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Waste Isolation Pilot Plant

CCDFGF Analysis Package for the AP-161 (PCS-2012) Performance Assessment

Revision 0

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WIPP:1.4.1.2:PA:QA-L:557393

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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.

Waste panel closures comprise a repository feature that has been represented in WIPP PA since the original Compliance Certification Application (CCA) of 1996. Panel closures are included in WIPP PA models principally because they are a part of the disposal system, not because they play a substantive role in inhibiting the release of radionuclides to the outside environment. The DOE stated in the CCA (DOE 1996) that *"The panel closure system was not designed or intended to support long-term repository performance."* The 1998 rulemaking that certified WIPP to receive transuranic waste placed conditions on the panel closure design to be implemented in the repository. The mandated design consists of a concrete block wall, an open drift section, and a concrete monolith, and was termed the "Option D" panel closure. Following the selection of the Option D design in 1998, the engineering of the panel closure has been re-assessed, and a revised design has been established that is simpler, cheaper, and easier to construct. The revised panel closure design, termed the Run-of-Mine Panel Closure System (ROMPCS), is comprised of 100 feet of ROM salt with barriers at each end. The ROM salt is generated from ongoing mining operations at the WIPP and may be compacted and/or moistened as it is emplaced in a panel entry. The barriers consist of ventilation bulkheads, similar to those currently used in the panels as room closures.

The DOE has submitted a planned change request (PCR) to the EPA requesting that EPA modify Condition 1 of the Final Certification Rulemaking for 40 CFR Part 194 (EPA, 1998) for the WIPP. The PCR submitted to EPA requests that Condition 1 be changed, and that the ROMPCS design be approved for use in all panels (DOE, 2011). In support of this rulemaking change, a performance assessment has been completed that incorporates the ROMPCS design into the current PA baseline established by the 2009 Performance Assessment Baseline Calculation (PABC-2009) (Clayton et al., 2010). The name given to this new panel closure PA is PCS-2012, and the plan for its execution is detailed in AP-161 (Camphouse 2012a). PCS-2012 PA results are compared to those obtained in the PABC-2009 as a means to quantify potential impacts due

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to the panel closure redesign. This analysis package consists of the CCDFGF component of the PCS-2012 PA.

2 METHODOLOGY

The performance assessment methodology accommodates both aleatory (i.e. stochastic) and epistemic (i.e. subjective) uncertainty in its constituent models. Aleatory uncertainty pertains to unknowable future events such as intrusion times and locations that may affect repository performance. It is accounted for by the generation of random sequences of future events. Epistemic uncertainty concerns parameter values that are assumed to be constants and the constants' true values are uncertain due to a lack of knowledge about the system. An example of a parameter with epistemic uncertainty is the permeability of a material. Epistemic uncertainty is accounted for by sampling of parameter values from assigned distributions. One set of sampled values required to run a WIPP PA calculation is termed a vector. The performance assessment models are executed for three replicates of 100 vectors, each vector being a realization resulting from a particular set of parameter values. A sample size of 10,000 possible sequences of future events is used in the calculations to estimate an exceedance probability of 0.001 (Helton et al. 1998). The releases for each of 10,000 possible sequences of future events are tabulated for each of the 300 vectors, totaling 3,000,000 possible sequences.

For a random variable, the complementary cumulative distribution function (CCDF) provides the probability of the variable being greater than a particular value. By regulation, performance assessment results are presented as a distribution of CCDFs of releases (U.S. EPA 1996). Each individual CCDF summarizes the likelihood of releases across all futures for one vector of parameter values. The uncertainty in parameter values results in a distribution of CCDFs.

Releases are quantified in terms of "EPA units". Releases in EPA units result from a normalization by radionuclide and the total inventory. For each radionuclide, the ratio of its 10,000 year cumulative release (in curies) to its release limit is calculated. The sum of these ratios is calculated across the set of radionuclides and normalized by the transuranic inventory (in curies) of α-emitters with half-lives greater than 20 years. Mathematically, the formula used to calculate releases in terms of EPA units is of the form

$$R = \frac{1 \times 10^6\, curies}{C} \sum_i \frac{Q_i}{L_i}$$

where R is the normalized release in EPA units. Quantity Q_i is the 10,000 year cumulative release (in curies) of radionuclide i. Quantity L_i is the release limit for radionuclide i, and C is the total transuranic inventory (in curies) of α-emitters with half-lives greater than 20 years.

Mean and quantile CCDFs are calculated to compare the distributions of CCDFs among replicates and to demonstrate sufficiency of sample size. At each value of normalized release R on the horizontal axis, the CCDFs for a single replicate define 100 values of probability. Forming the arithmetic mean of these 100 probabilities yields the mean probability that the release exceeds R. The curve defined by the mean probabilities for each value of R is the mean

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CCDF. The 10th and 90th quantile CCDFs for a particular replicate are determined from the sorted order of the 100 CCDFs found for that replicate.

The overall mean CCDF is computed as the arithmetic mean of the three mean CCDFs from each replicate. Confidence limits are computed about the overall mean CCDF using the Student's t-distribution, the mean CCDFs from each replicate, and the standard error based on the three replicate means. Confidence limits as they are implemented in PA are defined vertically about the mean, rather than horizontally. An artifact of this convention is that lower confidence limits can sometimes assume negative values, which cannot be plotted on a logarithmic scale. When this occurs, the resulting lower confidence curve appears incomplete.

CCDF curves and statistics are generated using the CCDFGF_Analysis database utility. A description of this utility can be found in Kirchner (2010). A DVD containing the data loaded into this utility resulting from PCS-2012 PA and PABC-2009 CCDFGF calculations, and subsequent SigmaPlot plots, are included as an attachment to this document.

2.1 Code Version

PRECCDFGF version 1.01 and CCDFGF version 5.02 were used for the PABC-2009 and the PCS-2012.

2.2 Random Seed in the CCDFGF Control Files

One of the features that the CCDFGF control file initializes is the random number generator in the code. Setting the random number seed in the control file determines the sequence of pseudo-random numbers used by CCDFGF. This sequence of numbers affects several stochastic parameters, such as the drilling location, depth, and type of plugging pattern, utilized when CCDFGF simulates the drilling of boreholes at the surface of the WIPP repository.

For the PCS-2012 PA, the same random seeds for CCDFGF were used as in the PABC-2009. This was done to allow a vector by vector comparison of the results of the PCS-2012 PA to those obtained in the PABC-2009. As the random seeds used to initialize the sampling of the epistemic parameters were unchanged in the PCS-2012 PA and the PABC-2009, any differences between the analyses can be attributed solely to the changes in parameters and geometry used in those calculations. Random seeds used in the PCS-2012 PA calculations are specified in the files CCGF_AP161_CONTROL_Rr.inp, where r = 1, 2, 3. These files are located in CMS library LIBAP161_CCGF.

2.3 Run Control

Run control, including code versions used and descriptions of code sequencing used to obtain CCDFGF results in the PCS-2012 PA, is documented in Camphouse et al. (2012c). PCS-2012 PA results generated by code CCDFGF have file names CCGF_AP161_Rr.OUT, where r (the replicate number) equals 1, 2, or 3. These files are located in CMS library LIBAP161_CCGF under class AP161-0. PABC-2009 results generated by CCDFGF have file names

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CCGF_PABC09_Rr.OUT, and are located in CMS library LIBPABC09_CCGF under class PABC09-0.

3 ANALYSIS AND RESULTS

Results obtained from PCS-2012 PA calculations are broken out in subsections for each component of release. At the conclusion of the subsection for each release component, results obtained for the PCS-2012 PA are compared to those found in the PABC-2009. Normalized releases for cuttings and cavings are discussed in Subsection 3.1. Spallings releases are presented in Subsection 3.2. Results found for direct brine releases are discussed in Subsection 3.3. New calculations for normalized transport releases through the Culebra were not performed as part of the PCS-2012 PA. BRAGFLO scenario S6-BF is used by PA code PANEL to determine the radionuclide source term to the Culebra. BRAGFLO scenario S6-BF results obtained in the PCS-2012 PA are virtually identical to those calculated in the PABC-2009 (Camphouse 2012b). Consequently, the radionuclide source term to the Culebra is unaffected by the change of the panel closure design from Option D to the ROMPCS. There have been no updates to the Culebra flow model, e.g. updated transmissivity fields, since the completion of the PABC-2009. As a result, it is reasonable and appropriate to incorporate Culebra transport results calculated in the PABC-2009 into the PCS-2012 PA.

Total normalized releases are shown in Subsection 3.5.

3.1 Cuttings and Cavings Normalized Releases

The change in panel closure design from Option D to the ROMPCS has no impact on cuttings and cavings releases. PA code CUTTINGS_S calculates cuttings and cavings release volumes, as well as spallings volumes. Spallings release volumes are potentially impacted by the panel closure redesign, and so are calculated as part of the PCS-2012 PA. As a result, cuttings and cavings releases are also calculated, even though they are identical to those obtained in the PABC-2009.

PCS-2012 PA cuttings and cavings releases are presented in this section and subsequently compared to results obtained in the PABC-2009. Figure 3-1, Figure 3-2, and Figure 3-3 contain PCS-2012 PA cuttings and cavings release CCDFs for replicates 1, 2, and 3, respectively. Mean and quantile CCDF distributions for the three replicates are shown together in Figure 3-4. As seen in that figure, the mean and quantile CCDFs obtained for the three replicates are nearly coincident. Figure 3-5 contains the 95 percent confidence limits about the overall cuttings and cavings mean. As is clear in that figure, the confidence limit is very tightly contained about the mean at all probabilities.

For the sake of reference, overall means of cuttings and cavings releases calculated in the PCS-2012 PA and the PABC-2009 are plotted simultaneously in Figure 3-6 and Figure 3-7. As seen in those figures, cuttings and cavings releases and volumes obtained for both analyses were identical as no changes were made to the underlying models or parameters used in their calculation for the PCS-2012 PA (Kicker 2012).

