SENSITIVITY OF WIPP PERFORMANCE ASSESSMENT RESULTS TO REGULATOR-PRESCRIBED CHANGES

Todd R. Zeitler and Brad A. Day

Sandia National Laboratories

Address: 4100 National Parks Hwy. Bldg. A, Carlsbad, NM, 88220

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Abstract

The U.S. Environmental Protection Agency (EPA) requested of the U.S. Department of Energy (DOE) a sensitivity study (CRA14_SEN4) of the current Waste Isolation Pilot Plant (WIPP) Performance Assessment (PA) model that incorporated several changes to the baseline WIPP PA model (CRA14), including: parameter changes, use of an updated code, and a revised computational grid. The modifications to the repository model resulted in increased releases in all primary release mechanisms. The impacts of each EPA-requested change to CRA14 were analyzed with respect to each release mechanism in the CRA14_SEN4 study. Overall, total high-probability (P[Release>R] = 0.1) predicted mean releases from the repository were increased by about 15%, which corresponds to a 0.6% reduction in the margin to the limit of 1. Total low-probability (P[Release>R] = 0.001) predicted mean releases were increased by about 107%, which corresponds to a 2.9% reduction in the margin to the limit of 10. The upper 95% confidence level on the mean increased for high-probability and low-probability releases by 18 and 119%, respectively. It is concluded that the EPA-requested changes to the CRA14 result in increases to the predicted total releases from the repository. However, releases calculated in the CRA14_SEN4 analysis remain below regulatory limits, demonstrating continued compliance of the WIPP.

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1. Introduction

The Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, has been developed by the U.S. Department of Energy (DOE) for the geologic (deep underground) disposal of transuranic (TRU) waste. Containment of TRU waste at the WIPP is regulated by the U.S. Environmental Protection Agency (EPA) according to the regulations set forth in Title 40 of the Code of Federal Regulations (CFR), Part 191. The DOE demonstrates compliance with the containment requirements according to the Certification Criteria in Title 40 CFR Part 194 by means of performance assessment (PA) calculations performed by Sandia National Laboratories (SNL). WIPP PA calculations estimate the probability and consequence of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure. The models used in PA are maintained and updated with new information as part of an ongoing process. Improved information regarding important WIPP features, events, and processes typically results in refinements and modifications to PA models and the parameters used in them. Planned changes to the repository and/or the components therein also result in updates to WIPP PA models. WIPP PA models are used to support the repository recertification process that occurs at five-year intervals following the receipt of the first waste shipment at the site in 1999.

A sensitivity evaluation of the CRA-2014 PA (CRA14) has been requested by the U.S. Environmental Protection Agency to investigate potential regulatory compliance impacts associated with the following: 1) changes to certain sampled and constant parameter values; 2) the use of an updated version of the DRSPALL code; and 3) a correction to the length of a panel closure representation in the BRAGFLO grid (Zeitler 2016a, Zeitler and Day 2016). The objective of the sensitivity analysis was to evaluate the cumulative effects of these changes on predicted releases from the repository during the 10,000-year regulatory period.

Modified parameters implemented herein were used to satisfy an official request by the EPA for this sensitivity study. As such, the parameter values modified for this analysis should not be interpreted as being developed by SNL. The use of an updated version of DRSPALL code (which corrects an error in DRSPALL v. 1.21) and the correction of the length of the northern-most panel closure representation in the BRAGFLO grid are supported by SNL. The CRA14_SEN4 sensitivity analysis was performed under AP-164, Analysis Plan for the 2014 WIPP Compliance Recertification Application Performance Assessment (Camphouse 2013).

2. Approach

The CRA14_SEN4 sensitivity study investigates the impacts of parameter changes, the use of an updated version of the DRSPALL code, and a correction to the length of a panel closure representation in the BRAGFLO grid. All of these changes are taken together for use in a single PA calculation consisting of 3 replicates. The following changes to CRA14 inputs have been requested by the EPA for CRA14_SEN4:

1. Use newly-developed actinide solubility uncertainty distributions for +III and +IV actinides based on the Data0.FM1 WIPP thermodynamic database (FM1 database) and the data sets selected by the EPA.
2. Use EPA-developed distribution for GLOBAL:PBRINE parameter.
3. Use BOREHOLE:TAUFAIL parameter distribution with a new lower bound (EPA-directed).
4. Use version 1.22 of the DRSPALL code.
5. Use correct representative length of northernmost set of panel closures.
6. Set stoichiometric coefficients concerning reactions of hydrogen sulfide with iron to zero (EPA-directed).

