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To: Records Center

12/11/12

From: Tom Kirchner, Todd Zeitler and Ross Kirkes

Subject: Evaluating the data in order to derive a value for GLOBAL:PBRINE

1. Introduction

The penetration of brine pockets during drilling intrusions of the WIPP repository can have significant consequences with respect to releases. The term "brine pocket" seems to imply that pools of pressurized brine exist in the Castile. However, Popielak et al. (1983) reviewed the geologic data acquired during the WIPP-12 and ERDA-6 well testing and other information related to the occurrences of pressurized brine in the Castile formation and concluded that pressurized brine is associated with near-vertical fractures. Borns (1983) confirms the near-vertical orientation of brine-producing fractures through study of core from the WIPP-12 borehole. Furthermore, they stated that these fractures are associated with a belt of deformation that parallels the Capitan reef. WIPP PA parameter GLOBAL:PBRINE (hereafter PBRINE) is used to specify the probability that a drilling intrusion into the excavated region of the repository encounters a region of pressurized brine below the repository. Currently, a uniform distribution between 0.01 and 0.60 with a mean value of 0.305 is assigned to this parameter. Initial development of this distribution was the result of an analysis of TDEM data (Rechard et al. 1991, Peake 1998).

This memo provides an alternative statistical interpretation of the TDEM data as reported in Peake (1998) and integrates it with 20 years of observations of brine pocket intrusions in wells drilled in the vicinity of the WIPP site. The aim is to incorporate additional data gathered over the last 20 years into the definition of parameter PBRINE so that it is more accurate and defensible. In particular, this memo provides a quantitative argument for the refinement of PBRINE by reexamining the TDEM data while including a greatly expanded set of drilling data for locations adjacent to the WIPP site than were available when the original analysis was performed in 1998. The approach documented herein is not just a rehash of earlier arguments using an expanded set of well data but is based on an examination of a sub-region that has a high-density cluster of drilling intrusions. That subset of data is used both to provide a conservative estimate of the probability of brine pocket intrusion based solely on the drilling data and to estimate a probability of encountering a brine pocket given that a well is drilled into a TDEM-identified region.

Sandia believes that the drilling data offer the best estimate of the probability of hitting a brine pocket. A concern raised in regard to the use of drilling data is that drilling logs may not record all instances where pressurized brine was encountered. Powers et al. (1996) did an extensive geostatistical analysis on the data available at that time and concluded that the probability of encountering pressurized brine under the waste panels was 0.08 with no estimate of uncertainty on that value. Powers et al. (1996) argued that pressurized brine pockets of a size sufficient to impact the repository would produce a large enough flow as to threaten overflow of the surface storage pits, and hence require measurement and intervention by the drillers. Therefore, such "non-reported" brine intercepts are of no consequence to WIPP performance. Additionally, a concern remained regarding the frequency of brine pocket intrusions in the region around the WIPP site being a suitable estimate for the WIPP site in particular. Powers et al. (1996) addressed that concern by examining spatial autocorrelations in the data and correlation with factors such as the thickness of the formations. The application of a regional frequency being used to estimate a WIPP-site specific probability is also addressed herein in two ways, 1) a subset of the drilling

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data is used to provide a conservative estimate of the frequency of brine pocket encounters and 2) a confidence interval is constructed for the estimate of the true probability based on the observed frequency drawing upon statistical theory for Bernoulli processes.

It is shown that a statistical analysis of the TDEM data and a conservative estimate of the probability of drilling yield distributions that are similar to each other, although having reduced ranges in comparison to the current distribution of PBRINE. Finally, drilling events are simulated using the new normal distribution of PBRINE and the frequencies of drilling intrusions into brine pockets and are tabulated for 1,000,000 futures. The resulting distribution extends from 0.0 to 1.00 and exceeds the range of PBRINE because of the effects of random sampling. This distribution of the realized frequencies of brine pocket intrusions is compared to the realized distribution of intrusions based on the current uniform distribution of PBRINE. The mode of the new distribution is shifted to the left in comparison to that based on the uniform distribution but both have tails that extend beyond the 0.60 frequency that is the upper bound on the current distribution of PBRINE.

2. Observed rates of brine pocket penetration on the WIPP site

A concern was raised in our recent meeting with EPA (Gross 2012) that having one brine encounter in three wells within the boundaries of the WIPP site might indicate that the probability of encountering brine there was higher than the average of the surrounding areas. This concern can be addressed by bounding the probability based on the three observations alone. These bounds will be large, due to the small sample size, but can nonetheless provide a reference for the analysis based on the regional data.

The probability of seeing one or more brine intrusions is equal to 1 minus the probability of seeing no brine intrusions. The probability of not hitting brine in one trial is $1-p_{brine}$, and the probability of not hitting brine in any of three trials is $(1-p_{brine})^3$. If α is the probability of not hitting brine in three trials, then $\alpha = (1-p_{brine})^3$. Thus the probability of hitting brine can be solved directly as $p_{brine} = 1 - \sqrt[3]{\alpha}$, where confidence is $1-\alpha$. For a 95% chance of seeing 1 or more brine hits in 3 trials, $p_{brine} = 0.632$. To bound the lower tail, a 5% chance of seeing 1 or more brine intrusions would occur for $p_{brine} = 0.017$. Thus any probability between about 0.02 and 0.63 has a reasonable chance of resulting in one out of three wells hitting brine, so values less than the nominal probability of 0.33 should not be discounted out of hand as being too low. In addition, this calculation shows that the current range for PBRINE is similar to what could be specified as a 90% confidence interval using only the three observations within the WIPP boundaries and ignoring the TDEM analysis and the extensive drilling logs entirely. The use of these additional data should be able to reduce the uncertainty and improve the credibility of the estimated distribution, resulting in a more defensible distribution for PBRINE.

3. The well drilling data

The number of Castile brine encounters within a geologically similar area surrounding the WIPP site is reported periodically. The data as of November 1, 2012 show 34 brine pocket intrusions out of 678 well drilled (Fig. 1).

In the discussion that follows, the penetration of brine pockets is assumed to be a Bernoulli process. This assumption is justified and reasonable because each drilling event can hit brine with probability p or miss hitting brine with probability $q=1-p$. The probability p is assumed to be constant and all trials are independent. Given this assumption, the expected distribution for the observed frequencies is binomial with mean np and variance npq, where n is the number of trials. Given that the observed ratio of 34/678 represents the best estimate of the true probability (0.0501), the expected distribution of frequencies can be computed using

$$f_{m(n,p)} = \frac{n!}{m!(n-m)!} p^m q^{n-m}$$

Here *m* is the number of brine encounters, *n* is the number of wells drilled, *p* is the probability of hitting a brine pocket and *q* is the probability that a brine pocket would not be encountered. The frequencies are computed for values of *m* between 0 to *n*. Using the region-wide brine pocket intrusion data and the equation above yields the distribution shown in Fig. 2. This distribution represents the variability that is expected to be observed due to random error[1] for a constant value of 0.0501 representing the probability of encountering brine.

There are two consequences of random error associated with intrusions into brine: 1) an observed frequency, such as the 34 brine intrusions out of 678 wells drilled, can be reasonably expected for a range of values of *p*, and 2) both the variability in PBRINE as sampled by LHS and the random error introduced because drilling intrusion is a stochastic process will contribute to the overall uncertainty in the frequencies of brine intrusions simulated in WIPP PA. The first consequence of random error is addressed by computing a confidence interval around the observed frequency of encountering brine. The impact of the second consequence is illustrated in Section 6 of this memo.