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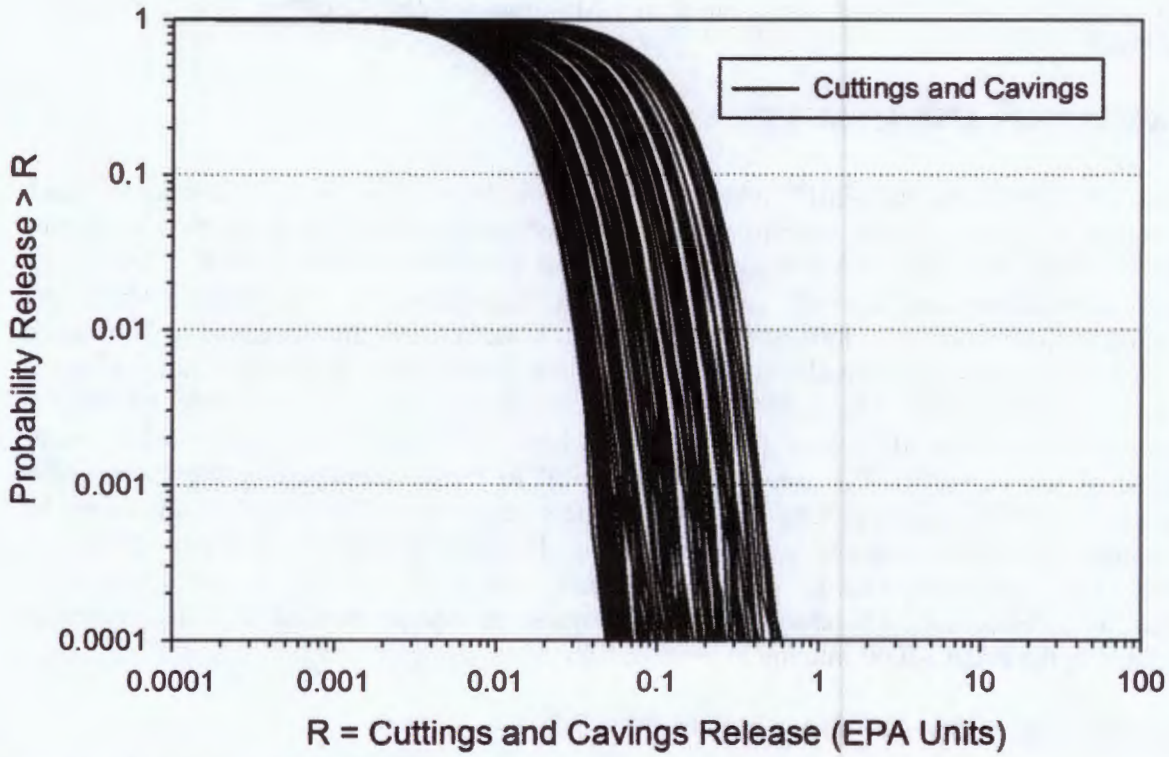

Figure 3-1: PCS-2012 PA Replicate 1 Cuttings and Cavings Normalized Releases

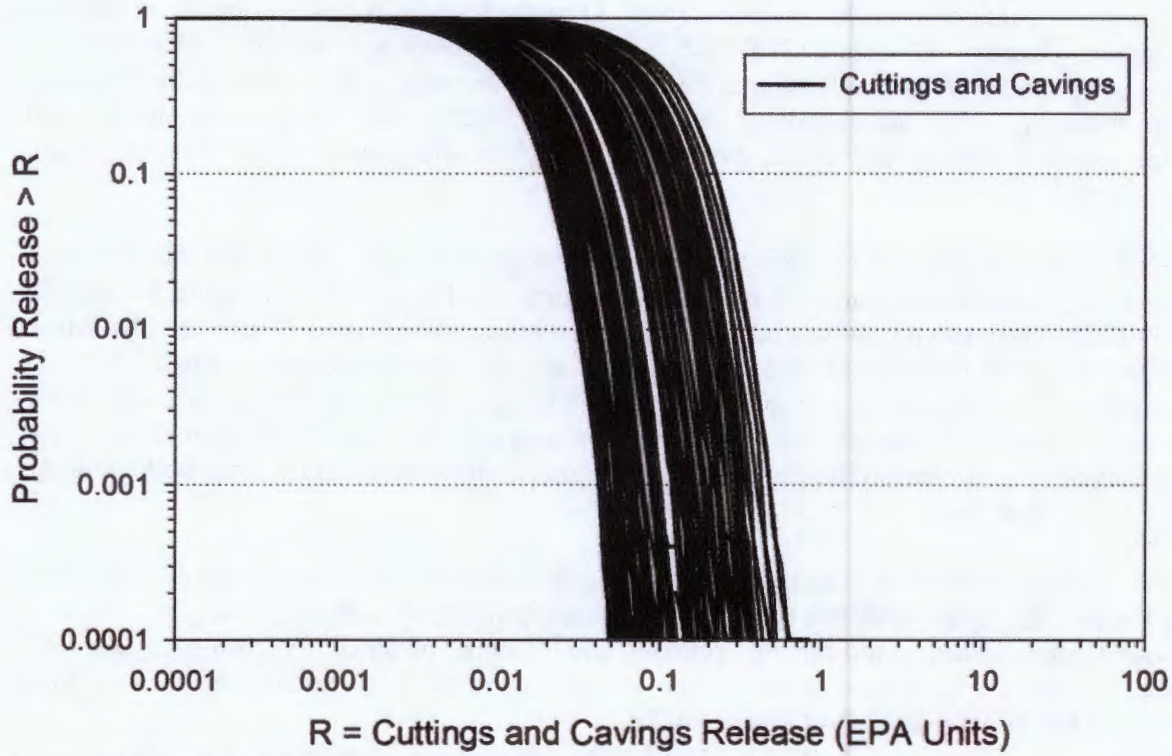

Figure 3-2: PCS-2012 PA Replicate 2 Cuttings and Cavings Normalized Releases

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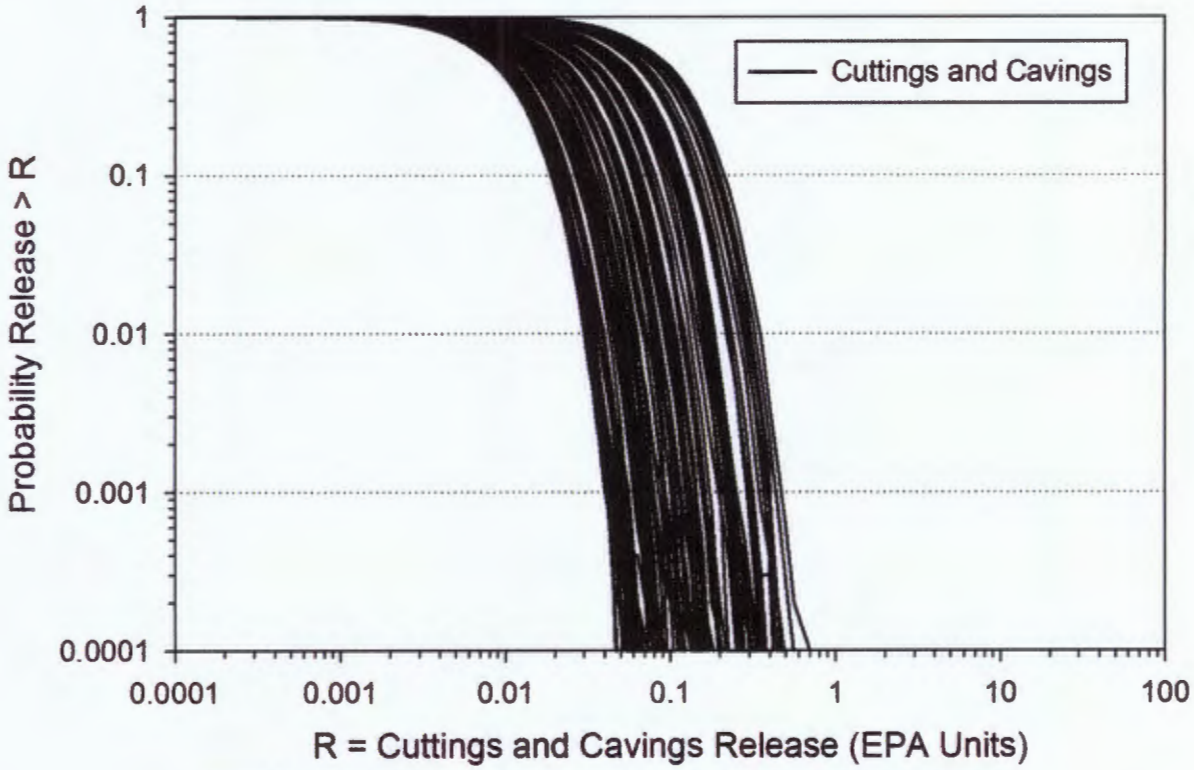

Figure 3-3: PCS-2012 PA Replicate 3 Cuttings and Cavings Normalized Releases

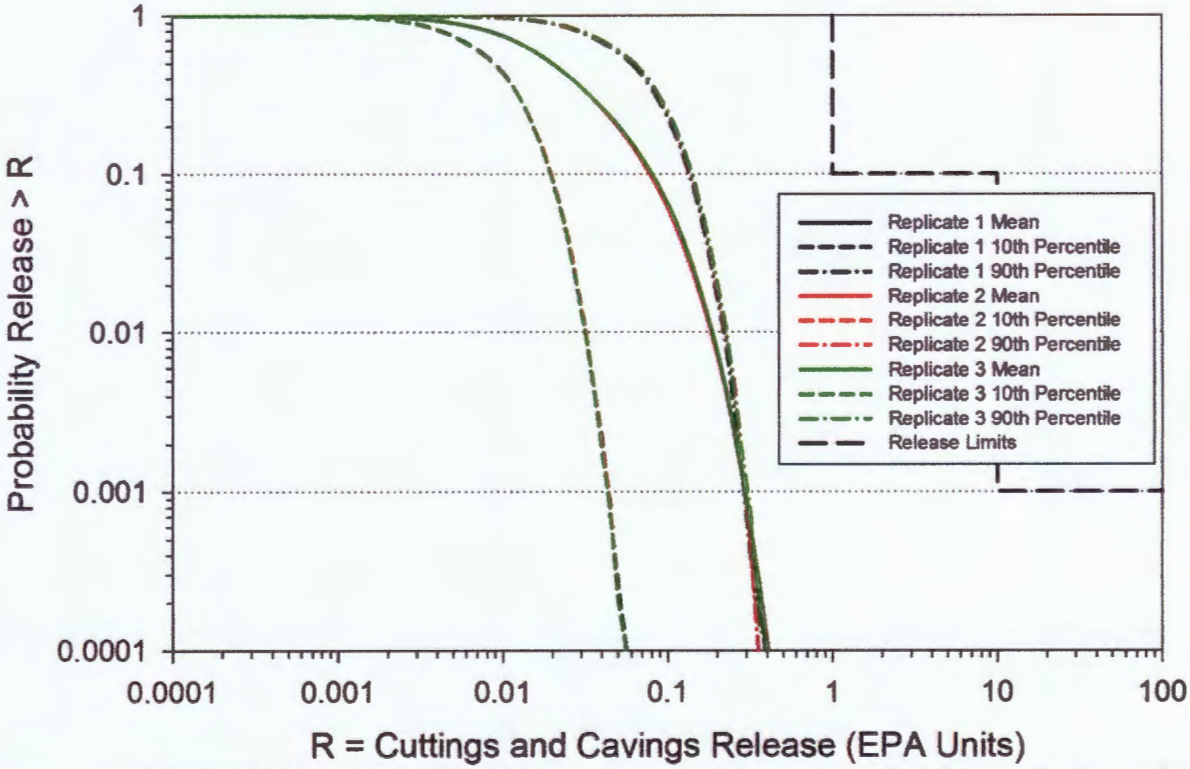

Figure 3-4: PCS-2012 PA Mean and Quantile CCDFs for Cuttings and Cavings Normalized Releases, Replicates 1-3

