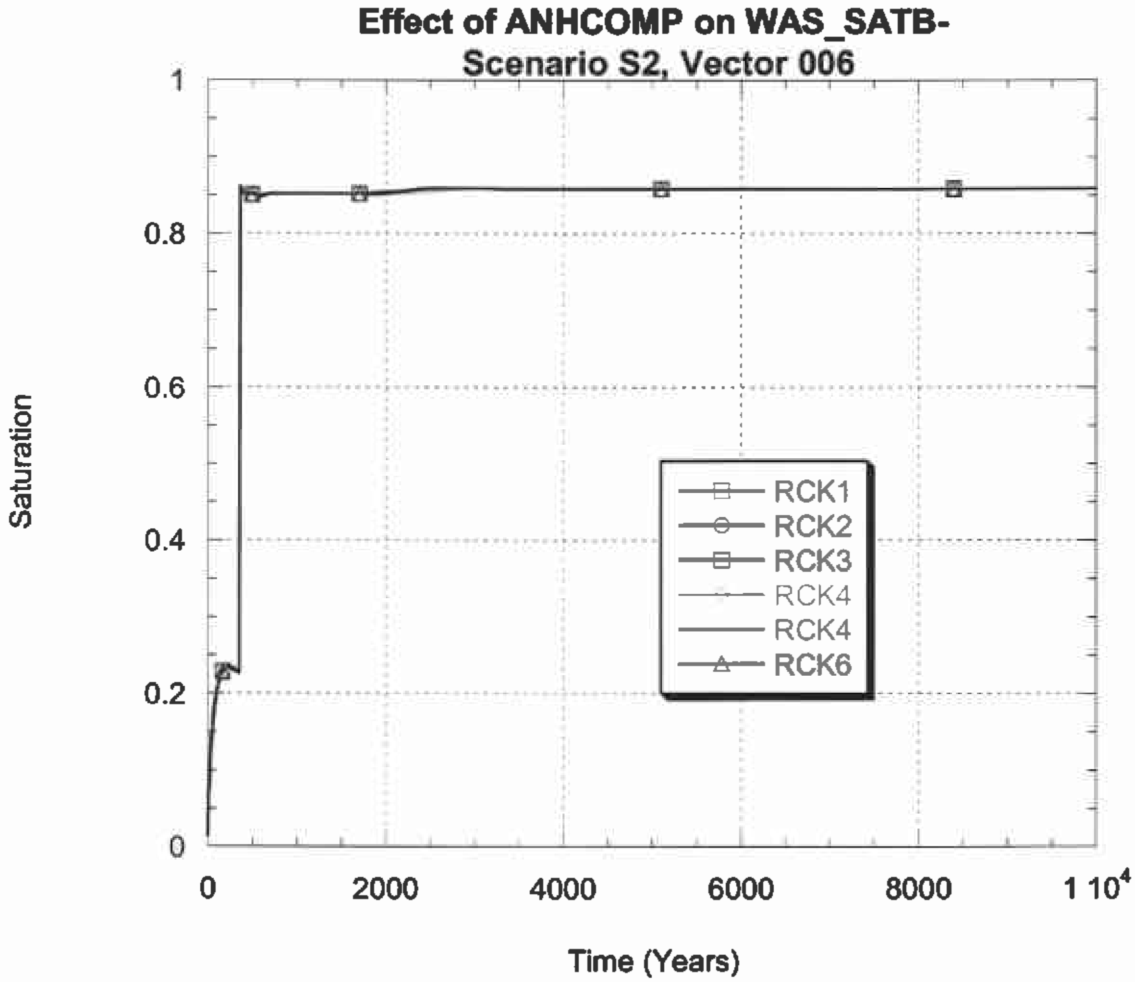

Figure 11 Brine Saturation vs. Time for Scenario S2, Vector 006.
ANHCOMP took on 6 different values, RCK1=2.75e-10 Pa^{-1}, RCK2=2.22e-10 Pa^{-1}, RCK3=1.69e-10 Pa^{-1}, RCK4=1.17e-10 Pa^{-1} RCK5=6.37e-11 Pa^{-1}, and RCK6=1.09e-11 Pa^{-1}. All other parameters were held constant for this vector. This figure displays the variability in brine saturation levels for a vector with moderate pressures.

For Scenario S1, brine saturation in vector 22 exhibited the most variability in response to varying the value of ANRGSSAT. Figure 12 shows that saturation levels remain within approximately 10% of the other saturation levels for this vector at most times.

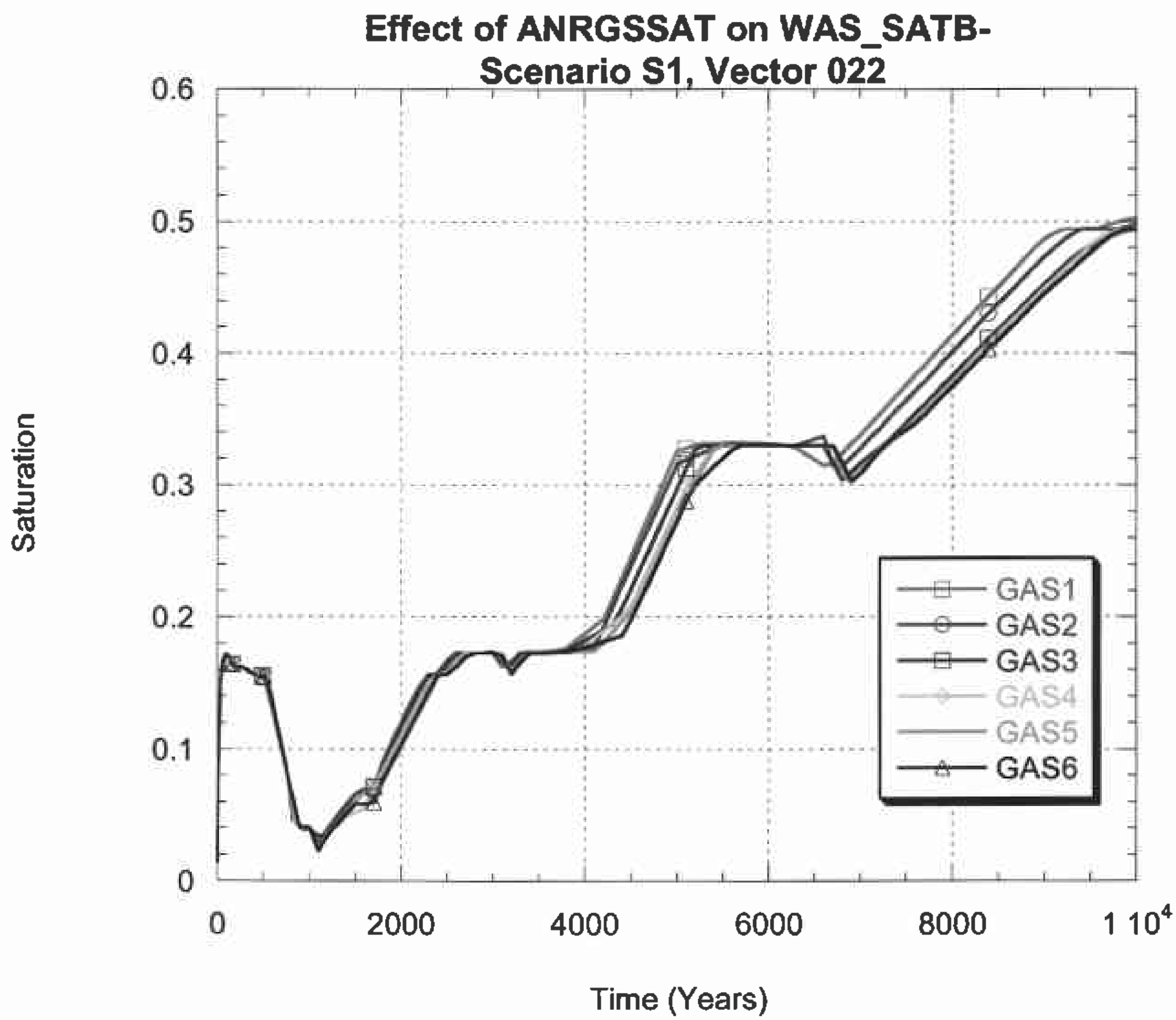

Figure 12 Brine Saturation vs. Time for Scenario S1, Vector 022.
ANRGSSAT took on 6 different dimensionless values, GAS1=1.97e-1, GAS2=1.61e-1, GAS3=1.24e-1, GAS4=8.73e-2, GAS5=5.06e-2, and GAS6=1.40e-2. All other parameters were held constant for this vector.

For scenario S2, brine saturation in vector 99 showed the most variability in response to varying the value of ANRGSSAT. Figure 13 shows that saturation levels for this vector are not significantly affected by variations in ANRGSSAT.