The requested changes to CRA14 are explained below in detail. Additionally, in order to maintain a greater flexibility in prescribing material properties to specific areas of the repository model in the future, the CRA14_SEN4 sensitivity study uses the material names and associated grid modifications implemented for the CRA14_SEN2 and CRA14_SEN3 sensitivity studies (Day 2016, Day and Zeitler 2016a); however, the material properties of those areas are set equivalent to those used in the CRA-2014 PA.

2.1 Baseline PA Analysis

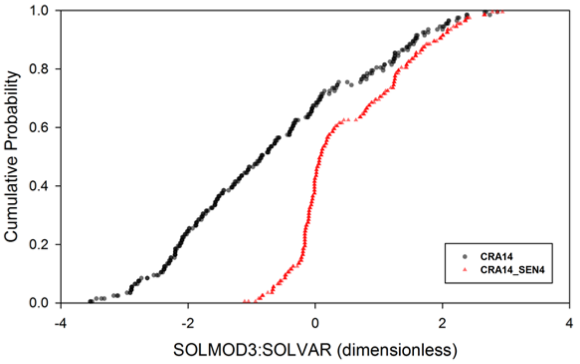
The most recent PA done to demonstrate WIPP regulatory compliance is that performed for the CRA-2014 (DOE 2014). The CRA-2014 PA considered four distinct cases with detailed descriptions of the four cases considered in the CRA-2014 PA found in Camphouse (2013) and a summary of results given in Camphouse et al. (2013). The final of the four cases considered in the CRA-2014 PA, identified as CRA14-0, is referenced herein as CRA14 and utilized as the baseline analysis for comparison with the sensitivity case called CRA14_SEN4. All three replicates evaluated under CRA14 are similarly run for CRA14_SEN4. Initial seed values for LHS and CCDFGF calculations were identical to those used in CRA14.

2.2 Modified Parameters

The original parameters used for CRA14 and the modified parameters implemented for CRA14_SEN4 in response to the EPA request can be found elsewhere (Zeitler and Day 2016).

2.2.1 Solubility Multipliers for Oxidation State III and IV Models (SOLMOD3:SOLVAR and SOLMOD4:SOLVAR)

As part of the EPA request for the CRA14_SEN4 analysis, the EPA has requested that actinide solubility uncertainty distributions be recalculated using the FM1 database and an updated list of references provided by the EPA (Zeitler 2016a). Baseline actinide solubilities were identical to those used in CRA14. A separate analysis has been performed in which new actinide solubility uncertainties have been calculated (Xiong and Domski 2016). The new analysis resulted in updated cumulative distributions for actinide solubility uncertainties, which are represented by the SOLMOD3:SOLVAR (+III oxidation state) and SOLMOD4:SOLVAR (+IV oxidation state) parameters. Comparisons for the values of SOLMOD3:SOLVAR and SOLMOD4:SOLVAR that were sampled in the CRA-2014 PA and CRA14_SEN4 analyses are shown in Figure 2-1 and Figure 2-2. For SOLMOD3:SOLVAR, the sampled values for CRA14_SEN4 are generally higher than



those for CRA14, while for SOLMOD4:SOLVAR, the sampled values for CRA14_SEN4 are lower than those for CRA14.

Figure 2-1: Comparison of LHS sampled values of the SOLMOD3:SOLVAR parameter for CRA14 and CRA14_SEN4 (300 sampled values for each analysis).