The frequencies of the binomial distribution can be normalized as probabilities (top axis of Fig. 2) and a confidence interval on the mean constructed as shown in Fig. 3. The confidence interval is constructed by finding the smallest value for p which results in a frequency of 34 out of 678 at the probability of 0.99 and the largest value of p that gives a frequency of 34 out of 678 at a probability of 0.01. These probability levels (0.99 and 0.01) were chosen because they are consistent with the probability levels used in the LHS sampling program to truncate continuous distributions. The resulting confidence interval is [0.0338, 0.0731]. This is not the range we are proposing to assign to PBRINE; it is computed here to provide a reference against which our more conservative estimate can be compared.

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[1] See Appendix I for more discussion of random error.

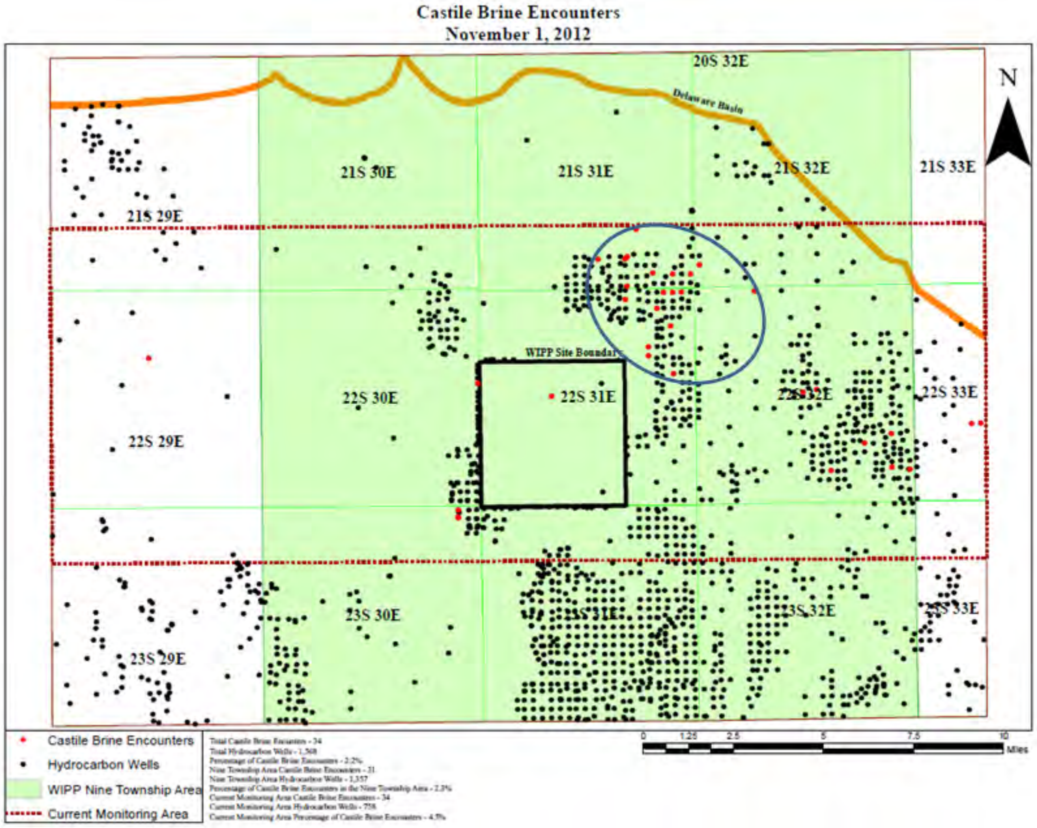

Figure 1. Map of brine pocket encounters on or near the WIPP site.

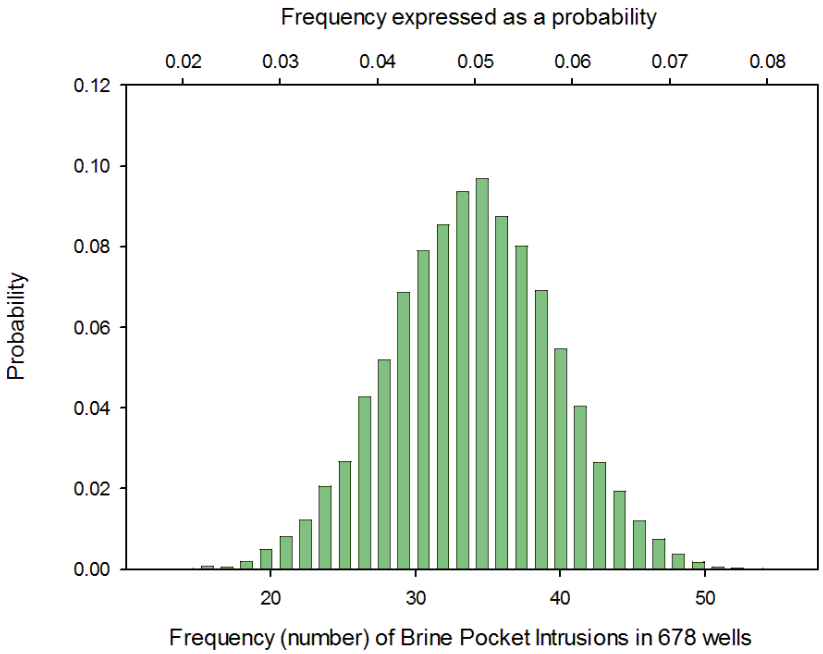

Figure 2. Expected frequency distribution for PBRINE.

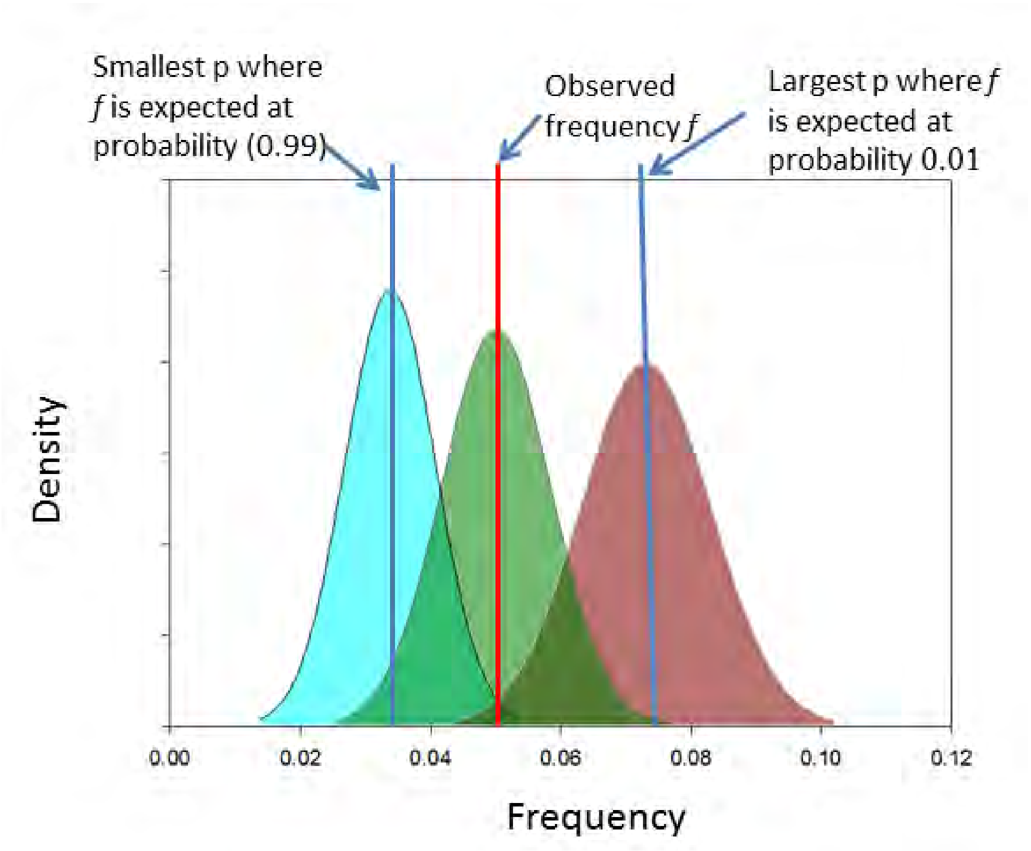

Figure 3. Confidence interval constructed around the observed frequency.