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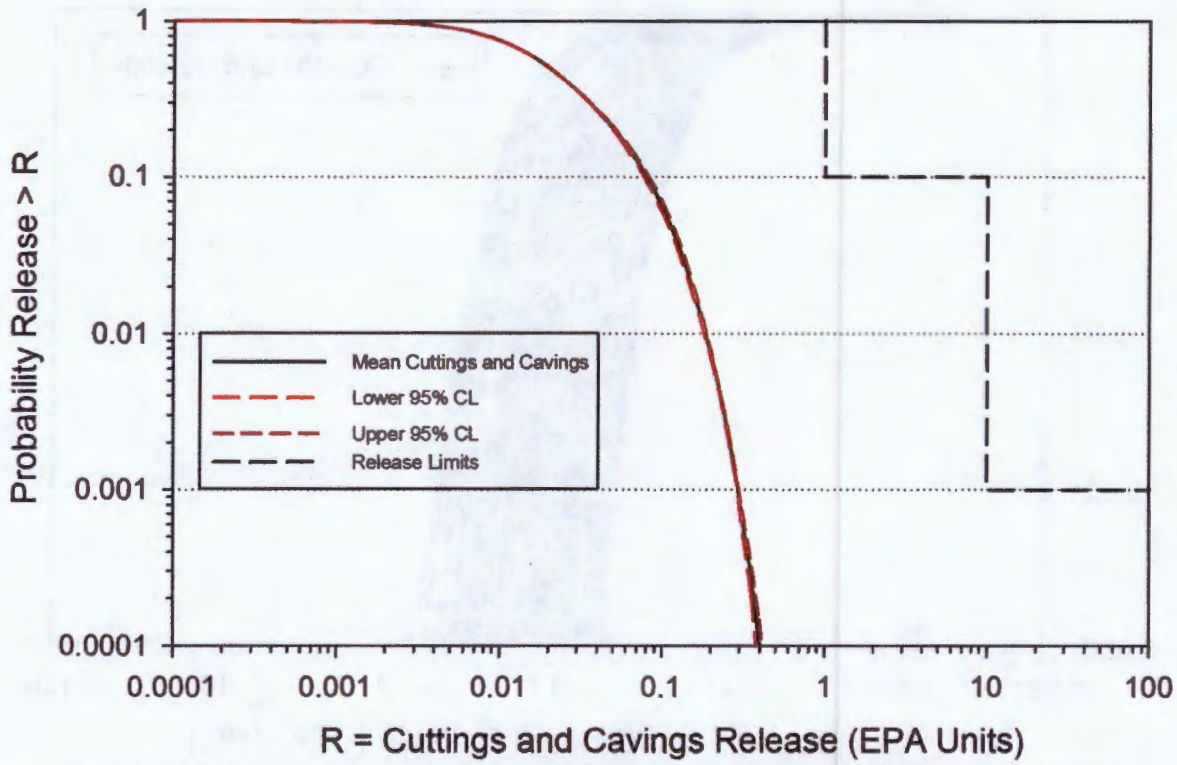

Figure 3-5: PCS-2012 PA Confidence Limits on Overall Mean for Cuttings and Cavings Normalized Releases

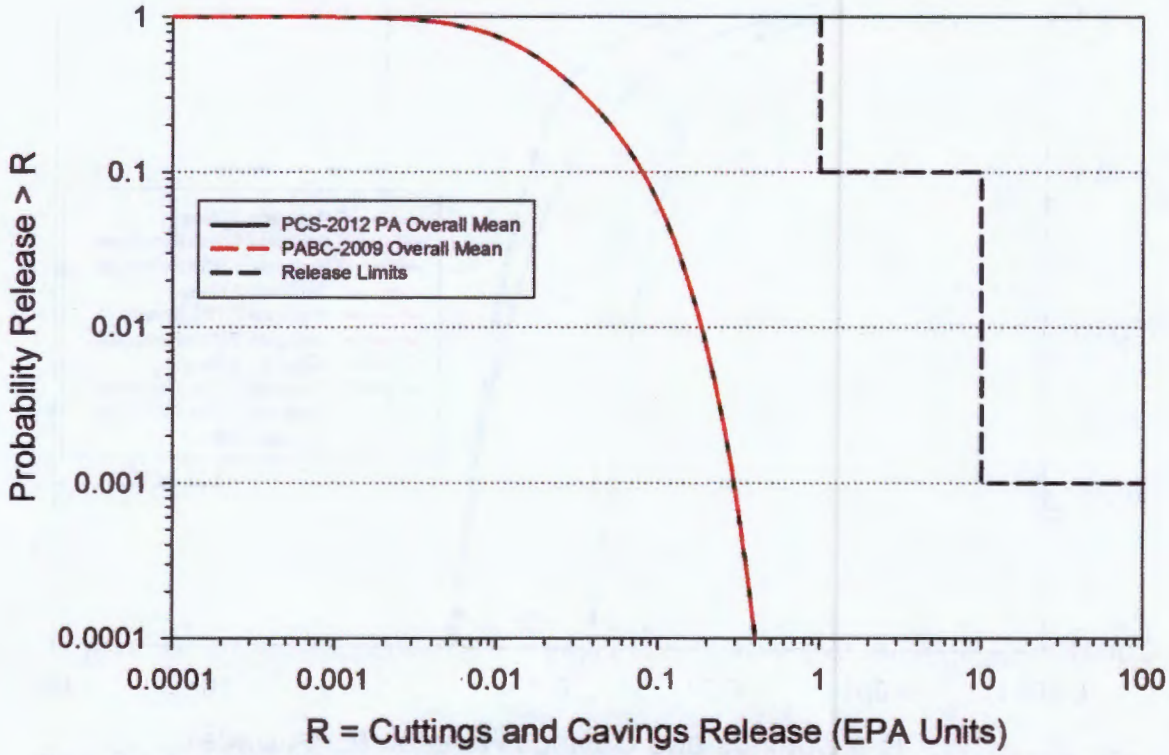

Figure 3-6: PCS-2012 PA and PABC-2009 Overall Mean CCDFs for Normalized Cuttings and Cavings Releases

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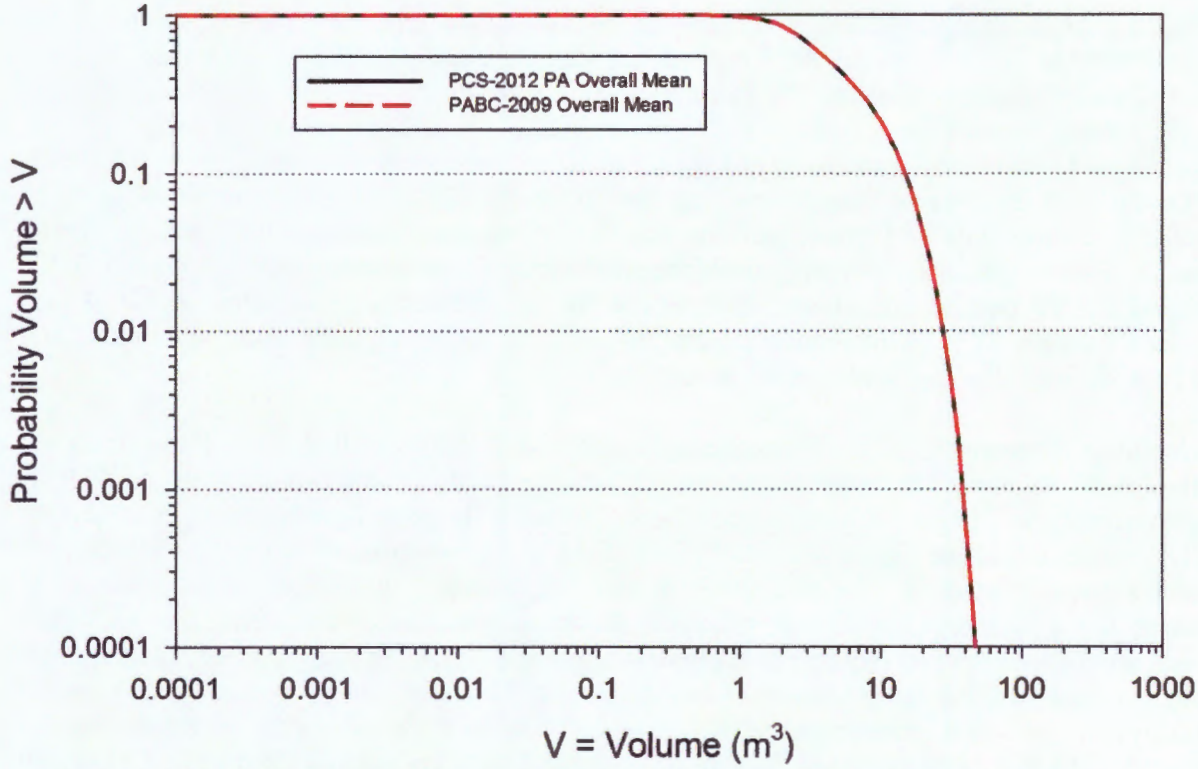

Figure 3-7: PCS-2012 PA and PABC-2009 Overall Mean CCDFs for Normalized Cuttings and Cavings Volumes

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3.2 Spallings Normalized Releases