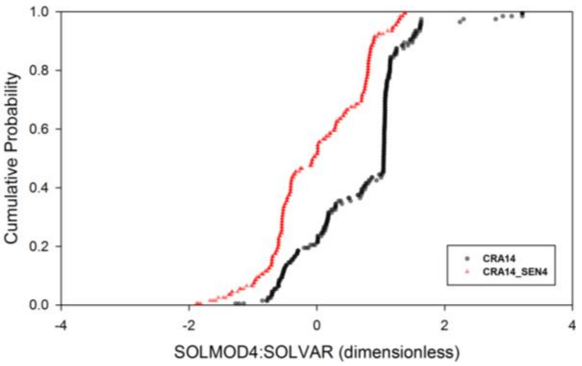


Figure 2-2: Comparison of LHS sampled values of the SOLMOD4:SOLVAR parameter for CRA14 and CRA14_SEN4 (300 sampled values for each analysis).

2.2.2 Probability that Drilling Intrusion in Excavated Area Encounters Pressurized Brine (GLOBAL:PBRINE)

For the CRA14_SEN4 sensitivity study, the EPA has requested the use of a revised distribution for the GLOBAL:PBRINE parameter (Zeitler 2016a). The GLOBAL:PBRINE parameter is a sampled parameter that represents the probability that an inadvertent human drilling intrusion intersecting the repository also intersects pressurized brine. A comparison of the values of GLOBAL:PBRINE that were sampled in CRA14 and CRA14_SEN4 is shown in Figure 2-3. The EPA-requested distribution of the GLOBAL:PBRINE parameter is given in the form of a cumulative distribution, while the distribution used in CRA14 was parameterized as a normal distribution. The range of values sampled from the CRA14_SEN4 distribution encompasses that from CRA14, but predominantly consists of values higher than those used in CRA14.

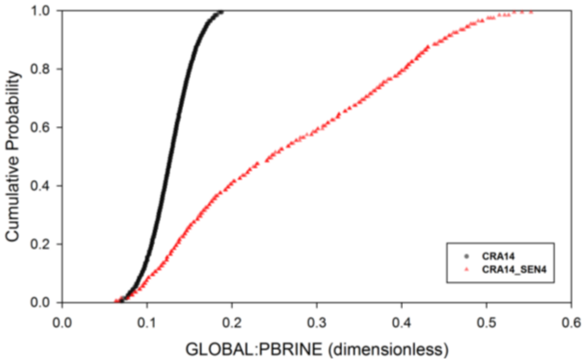


Figure 2-3: Comparison of LHS sampled values of the GLOBAL:PBRINE parameter for CRA14 and CRA14_SEN4 (300 sampled values for each analysis).

2.2.3 Effective Shear Strength for Erosion (BOREHOLE:TAUFAIL)

For the CRA14_SEN4 sensitivity study, the EPA has requested the use of a revised distribution for the BOREHOLE:TAUFAIL parameter. The BOREHOLE:TAUFAIL parameter is a sampled parameter that represents the shear strength of waste. The lower end of the uniform distribution was changed from 2.22 Pa to 1.60 Pa as specified by the EPA (Zeitler 2016a). A comparison of the values sampled in CRA14 and CRA14_SEN4 is shown in Figure 2-4. Because the lower end of the distribution is only slightly lowered for CRA14_SEN4, sampled values are only slightly lower than those used in CRA14.

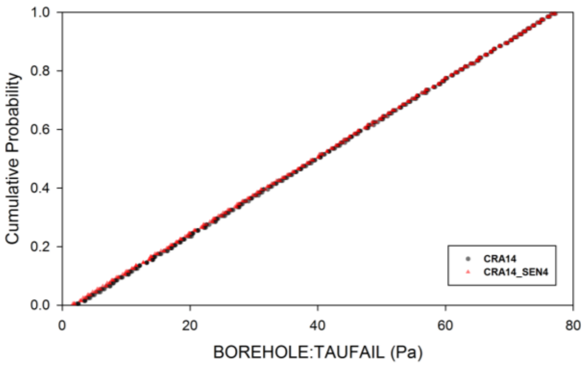


Figure 2-4: Comparison of LHS sampled values of the BOREHOLE:TAUFAIL parameter for CRA14 and CRA14_SEN4 (300 sampled values for each analysis).