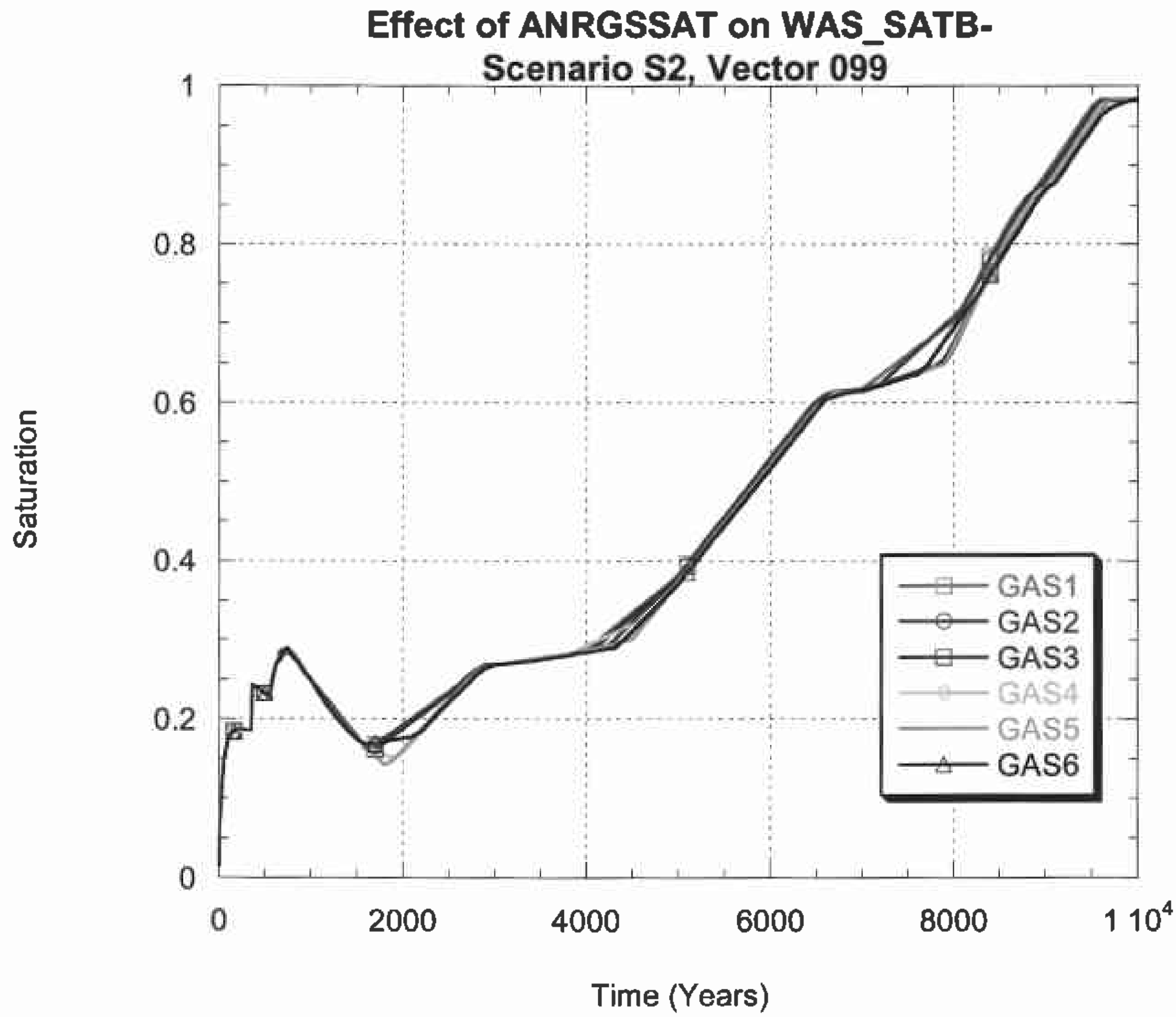

Figure 13 Brine Saturation vs. Time for Scenario S2, Vector 099.
ANRGSSAT took on 6 different dimensionless values, GAS1=1.97e-1, GAS2=1.61e-1, GAS3=1.24e-1, GAS4=8.73e-2, GAS5=5.06e-2, and GAS6=1.40e-2. All other parameters were held constant for this vector.

The figures displayed in this section show the instances of greatest variability. Vectors not shown expressed smaller ranges of variation in response to varying ANHCOMP and ANRGSSAT. These results suggest that model predictions of brine saturation are not very sensitive to changes in these parameters.

5.3 *Brine Outflow- step 1*

Two potential pathways exist for the release of brine containing radionuclides: 1) migration of radionuclides through the Salado along anhydrite marker beds to the land withdrawal boundary, and 2) migration of contaminated brine up a borehole in drilling-intrusion scenarios to the Culebra and then through the Culebra to the land withdrawal boundary. Total cumulative brine outflow in this analysis includes both types of brine flow away from the repository (into the marker beds and up the borehole and into the Culebra).

For both scenarios, vector 22 showed the greatest variation of brine outflow volumes when ANHCOMP was varied. Figure 14 shows that in scenario S1, the brine outflow volumes did not change much when ANHCOMP was varied. The brine outflow volume for vector 22 in scenario S2 varied slightly more, but the brine volume still remained within 6% of the other brine volume curves at most times (Figure 15). It is worth reiterating that the other vectors examined showed smaller ranges of variability than vector 22 when ANHCOMP was varied. These results suggest that model predictions of brine outflow are not very sensitive to changes in this parameter.

In Figure 14 and Figure 15 the BRAGFLO runs that use the largest ANHCOMP values tend to result in slightly higher brine outflow quantities. Marker beds start out with lithostatic pressure and as pressure lowers in response to atmospheric pressure in the waste rooms, volume of the marker beds actually decreases because of the weight of the overlying rock pushing down. The higher the compressibility the more the volume of bed decreases. Since the brine is much less compressible than the marker beds, it has a tendency to flow out of the beds toward the waste rooms. The greater the compressibility of the marker beds the greater the reduction in the volume of the marker beds in response to the pressure change and the greater amount of brine that will flow out of the beds. This process leads to an increase in brine flow into the repository from the marker beds, allowing for slightly higher brine outflow quantities.

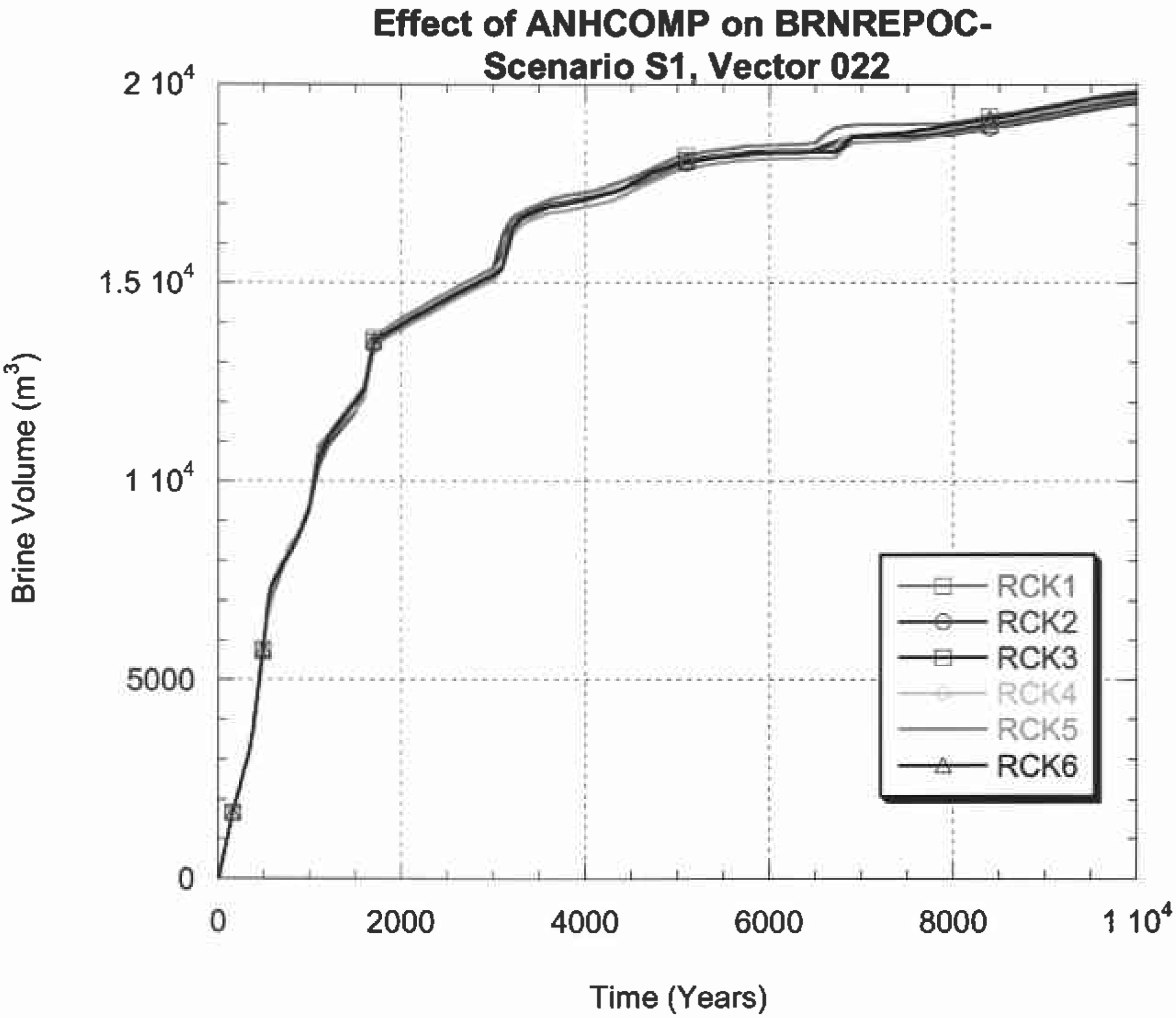

Figure 14 Brine Outflow vs. Time for Scenario S1, Vector 022.
ANHCOMP took on 6 different values, RCK1=2.75e-10 Pa^{-1}, RCK2=2.22e-10 Pa^{-1}, RCK3=1.69e-10 Pa^{-1}, RCK4=1.17e-10 Pa^{-1} RCK5=6.37e-11 Pa^{-1}, and RCK6=1.09e-11 Pa^{-1}. All other parameters were held constant for this vector.

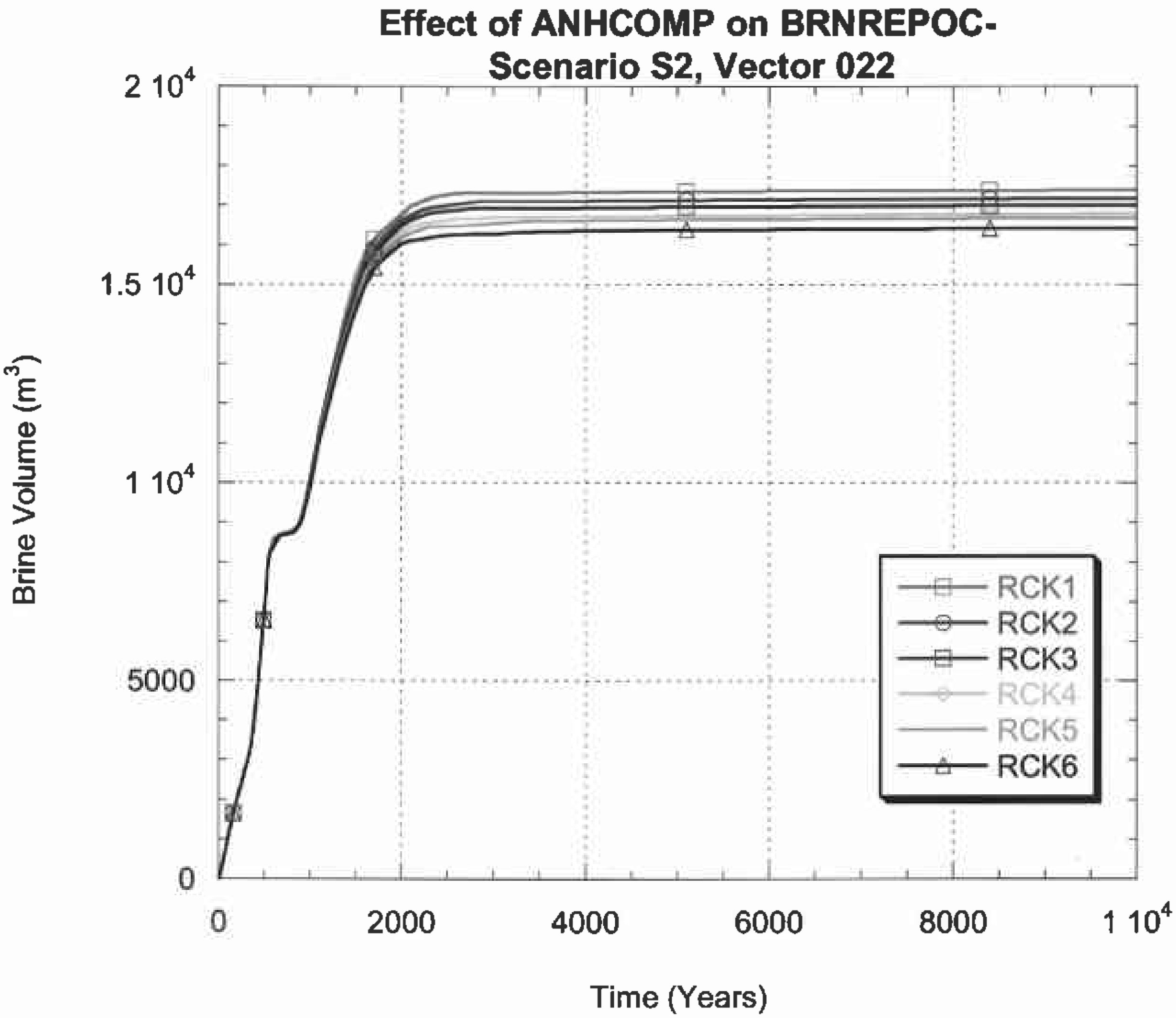

Figure 15 Brine Outflow vs. Time for Scenario S2, Vector 022.
ANHCOMP took on 6 different values, RCK1=2.75e-10 Pa^{-1}, RCK2=2.22e-10 Pa^{-1}, RCK3=1.69e-10 Pa^{-1}, RCK4=1.17e-10 Pa^{-1} RCK5=6.37e-11 Pa^{-1}, and RCK6=1.09e-11 Pa^{-1}. All other parameters were held constant for this vector.