PCS-2012 PA spallings releases are presented in this section and subsequently compared to results obtained in the PABC-2009. Figure 3-8, Figure 3-9, and Figure 3-10 contain PCS-2012 PA CCDFs for spallings releases. Mean and quantile CCDF distributions for the three replicates are shown together in Figure 3-11. As seen in that figure, the 10th percentiles for each replicate have releases sufficiently small as to not appear at all on the chosen axes. Moreover, the mean CCDF for each replicate becomes larger than the 90th percentile as releases increase. The large number of vectors with very small spallings releases causes the distribution to be heavily right-skewed. This results in a mean that exceeds the 90th percentile as releases increase. Figure 3-12 contains the 95 percent confidence limits about the spallings mean. In total, 38 % of the replicate 1 vector, 47 % of the replicate 2 vectors and 41 % of the replicate 3 vectors in the PCS-2012 PA showed non-zero spallings releases

To facilitate comparisons of spallings releases calculated in the PCS-2012 PA to those obtained in the PABC-2009, overall mean and volume CCDFs obtained in these two analyses are plotted simultaneously in Figure 3-13 and Figure 3-14. As seen in those figures, the PCS-2012 PA CCDF curves shown in Figure 3-13 and Figure 3-14 show increases in spallings releases and volumes when compared to PABC-2009 results. Spallings volumes, and their associated releases, are a function of repository pressure. A pressure increase in an intruded waste panel typically corresponds to an increase in spallings volumes. As nothing was changed regarding the waste inventory used in the PABC-2009 and the PCS-2012 PA, an increase in spallings volume results in an associated increase in spallings releases. The ROMPCS design implemented in the PCS-2012 PA has slightly lower long-term permeabilities (on average) than the Option D closures implemented in the PABC-2009. For intrusion scenarios that involve an encounter with a pressurized brine region below the repository, the reduction in closure permeability resulted in an increase in pressurization of the waste panel for a period of time following the intrusion. This increase in pressure translates directly to increases in PCS-2012 PA spallings volumes and releases as compared to the PABC-2009 results. For intrusion scenarios that do not involve an encounter with a region of pressurized brine below the repository, the mean average pressure in the intruded waste panel was higher in the PCS-2012 PA as compared to the PABC-2009. This increase in pressure also yields increases in spallings volumes and their associated releases. Increased pressure in repository waste areas is responsible for the increases seen in PCS-2012 PA spallings volumes and releases as compared to the PABC-2009 results (Kicker 2012).

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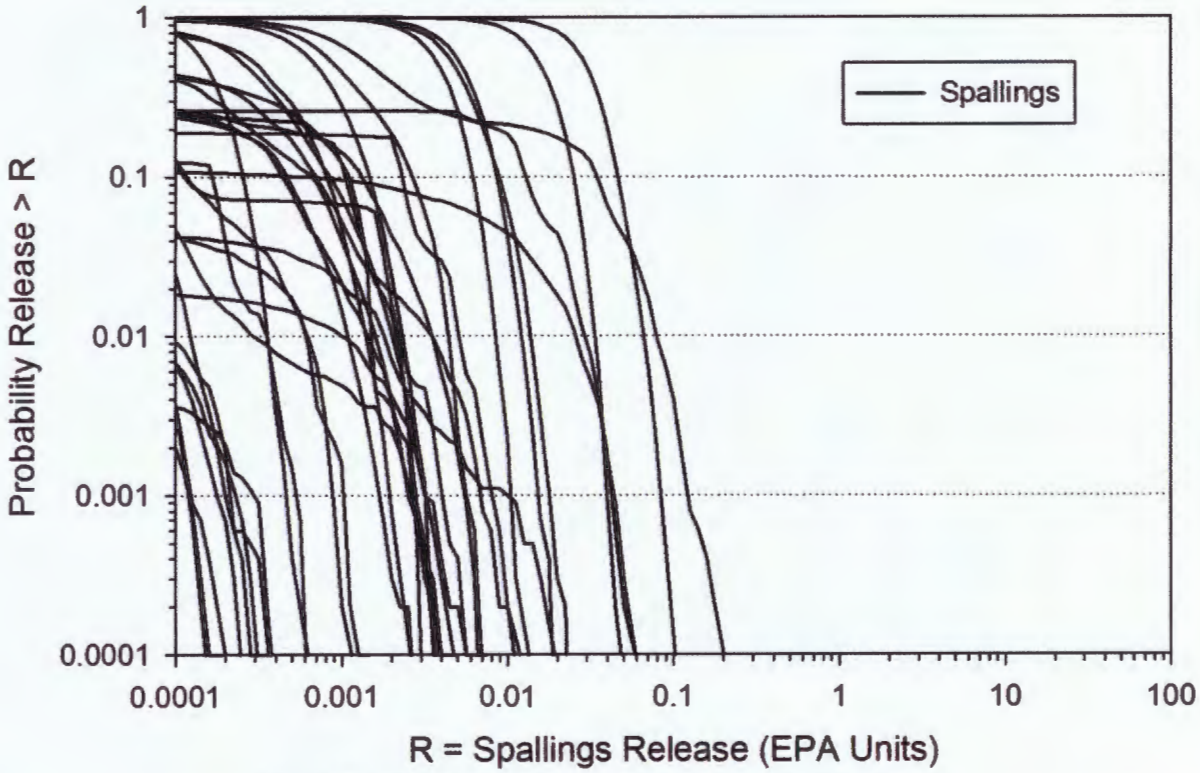

Figure 3-8: PCS-2012 PA Replicate 1 Spallings Normalized Releases

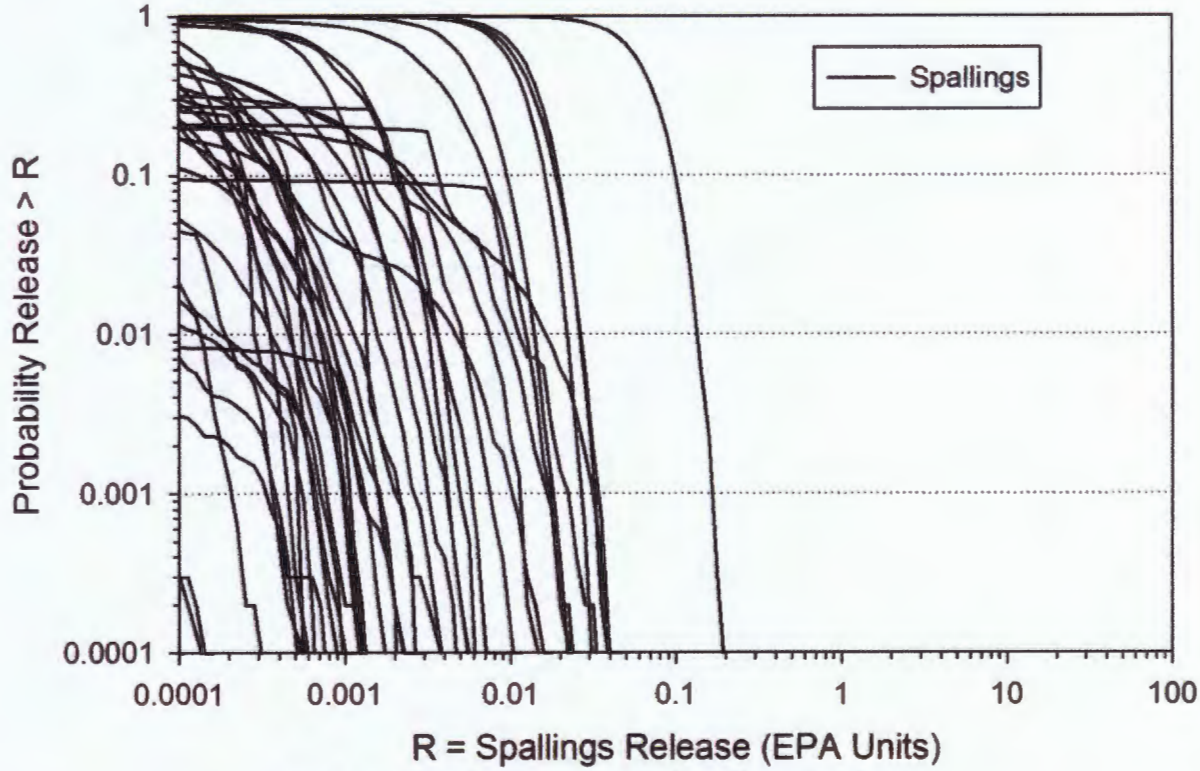

Figure 3-9: PCS-2012 PA Replicate 2 Spallings Normalized Releases

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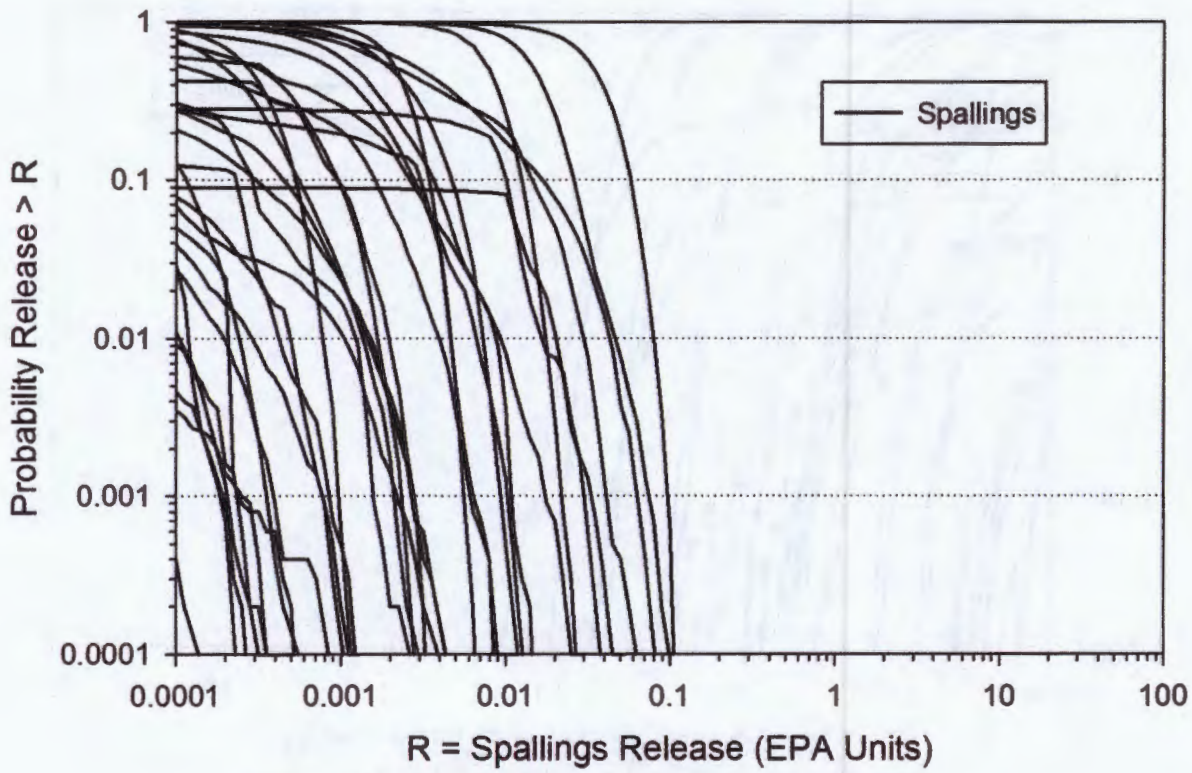