2.2.4 Stoichiometric Coefficients for Sulfidation Reactions (REFCON:STCO_31, STCO_32, STCO_35, STCO_36, STCO_43, STCO_46)

As part of the EPA request for the CRA14_SEN4 analysis, the EPA has requested that the chemistry reactions used in BRAGFLO, in which hydrogen sulfide (H_2S) interacts with iron, be eliminated.

Elimination of the sulfidation reactions is accomplished by setting the appropriate stoichiometric coefficients to zero. Reactions 3 and 4 in the chemistry model implemented in the BRAGFLO code include H_2S (WIPP PA 2012). Reaction 3 represents $Fe(OH)_2$ sulfidation and reaction 4 represents metallic Fe sulfidation (see reaction equations below).

$Fe(OH)_2(s) + H_2S(g) \rightarrow FeS(s) + 2\ H_2O(l)$. (BRAGFLO chemical reaction 3)

$Fe(s) + H_2S(g) \rightarrow FeS(s) + H_2(g)$, (BRAGFLO chemical reaction 4)

By removing these two reactions from the BRAGFLO chemistry model, the expected impact on PA calculations is that less hydrogen sulfide gas will be consumed and less water will be produced in the waste areas.

The stoichiometric coefficients for reactions 3 and 4 are represented by parameters REFCON:STCO_3x and REFCON:STCO_4x (where x ranges from 0 to 9 and represents one of ten compounds considered in the BRAGFLO chemical reactions), respectively. Of the twenty stoichiometric coefficients used to define reactions 3 and 4, fourteen had a value of zero in the CRA14. In order to comply with the EPA request for CRA14_SEN4, the following six coefficients were set to zero: STCO_31, STCO_32, STCO_35, STCO_36, STCO_43, and STCO_46 (Zeitler and Day 2016).

2.3 Use of Updated Version of DRSPALL

One of the requests from the EPA for CRA14_SEN4 is that DRSPALL v. 1.22 be used. When DRSPALL v. 1.22 was developed, in order to correct an error found in DRSPALL v. 1.21, a complete set of official DRSPALL calculations (including three replicates of 100 vectors each) was run using a current set of PA parameters as input (Kirchner et al. 2015). Results for DRSPALL v. 1.22 calculations were compared with those from v. 1.21 and documented in an impact assessment report (Kicker et al. 2015). Because PA parameter inputs for the DRSPALL code have not changed since those calculations were performed, and because the DRSPALL code does not rely on the output of any other code for its input, DRSPALL v. 1.22 was not rerun for CRA14_SEN4. Instead, the DRSPALL v. 1.22 output results from the calculations described in the impact assessment were used as input to the CUTTINGS_S code in CRA14_SEN4 calculations.

2.4 Modified Length of Northern Panel Closure

The proposed repository panel closures are modeled in BRAGFLO as three separate panel closure areas. The “northernmost” panel closure area separates the operations area from the “north rest of repository” (NROR) waste area, the “middle” panel closure separates the NROR from the “south rest of repository” (SROR), and the “southernmost” panel closure separates the SROR from the waste panel. The CRA14_SEN4 sensitivity study request (Zeitler 2016a) is consistent with that for the CRA14_SEN3 sensitivity study (Zeitler 2016b) and notes that the northernmost panel closure in the BRAGFLO grid should represent the length of two panel closures, 60.96 m. The CRA14 PA used a length of 30.48 m for the northernmost panel closure. The correction to the BRAGFLO grid has been made here. As part of the EPA completeness determination for CRA-2014, the issue of the length of the northernmost panel closure was broached by the EPA (EPA 2015). A PA calculation was done to examine the impact of doubling the length of the northernmost panel closure and negligible changes to the pressures and saturations in the waste areas were found (Zeitler 2015, DOE 2015).