For scenario S1, varying ANRGSSAT values resulted in the greatest range of variation of brine outflow volumes in vector 22. Figure 16 shows that the brine outflow curves varied very little when ANRGSSAT was varied. Figure 17 shows that the brine volumes were unaffected by varying ANRGSSAT in vector 17 for scenario S2. This vector showed more variation than any other vectors in S2. These results suggest that model predictions of brine outflow are not very sensitive to changes in this parameter.

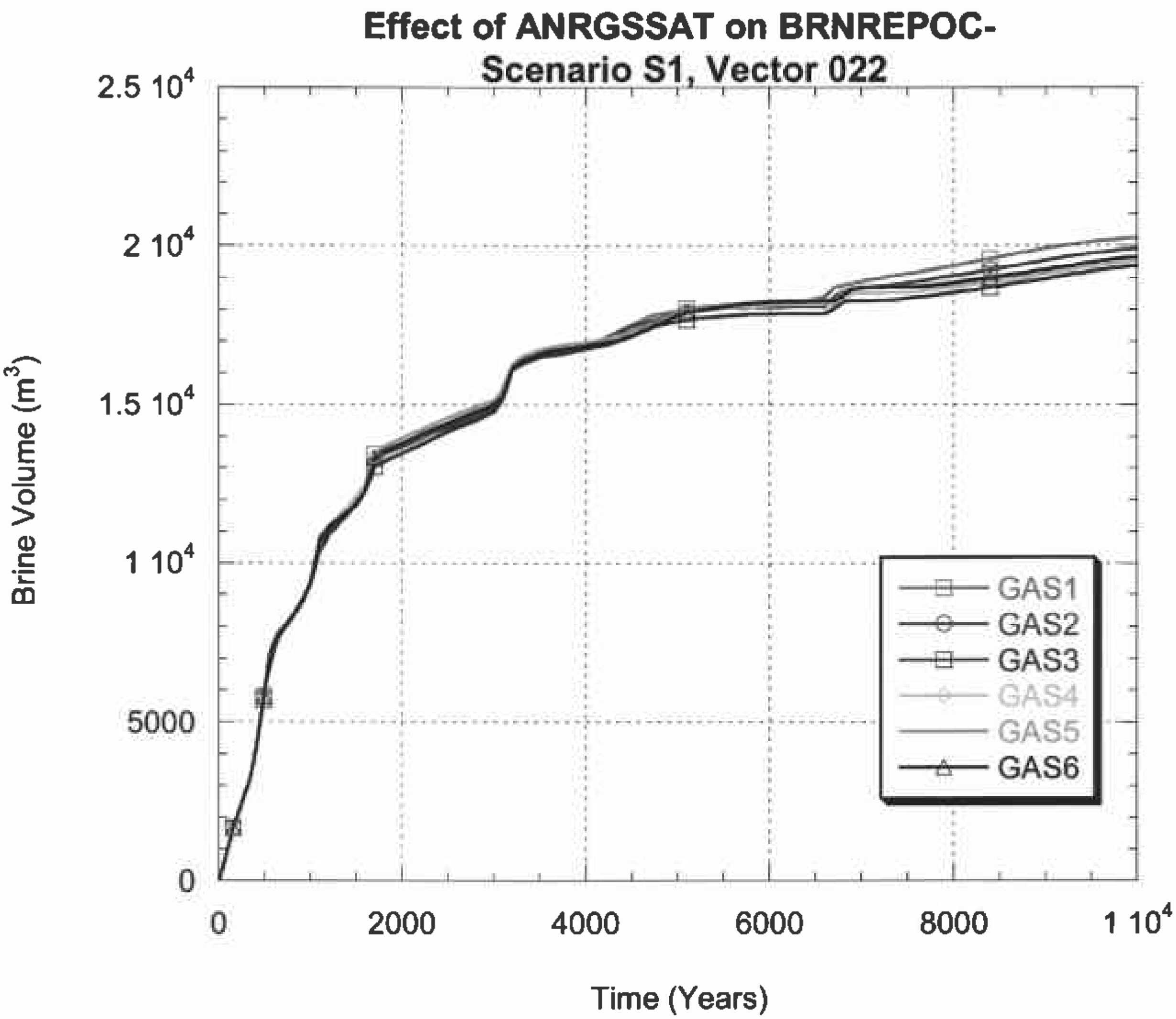

Figure 16 Brine Outflow vs. Time for Scenario S1, Vector 022.
ANRGSSAT took on 6 different dimensionless values, GAS1=1.97e-1, GAS2=1.61e-1, GAS3=1.24e-1, GAS4=8.73e-2, GAS5=5.06e-2, and GAS6=1.40e-2. All other parameters were held constant for this vector.

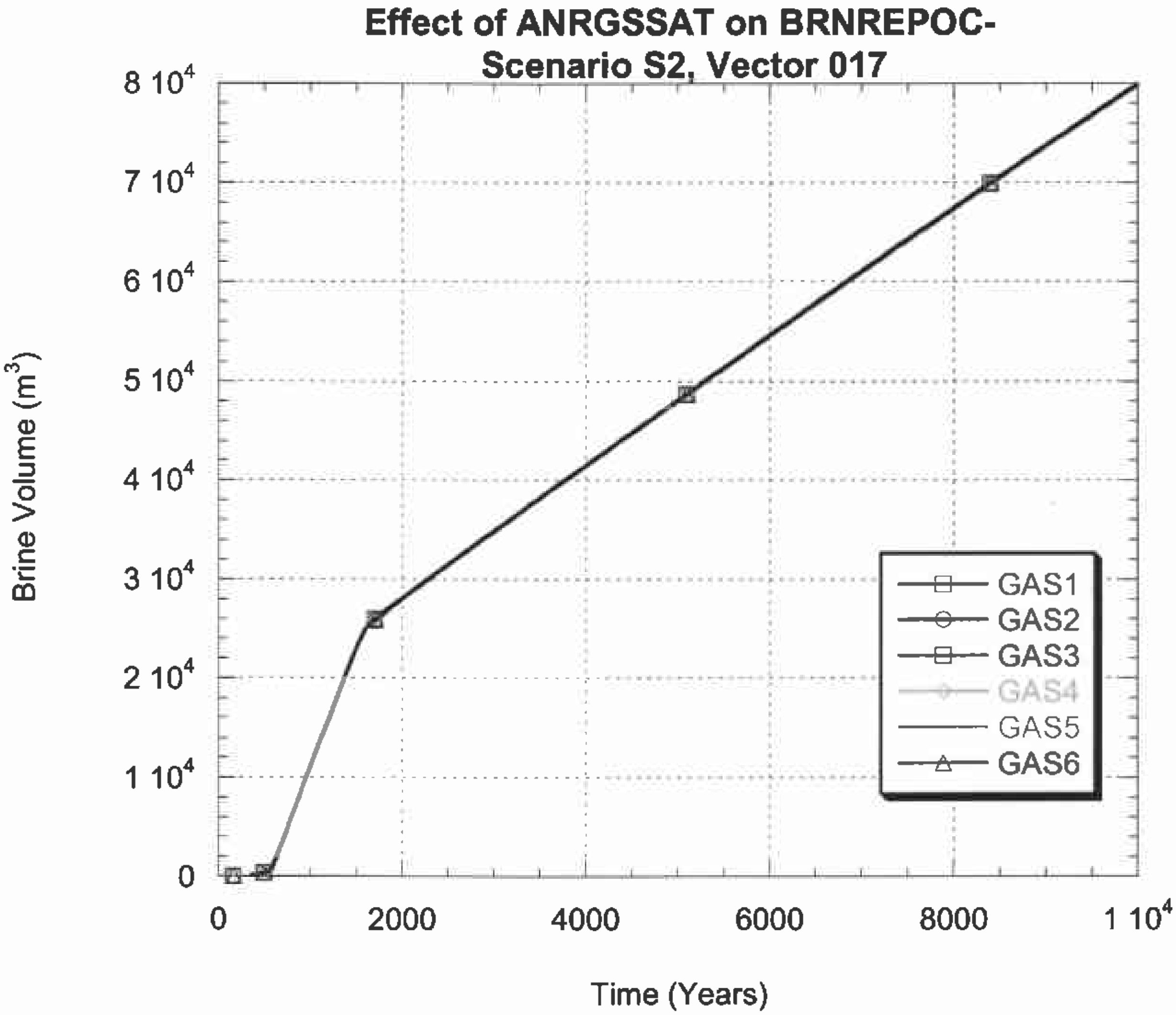

Figure 17 Brine Outflow vs. Time for Scenario S2, Vector 017.
ANRGSSAT took on 6 different dimensionless values, GAS1=1.97e-1, GAS2=1.61e-1, GAS3=1.24e-1, GAS4=8.73e-2, GAS5=5.06e-2, and GAS6=1.40e-2. All other parameters were held constant for this vector.

As a whole, the brine outflow volumes were not largely affected by variations in ANHCOMP and ANRGSSAT. It is unlikely that changes to ANRGSSAT and ANHCOMP would significantly affect flow to the Culebra, from the Culebra, or up the borehole in the event of an intrusion.

5.4 *Step 2 Results*

Since the step 1 results of the new parameter analysis did not indicate large variations in pressure, brine saturation, or outflow in response to varying ANHCOMP and ANRGSSAT, using constants to model these parameters is considered a suitable alternative to using student t-distributions. As discussed in Section 4.2, scenarios S1 and

S2 were run using the same constant values of ANHCOMP and ANRGSSAT for all vectors. This section assesses the impact of using constant values for these parameters on the predictions of pressure, brine saturation, brine outflow, and DBR volumes. Plots of high, low and average values are compared over the entire modeling period to evaluate the effects of the change on overall modeling results. These lines do not represent individual vectors but rather the statistics for all vectors as a function of time.