Fig. 3 represents the best estimate of PBRINE based on the drilling data and its uncertainty assuming that the regional average probability is applicable to the WIPP site. We suspect that this distribution is biased high, due to the higher frequency of brine intrusions to the north and east of the WIPP site in areas of deformation quite unlike the WIPP site (Powers et al. 1996). Nevertheless, one possible source of error in this approach is that the frequency observed in the surrounding region may not be representative of the frequency that might be observed if drilling were conducted on the WIPP site. For example, perhaps there are geologic factors associated with the presence of brine intrusions that are, in fact, also present on the WIPP site. As an example, the group of wells just to the northeast of the WIPP site has a higher than average frequency of brine intrusions (see Fig. 1). This higher frequency of intrusions is associated with the location being deformed into a major anticline (Powers et al. 1996, Section 5.2.2), which most likely caused the fractures in which pressurized brine is found. The WIPP site does not exhibit such deformation so is expected to show much less fracturing (Powers et al. 1996, Section 8.0) but this area can be used as a reference to develop a conservative estimate of the probability of intruding a brine pocket.

The blue ellipse that encompasses these locations in Fig. 1 is approximately the same area as the WIPP site and has a higher frequency of brine pocket hits than any other area adjacent to the WIPP site. The elliptical reference area was placed to maximize the number of intrusions. This reference area provides a conservative (maximizing brine encounters) subset of the drilling data. A count of the wells in that ellipse shows 19 intrusions (see Fig. 5) out of 150 wells, or a ratio of 0.127. The elliptical reference area contains a significantly ($p<0.001$) higher frequency of brine intrusions than the regional average of 0.0501. The confidence interval around 0.127 is [0.063, 0.190]. The normal distribution (mean=0.127, standard deviation=0.0272) representing the uncertainty in the probability of encountering brine is shown in Fig. 4. The normal distribution is used because the probability of encountering brine is estimated by the proportion of brine hits to wells drilled, and proportions converge to normal distributions when n and m are large (>10) (Hahn and Meeker 1991, p. 106). Inspection of the map (Fig. 1) shows one other area, well east of the WIPP site, having a similar but lower density cluster of brine intrusions. The normal distribution shown in Fig. 4 is therefore conservative as it is based on the highest density cluster associated with the brine intrusion data.

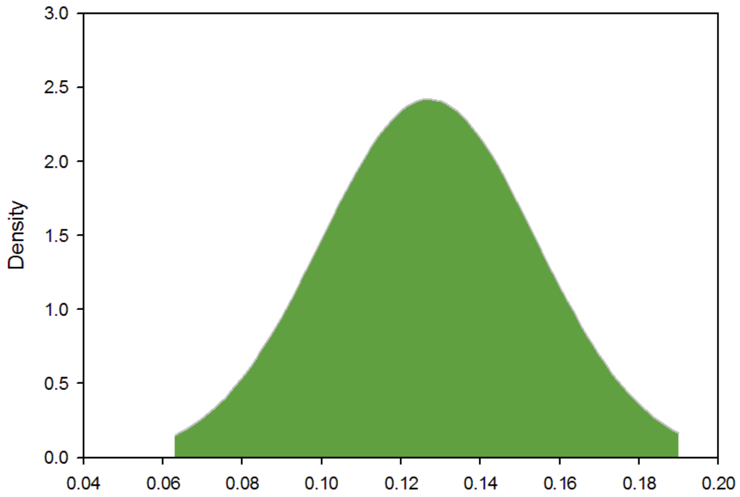

Figure 4. Normal distribution representing uncertainty in PBRINE.

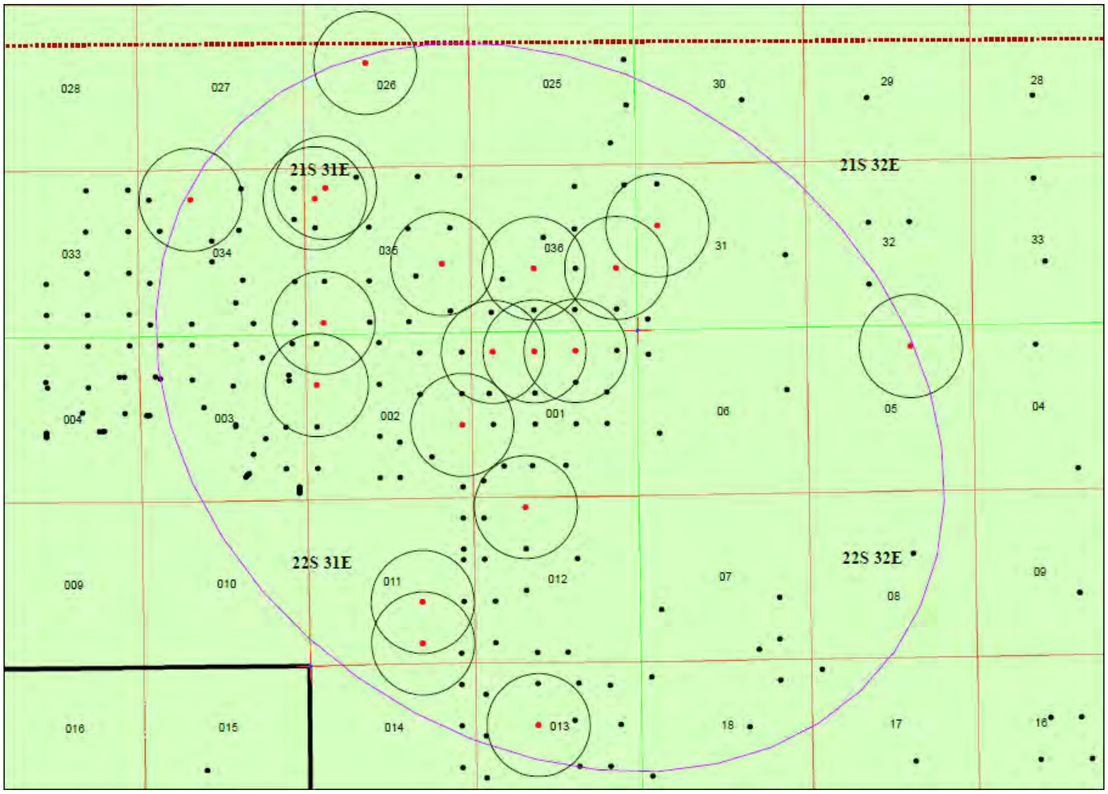

Figure 5. Close up view of reference area showing the circular subregions used to evaluate the probability of encountering brine adjacent within a TDEM region.

