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Subject: Normalized moles of Castile sulfate entering the repository and fraction of MgO lost due to brine flow out of the repository.

1.0 Executive Summary

Calculations were performed to address and quantify the amount of sulfate that could enter the repository from the Castile brine and the amount of MgO that could be lost due to dissolution in brine and subsequent movement of that brine out of the repository. A Monte Carlo approach was used to determine the probability distribution for each calculation. The results show that on average, enough sulfate enters the "worst case" waste panel to consume 2.4% or less of the carbon by sulfate reduction using Castile sulfate and that 0.8% of the MgO is lost due to brine flow out of the waste panel.

2.0 Introduction

On April 10, 2006, a planned change request was submitted to the U. S. Environmental Protection Agency (EPA) requesting approval to "emplace 1.2 moles of magnesium oxide (MgO) for every mole of consumable-organic carbon contained in the Waste Isolation Pilot Plane (WIPP)" (Moody, 2006). Currently the EPA requires the emplacement of 1.67 moles of MgO for every mole of consumable carbon in the emplaced cellulose, plastic, and rubber (CPR) materials. In response, EPA wrote a letter (Gitlin, 2006) asking the U. S. Department of Energy (DOE) to address the "uncertainties related to MgO effectiveness, the size of the uncertainties, and the potential impact of the uncertainties on long-term performance." Two sources of uncertainty, related to MgO effectiveness are the amount of sulfate that could enter the repository from the Castile brine and the amount of MgO that could be lost due to dissolution in brine and subsequent movement of that brine out of the repository. The amount of sulfate in the repository can affect the amount of CO_2 that is generated from the organic carbon and hence the amount of MgO needed. The objective of this memo is to address and quantify the uncertainties concerning these two issues.

To determine the amount of Castile sulfate and MgO lost to brine, a stochastic approach was used similar to the method used by the code CCDFGF to calculate releases

(Hansen, 2003). Futures of drilling events were generated using a Monte-Carlo simulation (see Section 3.0). The behavior of the repository in each future was taken from the 2004 Compliance Recertification Application (CRA-2004) Performance Assessment Baseline Calculation (PABC) BRAGFLO results (Nemer and Stein, 2005). All 300 vectors from all 3 replicates were used. For each future and vector, the amount of sulfate from the Castile and MgO lost to brine were determined. This was then used to produce cumulative probability distributions (using Microsoft Access® and Excel®) for the cumulative amount of Castile sulfate that entered the repository and the cumulative MgO lost to brine, in 10,000 years.

3.0 Calculation of repository drilling-intrusion futures

A Monte Carlo simulation using the commercial-off-the-shelf (COTS) software Crystal Ball® was used to generate 1000 distinct repository drilling-event futures. These futures contain sequences of drilling intrusions that penetrate the repository. The futures were calculated analogously to the method used by CCDFGF (Hansen, 2003). The choice of the number 1000 was to give a 95% confidence that up to the 99th percentile has been adequately represented (Hahn and Meeker, 1991).

Drilling is modeled as a Poisson process, with the rate of drilling events assumed to be 5.25e-003 intrusions/km^2/yr (GLOBAL:LAMBDAD). This rate counts all intrusions in the area covered by the berm 6.285e+005 m^2 (REFCON:ABERM); intrusions that hit waste areas are a subset of the total set of intrusions. Each drilling event was characterized by sampling the stochastic parameters listed in Table 1. The probabilities listed are conditional upon a drilling intrusion into the berm area.

Table 1. Drilling event characteristics with associated probability and justification.

Characteristic	Probability	Justification
Hit Waste Panel	0.202	Ratio of the waste area (REFCON: AREA_CH + REFCON: AREA_RH) to the area of the berm placed over the waste panel (REFCON: ABERM).
Hit Castile Brine Pocket	0.01 to 0.60	GLOBAL: PBRINE
Hit Panels 1-10	0.10	Uniform distribution between the 10 panels. This assumes the area of each panel is the same.
Plug Type 1	0.015	GLOBAL: ONEPLG
Plug Type 2	0.696	GLOBAL: TWOPLG
Plug Type 3	0.289	GLOBAL: THREEPLG

Based on the characteristics of each drilling event, the intrusions were classified as no change (not significantly changing repository behavior), an E1 type (where the brine pocket is hit) or an E2 type (where the brine pocket is not hit). This classification process is illustrated below in Table 2. The intrusion classification is the same as used in the code CCDFGF and was used to determine the impact on each calculation. The classification process was verified as shown in Appendix A.3.

Table 2. Intrusion classification criteria matrix.

Classification	Hit Waste	Hit Brine Pocket	Plug Type
No Change	No	Yes or No	1,2 or 3
	Yes	Yes or No	1
E1	Yes	Yes	2
E2	Yes	Yes	3
	Yes	No	2 or 3

4.0 Calculation of the state of an intruded panel

The post-processed BRAGFLO results from the CRA-2004 PABC (see Appendix A.2) were used to determine how much sulfate would enter the repository from the Castile, and how much MgO would be lost to brine and exit the repository. This was determined for each vector (100 vectors per replicate, replicates R1-R3) at 10,000 years. All of the scenarios (S1-S6, see Nemer and Stein, 2005) were either directly or indirectly used as explained below. Sulfate from the Castile is discussed below in Subsection 4.1. MgO lost to brine is discussed in Subsection 4.2. The calculation processes were verified as shown in Appendix A.

4.1 Sulfate inflow from the Castile

The BRAGFLO post-ALGEBRA files (Nemer and Stein, 2005) contain the variable BNBHLDRZ, which is the cumulative volumetric flow of brine (m^3) up the borehole from the brine pocket into the intruded panel. For this analysis, the cumulative volumetric flow at 10,000 years was taken for each of the 300 vectors (from all three replicates) and multiplied by 179 moles of sulfate per m^3 (see the file FMT_CRA1BC_ER6_HMAG_ORGS_011.OUT in the CMS library LIBCRA1BC_FMT, Long and Kanney, 2005). This sulfate concentration corresponds to that in Castile brine after equilibration with the minerals expected to be present in the repository. This value is conservative as it does not take credit for the magnesium or calcium in that brine. The total moles of sulfate from a single intrusion were then normalized by dividing by one half the estimated total moles of organic carbon per panel (1.1×10^9 moles organic carbon/10 panels/2, see Appendix A in Nemer and Stein, 2005), since 0.5 moles of SO_4^{2-} are required to produce 1 mole of CO_2 by sulfate reduction (see equation 2 in Nemer and Zelinski, 2005). This normalization results in $O(1)$ values, where 1.0 represents enough sulfate to consume 100% of the carbon by sulfate reduction using Castile sulfate. This analysis assumes that all of the sulfate that came up the borehole remained in the intruded panel and was not carried out by brine leaving the panel, and that no CO_2 generated by microbial respiration is carried out of the intruded panel by brine flow.