Figure 18 and Figure 19 show plots for maximum, minimum, and average pressures as a function of time for the new parameter analysis and the CRA . The pressure curves from the two analyses are indistinguishable. Furthermore, Figure 20 and Figure 21 show the maximum, minimum, and average brine saturations as a function of time for the new parameter analysis and the CRA. Once again, the brine saturation values from the two analyses display no significant differences. Figure 22 and Figure 23 indicate that the brine outflow levels are unaffected, as well. These results indicate that using constant values for these two parameters does not significantly affect BRAGFLO results.

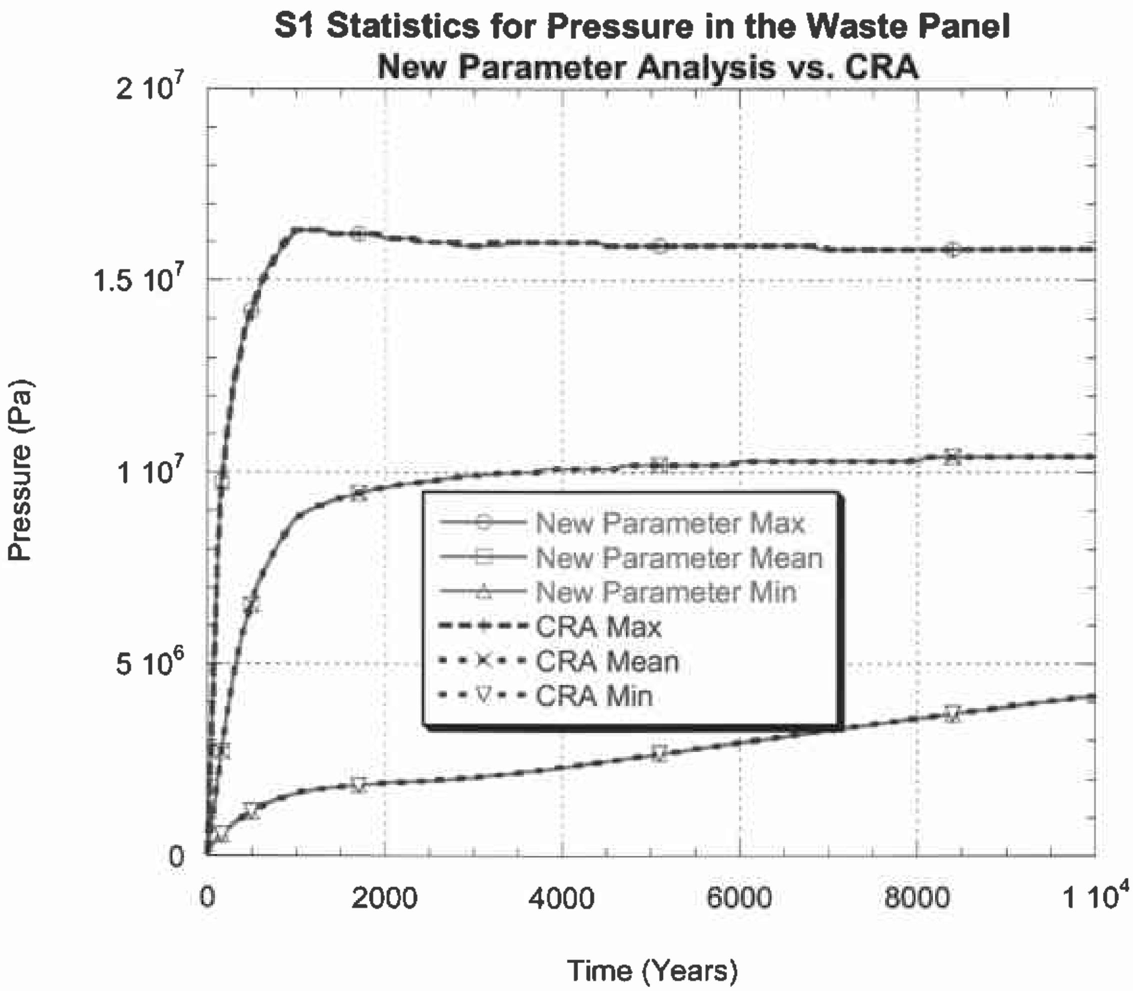

Figure 18 Pressure in the Waste Panel vs. Time: Scenario S1

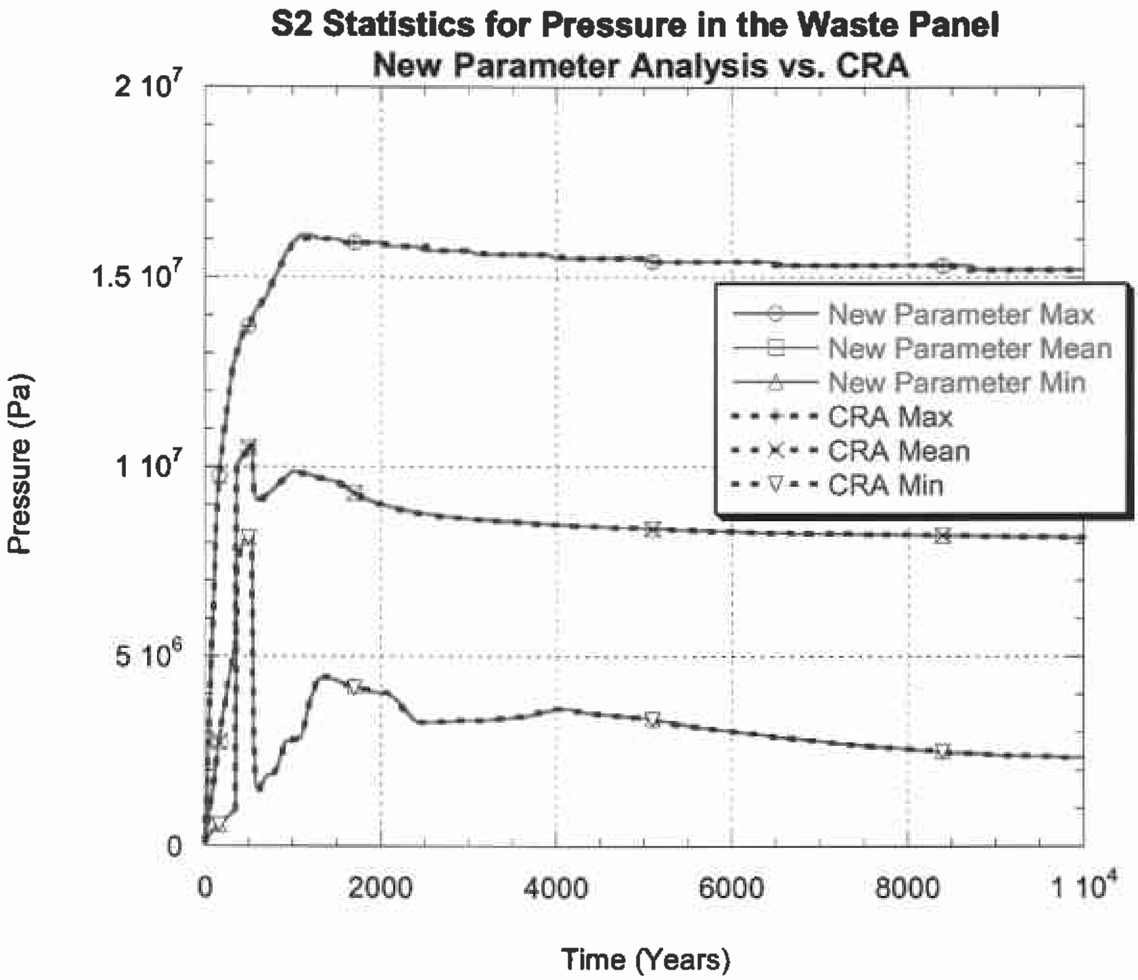

Figure 19 Pressure in the Waste Panel vs. Time: Scenario S2

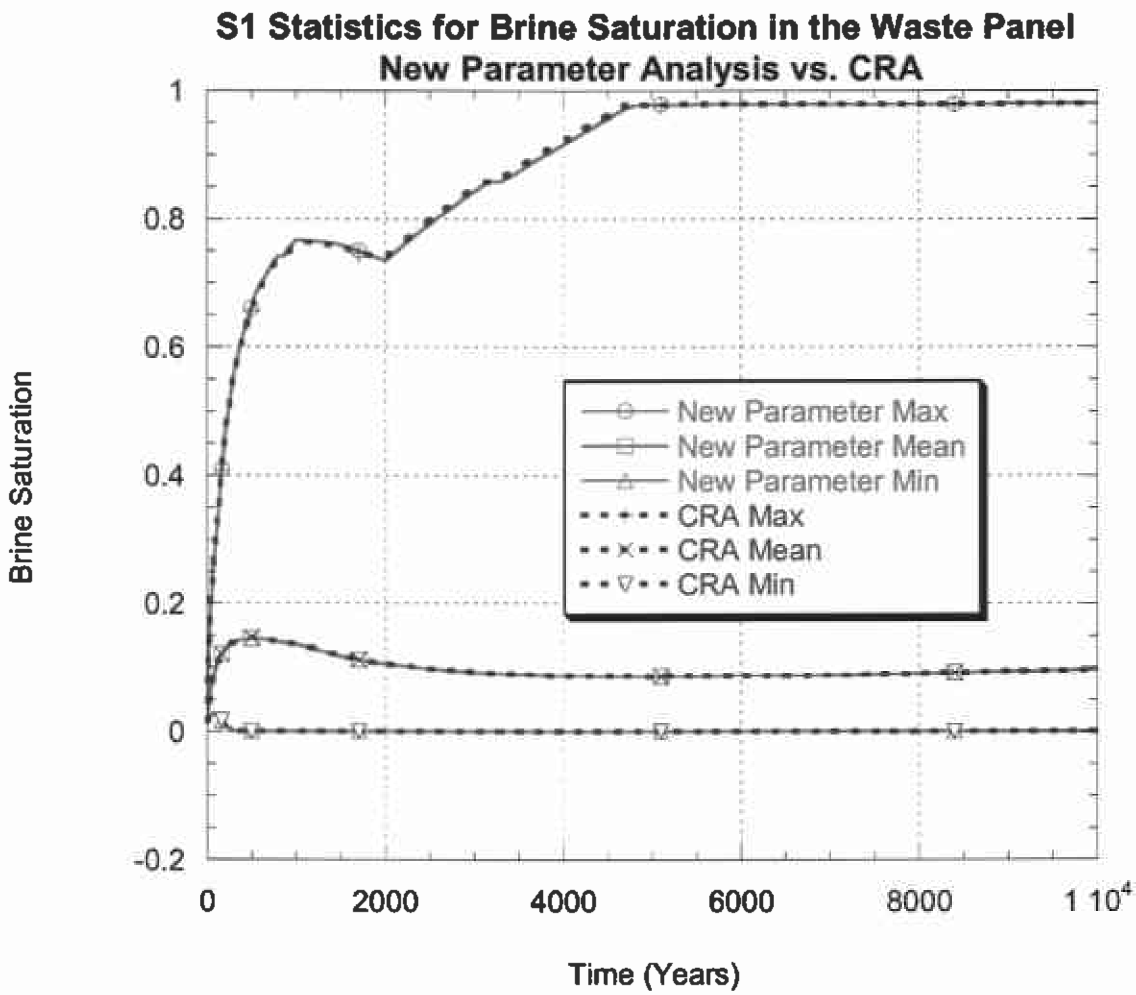

Figure 20 Brine Saturation in the Waste Panel vs. Time: Scenario S1

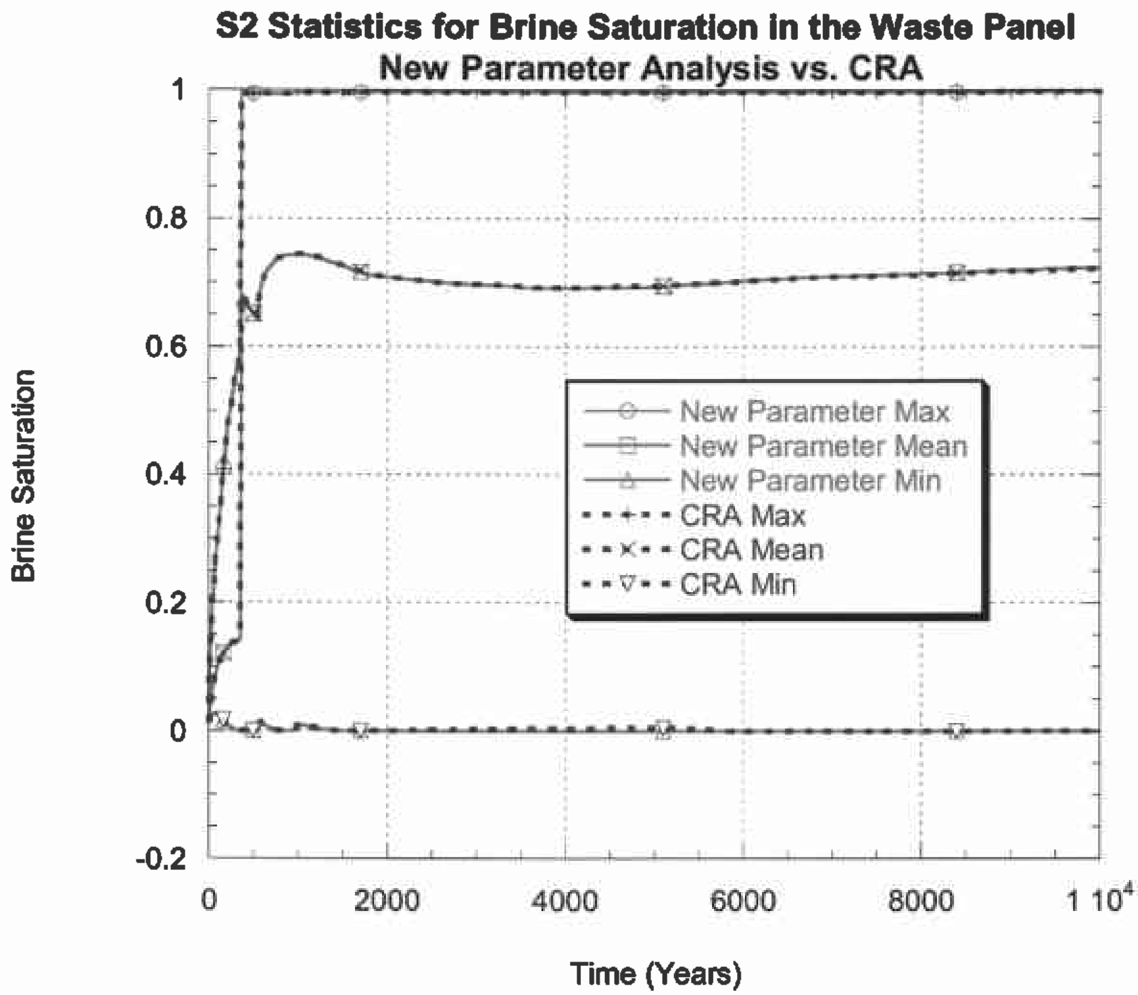

Figure 21 Brine Saturation in the Waste Panel vs. Time: Scenario S2