4. TDEM data

Rechard et al. (1991, page 5-3) reviewed the TDEM data and reported that 0 to 45% of the area of the repository is underlain by TDEM-identified high-conductivity regions that are assumed to represent locations where pressurized brine pockets exist. Their data, reproduced in Table 1, shows that the proportion of the area identified by TDEM is 43357/109354=0.396, or about 40% rather than the 45% they reported. An analysis of the uncertainties associated with the limited (36 sample points) data led to a conservative estimate of the area underlain by TDEM-identified regions of high conductivity of 25 to 55%. Borns (1996) evaluated the data and tabulated the percentage of the area underlain by brine as 10%, 25% and 55% at the maximum, mean and minimum depths (i.e. the mean depth ± 75 m).

Table 1. Percentages of disposal region underlain by TDEM-identified regions of high conductivity.

Panel	% TDEM	Area	TDEM Area	Panel	% TDEM	Area	TDEM Area
1	100	11530	11530	7	0	11530	0
2	73.08	11530	8426.124	8	52.86	11530	6094.758
3	18.23	11530	2101.919	9	3.24	8413	272.5812
4	75.57	11530	8713.221	10	45.29	8701	3940.683
5	19.76	11530	2278.328	Total		109354	43357.61
6	0	11530	0				

In a separate analysis of the TDEM data, EPA (Peake 1998) reported that the TDEM can be interpreted as indicating that between 50% and 88% of panels 1 and 8 (group 1) are underlain by brine and that between 10% and 50% of panels 5, 6, 7 and 9 (group 2) are underlain by brine[2]. WIPP PA code CCDFGF uses an average probability of intrusion for all panels rather than panel specific probabilities. The average probability of brine intrusion across all 10 panels can be computed as

$$p_{brine} = p\left[brine \,|\, TDEM\right] \times \sum_{i=1}^{2} p_i[borehole] \times p_i[TDEM]$$

where $p_i[borehole]$ is the probability of drilling into panel group i, $p_i[TDEM]$ is the probability of encountering the TDEM-identified brine region within panel group i, and $p[brine \mid TDEM]$ is the probability of hitting a brine pocket given a TDEM-identified brine region is intruded. In other words, the repository-wide probability of encountering a TDEM-identified area is the sum of the probabilities of encountering a TDEM region in the two groups weighted by the probability of drilling into a panel in each group and multiplied by the probability of hitting brine given that a TDEM region was penetrated. This repository-wide probability is used when simulating drilling events in all panels, even those that were identified as not being underlain by areas of high conductivity in the TDEM analysis.

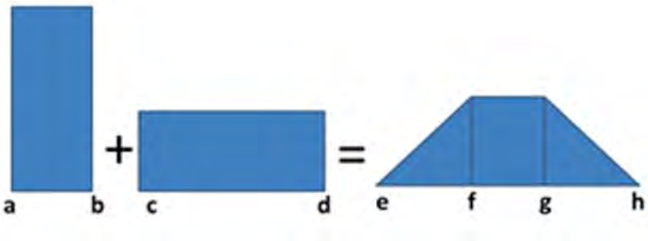

Figure 6. The sum of two non-identical distributions is a trapezoid distribution.

The probability of drilling into the panel groups, $p_i[borehole]$ is determined by their areas. The areas of panels 9 and 10 are somewhat smaller than the areas of the other panels but to keep things simple for this initial analysis all panels will be assumed to be equal in size. Hence $p_1[borehole]$=0.2 and $p_2[borehole]$=0.4 because group 1 has 2 panels and group 2 has 4 panels out of a total of 10 panels in the repository. The probabilities of encountering a TDEM-identified area are defined as ranges and will be assumed to be uniformly distributed within those ranges. The distributions resulting from multiplying the scalar probabilities p_i[borehole] and the uniform distribution for $p_i[TDEM]$ are also uniform. Using the U[min,max] notation for a uniform distribution and its associated minimum and maximum values, the resulting distributions can be simply found to be distributed as U[0.1, 0.176]=0.2×U[0.5,0.88] and U[0.04, 0.2]=0.4×U[0.10,0.50], where the limits of the uniform distributions on the right side of the equations are taken from Peake (1998). The probability of penetrating a TDEM-identified area across the panels is thus represented by the sum of these two uniform distributions. The sum of two non-identical uniform distributions produces a trapezoidal distribution (Fig. 6) (NCRP 2007, p. 442). In this figure, $e = a + c$, $f = b + c$, $g = a + d$ and $h = b + d$.

For the TDEM ranges presented by Peake (1998), the distribution for encountering a TDEM-defined area by a borehole penetrating the repository is shown in Fig. 7. It covers the range [0.14,0.376].

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[2] We believe that the panel numbers were assigned differently than in DOE's scheme, but that will have no impact on the analysis. The panel numbers used in Peake (1998) appear to be assigned counterclockwise from the NW corner whereas DOE numbers them clockwise from the NE corner.

To get the repository-wide probability of encountering brine, a value for *p*[*brine* | *TDEM*] is required. There are no data that speak directly to this but a value can be derived from a subset of the well drilling data, which is discussed in the next section.

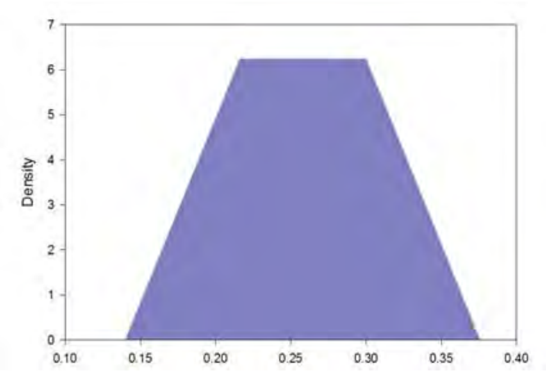

Figure 7. Distribution for the probability of hitting a TDEM-identified brine region.

5. Resolution of the differences between the TDEM and brine pocket intrusion data

One problem with the TDEM data is that it does not in itself provide an estimate for the probability of encountering brine; it identifies regions of high conductivity that are assumed to represent areas where brine pockets occur. In addition, there are no TDEM data for the region outside of the WIPP site where brine has been encountered by drilling so there are no data which can be used to correlate TDEM-identified regions with the likelihood of brine pocket intrusions by drilling. The near-vertical orientation of the brine pockets suggests that the likelihood of drilling into a pressurized brine pocket is lower than 100%. The overall frequency of brine encounters within the reference area can be used as an estimate for *p*[*brine* | *TDEM*] but could be biased low if the area encompasses patches of fractured and non-fractured salt. Presumably those wells that hit brine in the reference area are in a TDEM-type region. Thus, a conservative estimate of the probability of encountering brine can be gained by examining the frequency of brine hits within a radius around each well where brine was encountered, where the resulting circle is likely to encompass similar geologic conditions (Fig. 5). The TDEM data suggests that areas of high conductivity are patchy with the patches extending beyond the sampling domain (Fig. 8).