Figure 3-10: PCS-2012 PA Replicate 3 Spallings Normalized Releases

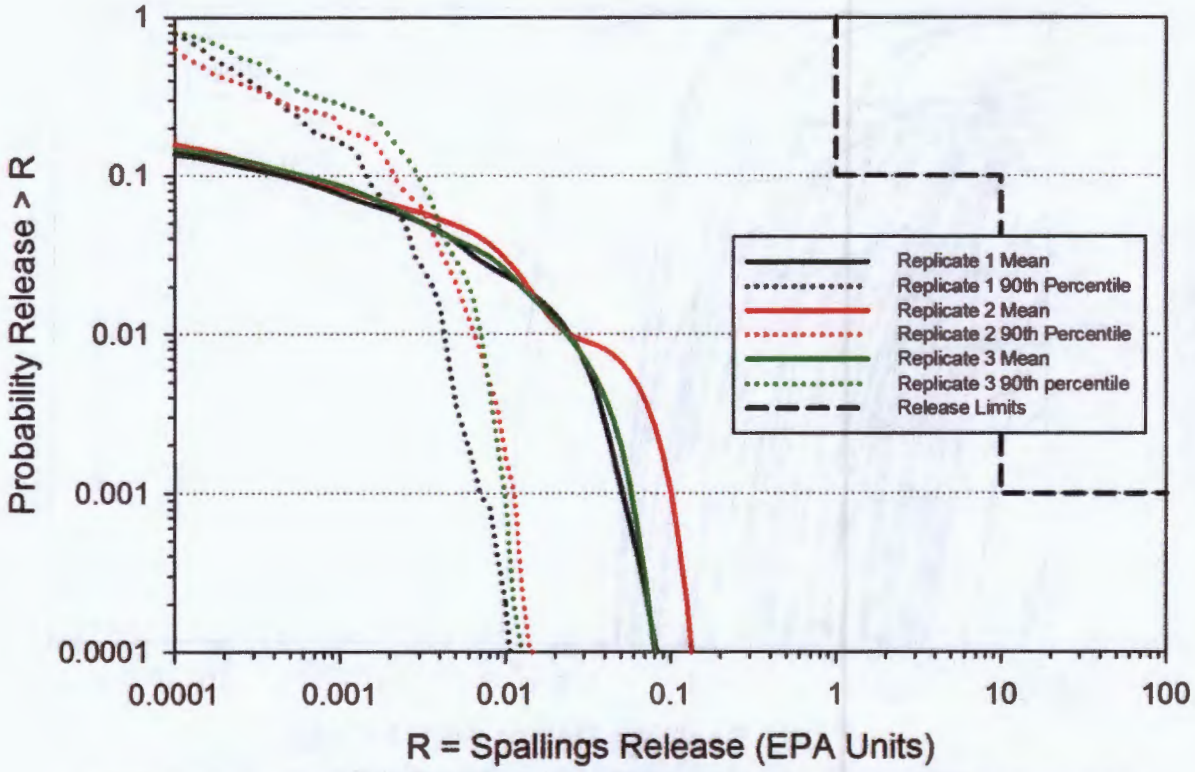

Figure 3-11: PCS-2012 PA Mean and Quantile CCDFs for Spallings Normalized Releases, Replicates 1-3

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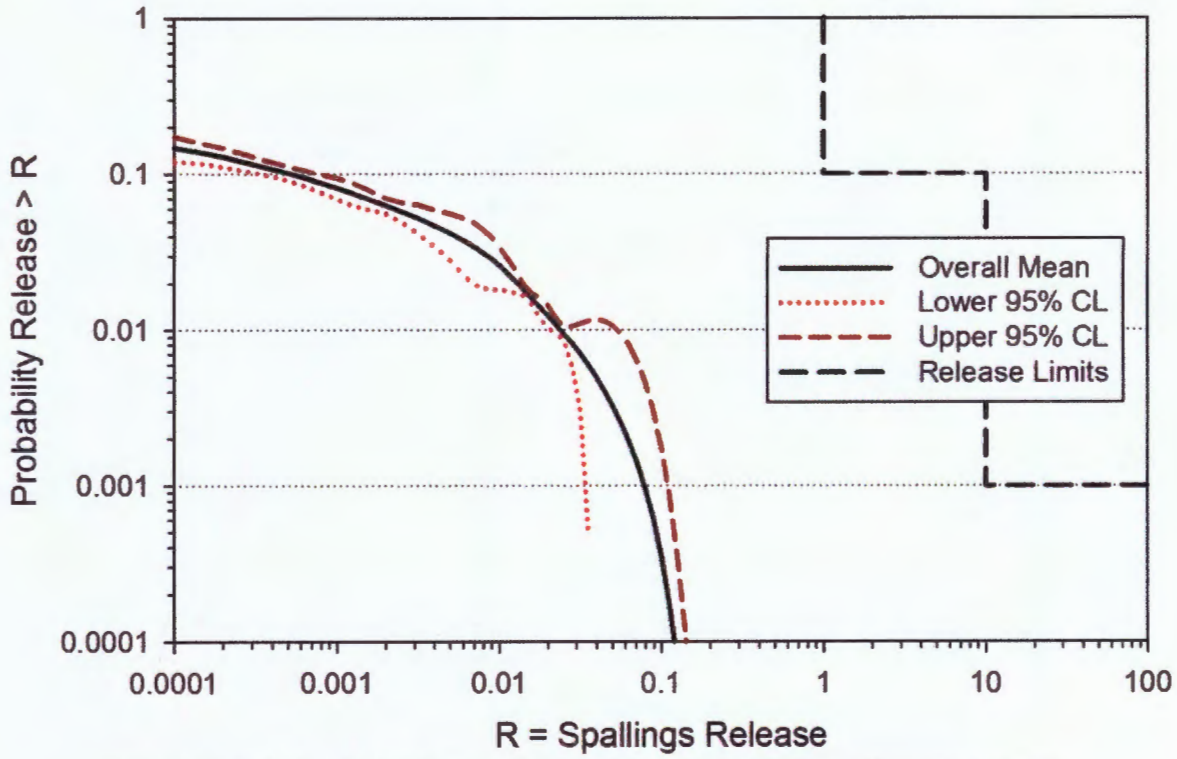

Figure 3-12: PCS-2012 PA Confidence Limits on Overall Mean for Spallings Normalized Releases

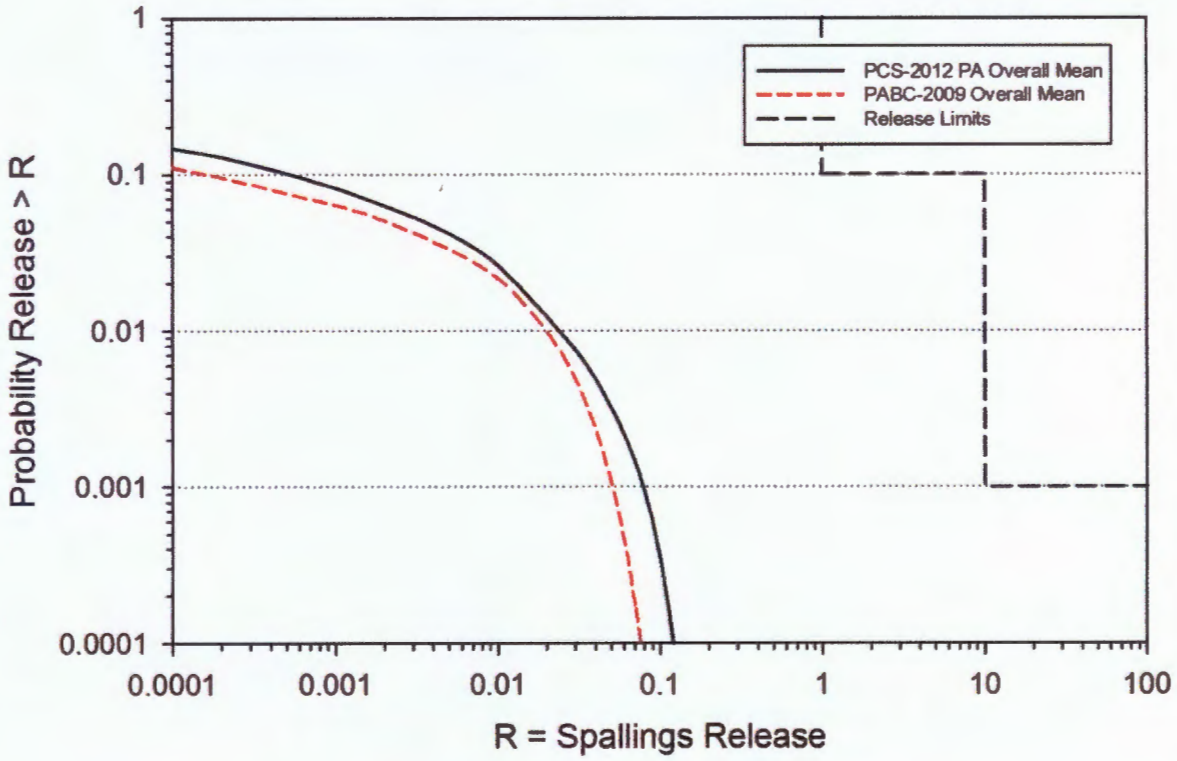

Figure 3-13: PCS-2012 PA and PABC-2009 Overall Mean CCDFs for Normalized Spallings Releases