For an intrusion to allow sulfate to enter the waste panel from the Castile, it needs to hit a brine pocket and allow brine to continue to flow up the borehole to the repository (E1 intrusion). The code BRAGFLO considers six drilling scenarios, and three of these scenarios were used explicitly in the sulfate distribution calculations. The S1 scenario represents the undisturbed scenario, and the S2 and S3 scenarios model E1 intrusions at 350 years and 1000 years, respectively. The cumulative amounts of Castile brine entering the panel at the end of the 10,000 year regulatory period were always smaller in Scenario S3 than S2 for each vector. This is expected and is due to the decrease in time for brine to flow up the borehole to the repository; 9650 years for the 350 year intrusion versus 9000 years for the 1000 year intrusion. The undisturbed scenario (S1) calculations, as well as the scenarios with E2 intrusions (S4 and S5), showed that no significant amount of sulfate would enter the panel from the brine pocket, since there is no connection to the brine pocket. Scenario S6 models an E2 intrusion (where the brine pocket is not hit) followed by an E1 intrusion. No significant increase in the volumetric flow of brine into the repository, for the S6 scenario, was observed in comparison with scenarios that model only one E1 intrusion (S2 and S3), so the effect of E2 intrusions were ignored in the calculations.

The drilling times simulated in the Monte Carlo analysis may occur at times other than 350 years or 1,000 years. For each vector, a piece-wise linear function was constructed to calculate the quantity of sulfate entering a panel from a single intrusion at any time between 100 and 10,000 years. For a single vector, Equation 1 gives the equation to determine the quantity of sulfate entering from Castile brine due to an intrusion at time t_i

$$S^j(t_i) = \begin{cases} S_2^j + \dfrac{S_3^j - S_2^j}{1{,}000 - 350}(t_i - 350), & 100 \le t_i < 1{,}000 \\ S_3^j + \dfrac{S_1^j - S_3^j}{10{,}000 - 1{,}000}(t_i - 1{,}000), & 1{,}000 \le t_i \le 10{,}000 \end{cases} \qquad (1)$$

S_1^j, S_2^j, and S_3^j denote the quantities of sulfate entering the panel from the Castile brine pocket for scenarios S1, S2, and S3, respectively, and $S^j(t_i)$ denotes the amount of sulfate entering the panel from an E1 intrusion at time t_i, for each vector j. This time-dependent function was calculated for each of the three hundred vectors.

4.2 MgO lost to brine

The BRAGFLO post-ALGEBRA files (Nemer and Stein 2005) contain the variable BRNWPOC which is the cumulative volumetric flow of brine (m^3) out of the intruded waste panel (WAS_AREA). Since the repository is modeled as having a 1° dip from the north to the south and the intruded waste panel is at the south end of the repository, ,the intruded waste panel should receive (and lose) the most brine. For scenarios S2, and S3, the cumulative volumetric flow at 10,000 years was taken for each of the 300 vectors and multiplied by a magnesium solubility of 157 moles per m^3 (the solubility of MgO in the Castile brine, see the file FMT_CRA1BC_ER6_HMAG_ORGS_011.OUT in the CMS library LIBCRA1BC_FMT, Long and Kanney, 2005) to calculate the loss of MgO for a single E1 intrusion. For scenarios S1, S4, and S5, the cumulative volumetric flow at 10,000 years was taken for each of the 300 vectors and multiplied by 578 moles of MgO per m^3 (the solubility of MgO in the Salado brine, see the file FMT_CRA1BC_GWB_HMAG_ORGS_007.OUT in the CMS library

LIBCRA1BC_FMT, Long and Kanney, 2005) to calculate the loss of brine due to a single E2 intrusion or no intrusion. These values were then normalized by dividing by the estimated total moles of organic carbon per panel ($1.1\text{x}10^9$ moles organic carbon/10 panels, see Appendix A in Nemer and Stein, 2005), which implicitly assumes that only one mole of MgO is emplaced per mole of organic carbon. This normalization results in $O(1)$ values, where 1.0 represents that all the MgO in a panel has migrated out of the waste panel. This calculation assumes that the MgO instantaneously dissolves to the equilibrium value in the brine and that none of the CO_2 is dissolved and lost. Furthermore, this calculation does not include the possibility that all the MgO had reacted with the CO_2 before the intrusion.

For this analysis MgO was considered lost if it dissolved into available brine and that brine subsequently migrated out of the waste panel. For an intrusion to allow significant amounts of MgO to leave the waste panel, it needs to have flow path that allows brine to continue to flow up the borehole to the Culebra. This corresponds to either an E1 (hit a brine pocket) or E2 (did not hit a brine pocket) type intrusion. Five of the BRAGFLO scenarios were used in the MgO brine loss distribution calculations: scenario S1, the undisturbed scenario, scenarios S2 and S3, with E1 intrusions occurring at 350 years and 1,000 years, respectively, and scenarios S4 and S5, with E2 intrusions occurring at 350 years and 1,000 years, respectively. For each vector, the S3 normalized amounts of MgO leaving the intruded waste panel were always smaller than the amount calculated for the S2 quantities. This is expected and is due to the decrease in time for brine to flow up the borehole to the Culebra; 9650 years for the 350 year intrusion versus 9000 years for the 1000 year intrusion. A similar trend was observed for the S4 and S5 scenarios. The undisturbed scenario (S1) calculation showed an order of magnitude decrease in the MgO that would leave the waste panel without an intrusion. The S6 scenario that models an E2 intrusion followed by an E1 intrusion was found to have an average that was less than the sum of the S3 and S4 averages. To simplify the analysis, the results from multiple E1 and E2 intrusions were summed together to give an upper bound.

To calculate the quantity of MgO lost due to brine outflow from a single E1 or E2 intrusion at time t_i, the following piece-wise linear functions were generated:

$$M_{E1}^{j}(t_i) = \begin{cases} M_2^j + \dfrac{M_3^j - M_2^j}{1{,}000 - 350}(t_i - 350), & 100 \le t_i < 1{,}000 \\ M_3^j + \dfrac{M_1^j - M_3^j}{10{,}000 - 1{,}000}(t_i - 1{,}000), & 1{,}000 \le t_i \le 10{,}000 \end{cases} \tag{2}$$

$$M_{E2}^{j}(t_i) = \begin{cases} M_4^j + \dfrac{M_5^j - M_4^j}{1{,}000 - 350}(t_i - 350), & 100 \le t_i < 1{,}000 \\ M_5^j + \dfrac{M_1^j - M_5^j}{10{,}000 - 1{,}000}(t_i - 1{,}000), & 1{,}000 \le t_i \le 10{,}000 \end{cases} \tag{3}$$

M_1^j, M_2^j, M_3^j, M_4^j ,and M_5^j denote the normalized quantities of MgO leaving the repository for scenarios S1, S2, S3, S4, and S5, respectively and $M_{E1}^j(t_i)$ and $M_{E2}^j(t_i)$

denote the amount of sulfate entering the panel from an E1 and E2 intrusion at time t_i, respectively, for each vector *j*. These time-dependent functions are calculated for each of the three hundred vectors.