2.5 Modified BRAGFLO Material Map

The code BRAGFLO is the WIPP PA code used to model brine and gas flow in and around the repository. The current disturbed rock zone (DRZ) above and below the operations and experimental (OPS/EXP) areas is modeled as the same material representing the DRZ above and below the waste areas. For the CRA14_SEN3 sensitivity study, EPA-requested parameter changes for DRZ properties above and below the OPS/EXP areas and the PCS required a change to the BRAGFLO material map in order to implement the requested parameter changes specific to those areas. The BRAGFLO grid and material map that incorporates the requested OPS/EXP area and PCS property changes has been correspondingly modified. This modification to the grid is an extension of that made for the CRA14_SEN2 sensitivity study (Day 2016). The changes in the BRAGFLO grid and material map that were implemented for CRA14_SEN3 have been kept for CRA14_SEN4. The modified grid separates the material in the DRZ, located above and below the OPS/EXP area and the PCS, so that they may be treated separately from the DRZ above and below the waste areas of the repository. The new material regions for the DRZ above and below the OPS/EXP and PCS areas as well as the pre-existing material regions for the PCS and OPS/EXP areas are thus available for any future parameter modifications. Although the BRAGFLO grid changes made here are the same as those made for the CRA14_SEN3 sensitivity study, material property values for those regions are the same as those used for the CRA14 analysis. The modified grid has been kept for flexibility in potential future parameter changes.

3. Results

Results for all release mechanisms are now presented and compared to those obtained in the CRA 2014 PA (CRA14). Results are discussed in terms of overall means. Overall means are obtained by forming the average of all realizations. In WIPP PA, a replicate consists of 100 calculated realizations. Three replicates are used to generate results for CRA14 and CRA14_SEN4. Means and statistics presented for the analyses are also calculated over all three replicates. The impacts of the requested modifications to CRA14 results include changes to all of the primary release mechanisms: cuttings and cavings, spallings, direct brine releases, and releases from the Culebra. Plots of releases for individual release mechanisms include lower and upper 95% confidence intervals on the means, as well as comparisons with results from CRA14. A summary of critical means and lower and upper confidence limits for individual release mechanisms at probabilities of 0.1 and 0.001 is presented in Section 3.5.

3.1 Cuttings and Cavings Releases

Cuttings and cavings releases are minimally increased due to the EPA requested modifications to CRA14 inputs (Figure 3-1). The reduction in the lower bound of the BOREHOLE:TAUFAIL parameter distribution resulted in the sampling of lower values of waste shear strength (Figure 2-4). The use of slightly reduced shear strength values resulted in minimally increased cavings releases for borehole intrusions into the repository that intersect waste.

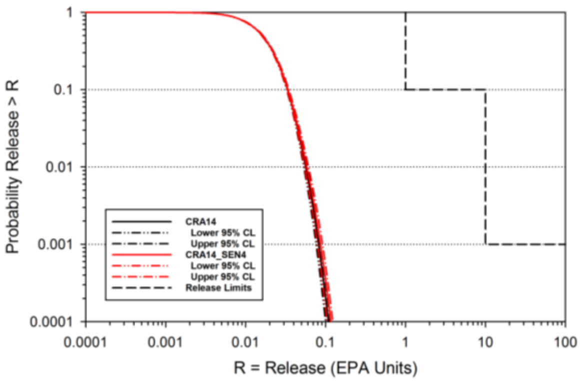


Figure 3-1: Confidence Interval on Overall Mean CCDFs for Cuttings and Cavings Releases: CRA14 and CRA14_SEN4

3.2 Spallings Releases

Spallings releases are a function of repository pressure at the time of intrusion. Increases in pressure necessarily translate to increased spallings release volumes. Changes to the northernmost panel closure length, the chemistry model (i.e., removal of sulfidation), and the GLOBAL:PBRINE parameter all impact repository pressure at the time of intrusion. Changing the northernmost panel closure length has been shown to be minimally impactful on waste panel pressures and saturations and not impactful on releases (DOE 2015).

The impact of removing sulfidation from the chemistry model has not been previously examined, but is shown here to slightly increase pressures and decrease saturations in the waste areas by comparing BRAGFLO results from CRA14, CRA14_SEN4, and the analysis done by DOE (2015). In the waste panel, there is little to no impact of the northernmost panel closure length on pressures and saturations. When the northernmost panel closure length is changed (lengthened) and sulfidation is removed in CRA14_SEN4, waste panel pressures are increased and brine saturations decreased—the increased pressure and decreased brine saturation can therefore be attributed to the removal of sulfidation. Increased pressure and gas volumes in the waste panel are consistent with reduced gas consumption associated with removing sulfidation reactions. Decreased brine saturation and brine volume in the waste panel are consistent with reduced water production associated with removing sulfidation reactions.