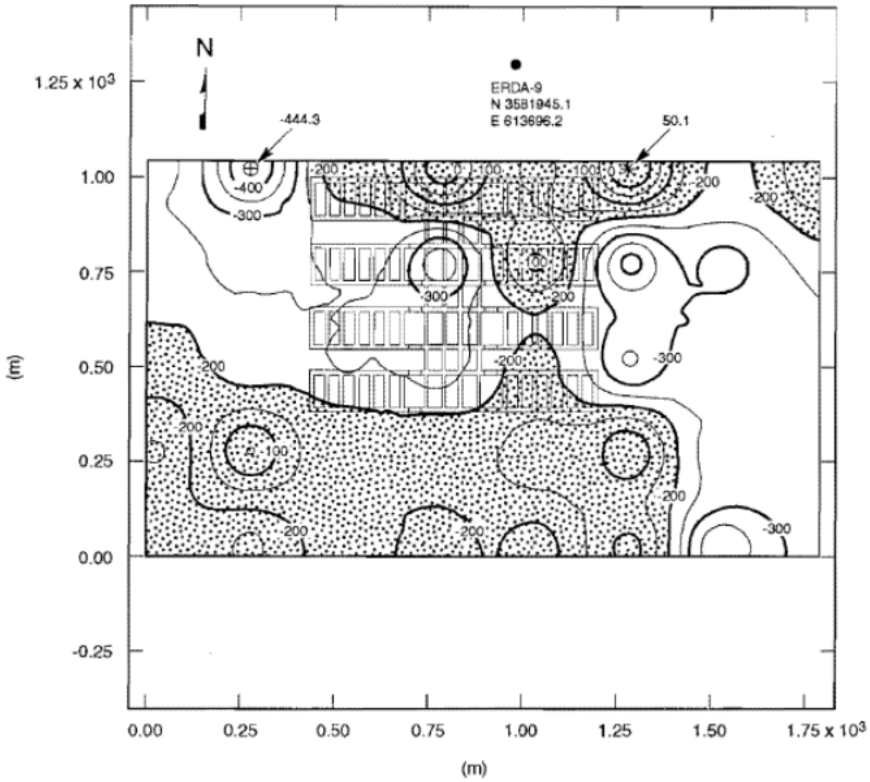

Figure 8. Conservative contour map of elevation above sea level of first major conductor below WIPP area.

Thus the size of such patches cannot be determined but a linear size of 1000 m appears reasonable. Circles having a diameter of 1000 m were drawn around each of the 19 wells in the reference area where brine was hit (Fig. 5). These circles are assumed to define regions of similar geology. The number of wells that hit brine or did not hit brine was tabulated (Table 2). Wells were included if the center of the dots showing their position fell within the circle. Cases where only the target well is within the circle give a ratio of 1. These could be excluded as being inadequate measures of the frequency of hitting brine but are included to provide a further level of conservatism in this procedure. The average of these ratios is 0.42 and represents a somewhat subjective but conservative estimate of the probability of hitting a brine pocket in an area where fracturing and brine pockets are abundant, i.e. *p*[*brine* | *TDEM*]. Although the 1000 m diameter of the circles is somewhat arbitrary, examination of Fig. 5 shows that increasing the diameter will most likely add more wells without brine intrusions than wells with intrusions, and thus drive the average ratio lower. Circles of a smaller diameter would result in many more cases of there being only a single well contained and thus be inadequate for estimating the ratio. Finally, smaller circles would not reflect minimum well spacing requirements for drilling in the Delaware Basin, and would exclude effectively all neighboring wells.

Table 2. Frequency of encountering brine within 500 m of a known brine intrusion.

Well	Number of encounters	Number of non-encounters	Ratio
1	1	0	1
2	2	4	0.333333
3	2	4	0.333333
4	2	4	0.333333
5	1	4	0.2
6	1	4	0.2
7	1	2	0.333333
8	1	2	0.333333
9	1	5	0.166667
10	3	2	0.6
11	2	4	0.333333
12	3	3	0.5
13	2	4	0.333333
14	1	0	1
15	1	5	0.166667
16	1	5	0.166667
17	2	1	0.666667
18	2	1	0.666667
19	1	2	0.333333
		Average	0.42

The estimation of $p[brine \mid TDEM]$ allows a comparison to be made of the probability of brine intrusions based on the well drilling data and the probability based on the TDEM data (Fig. 9). The trapezoid in Fig. 9 is the distribution of p_{brine} based on the distribution of the TDEM data (Fig. 7) which is multiplied by the estimate of the probability of hitting brine given that a TDEM area was penetrated (0.42). This distribution has the range $[0.0588, 0.1579]=0.42 \times [0.14, 0.376]$. Previously, no consideration was explicitly given to the probability of hitting brine within a TDEM data, effectively implying that this probability was 1. The drilling data from the reference area shows that a probability of 1 for $p[brine \mid TDEM]$ is unlikely.

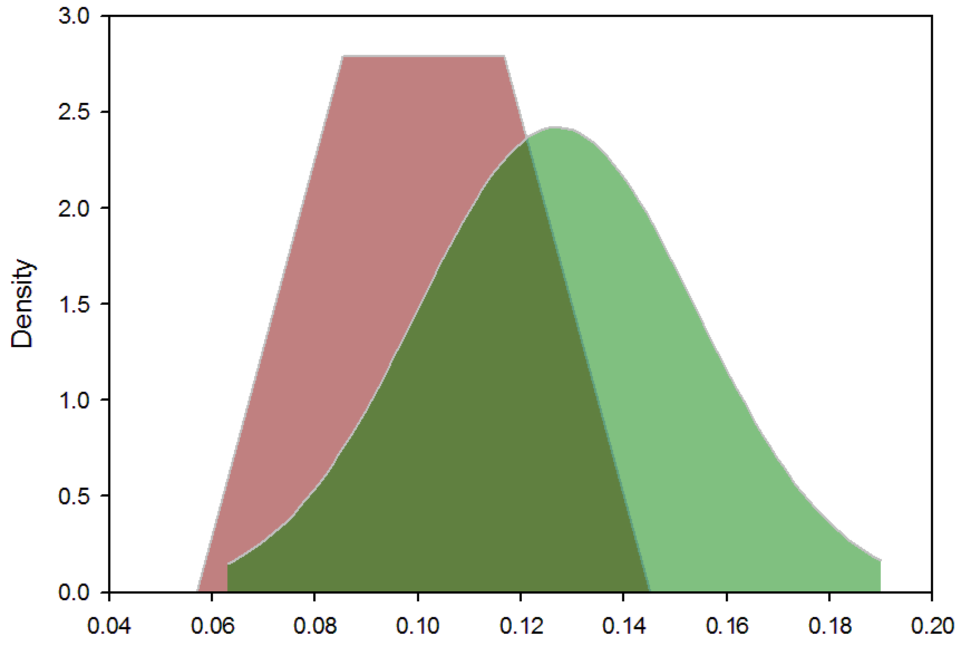

Figure 9. Distribution of PBRINE based on TDEM data (trapezoid) and derived probability of hitting brine within a TDEM-identified brine region overlaid by distribution derived from a subset of the data on drilling intrusions (normal curve).

6. Comparison of the TDEM and drilling data

As Fig. 9 reveals, a quantitative analysis of the two independent sets of data results in distributions that are remarkably similar. The construction of these distributions employed many conservative assumptions, so it is expected that the true probability is considerably lower than the lower bounds of either distribution. We propose to use the normal approximation of the binomial distribution derived from the subset of drilling data to the northeast of the site (shown in green in Fig. 9). These data are from a region that is expected to have a much higher proportion of the area showing the geologic deformation associated with brine pockets as compared to the WIPP site. Hence, this distribution represents a conservative estimate of PBRINE. Furthermore, it overlaps the distribution based on Peake's (1998) analysis of the TDEM data, after adjusting for the probability of encountering pressurized brine within a TDEM-identified region.