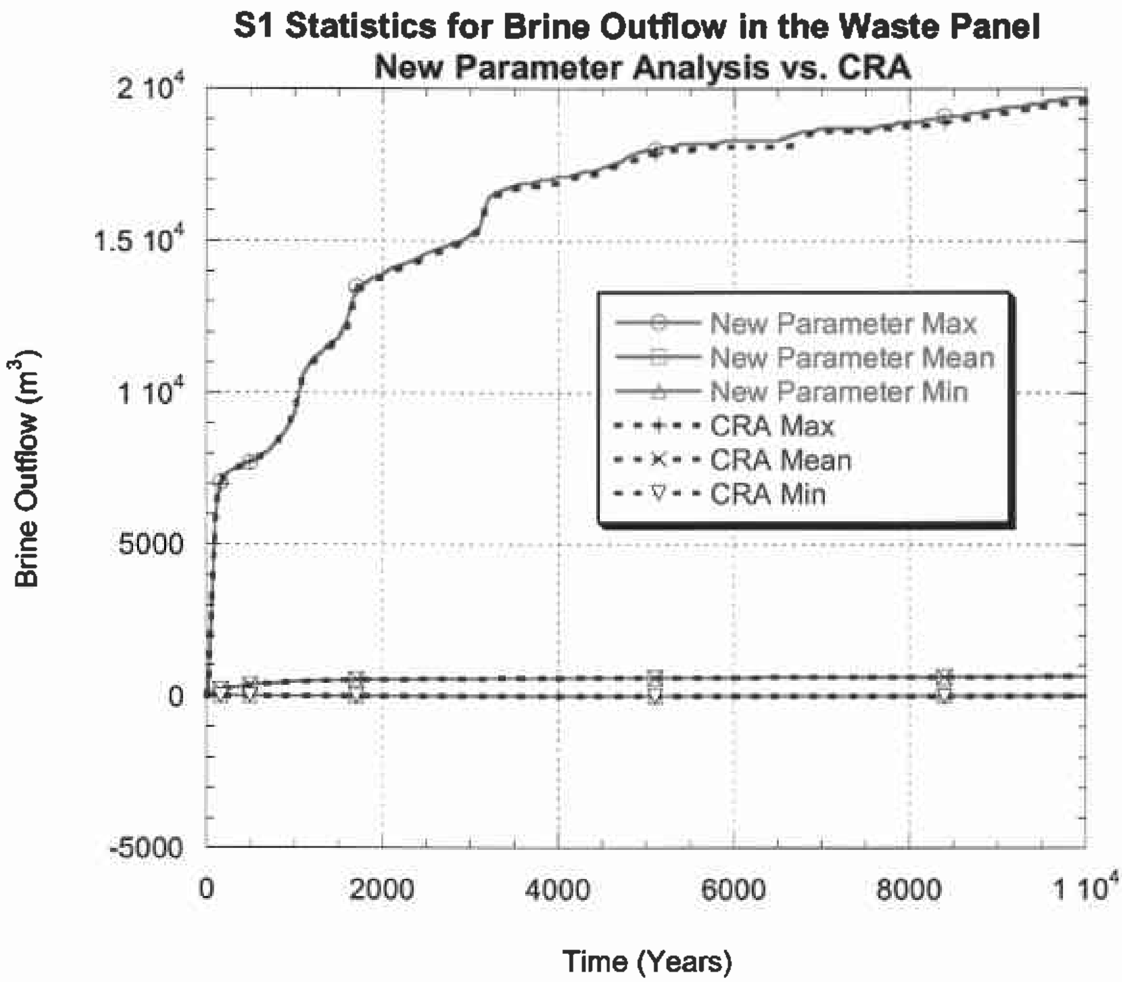

Figure 22 Cumulative Brine Outflow in the Waste Panel vs. Time: Scenario S1

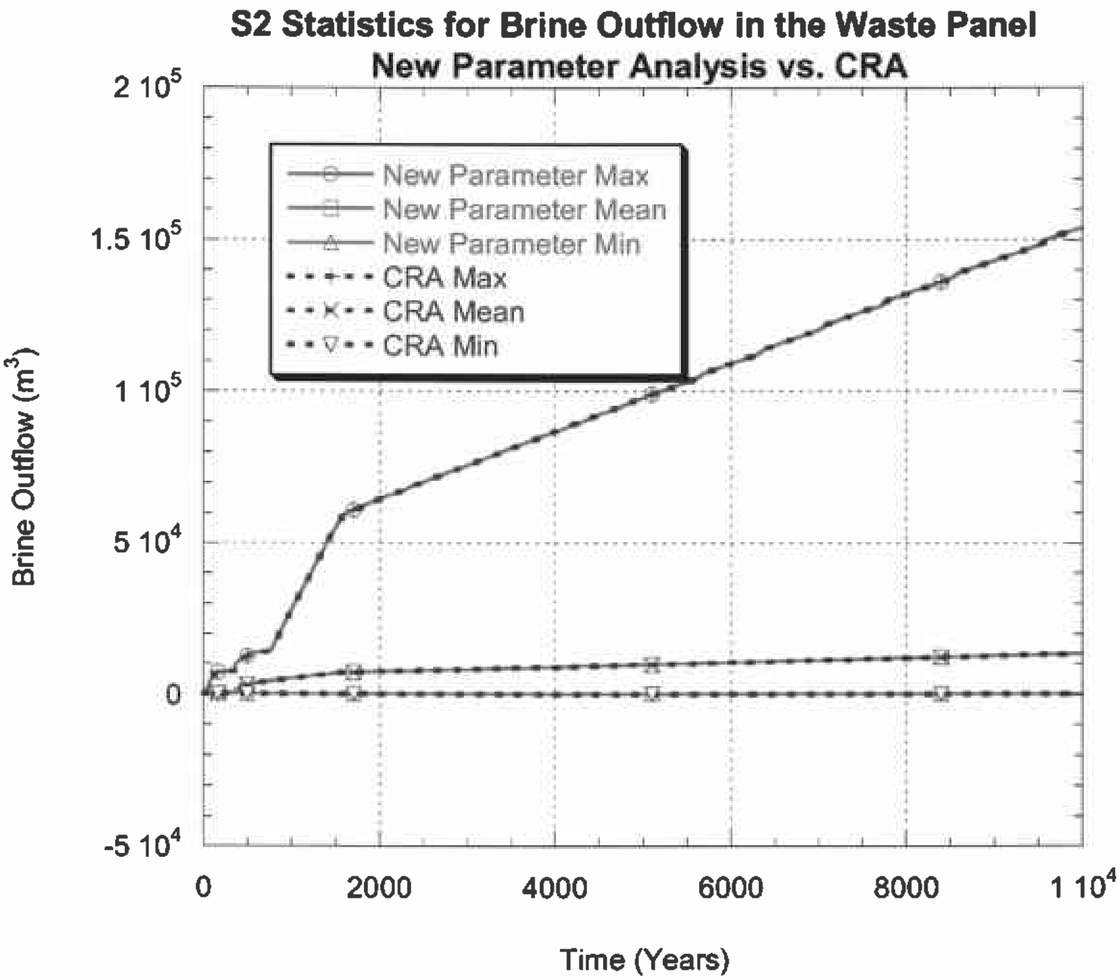

Figure 23 Cumulative Brine Outflow in the Waste Panel vs. Time: Scenario S2

The DBR calculations for scenarios S1 and S2 resulted in direct release calculations for 3,300 separate vector-scenario-time combinations. For a complete PA, these results (along with the results from scenarios S3-S5) would be input into the code CCDFGF that uses them to calculate a release for any vector-intrusion-time combination. This procedure is done by first, linearly interpolating modeled release volumes between the fixed intrusion times and second, multiplying the resulting intrusion–specific DBR volume with the radionuclide concentration calculated for that vector and intrusion time. The present analysis is restricted to the release volumes calculated for the prescribed intrusion times. For this analysis, non-zero releases are defined as releases that are greater than 10^{-7} m^3.