The shifting of the GLOBAL:PBRINE parameter distribution to generally higher values for CRA14_SEN4 leads to an increased number of intrusions into pressurized brine below the repository, which typically leads to increased pressure in the waste areas and therefore increased spallings. The impact of changing the GLOBAL:PBRINE distribution has not been examined independently of other changes.

An increase in spallings releases has been shown previously when DRSPALL v. 1.22, which has corrected an error in DRSPALL v. 1.21, is used (Kicker et al. 2015). Overall, spallings releases are increased with the application of all of the EPA requested changes, as compared to CRA14 results (Figure 3-2).

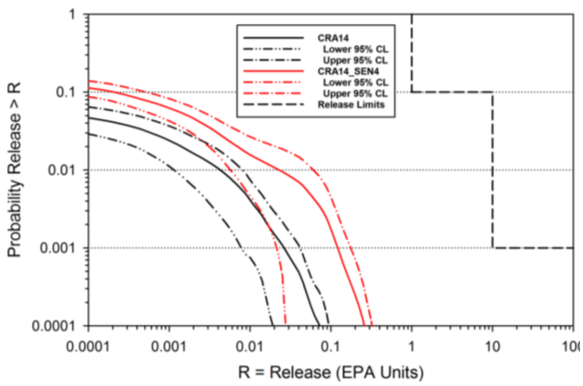


Figure 3-2: Confidence Interval on Overall Mean CCDFs for Spallings Releases: CRA14 and CRA14_SEN4

3.3 Releases from the Culebra

Transport releases through the Culebra and across the land withdrawal boundary are impacted by the amount of brine released to the Culebra, as well as actinide solubilities. Brine flows up the intrusion borehole obtained in CRA14_SEN4 are slightly decreased compared to those obtained in CRA14. Consequently, volumes of brine flowing up to the Culebra are slightly decreased, which is attributed to the modification to the northernmost panel closure and the removal of sulfidation (i.e., the only two changes in CRA14_SEN4 that could potentially impact BRAGFLO results).

Additionally, the change to the GLOBAL:PBRINE distribution leads to increased waste panel pressures following intrusion into pressurized brine below the repository (as discussed above for spallings releases), which tends to increase releases to the Culebra.

The differences in actinide solubilities between CRA14 and CRA14_SEN4 also contribute to releases from the Culebra. In general, increased solubilities lead to increased releases from the Culebra. However, because sampled values of SOLMOD3:SOLVAR have increased and those for SOLMOD4:SOLVAR have decreased, it is possible that the combined impacts of the solubility changes are to increase or decrease releases from the Culebra. The overall impact of the solubility changes on releases from the Culebra is dependent on the relative impacts due to the +III and +IV solubilities. The isolated impact of the solubility uncertainty changes (i.e., apart from all of the other changes made for CRA14_SEN4) has not been investigated. Overall, transport releases through the Culebra and across the land withdrawal boundary are slightly increased compared to results calculated for CRA14 (Figure 3-3). At very low probabilities (P[Release>R] < 0.0003), releases from the Culebra are decreased.

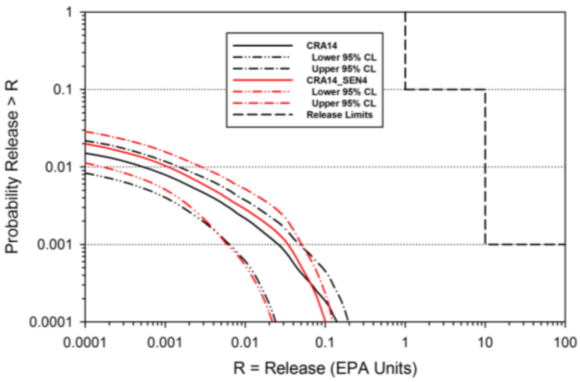


Figure 3-3: Confidence Interval on Overall Mean CCDFs for Releases from the Culebra: CRA14 and CRA14_SEN4