5.0 Procedure

Since 1,000 drilling futures were generated for this analysis, the probability of each future occurring is equally weighted, and each future is assigned a probability of 1/1,000. Similarly, since each time-dependent Castile sulfate or MgO lost to brine function is associated with one of 300 vectors, each function is equally weighted and assigned a probability of 1/300. Each particular future and vector combination is assigned the probability of 1/300,000 (1/1,000*1/300).

To calculate the quantity of Castile sulfate entering the intruded panel for a particular future and vector combination, the time of each E1 intrusion is input into Equation 1, corresponding to a specific vector, and the resulting Castile sulfate quantities are summed for each panel in each future, and rounded to the nearest 0.001 for plotting convenience. To calculate the quantity of MgO lost due to brine outflow for the intruded panel for a particular future and vector combination, the time of each E1 intrusion is input into Equation 2 and the time of each E2 intrusion is input into Equation 3, corresponding to a specific vector. The resulting normalized quantities of MgO lost to brine are summed for each panel, and rounded to the nearest 0.001 for plotting convenience. This is a conservative approach for multiple E1 and E2 intrusions, since it is expected that a previous E1 or E2 intrusion will reduce the effect of the next E1 or E2 intrusion by pressurizing the panel and filling the panel with brine. The panel with the maximum Castile sulfate or MgO lost in each future was chosen as the "worst case" and this value was then used for further calculations.

The probability distribution functions (PDFs) for Castile sulfate and MgO lost were used to determine complimentary cumulative distribution functions (CCDFs). The cumulative distribution function (CDF) is determined by summing the discrete probabilities up to a desired value of the independent variable X_n (i.e. X_n could be an amount of normalized sulfate or MgO lost-to brine),

$$P(X < X_n) = \sum_{i=1}^{n} p_i \quad , \tag{4}$$

where p_i is the discrete probability of obtaining the discrete variable X_i,

$$p_i = P(X = X_i) \, . \tag{5}$$

The CCDF is then

$$P(X > X_n) = 1 - P(X < X_n) \, . \tag{6}$$

The PDFs described above were used to calculate the expected result (average value) and the associated uncertainty (standard deviation). The average value and standard deviation were found by applying the following equations:

$$\overline{X} = \sum_{i=1}^{n} X_i p_i \tag{7}$$

$$\sigma^2 = \sum_{i=1}^{n} \left(X_i - \overline{X}\right)^2 p_i \tag{8}$$

where $\overline{X}$ is the mean of the independent variable and σ is the standard deviation of the variable distribution (Freund, 1992).

The normalized amount of MgO lost due to brine flow out of the waste panel was then converted to fraction of MgO lost, by dividing by the ratio of moles of MgO emplaced per mole of organic carbon emplaced in a panel, which for this calculation, a ratio of 1.2 moles of MgO emplaced per mole of carbon was used, as this is the amount proposed by DOE (Moody 2006). This was applied to the PDF of MgO lost due to brine flow to generate a PDF of the fraction of MgO lost due to brine flow. This procedure was applied to the data and verified as shown in Appendix A.3.

6.0 Results

The means and standard deviations of the normalized moles of Castile sulfate that enters the repository PDF and the fraction of MgO lost due to brine flow PDF are listed below in Table 3.

Table 3. Average and standard deviation for Castile sulfate that entered the repository and MgO lost to brine.

PDF	$\overline{X}$ (dimensionless)	σ (dimensionless)
Normalized Castile Sulfate	0.024	0.051
MgO lost to brine	0.008	0.019

The CCDF of the normalized moles of Castile sulfate that enters the intruded waste panel is shown in Figure1. As seen in Figure 1, there is a probability of less than 1% that enough sulfate enters the "worst case" waste panel to consume 27% or more of the carbon by sulfate reduction using Castile sulfate. In other words, there is a probability of 99% that enough sulfate enters the "worst case" waste panel to consume 27% or less of the carbon by sulfate reduction using Castile sulfate. There is a probability of 0.1% that enough sulfate enters the "worst case" waste panel to consume 53% or more of the carbon by sulfate reduction using Castile sulfate. As a result, there is a probability of 99.9% that enough sulfate enters the "worst case" waste panel to consume 53% or less of the carbon by sulfate reduction using Castile sulfate.

The CCDF of the fraction of MgO lost due to brine flow out of the waste panel is shown in Figure 2. As seen in Figure 2, there is a probability of less than 1%, that more than 10% of the MgO is lost due to brine flow out of the waste panel. Accordingly, there is a probability of 99%, that 10% or less of the MgO is lost due to brine flow out of the waste panel. There is a probability of 0.1%, that more than 19% of the MgO lost due to brine flow out of the waste panel. Therefore, there is a probability of 99.9% that 19% or less of the MgO is lost due to brine flow out of the waste panel.