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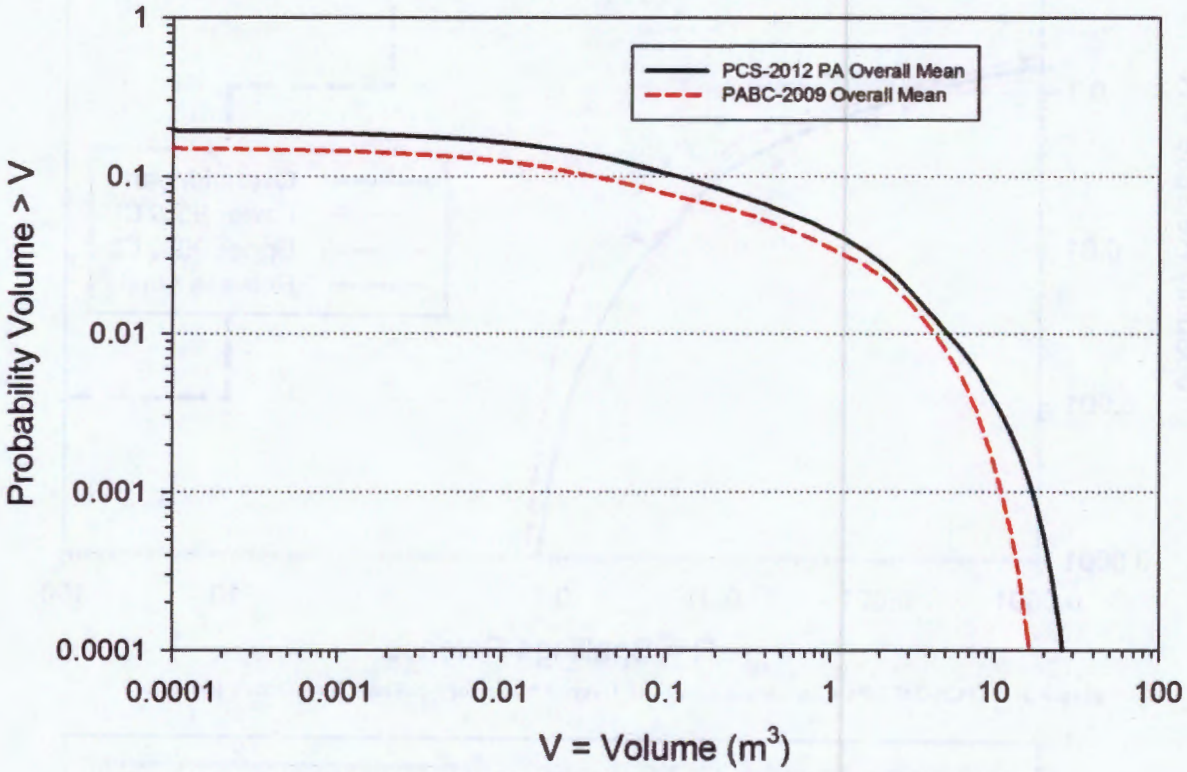

Figure 3-14: PCS-2012 PA and PABC-2009 Overall Mean CCDFs for Spallings Volumes

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3.3 Normalized Direct Brine Releases

PCS-2012 PA normalized direct brine releases are presented in this section and subsequently compared to results obtained in the PABC-2009. Figure 3-15, Figure 3-16, and Figure 3-17 contain PCS-2012 PA CCDFs for DBRs. Mean and quantile CCDF distributions for the three replicates are shown together in Figure 3-18. Figure 3-19 contains the 95 percent confidence limits about the DBR overall mean. As seen in Figure 3-19, the overall mean and its lower/upper 95% confidence limits are well below acceptable release limits.

To facilitate comparisons of DBRs calculated in the PCS-2012 PA to those obtained in the PABC-2009, overall mean and volume CCDFs obtained in these two analyses are plotted together in Figure 3-20 and Figure 3-21. As seen in Figure 3-20, the CCDF curve obtained for direct brine releases shows greater mean probabilities in the PCS-2012 PA for the majority of release values.

In the PCS-2012 PA, intrusion scenarios that involve drilling into a pressurized brine region underneath the repository exhibited an increase in the average pressure in the intruded waste panel when compared to the PABC-2009 results for a period of time following the intrusion (Malama 2012). Additionally, an increase in mean waste panel brine saturation was found for this type of intrusion (Malama 2012). The combination of an increase in waste panel pressure and brine saturation leads to an increase in DBR volumes, as well as a greater number of non-zero brine volume vectors for PCS-2012 PA compared to PABC-2009 (Camphouse 2012b). For intrusion scenarios that do not involve drilling into a pressurized brine region underneath the repository, there is an increase in mean waste panel pressure accompanied by a small decrease in brine saturation for the PCS-2012 PA compared to the PABC-2009 (Malama 2012). This results in an increase in maximum DBR volume for the PCS-2012 PA. This increase in pressure of the intruded panel as compared to the PABC-2009 impacted the number of DBR realizations used to calculate the DBR release tables (Malama 2012). The total number of nonzero DBR volumes increased from 2,999 in the PABC-2009 to 3,182 in the PCS-2012 PA, an increase of 183 realizations with a nonzero DBR volume (Malama 2012). For undisturbed conditions, the long-term mean waste panel pressure and brine pressure also increased from the PABC-2009 to the PCS-2012 PA. The is due to the implementation of the ROMPCS design, which allows greater brine flow into the waste panel than the Option D design, resulting in greater gas generation and thus mean waste panel pressure (Camphouse 2012b).

However, despite the greater number of nonzero DBR volumes found in the DBR analysis (Malama 2012), the number of nonzero DBR release vectors found in the CCDFGF analysis remains the same from the PABC-2009 to the PCS-2012 PA. The increase in mean DBR releases is due to increased releases in only a few vectors, and is not attributed to an overall increase in releases for a majority of vectors (Kirchner 2012). Additional evidence of the influence of a few vectors on the DBR volumes is found in Figures 5-1 to 5-10 of the PCS-2012 PA DBR report (Malama 2012), which show that the DBR volume distribution skews toward higher volumes only for the high end of the distribution. The final result is an increase in mean probabilities for the PCS-2012 PA compared to the PABC-2009 for the majority of DBR release values.

The overall mean CCDF curves for direct brine volumes obtained in the PCS-2012 PA and the PABC-2009 are shown together in Figure 3-21. For probabilities less than about 0.1, the mean

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DBR volume increased, most likely due to the increase in waste panel pressure observed in the Salado flow modeling results as compared to the PABC-2009. The increase in the number of realizations with a nonzero DBR volume combined with the increase in the maximum DBR volumes found in the Salado flow modeling results (Camphouse 2012b) explain the differences observed in the CCDF DBR volume curves obtained in the PABC-2009 and the PCS-2012 PA.