3.4 Direct Brine Releases

Direct brine releases (DBRs) require sufficient waste panel pressure and brine saturation in order to occur. The repository pressure near the drilling location must exceed the hydrostatic pressure of the drilling fluid, which is specified to be 8 MPa in WIPP PA. The brine saturation in the intruded panel must exceed the residual brine saturation of the waste, a sampled parameter in WIPP PA. The changes to the CRA14 analysis that have been implemented for the CRA14_SEN4 sensitivity analysis result in slightly increased waste region pressure and very slightly decreased waste region brine saturation.

The change to the GLOBAL:PBRINE distribution results in increased intrusions into pressurized brine below the repository, which increases pressures and saturations in waste areas—the net result of this change is increased direct brine volumes.

Additionally, the changes to actinide solubilities impact actinide concentrations in DBR releases. In general, increased solubilities lead to increased DBR releases. However, because sampled values of SOLMOD3:SOLVAR have increased and those for SOLMOD4:SOLVAR have decreased, it is possible that the combined impacts of the solubility changes are to increase or decrease DBRs. The overall impact of the solubility changes on DBRs is dependent on the relative impacts due to the +III and +IV solubilities. The isolated impact of the solubility uncertainty changes (i.e., apart from all of the other changes made for CRA14_SEN4) has not been investigated. The net result of all of the changes introduced in CRA14_SEN4 is an increase in DBRs at all probabilities (Figure 3-4).

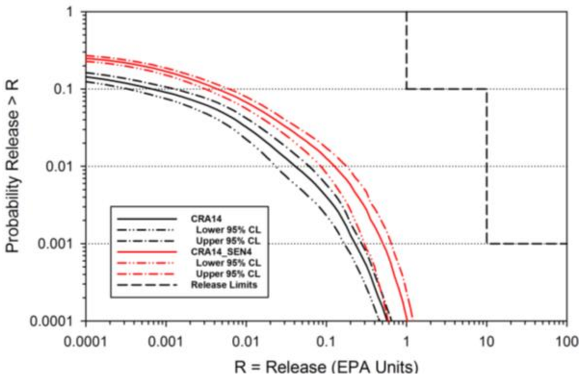


Figure 3-4: Confidence Interval on Overall Mean CCDFs for Direct Brine Releases: CRA14 and CRA14_SEN4

3.5 Total Releases

Total releases are calculated by totaling the releases from each release pathway: cuttings and cavings releases, spallings releases, DBRs, and transport releases (there were no undisturbed releases to contribute to total release). CRA14_SEN4 CCDFs for total releases obtained in replicates 1, 2, and 3 are plotted together in Figure 3-5. The overall mean CCDF is computed as the arithmetic mean of the mean CCDFs from each replicate. A confidence interval is computed about the overall mean CCDF using the Student's t-distribution and the mean CCDFs from each replicate. Figure 3-6 shows 95% confidence intervals about the overall mean for CRA14 and CRA14_SEN4.

Mean CCDFs of the individual release mechanisms that comprise total normalized releases are plotted together in Figure 3-7, as well as the CRA14_SEN4 total release overall mean. As seen in that figure, total normalized releases obtained for CRA14_SEN4 are dominated by cuttings and cavings releases and DBRs. Contributions to total releases from spallings and Culebra transport are not dominant, although spallings and Culebra transport releases have been increased in comparison to CRA14.

Overall means for total normalized releases obtained for CRA14 and CRA14_SEN4 are plotted together in Figure 3-6. Overall, total normalized releases increase from CRA14 to CRA14_SEN4 due to increases in all contributing release components. Total normalized releases increase at low probabilities (below 0.1) from CRA14 to CRA14_SEN4 principally due to increased DBRs. A comparison of the statistics on the overall mean for total normalized releases obtained for CRA14 and CRA14_SEN4 is now made. At a probability of 0.1, values obtained for the mean total release and upper 95% confidence interval for CRA14_SEN4 are increased in comparison to CRA14 (15 and 18%, respectively). At a probability of 0.001, the mean total release and upper 95% confidence level are higher for CRA14_SEN4 in comparison to CRA14 (107 and 119%, respectively).