Table 8 shows that the new parameter analysis had 291 runs out of 3,300 (8.82%) that resulted in non-zero DBR volumes and 136 runs out 3,300 (4.12%) that resulted in DBR volumes larger than 10 m^3. This compares with 290 (8.79%) CRA runs that had non-zero

DBR volumes and 135 (4.09%) that had DBR volumes larger than 10 m^3. (This only considers scenarios S1 and S2 from replicate R1.)

The largest DBR volume for the new parameter analysis is 78.4 m^3, whereas the largest DBR volume from the CRA analysis was 75.8 m^3. (This number is the largest DBR volume from scenarios S1 and S2 in the CRA.)

These results suggest that model predictions of direct brine releases are not very sensitive to changes in these parameters.

Table 8 DBR Statistics for the New Parameter Analysis and the CRA

Analysis	Total Runs	Runs/Percentage Resulting in Non-zero DBR volumes	Runs/Percentage w/DBR Volumes Exceeding 10 m^3	Maximum DBR Volume (m^3)
New Parameter Analysis	3,300	291 / 8.82%	136 / 4.12%	78.4
CRA Analysis (Stein 2005)	3,300	290 / 8.79%	135 / 4.09%	75.8

6.0 Conclusions

Pressure, brine saturation, and brine outflow for individual vectors show minor variations when either ANHCOMP or ANRGSSAT is varied. However, when considering all vectors, pressure, brine saturation, brine outflow, and DBR volumes are not significantly affected when the values for ANHCOMP and ANRGSSAT are modeled as constants. Consequently, neither DBRs nor spallings releases would be significantly affected by treating these two parameters as constants.

This analysis concludes that using constants to model ANHCOMP and ANRGSSAT is considered a suitable alternative to using student t-distributions. This analysis recommends using the median values, 2.230e-11 Pa^{-1} for ANHCOMP and 5.495e-2 for ANRGSSAT, and these changes should be implemented by updating their entries in the PAPDB.

It should be noted that when S_MB139:COMP_RCK was sampled by the code LHS for the CCA and CRA, a rank correlation was imposed between S_MB139:COMP_RCK and S_MB139:PRMX_LOG (ANHPERM) (Helton et. al. 2000, U.S. DOE 2004). A thorough review was conducted to determine the justification for imposing this correlation, and no record could be found justifying this correlation. Correlations observed between average permeability and average specific storage in Roberts et al. (1999- see Appendix C) do not support a strong correlation between S_MB139:COMP_RCK and S_MB139:PRMX_LOG . Furthermore, constants cannot be correlated with other parameters, so this analysis concludes that all correlations between S_MB139:COMP_RCK and other parameters should be removed in future PAs when S_MB139:COMP_RCK is modeled as a constant.

7.0 Run Control

Digital Command Language (DCL) scripts, referred to here as EVAL run scripts, are used to implement and document the running of all software codes. These scripts, which are the basis for the WIPP PA run control system, are stored in the CMS library LIBAP118. All inputs are fetched at run time by the scripts, and outputs and run logs are automatically stored in the library LIBAP118.

Table 9 details the run control for the step 1 analysis. Two classes, AP118 and AP118A, were formed for the step 1 analysis. Table 10 outlines the step 2 analysis, and the class CONST was used to label the relevant files for this analysis. Each table is labeled with the main code, and process step (if applicable). Many code sets are broken down into a first step (step 1) which runs utility codes such as Genmesh (GM), Matset (MS), LHS, etc., and subsequent steps (step 2, …) which run the primary code along with any pre and post processors. Step 1 codes are generally run once, or once per replicate, while step 2 codes are generally run once per vector.

Run control tables are intended to provide all the information required to document a calculation. The tables contain five columns:

Code — the descriptive common code name (ICSET, ALGEBRACDB, BRAGFLO, etc.) indicating the row relates to that code, "Script" indicating the row relates to the run control system, or blank indicating the row relates to the previous code label. Completely blank rows are for visual separation only.

Filename — VMS filename in the form <filename>.<extension>. Placeholders are included when multiple replicates, scenarios, vectors, … are being represented (see footnote below).

File Type — the type of file being identified from the point of view of the current step of the run control system. These include script, executable, input, output, and scratch. Note that the output of one step may become the input of an ensuing step.

CMS LIBRARY, CLASS — the CMS library and class where the controlled version of the file can be found, "temporary (wd)" indicating the file is not stored in CMS (many files generated by a calculation are for debug purposes, or are intermediate in nature, and are not retained after execution), "(wd)" or "(ad)" following a CMS library name indicating the input, though stored in CMS, is pulled from the temporary working directory or analysis directory (respectively) for convenience, other lowercase strings indicating the VMS directory pathname where the file (generally an executable) is located.

Table 9 Run Control for Step 1 of the New Parameter Analysis.

Code	Filename	File Type	CMS LIBRARY, location, CLASS
BRAGFLO Step 1a	*run for each replicate. A1 = R1S1 = one run*		
Script	EVAL_BF_AP118_RUN.COM	script	LIBAP118 class AP118
	EVAL_BF_AP118_RUN_MASTER.COM	script	LIBAP118 class AP118
	EVAL_BF_AP118_STEP1A.INP	script	LIBAP118 class AP118
	BF_AP118_R1_S1_STEP1A.LOG	output	LIBAP118 class AP118
GENMESH	gm_PA96.exe	Executable	wp$prodroot:[gm.exe]
	GM_BF_AP118.INP	Input	LIBAP118 class AP118
	GM_BF_AP118.CDB	Output	LIBAP118 class AP118
	GM_BF_AP118.DBG	Output	Temporary (WD)
MATSET	matset_qa0910.exe	Executable	wp$prodroot:[ms.exe]
	MS_BF_AP118.INP	Input	LIBAP118 class AP118
	GM_BF_AP118.CDB	Input	LIBAP118 class AP118 (WD)
	MS_BF_AP118.CDB	Output	LIBAP118 class AP118
	MS_DBG$OUTPUT.DAT	Output	Temporary (WD)
PRELHS	prelhs_qa0230.exe	Executable	wp$prodroot:[lhs.exe]
	LHS1_BF_AP118_A1.INP	Input	LIBAP118 class AP118
	LHS1_BF_AP118_TRN_A1.OUT	Output	LIBAP118 class AP118
	LHS1_BF_AP118_A1.OUT	Output	LIBAP118 class AP118
LHS	lhs_PA96.exe	Executable	wp$prodroot:[lhs.exe]
	LHS1_BF_AP118_A1_TRN.OUT	Input	LIBAP118 class AP118 (WD)
	LHS2_BF_AP118_TRN_A1.OUT	Output	LIBAP118 class AP118
	LHS2_BF_AP118_DBG_A1.OUT	Output	LIBAP118 class AP118
Code	**Filename**	**File Type**	**CMS LIBRARY, location**

BRAGFLO Step 1b	*run for each replicate. A1 = R1S1 = one run*		
Script	EVAL_BF_AP118_RUN.COM	script	LIBAP118 class AP118
	EVAL_BF_AP118_RUN_MASTER.COM	script	LIBAP118 class AP118
	EVAL_BF_AP118_STEP1B.INP	script	LIBAP118 class AP118
	EVAL_BF_AP118A_STEP1B.INP	script	LIBAP118 class AP118A
	BF_AP118_(_R1_S1_STEP1B.LOG	output	LIBAP118 class AP118
POSTLHS	postlhs_PA96.exe	Executable	wp$prodroot:[lhs.exe]
	MS_BF_AP118.CDB	Input	LIBAP118 class AP118
	LHS2_AP118_(_TRN_A1.OUT	Input	LIBAP118 class AP118
	LHS3_AP118.INP	Input	LIBAP118 class AP118
	LHS3_AP118_(_A1_R^.CDB	Output	LIBAP118 class AP118
	LHS3_AP118_(.DBG	Output	Temporary (WD)
	LHS3_AP118_(_1.SCR	Output	Temporary (WD)
	LHS3_AP118_(_2.SCR	Output	Temporary (WD)
ICSET	icset_PA96.exe	Executable	wp$prodroot:[ic.exe]
	LHS3_AP118_(_A1_R^.CDB	Input	LIBAP118 class AP118 (WD)
	IC_BF_AP118.INP	Input	LIBAP118 class AP118
	IC_BF_AP118_(_R1_V^.CDB	Output	Temporary (WD)
	IC_BF_AP118_(_R1_V^.DBG	Output	Temporary (WD)
ALGEBRACDB	algebracdb_PA96.exe	Executable	wp$prodroot:[alg.exe]
	IC_BF_AP118_(_R1_V^.CDB	Input	Working Directory
	ALG1_BF_AP118.INP	Input	LIBAP118 class AP118
	ALG1_BF_AP118_(_R1_V^.CDB	Output	LIBAP118 class AP118
	ALG1_BF_AP118_(_R1_V^.DBG	Output	Temporary (WD)
BRAGFLO Step 2	*Run for each replicate (R1), scenario (S1-S2), vector (V001-V100) = 200 runs*		
Code	**Filename**	**File Type**	**CMS LIBRARY, location**
Script	EVAL_BF_AP118_RUN.COM	script	LIBAP118 class AP118

	EVAL_BF_AP118_RUN_MASTER.COM	script	LIBAP118 class AP118
	EVAL_BF_AP118_STEP2.INP	script	LIBAP118 class AP118
	EVAL_BF_AP118A_STEP2.INP	script	LIBAP118 class AP118A
	BF_AP118_(_R1S%V^.LOG	output	LIBAP118 class AP118
PREBRAG	prebrag_qb0700.exe	Executable	wp$prodroot:[bf.exe]
	BF1_AP118_S%.INP	Input	LIBAP118 class AP118
	ALG1_BF_AP118_(_R1_V^.CDB	Input	LIBAP118 class AP118
	BF1_AP118_(_R1_S%_V^.DBG	Output	Temporary (WD)
	BF2_AP118_(_R1_S%_V^.INP	Output	LIBAP118 class AP118
BRAGFLO Step 3	*Run for each replicate (R1), scenario (S1-S2), vector (V001-V100) = 200 runs*		
Code	**Filename**	**File Type**	**CMS LIBRARY, location**
Script	EVAL_BF_AP118_RUN.COM	script	LIBAP118 class AP118
	EVAL_BF_AP118_RUN_MASTER.COM	script	LIBAP118 class AP118
	EVAL_BF_AP118_STEP3.INP	script	LIBAP118 class AP118
	EVAL_BF_AP118A_STEP3.INP	script	LIBAP118 class AP118A
	BF_ALG2_AP118_(_R1S%V^_STEP3.LOG	output	LIBAP118 class AP118
BRAGFLO	bragflo_qa0500.exe	Executable	wp$prodroot:[bf.exe]
	BF2_AP118_(_R1_S%_V^.INP	Input	LIBAP118 class AP118 (WD)
	BF2_AP118_CLOSURE.DAT	Input	LIBAP118 class AP118
	BF2_AP118_(_R1_S%_V^.OUT	Output	LIBAP118 class AP118
	BF2_AP118_(_R1_S%_V^.SUM	Output	LIBAP118 class AP118
	BF2_AP118_(_R1_S%_V^.BIN	Output	Temporary (WD)
	BF2_AP118_(_R1_S%_V^.ROT	Output	Temporary (WD)
	BF2_AP118_(_R1_S%_V^.RIN	Output	Temporary (WD)
POSTBRAG	postbrag_PA96.exe	Executable	wp$prodroot:[bf.exe]
	BF2_AP118_(_R1_S%_V^.BIN	Input	LIBAP118 class AP118 (WD)
	ALG1_BF_AP118_(_R1_V^.CDB	Input	LIBAP118 class AP118 (WD)