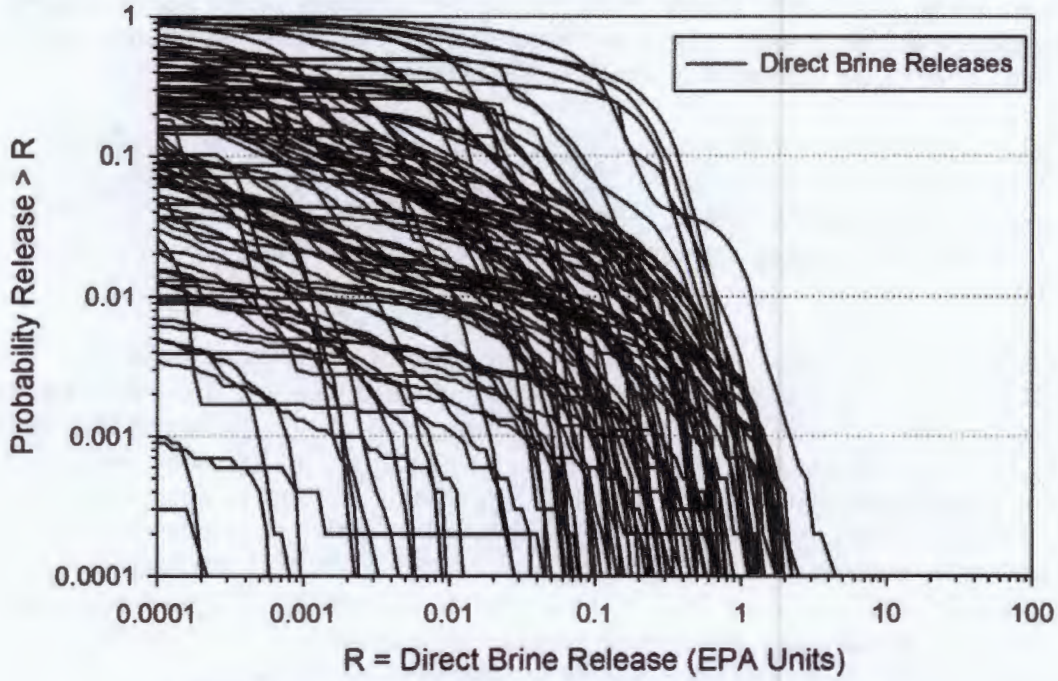

Figure 3-15: PCS-2012 PA Replicate 1 Normalized Direct Brine Releases

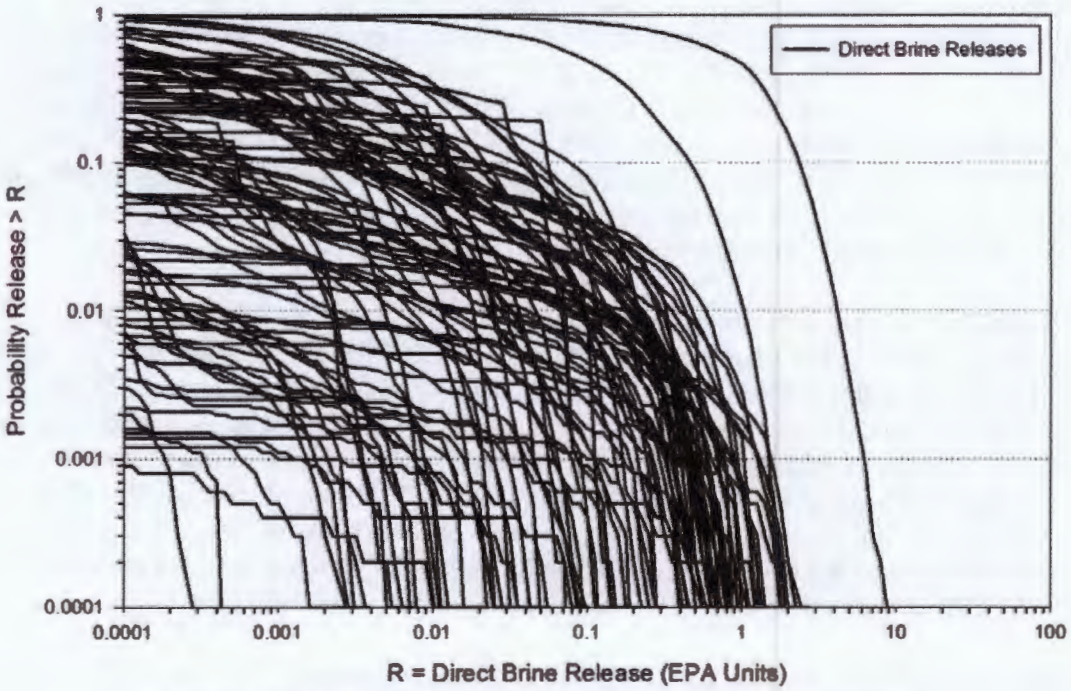

Figure 3-16: PCS-2012 PA Replicate 2 Normalized Direct Brine Releases

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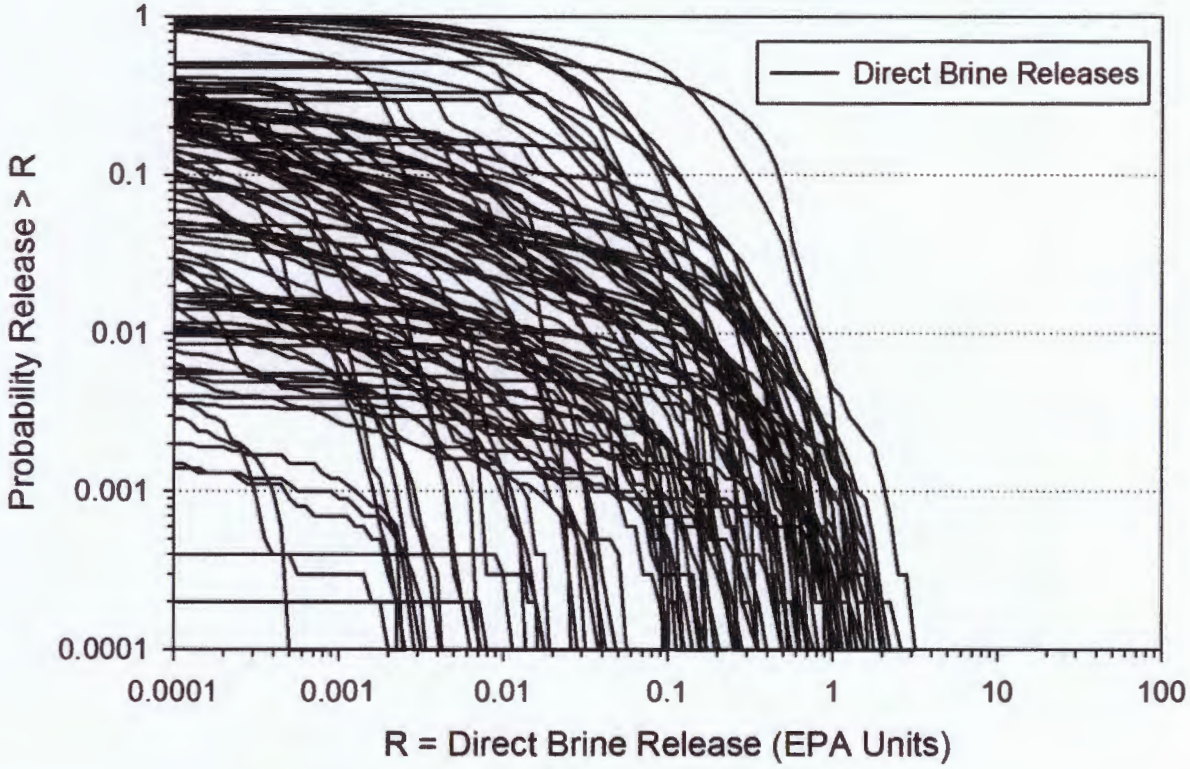

Figure 3-17: PCS-2012 PA Replicate 3 Normalized Direct Brine Releases

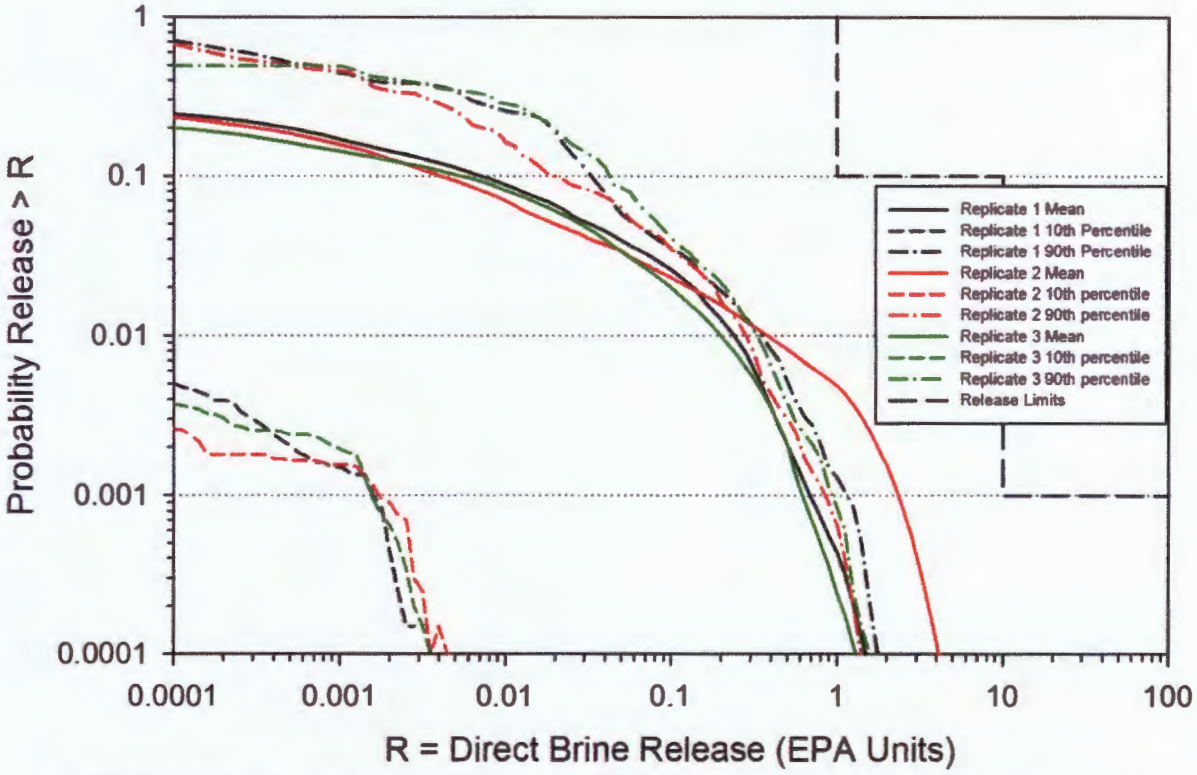

Figure 3-18: PCS-2012 PA Mean and Quantile CCDFs for Normalized Direct Brine Releases, Replicates 1-3

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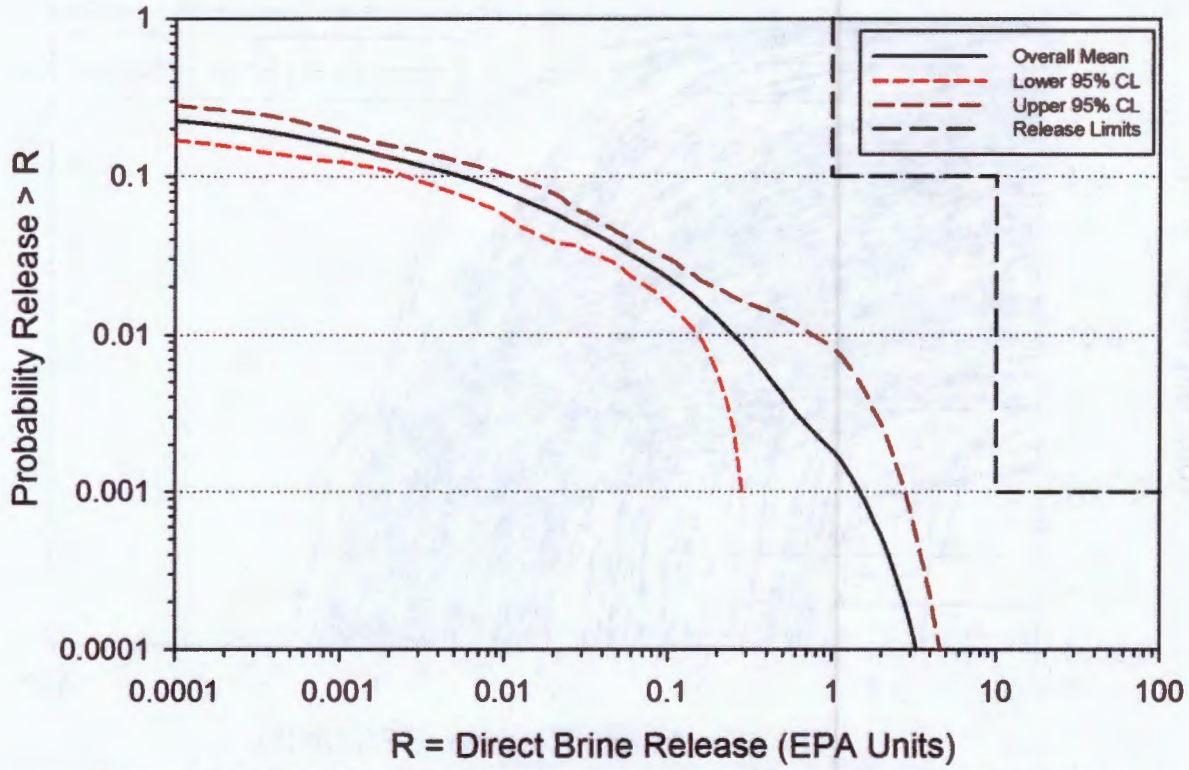