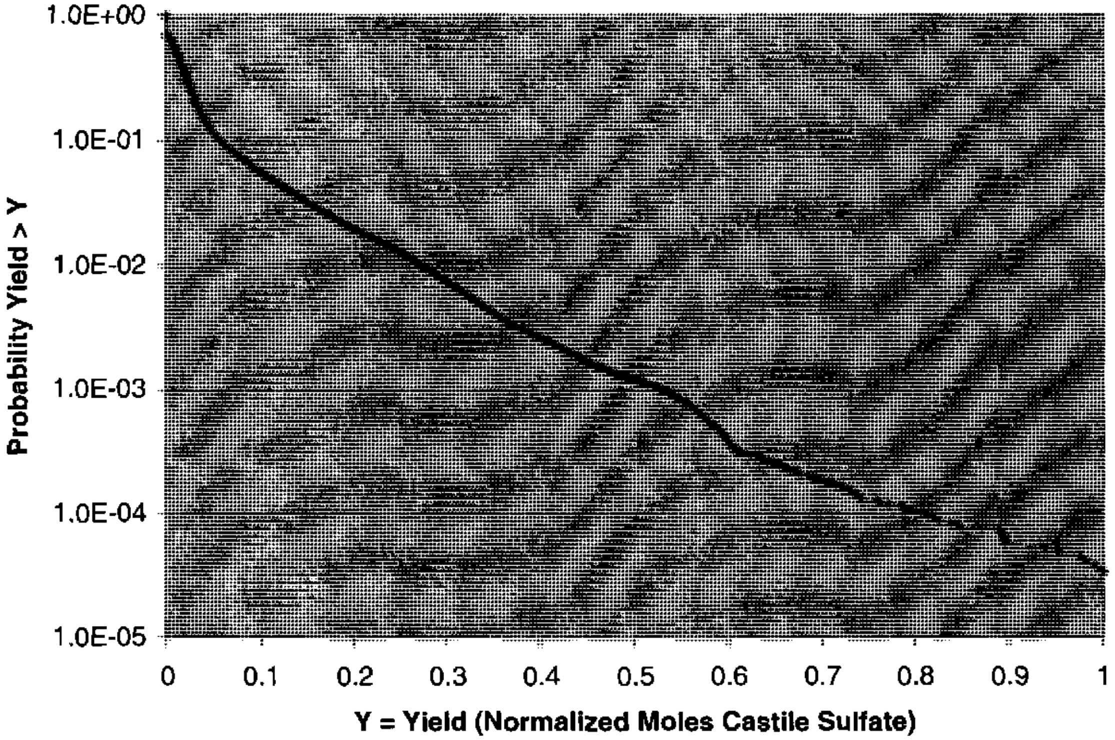


Figure 1. CCDF of normalized moles of Castile sulfate that enters the waste panel.

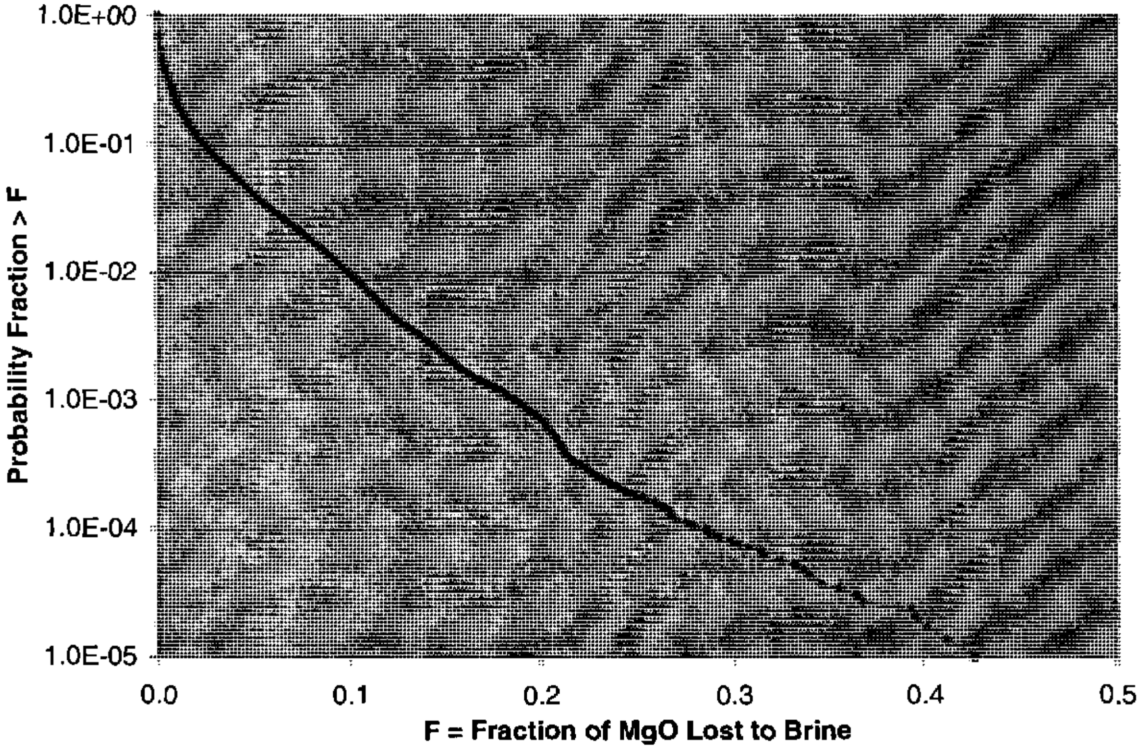


Figure 2. CCDF of fraction of MgO lost to brine flow out of the waste panel.

7.0 References

Freund, J. E. 1992. *Mathematical Statistics*. New Jersey: Prentice Hall, Inc.

Gitlin, B.C. 2006. Letter to D.C. Moody Concerning the DOE's Request to Reduce the MgO Excess Factor from 1.67 to 1.2, dated April 28, 2006.

Hansen, C.W. 2003. "Design Document and User's Manual for CCDFGF, Version 5.00." Carlsbad, NM: Sandia National Laboratory. ERMS 540471.

Hahn, G. J. and W. Q. Meeker. 1991. *Statistical Intervals: A Guide for Practitioners*. New York, NY: John Wiley and Sons.

Long, J. and J. F. Kanney. October 12, 2005. "Execution of Performance Assessment Codes for the CRA-2004 Performance Assessment Baseline Calculation, Revision 0." Carlsbad, NM: Sandia National Laboratory. ERMS 541394

Moody, D.C. 2006. Letter to E.A. Cotsworth Requesting a Reduction in the MgO Excess Factor from 1.67 to 1.2, dated April 10, 2006.

Nemer, M. B. and J. S. Stein. 2005. "Analysis Package for BRAGFLO: 2004 Compliance Recertification Application Performance Assessment Baseline Calculation." Analysis Report, June 28, 2005. Carlsbad, NM: Sandia National Laboratories. ERMS 540527.

Nemer, M. B. and W. Zelinski. 2005. "Analysis Report for BRAGFLO Modeling Results with the removal of Methanogenesis from the Microbial-Gas-Generation Model." Carlsbad, NM: Sandia National Laboratory. ERMS 538748.

Appendix A. Verification of Calculations

The results generated in this report were verified through each step in the analysis. A discussion of the verification process is given below. First, the verification for the future generation process is discussed. Next, the verification process of the piece-wise linear functions calculated from the BRAGFLO results is shown. Finally, the verification process used to verify the Microsoft Access® calculations and further calculations in Microsoft Excel® is given.

A.1 Drilling Event Futures

The drilling event futures generated by the commercial-off-the-shelf (COTS) software Crystal Ball® used the stochastic parameters listed in Table 1. The Crystal Ball® software must be installed in Excel® in order to generate the drilling event futures. The parameters were taken from the parameter database and entered into the input file *Martins_CB_Intervals.xls*. A visual inspection of the input file confirmed that the correct values were taken from the parameter database. The output Excel® file generated by Crystal Ball® was labeled *MartinsCCDFGF_Intervals_1000Trials.xls* and loaded into the *sulfate.mdb* and *brineloss.mdb* databases as a table labeled "*Futures*". These Excel® files are located on the attached CD.