The observed or realized frequency of intrusions into brine pockets for any given future or realization simulated by CCDFGF can exceed the range of the mean probability (the normal distribution sampled by LHS). This result is due to simulating the penetration of a brine pocket as a stochastic process in the CCDFGF code. In other words, the distribution of the frequencies of brine pocket intrusions per future will have a larger range than that of PBRINE due to random sampling error. To further illustrate that the observed frequency of intrusions can easily exceed the range of mean probabilities, we simulated the intrusion of brine pockets by using LHS 2.42 to sample both the previous uniform distribution and the new normal distribution (Fig. 9) and then using a utility code (HPI, Appendix 2) to simulate the stochastic events that control brine pocket intrusions, based on the methodology employed in CCDFGF 5.02. As expected, the observed frequencies for intruding brine pockets in both cases ranged from 0 to 1.00 (Fig. 10). In other words, futures were seen where no drilling intrusions resulted in a brine pocket encounter, as well as futures where every drilling intrusion resulted in a brine pocket encounter.

The irregular shapes of the distributions in Fig.10 arise because the frequencies are computed as the ratio of small integer values, i.e. the ratio of the number of brine intrusions to the intrusions and the number intrusions into the waste panel. Some ratios, e.g. 14/15, will be uncommon whereas others, e.g. 1/2, will be common because there are lots of combinations that can produce the same ratio, e.g. 2/4, 3/6, 4/8, etc. Up to 21 intrusions per future were observed. The cases where there were zero penetrations are excluded for clarity; the number of zero cases is 251514 (25%) for the uniform distribution and 461532 (46%) for the normal distribution. The contribution of random error to the realized distribution of brine pocket intrusion frequencies is clearly important.

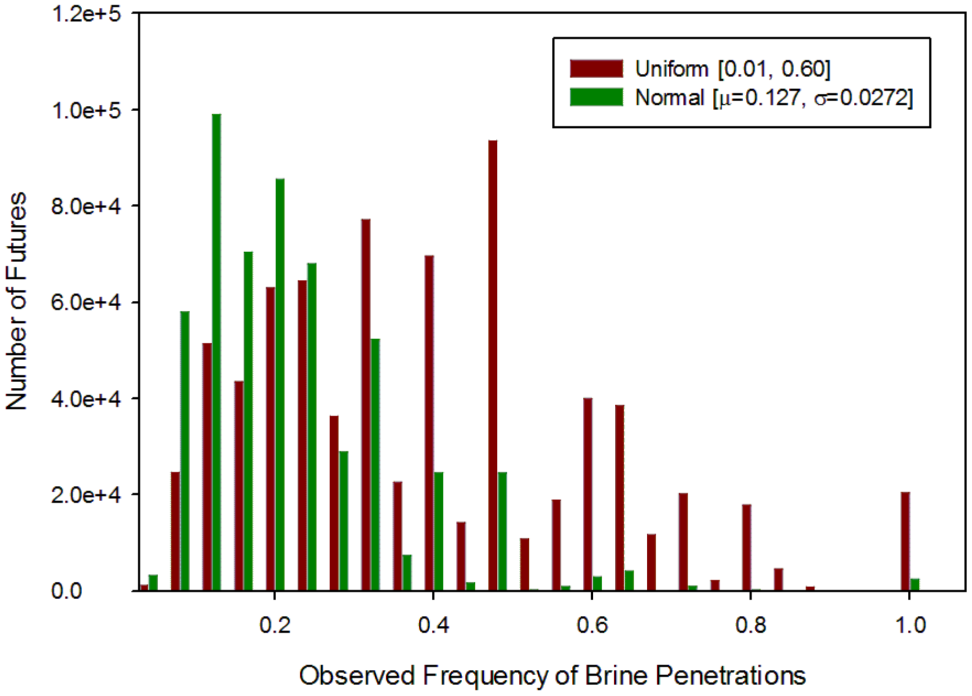

Figure 10. Observed frequencies of brine pocket penetration (number of futures out of 1 million) based on sampling PBRINE as uniform[0.01, 0.60] and normal[μ=0.127, σ=0.0172] distributions. The frequencies of zero are excluded.

7. Summary

This analysis was undertaken as part of the review of parameter values to be used in the CRA-2014. An extensive geo-statistical analysis of drilling data by Powers et al. (1996) concluded that the best estimate of hitting brine by an intrusion into a panel was 0.08, equivalent to the regional frequency of brine intrusions. To address concerns raised by the EPA, parameter GLOBAL:PBRINE was later assigned a uniform distribution with a range of 0.01 to 0.6. The upper and lower bounds of the distribution were based on the TDEM results but with a limited analysis of the probabilities. Since that time a considerable number of new wells have been drilled in the region around the WIPP site, providing more data for an analysis of drilling intrusions into pressurized brine pockets. In addition, a reexamination of the interpretation of the TDEM data was also undertaken.

This memo describes the process to refine the current distribution of PBRINE and gives estimates of the mean and standard deviation based on current well data. The regional frequency of brine intrusions based on recent data is 0.0501 with a confidence interval of [0.0338, 0.0731].This estimate is conservative because it includes data from deformed areas to the north and east of the WIPP site that show a higher frequency of brine encounters than are expected at the WIPP site based on the geology of the region. We believe that this is the best estimate for the probability of intruding brine pockets in the WIPP repository panels. However, to ensure that possible geological associations are considered, a distribution for PBRINE was developed based solely on the frequency of brine intrusions from the deformed area to the northeast of the site. This produced an estimate of the probability of encountering brine of 0.127 with uncertainty bounds of [0.063, 0.190]. A reexamination of the TDEM analysis using ranges of uncertainty reported by EPA (Peake 1998) combined with an estimate of the probability of hitting brine for wells drilled into a TDEM region produced a trapezoidal distribution having the range [0.0588, 0.1579]. Thus the ranges covered by the distribution based on the TDEM data and the distribution based on the conservative subset of the drilling data overlap, with the drilling data having a more conservative range of values. When simulated in PA, the observed frequencies of drilling intrusions will range between 0 and 1.00 as in previous PA calculations. The extended range of the observed frequencies compared to the range of PBRINE is due to the additional source of random error that is inherent in the implementation of the intrusion scenarios in CCDFGF. Thus sampling the normal approximation (Fig.7) of the distribution of PBRINE (mean=0.127, SD=0.0272) will result in simulated frequencies of brine intrusions that cover the same range as that produced using the uniform distribution ([0.01, 0.60]) but showing a greater degree of positive skewness, i.e. showing a mode that is shifted to the left.

8. References

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Appendix 1: Random Error

The concept of random error and the binomial distribution can be illustrated using the example of flipping a fair coin. A success will be the case where the coin shows heads. The probability of a head is 0.5. However, the actual frequency of heads can vary from 0.5 due to random error. For example, in four tosses of the coin, the number of heads can vary between 0 and 4. The probability for each of these cases can be computed using the formula

$$f_{m(n,p)} = \binom{n}{m} p^m q^{n-m} = \frac{n!}{m!(n-m)!} p^m q^{n-m}$$

for the binomial distribution. In this case the expected frequencies are:

Number of heads	Proportion of heads	Expected frequency
0	0	1/16
1	0.25	1/4
2	0.50	3/8
3	0.75	1/4
4	1	1/16

Thus for a value of *p* for an event that is constant the realized frequency of that event will vary just due to the stochastic nature of the process. In this example, the proportion of heads ranges from 0 to 1 even though the probability of getting a head in one trial is 0.5. This source of uncertainty is unpredictable and irreducible.