	BF3_AP118_(_R1_S%_V^.CDB	Output	LIBAP118 class AP118 (WD)
	BF3_AP118_(_R1_S%_V^.DBG	Output	Temporary (WD)
BRAGFLO Step 4	*Run for each replicate (R1), scenario (S1-S2), vector (V001-V100) = 200 runs*		
Code	**Filename**	**File Type**	**CMS LIBRARY, location**
Script	EVAL_BF_AP118_RUN.COM	script	LIBAP118 class AP118
	EVAL_BF_AP118_RUN_MASTER.COM	script	LIBAP118 class AP118
	EVAL_BF_AP118_STEP4.INP	script	LIBAP118 class AP118
	EVAL_BF_AP118A_STEP4.INP	script	LIBAP118 class AP118A
	BF_ALG2_AP118_(_R1S%V^_STEP4.LOG	output	LIBAP118 class AP118
ALGEBRACDB_2 (POSTALG)	algebracdb_PA96.exe	Executable	wp$prodroot:[alg.exe]
	BF3_AP118_(_R1_S%_V^.CDB	Input	LIBAP118 class AP118 (AD)
	ALG2_BF_AP118.INP	Input	LIBAP118 class AP118
	ALG2_AP118_(_R1_S%_V^.CDB	Output	LIBAP118 class AP118
	ALG2_BF_AP118_(_R1S%V^.DBG	Output	Temporary (WD)

- S%—used to denote multiple scenarios.
- V^—used to denote multiple vectors.
- (—used to denote use of a specific value for ANHCOMP or ANRGSSAT. See Table 6 and Table 7.
- T! — used to denote multiple time intrusions.
- (wd)—working_dir
- (ad)—analysis_dir

Table 10 Run Control for Step 2 of the New Parameter Analysis

Code	Filename	File Type	CMS LIBRARY, CLASS
BRAGFLO Step 1	*run for each replicate. R1 = one run*		
Script	EVAL_BF_AP118_CONST_RUN.COM	script	AP118, CONST
	EVAL_BF_AP118_CONST_RUN_MASTER.COM	script	AP118, CONST
	EVAL_BF_AP118_CONST_STEP1.INP	script	AP118, CONST
	BF_AP118_CONST_R1_S%_STEP1.LOG	output	AP118, CONST
POSTLHS	postlhs_PA96.exe	Executable	wp$prodroot:[lhs.exe]
	MS_BF_CRA1.CDB	Input	AP118, CONST
	LHS2_AP118_CONST_TRN_A1.OUT	Input	AP118, CONST
	LHS3_CRA1.INP	Input	AP118, CONST
	LHS3_AP118_CONST_A1_R^.CDB	Output	AP118, CONST
	LHS3_AP118_CONST.DBG	Output	Temporary (WD)
	LHS3_AP118_CONST_1.SCR	Output	Temporary (WD)
	LHS3_AP118_CONST_2.SCR	Output	Temporary (WD)
ICSET	icset_PA96.exe	Executable	wp$prodroot:[ic.exe]
	LHS3_AP118_CONST_A1_R^.CDB	Input	AP118, CONST (WD)
	IC_BF_CRA1.INP	Input	AP118, CONST
	IC_BF_AP118_CONST_R1_V^.CDB	Output	Temporary (WD)
	IC_BF_AP118_CONST_R1_V^.DBG	Output	Temporary (WD)
ALGEBRACDB	algebracdb_PA96.exe	Executable	wp$prodroot:[alg.exe]
	IC_BF_AP118_CONST_R1_V^.CDB	Input	AP118, CONST (WD)
	ALG1_BF_CRA1.INP	Input	AP118, CONST
	ALG1_BF_AP118_CONST_R1_V^.CDB	Output	AP118, CONST
	ALG1_BF_AP118_CONST_R1_V^.DBG	Output	Temporary (WD)

BRAGFLO Step 2	*Run for each replicate (R1), scenario (S1-S2), vector (V001-V100) = 200 runs*		
Code	**Filename**	**File Type**	**CMS LIBRARY, location**
Script	EVAL_BF_AP118_CONST_RUN.COM	script	AP118, CONST
	EVAL_BF_AP118_CONST_RUN_MASTER.COM	script	AP118, CONST
	EVAL_BF_AP118_CONST_STEP2.INP	script	AP118, CONST
	BF_AP118_CONST_R1S%V^.LOG	output	AP118, CONST
PREBRAG	prebrag_qb0700.exe	Executable	wp$prodroot:[bf.exe]
	BF1_CRA1_S%.INP	Input	AP118, CONST
	ALG1_BF_AP118_CONST_R1_V^.CDB	Input	AP118, CONST
	BF1_AP118_CONST_R1_S%_V^.DBG	Output	Temporary (WD)
	BF2_AP118_CONS_R1_S%_V^.INP	Output	AP118, CONST
BRAGFLO Step 3	*Run for each replicate (R1), scenario (S1-S2), vector (V001-V100) = 200 runs*		
Code	**Filename**	**File Type**	**CMS LIBRARY, location**
Script	EVAL_BF_AP118_CONST_RUN.COM	script	AP118, CONST
	EVAL_BF_AP118_CONST_RUN_MASTER.COM	script	AP118, CONST
	EVAL_BF_AP118_CONST_STEP3.INP	script	AP118, CONST
	BF_ALG2_AP118_CONST_R1S%V^_STEP3.LOG	output	AP118, CONST
BRAGFLO	bragflo_qa0500.exe	Executable	wp$prodroot:[bf.exe]
	BF2_AP118_CONST_R1_S%_V^.INP	Input	AP118, CONST (WD)
	BF2_CRA1_CLOSURE.DAT	Input	AP118, CONST
	BF2_AP118_CONST_R1_S%_V^.OUT	Output	AP118, CONST
	BF2_AP118_CONST_R1_S%_V^.SUM	Output	AP118, CONST
	BF2_AP118_CONST_R1_S%_V^.BIN	Output	Temporary (WD)
	BF2_AP118_CONST_R1_S%_V^.ROT	Output	Temporary (WD)
	BF2_AP118_CONST_R1_S%_V^.RIN	Output	Temporary (WD)

POSTBRAG	postbrag_PA96.exe	Executable	wp$prodroot:[bf.exe]
	BF2_AP118_CONST_R1_S%_V^.BIN	Input	Temporary (WD)
	ALG1_BF_AP118_CONST_R1_V^.CDB	Input	AP118, CONST (WD)
	BF3_AP118_CONST_R1_S%_V^.CDB	Output	AP118, CONST
	BF3_AP118_CONST_R1_S%_V^.DBG	Output	Temporary (WD)
BRAGFLO Step 4	*Run for each replicate (R1), scenario (S1-S2), vector (V001-V100) = 200 runs*		
Code	**Filename**	**File Type**	**CMS LIBRARY, location**
Script	EVAL_BF_AP118_CONST_RUN.COM	script	AP118, CONST
	EVAL_BF_AP118_CONST_RUN_MASTER.COM	script	AP118, CONST
	EVAL_BF_AP118_CONST_STEP4.INP	script	AP118, CONST
	BF_ALG2_AP118_CONST_R1S%V^_STEP4.LOG	output	AP118, CONST
ALGEBRACDB_2 (POSTALG)	algebracdb_PA96.exe	Executable	wp$prodroot:[alg.exe]
	BF3_AP118_CONST_R1_S%_V^.CDB	Input	AP118, CONST (WD)
	ALG2_BF_CRA1.INP	Input	AP118, CONST
	ALG2_AP118_CONST_R1_S%_V^.CDB	Output	AP118, CONST
	ALG2_BF_AP118_CONST_R1S%V^.DBG	Output	Temporary (WD)
BRAGFLO Step 3 Mod	**Exception Runs: R1S1V018, R1S2V018, R1S2V098**		
Code	**Filename**	**File Type**	**CMS LIBRARY, location**
Script	EVAL_BF_AP118_CONST_RUN.COM	script	AP118, CONST
	EVAL_BF_AP118_CONST_RUN_MASTER.COM	script	AP118, CONST
	EVAL_BF_AP118_CONST_STEP3_GENERIC_MOD.INP	script	AP118, CONST
	BF_ALG2_AP118_CONST_R1S%V^_STEP3.LOG	output	AP118, CONST

BRAGFLO	bragflo_qa0500.exe	Executable	wp$prodroot:[bf.exe]
	BF2_AP118_CONST_R1_S%_V^_MOD.INP	Input	AP118, CONST
	BF2_CRA1_CLOSURE.DAT	Input	AP118, CONST
	BF2_AP118_CONST_R1_S%_V^.OUT	Output	Temporary (WD)
	BF2_AP118_CONST_R1_S%_V^.SUM	Output	Temporary (WD)
	BF2_AP118_CONST_R1_S%_V^.BIN	Output	Temporary (WD)
	BF2_AP118_CONST_R1_S%_V^.ROT	Output	Temporary (WD)
	BF2_AP118_CONST_R1_S%_V^.RIN	Output	Temporary (WD)
POSTBRAG	postbrag_PA96.exe	Executable	wp$prodroot:[bf.exe]
	BF2_AP118_CONST_R1_S%_V^.BIN	Input	WD
	ALG1_BF_AP118_CONST_R1_V^.CDB	Input	AP118, CONST (WD)
	BF3_AP118_CONST_R1_S%_V^.CDB	Output	AP118, CONST
	BF3_AP118_CONST_R1_S%_V^.DBG	Output	Temporary (WD)
Code	**Filename**	**File Type**	**CMS LIBRARY, CLASS**
CUTTINGS_S Step 2	*Run for each replicate (R1), scenario (S1-S2), vector (V001-V100), cavity (U,M,L), time intrusion (100, 350, 550, 750, 1000, 2000, 3000, 4000, 5000, 10000) = 3300 runs*		
Script	EVAL_CUSP_AP118_RUN.COM	script	AP118, CONST
	EVAL_CUSP_AP118_RUN_MASTER.COM	script	AP118, CONST
	EVAL_CUSP_AP118_STEP2.INP	script	AP118, CONST
	CUSP_AP118_CONST_R1S%V^(T!_STEP2.LOG	output	AP118, CONST