A.2 Piece-Wise Linear Functions

The piece-wise linear functions were generated from the ALGEBRA2 files, that were obtained during BRAGFLO post-processing (Nemer and Stein, 2005) of the 2004 Compliance Recertification Application (CRA-2004) Performance Assessment Baseline Calculation (PABC). These files are named ALG2_BF_CRA1BC_RxSy_Vzzz.CDB (1800 files), where R is the replicate and x = 1, 2 or 3, S is the scenario where y = 1 to 6, and V is vector where zzz = 001 to 100 (Long and Kanney, 2005). These files were fetched from the 18 CMS libraries LIBCRA1BC_BFRxSy. The values of the variables BNBHLDRZ and BRNWPOC (along with some others as well) at 10,000 years were extracted for each replicate, scenario and vector using the SUMMARIZE program with 18 input files labeled BOREHOLERxSy.SMZ, which are located in the CMS library LIBMGORED. This generated 18 output files named BOREHOLERxSy.TBL which are also located in the CMS library LIBMGORED. The output files were loaded into the Microsoft Excel® files *Borehole Brine Loss Calculations.xls* and *Borehole Sulfate Calculations.xls*, with each of the 18 files loaded as 18 separate sheets labeled "*BOREHOLERxSy*", respectively in the Excel® file.

The piece-wise linear functions for the Castile sulfate were generated in the *Borehole Sulfate Calculations.xls* file. First, in each of the imported file sheets labeled "*BOREHOLERxSy*", the normalized amount of Castile sulfate that entered the waste (S) panel was calculated by the following equation:

$$S^j = \frac{BNBHLDRZ^j \cdot 179}{1.1e9 \big/ (10 \cdot 2)} \tag{A.1}$$

for each vector *j*. This equation was visually confirmed and can be seen in column N in each of the "*BOREHOLERxSy*" sheets. Next the normalized sulfate for each sheet was summarized in the "*Summary*" sheet, where the terms in the piece-wise functions were calculated, in columns U through AF. These terms are shown in Equation 1,

$$S^j(t_i)=\begin{cases} S_2^j+\dfrac{S_3^j-S_2^j}{1{,}000-350}(t_i-350), & 100\le t_i<1{,}000 \\ S_3^j+\dfrac{S_1^j-S_3^j}{10{,}000-1{,}000}(t_i-1{,}000), & 1{,}000\le t_i\le 10{,}000 \end{cases} \tag{1}$$

where the columns labeled Region1 refer to the S_2^j terms, the columns labeled Slope1 refer to the $\dfrac{S_3^j-S_2^j}{1{,}000-350}$ terms, the columns labeled Region2 refer to the S_3^j terms, and the columns labeled Slope2 refer to the $\dfrac{S_1^j-S_3^j}{10{,}000-1{,}000}$ terms, for each vector *j*. A visual inspection of the formulas for the terms confirmed the calculations in the "*Summary*" sheet of the *Borehole Sulfate Calculations.xls* file. The terms were then complied on the "*Sulfate_Adj_Slope*" sheet to be loaded in to the *sulfate.mdb* database as a table labeled "*Sulfate_Adj_Slope*". The *Borehole Sulfate Calculations.xls* file and *sulfate.mdb* database are located on the attached CD.

The piece-wise linear functions for the MgO lost to brine were generated in the *Borehole Brine Loss Calculations.xls* file. First, in each of the imported file sheets labeled "*BOREHOLERxSy*", the normalized amount of MgO that left the waste panel was calculated by the following equations for the E1 intrusion scenarios (M_{E1}, scenarios S2, S3, S6) and the E2 intrusion scenarios (M_{E2}, scenarios S1, S4, S5):

$$M_{E1}^j=\frac{BRNWPOC^j\cdot 157}{1.1e9/10} \tag{A.2}$$

$$M_{E2}^j=\frac{BRNWPOC^j\cdot 578}{1.1e9/10} \tag{A.3}$$

for each vector *j*. These equations were visually confirmed and can be seen in column N for each of the "*BOREHOLERxSy*" sheets. Next the normalized MgO lost for each sheet was summarized in the "*Summary*" sheet, where the terms in the piece-wise functions were calculated, in columns U through AR. These terms are shown in Equations 2 and 3,

$$M_{E1}^j(t_i)=\begin{cases} M_2^j+\dfrac{M_3^j-M_2^j}{1{,}000-350}(t_i-350), & 100\le t_i<1{,}000 \\ M_3^j+\dfrac{M_1^j-M_3^j}{10{,}000-1{,}000}(t_i-1{,}000), & 1{,}000\le t_i\le 10{,}000 \end{cases} \tag{2}$$

$$M_{E2}^{j}(t_i)=\begin{cases} M_4^j+\dfrac{M_5^j-M_4^j}{1{,}000-350}(t_i-350), & 100\le t_i<1{,}000 \\ M_5^j+\dfrac{M_1^j-M_5^j}{10{,}000-1{,}000}(t_i-1{,}000), & 1{,}000\le t_i\le 10{,}000 \end{cases} \tag{3}$$

where the columns labeled "E1 Region1" refer to the M_2^j terms, the columns labeled "E1 Slope1" refer to the $\dfrac{M_3^j-M_2^j}{1{,}000-350}$ terms, the columns labeled "E1 Region2" refer to the M_3^j terms, the columns labeled "E1 Slope2" refer to the $\dfrac{M_1^j-M_3^j}{10{,}000-1{,}000}$ terms, the columns labeled "E2 Region1" refer to the M_4^j terms, the columns labeled "E2 Slope1" refer to the $\dfrac{M_5^j-M_4^j}{1{,}000-350}$ terms, the columns labeled "E2 Region2" refer to the M_5^j terms, the columns labeled "E2 Slope2" refer to the $\dfrac{M_1^j-M_5^j}{10{,}000-1{,}000}$ terms, for each vector *j*. A visual inspection of the formulas for the terms confirmed the calculations in the "*Summary*" sheet of the *Borehole Brine Loss Calculations.xls* file. The terms were then complied on the "*Brine_Loss_Slope*" sheet to be loaded in to the *brineloss.mdb* database as a table labeled "*Brine_Loss_Slope*". The *Borehole Brine Loss Calculations.xls* file and *brineloss.mdb* database are located on the attached CD.

A.3 Microsoft Access® and Excel® Processing

The classification of the drilling-events in each future was done in Microsoft Access®. The drilling-events were classified, by the criteria matrix shown in Table 2, as no change, E1 or E2 events. Furthermore, the drilling-events were classified by the time they occurred to determine which part of the piece-wise functions would be used. Drilling-events that occurred between 100 and 1,000 years were classified as Time region 1 (T1) and drilling-events that occurred on and between 1,000 and 10,000 years were classified as Time region 2 (T2). For the following examples, two futures will be used, labeled 2 and 89, which were selected as representative futures. The results from Crystal Ball® for futures 2 and 89 are shown in Tables A1 and A2, respectively. The classification of the drilling-event is represented by both color coding and the last four columns in each table. The classification was performed in the "*Validation*" sheets in the files *Borehole Brine Loss Calculations.xls* and *Borehole Sulfate Calculations.xls*. The white rows, as well as zeros in the last four columns indicate that there was no change to the repository due to the drilling-event. The dark grey rows, as well as a one in the E1 T1 or E1 T2 columns, indicate that the drilling-event represents an E1 intrusion. The lighter grey rows, as well as a one in the E2 T1 or E2 T2 columns, indicate that the drilling-event represents an E2 intrusion. The classification between T1 and T2 is shown for each intrusion in the last four columns in the tables.