Appendix 2: The HPI Code

The intrusion of brine pockets was simulated using the HPI utility code. The code was constructed to match the implementation of the penetration of brine pockets employed in the PA code CCDFGF. The random number functions were taken from the CCDFGF code. The LHS input and output files, the code and its input and output files and the spreadsheet used to find the confidence limits are stored in CMS as LIBCRA14_FILES class CRA14-0 (PACMS3:[CMS_CRA14.CRA14_FILES]) in the archive file PBRINE.ZIP

The program determines for a given intrusion whether that intrusion takes place in the excavated area using the ratio of excavated area to berm area as the probability for hitting an excavated area. For an intrusion into the excavated area (a “hit”), it determines whether the intrusion encounters pressurized brine (PBRINE). A single value of PBRINE is sampled for each of 100 vectors via LHS, and 10,000 futures are simulated per vector. Each future may have multiple intrusions. The ratio of brine hits to total hits (having a possible range of 0 to 1) is calculated for each future. A total of 10^6 futures are considered (100 vectors*10,000 futures/vector). The program produces a column of binned ratio data over the entire range of 0 to 1. Finally, the total number of drilling intrusions, excavated intrusions, and brine hits are output.

```
      PROGRAM HPI
      Implicit None
!.....Purpose:Calculate # of hits per future
!.....with or without brine
!     Author: Modified by Todd R. Zeitler
!     Date: 11/30/2012

!.....DECLARE STUFF
      Double Precision ProbabilityOfEncounterExcavated
      REAL*4 LBOUND, UBOUND, RATIO, ISEED
      Double Precision FinalDrillingRate
      Double Precision TIME

      Integer NumberOfObservations
      Integer NumberOfFutures, Future
      Integer I, J
      Double Precision ContactHandledWasteArea
      Double Precision RemoteHandledWasteArea
      Double Precision BermArea
      Integer BINSIZE
      Double Precision NumberDrillingIntrusions
      Double Precision TotalNumberDrillingIntrusions
      Double Precision NumberExcavatedHits
      Double Precision TotalNumberExcavatedHits
      Double Precision NumberUnexcavatedHits
      Double Precision TotalNumberUnexcavatedHits
      Double Precision NumberBrineHits
      Double Precision TotalNumberBrineHits
      Double Precision TEND

      Double Precision SBIN(26)
      Double Precision PBRINE(100)

!.....Function declarations
      Double Precision ExponentialVariate
      Double Precision RAN3             !Function that returns a pseudorandom number
      Double Precision Hits(26,26)

      Common/RandNumGen/MA(55), IFF, INEXT, INEXTP
      Integer MA, IFF, INEXT, INEXTP, MJ, NB, NE

!.....PARAMETERS
      NumberOfObservations = 100
      NumberOfFutures = 10000
      TEND = 10000
      ProbabilityOfEncounterExcavated = 0.0
      ContactHandledWasteArea = 111500
      RemoteHandledWasteArea = 15760
      BermArea = 628500
      BINSIZE = 25
      FinalDrillingRate = 0.002941
      ISEED =127987

!.....Read in PBRINE from LHS_DATA_0133.CSV
      OPEN (101, FILE="LHS_DATA$CSV", STATUS='OLD')
          DO J=1,100
             READ (101,*) PBRINE(J)
             WRITE (*,*) PBRINE(J)
          ENDDO
      CLOSE (101)

!.....Open output file.
      OPEN (102, FILE="HPIOut$out", STATUS='NEW')
      Write (102,*) 'LowerBound ', 'UpperBound ', 'FractionBrineHits '
```

```
      ProbabilityOfEncounterExcavated=                                  &
     &     (ContactHandledWasteArea+RemoteHandledWasteArea)/BermArea

      write(*,*) 'ProbabiExcavated = ', ProbabilityOfEncounterExcavated



!.....Initialize random number generator according to seed
      Call RanInit(ISEED)

      TotalNumberDrillingIntrusions = 0.0
      TotalNumberExcavatedHits = 0.0
      TotalNumberUnexcavatedHits = 0.0
      TotalNumberBrineHits = 0.0
      Do i=1,26
          Do J=1,26
              Hits(i,j)=0
          end do
      End Do
!.....Loop over observations (vectors)
      Do I = 1, NumberOfObservations

         write (*,*) 'Vector ', I

!         TIME = 0.0

!.......Loop over futures
         Do Future=1,NumberOfFutures

             TIME = 0.0

!...........Initialize Counters
             NumberDrillingIntrusions = 0
             NumberExcavatedHits = 0
             NumberUnexcavatedHits = 0
             NumberBrineHits = 0

!............Calculate next drill time based on previous drill time,
!             subsequent administrative control time, and final drilling rate

!...........Loop over intrusions
             Do While (TIME .LT. TEND)

!............Calculate next drill time based on previous drill time,
!             subsequent administrative control time, and final drilling rate
!................Assume an exponential distribution of interval lengths
                TIME=TIME + ExponentialVariate(FinalDrillingRate)

                NumberDrillingIntrusions = NumberDrillingIntrusions + 1
                TotalNumberDrillingIntrusions =                         &
     &            TotalNumberDrillingIntrusions + 1

!................Determine whether drilling intrusion penetrates excavated region.
                If (RAN3("DBH1").LE.ProbabilityOfEncounterExcavated)
     &             Then !hit excavated area

                   NumberExcavatedHits = NumberExcavatedHits + 1
                   TotalNumberExcavatedHits =TotalNumberExcavatedHits+1

                   If (RAN3("DBH1") .LE. PBRINE(I)) Then !hit brine
                      NumberBrineHits = NumberBrineHits + 1
                      TotalNumberBrineHits =TotalNumberBrineHits + 1

!                      write(*,*) 'hit brine'
                   End if

                Else    !hit unexcavated area
                   NumberUnexcavatedHits = NumberUnexcavatedHits + 1
                   TotalNumberUnexcavatedHits=
     &                 TotalNumberUnexcavatedHits+1
                End if
```

```
             End Do


!............Calculate ratio of brine hits to all hits and bin
             NE=Int(NumberExcavatedHits+0.0001)+1
             NB=Int(NumberBrineHits+0.0001)+1
             if (NB.GT.NE) Then
                 write(*,*) "Error:",NE, "<",NB
             END if
             if (NE.LE.26) Then
                 Hits(NE,NB)=Hits(NE,NB)+1
             end if
             If (NumberExcavatedHits.gt.0.0) then
                RATIO = NumberBrineHits / NumberExcavatedHits
             Else
                RATIO = -1.0
             End If

             If (RATIO.ge.0.0) Then
               Do J=1,BINSIZE+1
                  LBOUND = (J-1)/REAL(BINSIZE)
                  UBOUND = J/REAL(BINSIZE)
                  If ((RATIO.GE.LBOUND) .and. (RATIO.LT.UBOUND) ) Then !this is the bin
                     SBIN(J) = SBIN(J) + 1
                  End If
               End Do
             End If

         END DO

      END DO

!.....Print output
      DO J=1,BINSIZE+1
         LBOUND = (J-1)/REAL(BINSIZE)
         UBOUND = J/REAL(BINSIZE)
         Write (102,*) LBOUND, UBOUND, SBIN(J)
      END DO
      write (102,*) 'total # drilling intrusions',                      &
     &  TotalNumberDrillingIntrusions
      write (102,*) 'total # excavated hits ',TotalNumberExcavatedHits
      write (102,*) 'total # unexcavated hits',                         &
     &  TotalNumberUnexcavatedHits
      write (102,*) 'total # brine hits', TotalNumberBrineHits
      do i=1, 26
        write(102,'(" ",i2,5(5(",",i6),/,"  "))') i-1,(int(Hits(i,j)+
     & .001),j=1,26)
      end do

      CLOSE (102)
      End
      Function ExponentialVariate(Rate)
!.....Purpose: Return an exponential variate
!     Author: T. B. Kirchner
!     Date: 6/11/03
      Implicit None
        Double Precision ExponentialVariate !Returns: Exponetial variate
        Double Precision Rate               !Input: Rate constant

!.....Function declaration
        Double Precision RAN3

        ExponentialVariate = -Log(1.0D0-RAN3("EVR1")) / Rate

        Return
      End
      Function RAN3 (Tag)
!.....Purpose: Returns a uniform random deviate between 0.0 and 1.0.
!              Based on method in W. H. Press et al., Numerical recipes
!              in Fortran (1992), pp. 273-4)
```

```
!     Author: re-written by T. B. Kirchner
!     Date: 6/11/03
      Implicit None
        Character*4 Tag         !Input: A label used when storing a value to ind
icate
                            !       where it was used
!.....Local variables
!        Character*4 Tg  !A label used when storing a value to indicate where it
                        !was used
        Double Precision RAN3
      Integer MBIG, MSEED, MZ
        Double Precision FAC, Value
        Parameter (MBIG=1000000000, MSEED=161803398, MZ=0, FAC=1.0/MBIG)

        Common/RandNumGen/MA(55), IFF, INEXT, INEXTP
      Integer MA, IFF, INEXT, INEXTP, MJ

      INEXT=INEXT + 1
      If (INEXT .EQ. 56) INEXT=1
      INEXTP=INEXTP + 1
      If (INEXTP .EQ. 56) INEXTP=1
      MJ=MA(INEXT) - MA(INEXTP)
      If (MJ .LT. MZ) MJ=MJ + MBIG
      MA(INEXT)=MJ
      RAN3=MJ * FAC


      Return
!.....Formats
  100 Format(D12.6,1x,A)
  200 Format(f18.16,1x,A)

!.....Errors
 9000 Continue
      Write(*,*) "Out of input data in RAN3. Terminating"
      Write(11,*) "Out of input data in RAN3. Terminating"
        Stop

      End
        Subroutine RanInit(Seed)
!.....Purpose: Initialize the random number generator
!     Author: T. B. Kirchner
!     Date: 6/2/03

      Implicit None
        Integer SEED    !Input: The seed for the random number sequence

!       Include "ccgf_Control.fi"

!.....Local variables
      Integer MBIG, MSEED, MZ
        Double Precision FAC, Value
        Parameter (MBIG=1000000000, MSEED=161803398, MZ=0)
        Common/RandNumGen/MA(55), IFF, INEXT, INEXTP
      Integer MA, IFF, INEXT, INEXTP
        Integer MJ, MK, I, II, K

      Data IFF / 0 /

      SEED = Max0(IABS(SEED),1)

!.....Initialize or reinitialize sequence
      IFF=1
      MJ=MSEED - SEED
      MJ=MOD(MJ,MBIG)
      MA(55)=MJ
      MK=1

      Do I=1,54   !Fill the array of random numbers
          II=MOD (21*I, 55)
          MA(II)=MK
```

```
          MK=MJ - MK
          If (MK .LT. MZ) MK=MK + MBIG
          MJ=MA(II)
      End Do

      Do K=1,4
          Do I=1,55
              MA(I)=MA(I) - MA(1+MOD(I+30,55))
              If (MA(I) .LT. MZ) MA(I)=MA(I) + MBIG
          End Do
      End Do

      INEXT=0
      INEXTP=31
      SEED=1
      Return
        End
```