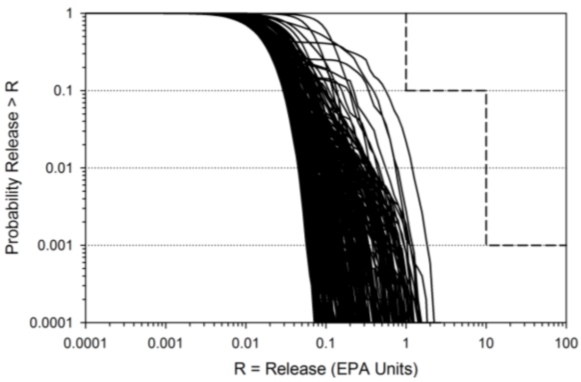


Figure 3-5: Total Normalized Releases, Replicates R1, R2, and R3, CRA14_SEN4

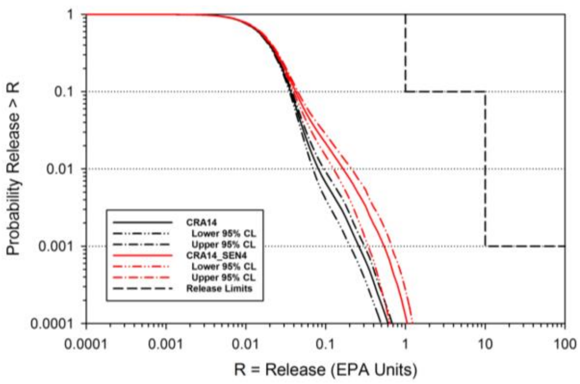


Figure 3-6: Confidence Interval on Overall Mean CCDFs for Total Normalized Releases: CRA14 and CRA14_SEN4

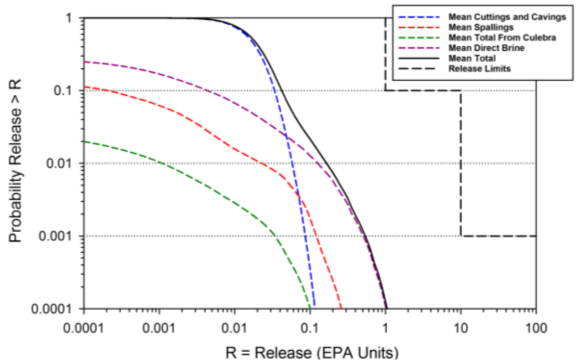


Figure 3-7: Comparison of Overall Means for Release Components of CRA14_SEN4

4. Summary

The application of EPA-requested modified parameters has been incorporated into a sensitivity analysis (CRA14_SEN4) and compared to the most recent PA done in support of WIPP recertification (CRA14). A minimal increase in cuttings and cavings releases was found due to a change to the BOREHOLE:TAUFAIL parameter distribution. Spallings releases were increased as a result of a combination of changes to the northernmost panel closure length and GLOBAL:PBRINE parameter distribution, as well as a correction to the DRSPALL code and removal of sulfidation from the chemistry model. Total releases from the Culebra were increased as a result of a combination of changes to the northernmost panel closure length, actinide solubility uncertainties, and GLOBAL:PBRINE parameter distribution, as well as removal of sulfidation from the chemistry model. Direct brine releases were increased as a result of a combination of changes to the GLOBAL:PBRINE and actinide solubility uncertainties. Overall, total high-probability (P[Release>R] = 0.1) predicted mean releases from the repository were increased by about 15%, which corresponds to a 0.6% reduction in the margin to the limit of 1. Total low-probability (P[Release>R] = 0.001) predicted mean releases were increased by about 107%, which corresponds to a 2.9% reduction in the margin to the limit of 10. The upper 95% confidence level on the mean increased for high-probability and low-probability releases by 18 and 119%, respectively. It is concluded that the EPA-requested changes to the CRA14 result in increases to the predicted total releases from the repository, but with those increased releases, the CRA14_SEN4 analysis continues to demonstrate that WIPP complies with the regulatory limits.

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