Table A1. Drilling-event history for future 2, along with classification.

Future	Intrusion	Hit Waste	Hit Brine	Plugging Pattern	Time (year)	Panel #	E1 T1	E1 T2	E2 T1	E2 T2
2	1	0	1	2	490	5	0	0	0	0
2	2	0	0	3	849	3	0	0	0	0
2	3	1	0	2	1432	8	0	0	0	1
2	4	0	0	2	1858	1	0	0	0	0
2	5	0	0	2	1886	9	0	0	0	0
2	6	0	1	3	1922	2	0	0	0	0
2	7	0	1	2	2308	3	0	0	0	0
2	8	0	0	2	2519	5	0	0	0	0
2	9	0	0	2	2771	9	0	0	0	0
2	10	0	0	3	2795	5	0	0	0	0
2	11	1	0	2	3025	7	0	0	0	1
2	12	0	0	3	3271	7	0	0	0	0
2	13	0	0	3	4036	3	0	0	0	0
2	14	0	0	2	4383	10	0	0	0	0
2	15	0	0	2	4714	5	0	0	0	0
2	16	0	0	2	4927	10	0	0	0	0
2	17	0	0	3	4934	7	0	0	0	0
2	18	0	0	2	5025	1	0	0	0	0
2	19	0	0	3	5170	9	0	0	0	0
2	20	0	1	2	5375	4	0	0	0	0
2	21	0	0	3	5378	8	0	0	0	0
2	22	0	0	2	5406	2	0	0	0	0
2	23	1	1	2	5663	3	0	1	0	0
2	24	0	1	2	5804	7	0	0	0	0
2	25	0	0	2	6501	1	0	0	0	0
2	26	1	0	2	6682	5	0	0	0	1
2	27	1	0	3	6940	1	0	0	0	1
2	28	0	0	3	7203	1	0	0	0	0
2	29	0	1	2	7337	5	0	0	0	0
2	30	0	0	2	8074	4	0	0	0	0
2	31	0	0	2	8371	6	0	0	0	0
2	32	0	0	2	8642	7	0	0	0	0
2	33	0	0	3	8992	2	0	0	0	0
2	34	0	1	2	9232	10	0	0	0	0
2	35	0	0	2	9408	6	0	0	0	0
2	36	0	0	3	9479	5	0	0	0	0
2	37	0	0	3	9558	8	0	0	0	0
2	38	0	0	2	9592	10	0	0	0	0
2	39	0	1	2	9636	9	0	0	0	0

Table A2. Drilling-event history for future 89, along with classification.

Future	Intrusion	Hit Waste	Hit Brine	Plugging Pattern	Time (year)	Panel #	E1 T1	E1 T2	E2 T1	E2 T2
89	1	1	1	2	368	6	1	0	0	0
89	2	1	1	3	630	2	0	0	1	0
89	3	0	0	2	853	8	0	0	0	0
89	4	0	0	2	1352	4	0	0	0	0
89	5	0	0	2	1704	5	0	0	0	0
89	6	0	0	3	2151	9	0	0	0	0
89	7	0	0	3	2282	1	0	0	0	0

89	8	0	1	2	2436	10	0	0	0	0
89	9	0	0	3	2892	4	0	0	0	0
89	10	1	1	2	3189	6	0	1	0	0
89	11	0	0	2	3310	4	0	0	0	0
89	12	0	0	2	4228	9	0	0	0	0
89	13	0	0	2	4302	4	0	0	0	0
89	14	0	1	3	4744	3	0	0	0	0
89	15	0	0	3	4964	3	0	0	0	0
89	16	0	0	1	5008	10	0	0	0	0
89	17	1	1	2	5286	2	0	1	0	0
89	18	0	0	2	5298	6	0	0	0	0
89	19	0	1	2	5483	3	0	0	0	0
89	20	0	0	3	5636	9	0	0	0	0
89	21	0	1	2	5719	4	0	0	0	0
89	22	0	1	2	5776	4	0	0	0	0
89	23	0	1	2	5816	8	0	0	0	0
89	24	0	0	3	6430	8	0	0	0	0
89	25	0	0	2	6909	6	0	0	0	0
89	26	0	0	3	7855	2	0	0	0	0
89	27	0	0	3	8391	7	0	0	0	0
89	28	0	1	3	8565	9	0	0	0	0
89	29	0	1	2	8792	9	0	0	0	0
89	30	0	1	2	8841	7	0	0	0	0
89	31	0	0	2	9056	9	0	0	0	0
89	32	0	1	2	9734	9	0	0	0	0
89	33	0	0	2	9836	1	0	0	0	0
89	34	1	1	2	9919	3	0	1	0	0

A.3.1 Castile sulfate calculations

In the *sulfate.mdb* database, the queries "*SelectedFuturesE1*", "*Region1E1*", "*Region2E1*" and "*Combined_Regions*" were used for the classification process for the Castile sulfate calculations. The "*SelectedFuturesE1*" query filters the table "*Futures*" for all of the E1 intrusions. The "*Region1E1*" and "*Region2E1*" queries each filter the "*SelectedFuturesE1*" query based on the intrusion time. The "*Combined_Regions*" query combines the results from the "*Region1E1*" and "*Region2E1*" queries and fills in zeros for the other entries. Table A3 shows the results of the "*Combined_Regions*" query in the *sulfate.mdb* database for futures 2 and 89. Review of Tables A1, A2 and A3 show that the drilling-event classification is being calculated correctly in the *sulfate.mdb* database.

Table A3. Results from the "*Combined_Regions*" query in the *sulfate.mdb* database for futures 2 and 89.

Future	Cumulative Time	Panel Number	Region1 E1	Region2 E1
2	5663	3	0	1
89	368	6	1	0
89	3189	6	0	1
89	5286	2	0	1
89	9919	3	0	1

Next, the Castile sulfate amount is calculated for each event and for each piece-wise linear function. For the following example, the piece-wise linear functions from vectors 17 and 66 will be used. The piece-wise linear Castile sulfate function terms for vectors 17 and 66 are shown below in Table A4 from the "*Sulfate_Adj_Slope*" table in the *sulfate.mdb* database. Using the piece-wise linear functions shown in Table A4, the Castile sulfate was calculated for each event in futures 2 and 89, for both vectors 17 and 66, in the "*Validation*" sheet in the *Borehole Sulfate Calculations.xls*. The results are shown in Table A5.