Qualification of the code

The functioning of the code was verified by comparing the frequencies of brine pocket intrusions that it computes against the expected frequencies computed using the binomial distribution function in Microsoft Excel. The observed counts were tallied by the HPI code and translated into proportions in Excel. The expected and observed frequencies of brine intrusions, shown in the tables below, are very close and thus the code has worked as designed.

As a further verification of the program’s results, the total number of drilling intrusions, excavated intrusions, and brine hits are compared below to the predicted results. The differences between the simulated and predicted results agree to within about 3%, which is reasonable.

	Predicted Frequencies						
	Number of panel intrusions						
n brine intrusions	4	5	6	7	8	9	10
0	0.0625	0.03125	0.015625	0.007813	0.003906	0.001953	0.000977
1	0.25	0.15625	0.09375	0.054688	0.03125	0.017578	0.009766
2	0.375	0.3125	0.234375	0.164063	0.109375	0.070313	0.043945
3	0.25	0.3125	0.3125	0.273438	0.21875	0.164063	0.117188
4	0.0625	0.15625	0.234375	0.273438	0.273438	0.246094	0.205078
5		0.03125	0.09375	0.164063	0.21875	0.246094	0.246094
6			0.015625	0.054688	0.109375	0.164063	0.205078
7				0.007813	0.03125	0.070313	0.117188
8					0.003906	0.017578	0.043945
9						0.001953	0.009766
10							0.000977

	Simulated Results						
	Number of panel intrusions						
n brine intrusions	4	5	6	7	8	9	10

0	7896	4822	2479	1096	400	171	50
1	31673	24620	15181	7845	3493	1315	470
2	47401	49112	37483	23390	12097	5229	2008
3	31601	49431	49921	38717	23673	12207	5269
4	8025	24557	37666	38780	29747	18425	9405
5		4796	15008	23264	23763	18142	11223
6			2504	7784	11831	12124	9147
7				1100	3381	5144	5303
8					424	1294	2035
9						142	452
10							40
Total intrusions	126596	157338	160242	141976	108809	74193	45402

	Simulated Frequencies						
	Number of panel intrusions						
n brine intrusions	4	5	6	7	8	9	10
0	0.062372	0.030647	0.01547	0.00772	0.003676	0.002305	0.001101
1	0.25019	0.156478	0.094738	0.055256	0.032102	0.017724	0.010352
2	0.374427	0.312143	0.233915	0.164746	0.111176	0.070478	0.044227
3	0.249621	0.314171	0.311535	0.272701	0.217565	0.16453	0.116052
4	0.063391	0.156078	0.235057	0.273145	0.273387	0.248339	0.207149
5	0	0.030482	0.093658	0.163859	0.218392	0.244524	0.247192
6	0	0	0.015626	0.054826	0.108732	0.163412	0.201467
7	0	0	0	0.007748	0.031073	0.069333	0.116801
8	0	0	0	0	0.003897	0.017441	0.044822
9	0	0	0	0	0	0.001914	0.009956
10	0	0	0	0	0	0	0.000881

Total Number of Intrusions

The expected number of total intrusions is calculated as the drilling rate (GLOBAL:LAMBDAD) multiplied by the area of the WIPP footprint (REFCON:ABERM), the number of years (10,000), and the number of futures (10^6).

Expected total # of intrusions = ($4.68*10^{-3}$ intrusions/km^2/yr)*(0.6285 km^2)*(10,000 yrs)*(10^6 futures) = $29.4*10^6$ intrusions

Simulated number of intrusions = $30.4*10^6$ intrusions

Total Number of Intrusions into the Excavated Area

The expected number of intrusions into the excavated area is simply the total number of intrusions multiplied by the fraction of footprint area ((REFCON:AREA_CH + REFCON:AREA_RH)/REFCON:ABERM) excavated.

Expected number of excavated intrusions = ($29.4*10^6$ intrusions)*(0.1115+0.01576 km^2)/(0.6285 km^2) = $6.0*10^6$ excavated intrusions

Simulated number of excavated intrusions = $6.2*10^6$ excavated intrusions

Total Number of Brine Hits

The expected number of total brine hits is equal to the number of excavated intrusions multiplied by the mean value of PBRINE. The mean value of PBRINE is 0.127 brine hits/intrusion.

Expected number of brine hits = ($6.0*10^6$ excavated intrusions)*(0.127 brine hits/intrusion) = $7.6*10^5$ brine hits

Simulated number of brine hits = $7.8*10^5$ brine hits