CUTTINGS_S	cuttings_s_qa0510.exe	Executable	wp$prodroot:[cusp.exe]
	CUSP_CRA1_S%_(_T!.INP	Input	AP118, CONST
	LHS3_CRA1_CUSP_A1_R^.CDB	Input	AP118, CONST
	CUSP_CRA1_SDB.ASC	Input	AP118, CONST
	BF3_AP118_CONST_R1_S%_V^.CDB	Input	AP118, CONST
	SUM_DRS_SPLV0L2.TBL	Input	AP118, CONST
	CUSP_AP118_CONST_R1_S%_V^_(_T!.DBG	Output	Temporary (WD)
	CUSP_AP118_CONST_R1_S%_V^_(_T!.CDB	Output	AP118, CONST
Code	**Filename**	**File Type**	**CMS LIBRARY, CLASS**
DBR Step 2_3	*Run for each replicate (R1), scenario (S1-S2), vector (V001-V100), cavity (U,M,L), time intrusion (100, 350, 550, 750, 1000, 2000, 3000, 4000, 5000, 10000) = 3300 runs*		
Script	EVAL_DBR_AP118_CONST_RUN.COM	script	AP118, CONST
	EVAL_DBR_AP118_CONST_RUN_MASTER.COM	script	AP118, CONST
	EVAL_DBR_AP118_CONST_STEP2_3.INP	script	AP118, CONST
	DBR_AP118_CONST_R1S%V^(T!_STEP2_3.LOG	output	AP118, CONST
ALGEBRACDB	algebracdb_pa96.exe	Executable	wp$prodroot:[alg.exe]
	CUSP_AP118_CONST_R1_S%_V^_L_T!.CDB	Input	AP118, CONST
	ALG_DBR_CRA1_PRECUSP_DIR_REL.INP	Input	AP118, CONST
	DBR_AP118_CONST_R1S%_V^_T!.CDB	Output	Temporary (WD)
	DBR_AP118_CONST_R1S%_V^_T!.DBG	Output	Temporary (WD)
RELATE_1	relate_pa96.exe	Executable	wp$prodroot:[rel.exe]
	DBR_AP118_CONST_R1S%_V^_T!.CDB	Input	AP118, CONST
	MS_DBR_CRA1_DIR_REL.CDB	Input	AP118, CONST
	REL_DBR_CUSP_CRA1_DIR_REL.INP	Input	AP118, CONST
	REL1_DBR_AP118_CONST_R1S%_V^_T!.CDB	Output	Temporary (WD)
	REL1_DBR_AP118_CONST_R1S%_V^_T!.DBG	Output	Temporary (WD)

RELATE_2	relate_pa96.exe	Executable	wp$prodroot:[rel.exe]
	REL1_DBR_AP118_CONST_R1S%_V^_T!.CDB	Input	Temporary (WD)
	REL_DBR_BRAG_CRA1_DIR_REL_S%.INP	Input	AP118, CONST
	BF3_AP118_CONST_R1_S%_V^.CDB	Input	AP118, CONST
	REL2_AP118_CONST_R1S%_V^_T!.CDB	Output	Temporary (WD)
	REL2_AP118_CONST_R1S%_V^_T!.DBG	Output	Temporary (WD)
ICSET	icset_pa96.exe	Executable	wp$prodroot:[ic.exe]
	REL2_AP118_CONST_R1S%_V^_T!.CDB	Input	Temporary (WD)
	IC_DBR_CRA1_DIR_REL_S%.INP	Input	AP118, CONST
	IC_DBR_AP118_CONST_R1S%_V^_T!.CDB	Output	Temporary (WD)
	IC_DBR_AP118_CONST_R1S%_V^_T!.DBG	Output	Temporary (WD)
ALGEBRACDB_2	algebracdb_pa96.exe	Executable	wp$prodroot:[alg.exe]
	IC_DBR_AP118_CONST_R1S%_V^_T!.CDB	Input	Temporary (WD)
	ALG_DBR_CRA1_PRE_DIR_REL_S%.INP	Input	AP118, CONST
	ALG_2_DBR_AP118_CONST_R1S%_V^_T!.CDB	Output	Temporary (WD)
	ALG_2_DBG_AP118_CONST_R1S%_V^_T!.DBG	Output	Temporary (WD)
PREBRAG	prebrag_qb0700.exe	Executable	wp$prodroot:[bf.exe]
	ALG_2_DBR_AP118_CONST_R1S%_V^_T!.CDB	Input	Temporary (WD)
	DBR_BF1_CRA1_DIR_REL_S%_(.INP	Input	AP118, CONST
	BF1_DBR_AP118_CONST_R1S%_V^_(_T!.DBG	Output	Temporary (WD)
	DBR_AP118_CONST_R1S%_V^_(_T!.INP	Output	AP118, CONST
BRAGFLO	bragflo_qa0500.exe	Executable	wp$prodroot:[bf.exe]
	DBR_AP118_CONST_R1S%_V^_(_T!.INP	Input	AP118, CONST (WD)
	DBR_AP118_CONST_R1S%_V^_(_T!.OUT	Output	Temporary (WD)
	DBR_AP118_CONST_R1S%_V^_(_T!.SUM	Output	Temporary (WD)
	DBR_AP118_CONST_R1S%_V^_(_T!.BIN	Output	Temporary (WD)
	DBR_AP118_CONST_R1S%_V^_(_T!.ROT	Output	Temporary (WD)
	DBR_AP118_CONST_R1S%_V^_(_T!.RIN	Output	Temporary (WD)

POSTBRAG	postbrag_pa96.exe	Executable	wp$prodroot:[bf.exe]
	ALG_2_DBR_AP118_CONST_R1S%_V^_T!.CDB	Input	Temporary (WD)
	DBR_AP118_CONST_R1S%_V^_(_T!.BIN	Input	Temporary (WD)
	BF3_DBR_AP118_CONST_R1S%_V^_(_T!.CDB	Output	AP118, CONST
	BF3_DBR_AP118_CONST_R1S%_V^_(_T!.DBG	Output	Temporary (WD)
SUMMARIZE for DBR	*Run for each replicate (R1), scenario (S1-S2), vector (V001-V100), cavity (U,M,L), time intrusion (100, 350, 550, 750, 1000, 2000, 3000, 4000, 5000, 10000) = 3300 runs*		
Code	**Filename**	**File Type**	**CMS LIBRARY, location**
Script	EVAL_SUM_DBR_AP118_RUN.COM	script	AP118, CONST
	EVAL_SUM_DBR_AP118_RUN_MASTER.COM	script	AP118, CONST
	EVAL_SUM_DBR_AP118.INP	script	AP118, CONST
	SUM_DBR_AP118_CONSTR1S%_T!.LOG	output	AP118, CONST
SUMMARIZE	summarize_qa0220.exe	Executable	wp$prodroot:[sum.exe]
	SUM_DBR_AP118_CONST_R1_S%_(_T!.INP	Input	AP118, CONST
	DBR_POST_AP118_CONST_R1_S%_V^_(_T!.CDB	Input	AP118, CONST
	SUM_DBR_AP118_CONST_R1_S%_(_T!.TBL	Output	Temporary (WD)
	SUM_DBR_AP118_CONST_R1_S%_(_T!.LOG	Output	Temporary (WD)
	SUM_DBR_AP118_CONST_R1_S%_(_T!_ERROR.LOG	Output	Temporary (WD)

- S%—used to denote multiple scenarios.
- V^—used to denote multiple vectors.
- (—used to denote multiple cavities.
- T! — used to denote multiple time intrusions.
- (wd)—working_dir
- (ad)—analysis_dir

8.0 References

Hansen, C. 2004. Software Problem Report 04-003. Sandia National Laboratories. Carlsbad,NM. ERMS #535667.

Helton, J., Martell, M.-A., and M. Tierney. 2000."Characterization of Subjective Uncertainty in the 1996 Performance Assessment for the Waste Isolation Pilot Plant." Reliability Engineering and System Safety, 69. p.191–204.

Long, J. 2004. Execution of Performance Assessment for the Advanced Mixed Waste Calculations, Revision 1. Sandia National Laboratories. Carlsbad, NM. ERMS #534194.

Roberts, R., Beauheim, R., and P. Domski. Hydraulic Testing of Salado Formation Evaporites at the Waste Isolation Pilot Plant Site: Final Report. Sandia National Laboratories. Carlsbad, NM. SAND98-2537.

Stein, J. and Zelinski, W. 2003. Analysis Package for Direct Brine Releases: Compliance Recertification Application Rev 1. Sandia National Laboratories. Carlsbad, NM. ERMS # 532344.

Stein, J. 2005. Memo to Records: Error found in table included in CRA DBR Analysis Report. Sandia National Laboratories. Carlsbad, NM. ERMS # 539116.

U. S. Congress. 1992. Waste Isolation Pilot Plant Land Withdrawl Act. Public Law 102-579, as amended by Public Law 104-201. September 1996. 104th Congress, Washington D.C.

U.S. DOE. 2004. Title 40 CFR Part 191 Compliance Recertification Application for the Waste Isolation Pilot. DOE/WIPP 2004-3231, U.S. Department of Energy Waste Isolation Pilot Plant, Carlsbad Field Office, Carlsbad, NM.

U.S. EPA. 1993. 40 CFR 191. Environmental Radiation Protection Standards for Management and Disposal of Spent Nuclear Fuel, High-Level and Transuranic Radioactive Wastes: Final Rule. U.S. Environmental Protection Agency, Washington, DC.

U.S. EPA. 1996. 40 CFR 194. Criteria for the Certification and Recertification of the Waste Isolation Pilot Plant's Compliance with the 40 CFR Part 191 Disposal Regulations. U.S. Environmental Protection Agency, Washington, DC.

Vugrin, E. 2005. Change Control Form for LHS version 2.41 to LHS version 2.42. Sandia National Laboratories. Carlsbad, NM. ERMS# 538375.

Vugrin, E. and T. Kirchner. 2005. Analysis Plan for Modifying Parameter Distributions for S_MB139:COMP_RCK and S_MB139:SATRGAS. Sandia National Laboratories. Carlsbad, NM. ERMS# 538607.

WIPP-PA (Performance Assessment). 2004. User's Manual for LHS Version 2.41. Sandia National Laboratories. Carlsbad, NM. ERMS# 230732.

WIPP-PA (Performance Assessment). 2003. User's Manual for BRAGFLO Version 5.00. Sandia National Laboratories. Carlsbad, NM. ERMS# 525702.

EV 3/31/05

Vugrin, Eric D

From: Stein, Joshua Stephenson
Sent: Thursday, March 31, 2005 12:39 PM
To: Vugrin, Eric D
Subject: Signature authority for COMP_RCK report

Eric,

I grant you signature authority in my absence for the report entitled: "Analysis Report for Modifying Parameter Distributions for S_MB139:COMP_RCK and S_MB139:SAT_RGAS". Please sign-off for me as a co-author

Thanks,
-Josh

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