Table A4. Piece-wise linear Castile sulfate function terms for vectors 17 and 66.

Vector	Region 1	Slope 1	Region 2	Slope 2
17	0.6003	-4.95E-05	0.5682	-6.31E-05
66	0.1223	-2.19E-05	0.1080	-1.20E-05

Table A5. Results from the verification calculations for the Castile sulfate for futures 2 and 89, vectors 17 and 66.

Vector	Future	Time	Panel Number	Sulfate
17	2	5663	3	0.2738
17	89	368	6	0.5994
17	89	3189	6	0.4300
17	89	5286	2	0.2976
17	89	9919	3	0.0051
66	2	5663	3	0.0521
66	89	368	6	0.1219
66	89	3189	6	0.0817
66	89	5286	2	0.0566
66	89	9919	3	0.0010

The "*Sulfate*" query takes the results of the "*Combined_Regions*" query and applies the piece-wise linear function to each event for each vector. The results from the "*Sulfate*" query in the *sulfate.mdb* database are shown in Table A6 for futures 2 and 89, for vectors 17 and 66. Review of Tables A5 and A6 show that the piece-wise linear functions are correctly applied to each intrusion event.

Table A6. Results from the "*Sulfate*" query in the *sulfate.mdb* database for futures 2 and 89, for vectors 17 and 66.

Vector	Future	Cumulative Time	Panel Number	Sulfate
17	2	5663	3	0.2738
17	89	368	6	0.5994
17	89	3189	6	0.4300
17	89	5286	2	0.2976
17	89	9919	3	0.0051
66	2	5663	3	0.0521
66	89	368	6	0.1219
66	89	3189	6	0.0817
66	89	5286	2	0.0566

66	89	9919	3	0.0010

The "*SulfatebyFbyP*" query in the *sulfate.mdb* database takes the results from the "*Sulfate*" query and sums the events to get a total amount for each panel. The results from the "*SulfatebyFbyP*" query in the *sulfate.mdb* database are shown in Table A7 for futures 2 and 89, for vectors 17 and 66. As seen in Table A6, there are two events in future 89, panel 6. The other panels each only had only one (or zero) events in these futures. As seen in Table A7, the Castile sulfate amounts for each vector-future-panel combination are the same as shown in Table A6, except for future 89, panel 6, where the Castile sulfate amount is the sum of the two events seen in Table A6 for both vectors.

Table A7. Results from the "*SulfatebyFbyP*" query in the *sulfate.mdb* database for futures 2 and 89, for vectors 17 and 66.

Vector	Future	Panel Number	SumOfSulfate
17	2	3	0.2738
17	89	2	0.2976
17	89	3	0.0051
17	89	6	1.0294
66	2	3	0.0521
66	89	2	0.0566
66	89	3	0.0010
66	89	6	0.2036

The "*WorstCasebyFuture*" query in the *sulfate.mdb* database takes the results from the "*SulfatebyFbyP*" query and finds the maximum Castile sulfate in a panel for each future. The "*WorstCasebyFutureRounded*" query takes the results from the "*WorstCasebyFuture*" query and rounds them to the nearest 0.001. The "*WorstCasebyFuturePlusZero*" query takes the results from the "*WorstCasebyFutureRounded*" query and fills in zeros for the futures that had no events and assigns a probability (1/300*1/1,000) for each future-vector combination. The results from the "*WorstCasebyFuturePlusZero*" query are shown in Table A8 for futures 2 and 89, for vectors 17 and 66. As seen by comparing Tables A7 and A8, the maximum value from each future-vector combination was chosen.

Table A8. Results from the "*WorstCasebyFuturePlusZero*" query in the *sulfate.mdb* database for futures 2 and 89, for vectors 17 and 66.

Vector	Future	Probability	Sulfate
17	2	3.33E-06	0.274
17	89	3.33E-06	1.029
66	2	3.33E-06	0.052
66	89	3.33E-06	0.204

The "*SulfatePlot*" query in the *sulfate.mdb* database takes the results from the "*WorstCasebyFuturePlusZero*" query and combines all of the vector-future combinations that calculate the same Castile sulfate value and sums their probabilities. This condensed list of Castile sulfate amounts versus probability is output to the Excel® file labeled

SulfatePlot_DJC.xls in the sheet "*SulfatePlot*". In the *SulfatePlot_DJC.xls* file the CCDF, mean and standard deviation are calculated in the "*Total Effect*" sheet and the resulting plot is generated in the "*Plot*" sheet as seen in Figure 1. A visual inspection of the *SulfatePlot_DJC.xls* file shows that the procedure was implemented correctly.

A.3.2 MgO lost to brine flow calculations

In the *brineloss.mdb* database, the queries "*SelectedFutures*", "*SelectedFuturesE1*", "*SelectedFuturesE2*", "*Region1E1*", "*Region2E1*", "*Region1E2*", "*Region2E2*" and "*Combined_Regions*" were used for the classification process for the MgO lost to brine flow calculations. The "*SelectedFuturesE1*" and "*SelectedFuturesE2*" queries filter the table "*Futures*" for all of the E1 and E2 intrusions, respectively, while the "*SelectedFutures*" query filters the table "*Futures*" for all of the E1 and E2 intrusions together. Based on the intrusion time, the "*Region1E1*" and "*Region2E1*" queries each filter the "*SelectedFuturesE1*" query, while the "*Region1E2*" and "*Region2E2*" queries each filter the "*SelectedFuturesE2*" query. The "*Combined_Regions*" query combines the results from the "*Region1E1*", "*Region2E1*", "*Region1E2*" and "*Region2E2*" queries and fills in the zeros for the other entries. Table A9 shows the results of the "*Combined_Regions*" query in the *brineloss.mdb* database for futures 2 and 89. Review of Tables A1, A2 and A9 show that the drilling-event classification is being calculated correctly in the *brineloss.mdb* database.

Table A9. Results from the "*Combined_Regions*" query in the *brineloss.mdb* database for futures 2 and 89.

Future	Cumulative Time	Panel Number	Region1 E1	Region2 E1	Region1 E2	Region2 E2
2	1432	8	0	0	0	1
2	3025	7	0	0	0	1
2	5663	3	0	1	0	0
2	6682	5	0	0	0	1
2	6940	1	0	0	0	1
89	368	6	1	0	0	0
89	630	2	0	0	1	0
89	3189	6	0	1	0	0
89	5286	2	0	1	0	0
89	9919	3	0	1	0	0

Next, the MgO lost to brine flow is calculated for each event and for each piece-wise linear function. For the following example, the piece-wise linear functions from vectors 17 and 66 will be used. The piece-wise linear MgO lost function terms for vectors 17 and 66 are shown below in Table A10 from the "*Brine_Loss_Slope*" table in the *brineloss.mdb* database. Using the piece-wise linear functions shown in Table A10, the MgO lost to brine flow was calculated for each event in futures 2 and 89, for both vectors 17 and 66, in the "*Validation*" sheet in the *Borehole Brine Loss Calculations.xls*. The results are shown in Table A11.

Table A10. Piece-wise linear MgO lost to brine flow function terms for vectors 17 and 66.

Vector	E1 Loss Region1	E1 Slope Region1	E2 Loss Region1	E2 Slope Region1	E1 Loss Region2	E1 Slope Region2	E2 Loss Region2	E2 Slope Region2
17	0.2552	-2.20E-05	0.0153	-7.83E-06	0.2409	-2.67E-05	0.0102	-1.08E-06
66	0.0442	-9.49E-06	0.0698	-5.08E-06	0.0380	-4.22E-06	0.0665	-7.39E-06

Table A11. Results from the verification calculations for the MgO lost to brine flow for futures 2 and 89, vectors 17 and 66.

Vector	Future	Time	Panel Number	Brine Loss
17	2	1432	8	0.0098
17	2	3025	7	0.0081
17	2	5663	3	0.1164
17	2	6682	5	0.0041
17	2	6940	1	0.0038
17	89	368	6	0.2548
17	89	630	2	0.0131
17	89	3189	6	0.1824
17	89	5286	2	0.1264
17	89	9919	3	0.0027
66	2	1432	8	0.0633
66	2	3025	7	0.0515
66	2	5663	3	0.0183
66	2	6682	5	0.0245
66	2	6940	1	0.0226
66	89	368	6	0.0440
66	89	630	2	0.0684
66	89	3189	6	0.0288
66	89	5286	2	0.0199
66	89	9919	3	0.0003

The "*Brineloss*" query takes the results of the "*Combined_Regions*" query and applies the piece-wise linear function to each event for each vector. The results from the "*Brineloss*" query in the *brineloss.mdb* database are shown in Table A12 for futures 2 and 89, for vectors 17 and 66. Review of Tables A11 and A12 show that the piece-wise linear functions are correctly applied to each intrusion event.

Table A12. Results from the "*Brineloss*" query in the *brineloss.mdb* database for futures 2 and 89, for vectors 17 and 66.

Vector	Future	Cumulative Time	Panel Number	Brineloss
17	2	1432	8	0.0098
17	2	3025	7	0.0081
17	2	5663	3	0.1164
17	2	6682	5	0.0041
17	2	6940	1	0.0038
17	89	368	6	0.2548

17	89	630	2	0.0131
17	89	3189	6	0.1824
17	89	5286	2	0.1264
17	89	9919	3	0.0027
66	2	1432	8	0.0633
66	2	3025	7	0.0515
66	2	5663	3	0.0183
66	2	6682	5	0.0245
66	2	6940	1	0.0226
66	89	368	6	0.0440
66	89	630	2	0.0684
66	89	3189	6	0.0288
66	89	5286	2	0.0199
66	89	9919	3	0.0003

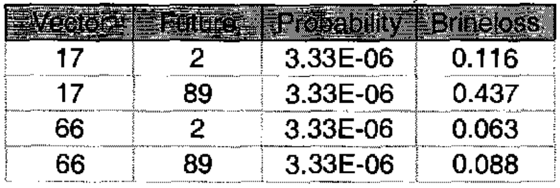
The "*BrinelossbyFbyP*" query in the *brineloss.mdb* database takes the results from the "*Brineloss*" query and sums the events to get a total amount for each panel. The results from the "*BrinelossbyFbyP*" query in the *brineloss.mdb* database are shown in Table A13 for futures 2 and 89, for vectors 17 and 66. As seen in Table A12, there are two events in future 89, panel 2 and panel 6. The other panels each only had only one (or zero) events in these futures. As seen in Table A13, the MgO lost to brine flow for each vector-future-panel combination are the same as shown in Table A12, except for future 89, panels 2 and 6, where the MgO lost to brine flow is the sum of the two events seen in Table A12 for both vectors.

Table A13. Results from the "*BrinelossbyFbyP*" query in the *brineloss.mdb* database for futures 2 and 89, for vectors 17 and 66.

Vector	Future	Panel Number	SumOfBrineloss
17	2	1	0.0038
17	2	3	0.1164
17	2	5	0.0041
17	2	7	0.0081
17	2	8	0.0098
17	89	2	0.1395
17	89	3	0.0027
17	89	6	0.4372
66	2	1	0.0226
66	2	3	0.0183
66	2	5	0.0245
66	2	7	0.0515
66	2	8	0.0633
66	89	2	0.0883
66	89	3	0.0003
66	89	6	0.0727

The "*WorstCasebyFuture*" query in the *brineloss.mdb* database takes the results from the "*BrinelossbyFbyP*" query and finds the maximum MgO lost to brine flow in a panel for each future. The "*WorstCasebyFutureRounded*" query takes the results from the "*WorstCasebyFuture*" query and rounds them to the nearest 0.001. The "*WorstCasebyFuturePlusZero*" query takes the results from the "*WorstCasebyFutureRounded*" query and fills in zeros for the futures that had no events and assigns a probability (1/300*1/1,000) for each future-vector combination. The results from the "*WorstCasebyFuturePlusZero*" query are shown in Table A14 for futures 2 and 89, for vectors 17 and 66. As seen by comparing Tables A13 and A14, the maximum value from each future-vector combination was chosen.

Table A14. Results from the "*WorstCasebyFuturePlusZero*" query in the *brineloss.mdb* database for futures 2 and 89, for vectors 17 and 66.



Vector	Future	Probability	Brineloss
17	2	3.33E-06	0.116
17	89	3.33E-06	0.437
66	2	3.33E-06	0.063
66	89	3.33E-06	0.088

The "*BrinelossPlot*" query in the *brineloss.mdb* database takes the results from the "*WorstCasebyFuturePlusZero*" query and combines all of the vector-future combinations that calculate the same MgO lost to brine flow value and sums their probabilities. This condensed list of MgO lost to brine flow amounts versus probability is output to the Excel® file labeled *BrinelossPlot_DJC.xls* in the sheet "*BrinelossPlot*". In the *BrinelossPlot_DJC.xls* file the CCDF, mean and standard deviation are calculated in the "*Total Effect*" sheet and the resulting plot is generated in the "*Plot*" sheet as seen in Figure 2. The values are divided by the ratio of 1.2 moles of MgO emplaced per mole of carbon was used, as this is the amount proposed by DOE (Moody 2006). A visual inspection of the *BrinelossPlot_DJC.xls* file shows that the procedure was implemented correctly.