Figure 3-19: PCS-2012 PA Confidence Limits on Overall Mean for Normalized Direct Brine Releases

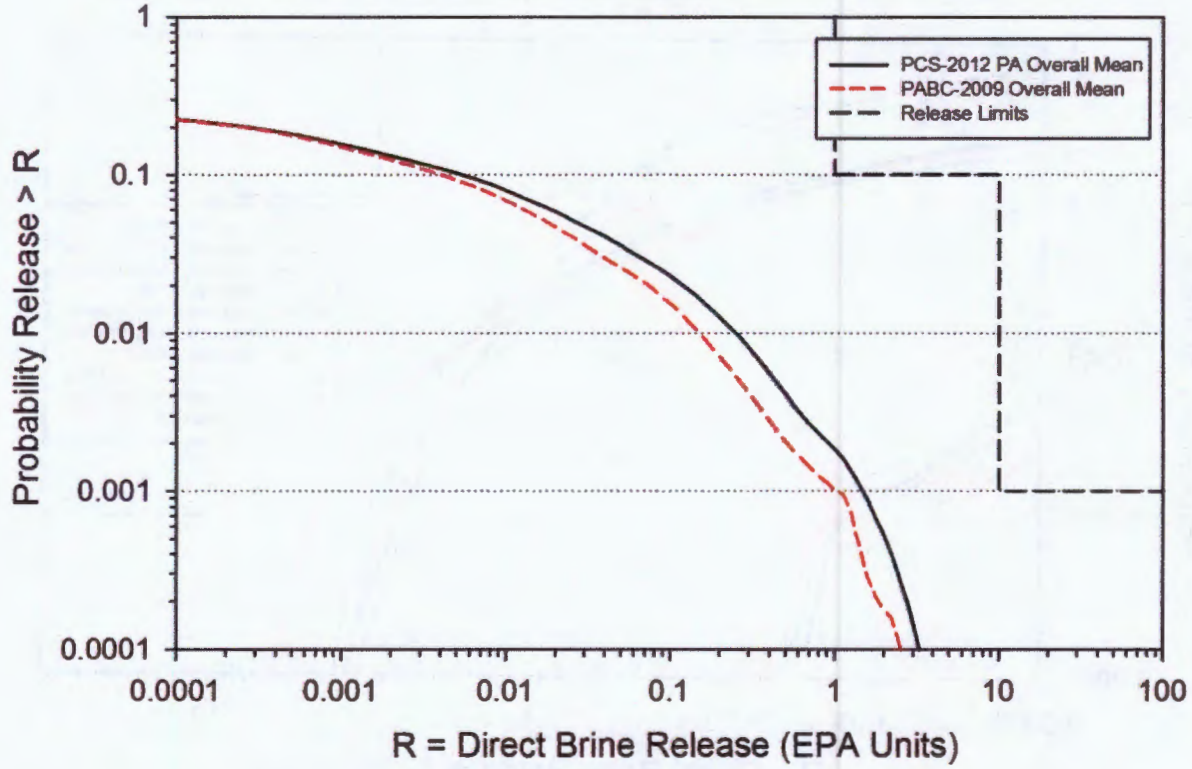

Figure 3-20: PCS-2012 PA and PABC-2009 Overall Mean CCDFs for Normalized Direct Brine Releases

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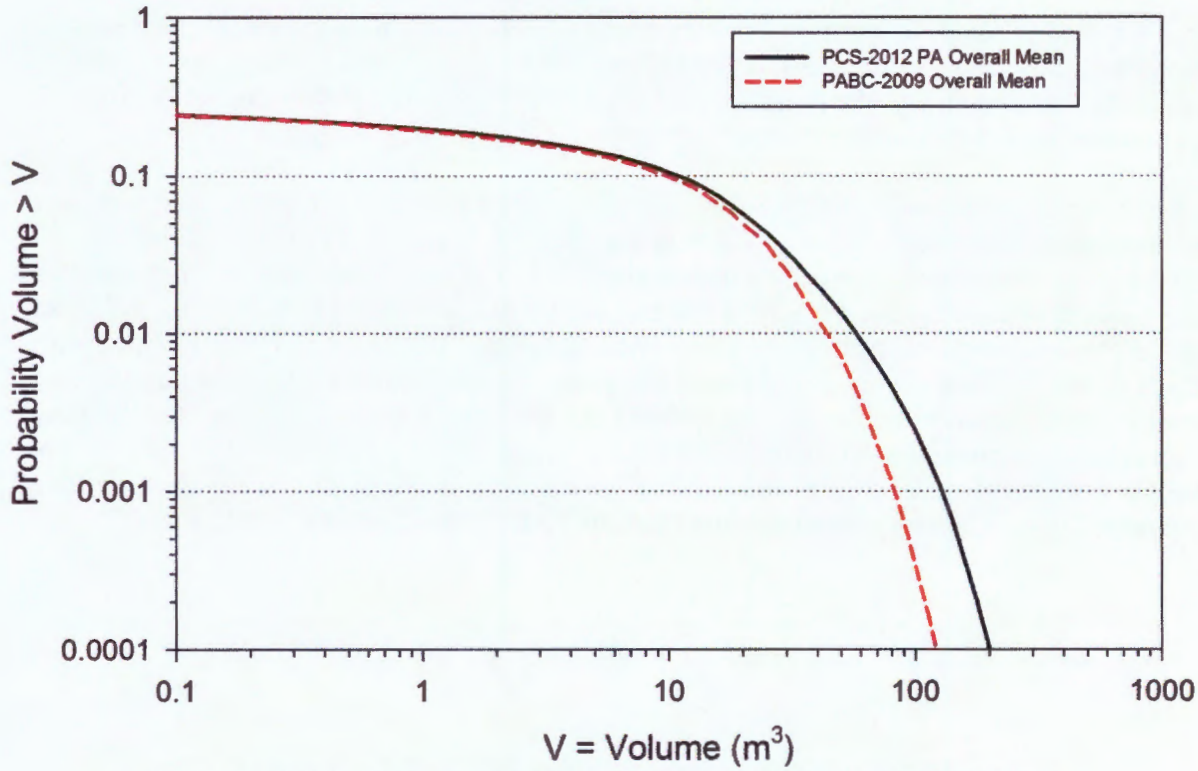

Figure 3-21: PCS-2012 PA and PABC-2009 Overall Mean CCDFs for Direct Brine Volumes

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3.4 Normalized Transport Releases to the Culebra

PCS-2012 PA normalized transport releases to the Culebra are discussed in this section and compared to those seen in the PABC-2009. These results are included primarily as a means to validate the expectation that the proposed changes to the PCS investigated in the PCS-2012 PA have minimal impact on Culebra transport releases.

Replicate means obtained in the PCS-2012 PA and the PABC-2009 for normalized transport releases to the Culebra are shown together in Figure 3-22. As seen in that figure, the means obtained in the two analyses for each replicate are identical. Overall means of transport releases to the Culebra obtained in the PCS-2012 PA and the PABC-2009 are shown together in Figure 3-23. As is evident from that figure, there is no difference in the overall mean of transport releases to the Culebra obtained in the two analyses. The individual replicate means and the overall mean of transport releases to the Culebra are primarily unaffected by the panel closure design changes implemented in the PCS-2012 PA. As a result, it is reasonable to conclude that normalized transport releases from the Culebra be primarily unchanged as well, since nothing was changed in the Culebra transport model from the PABC-2009 to the PCS-2012 PA.

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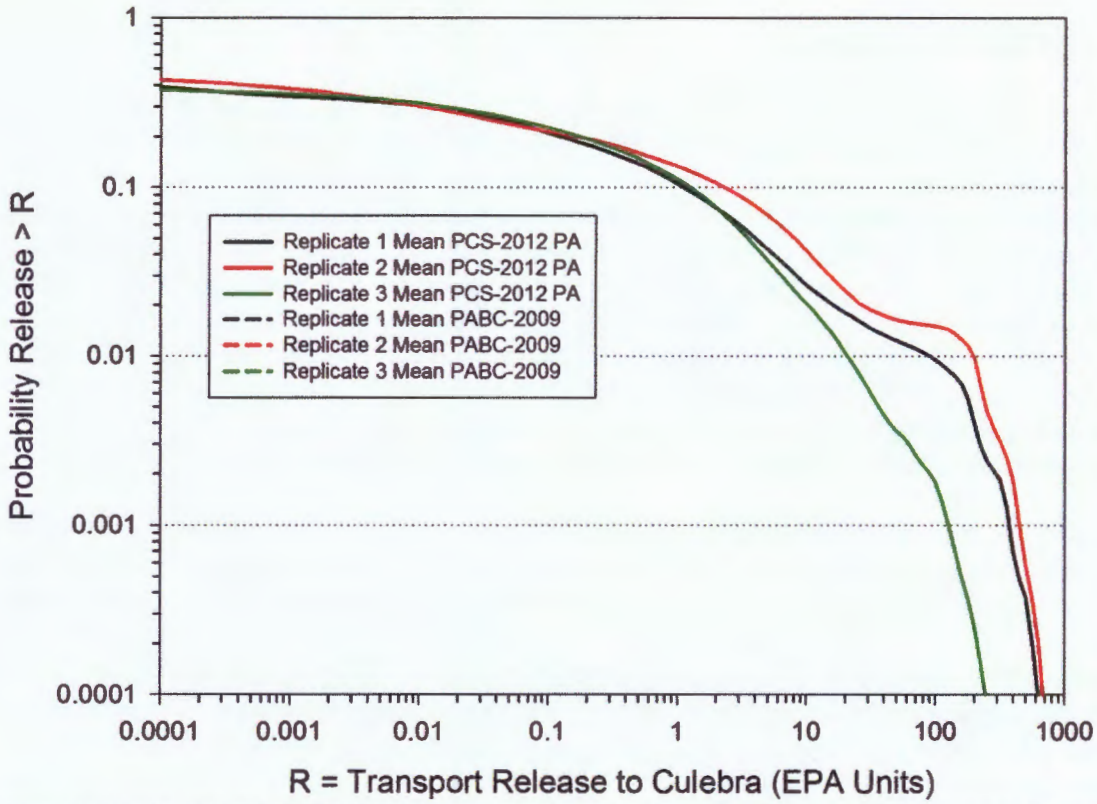

Figure 3-22: PCS-2012 PA and PABC-2009 Replicate Means for Normalized Transport Releases to the Culebra

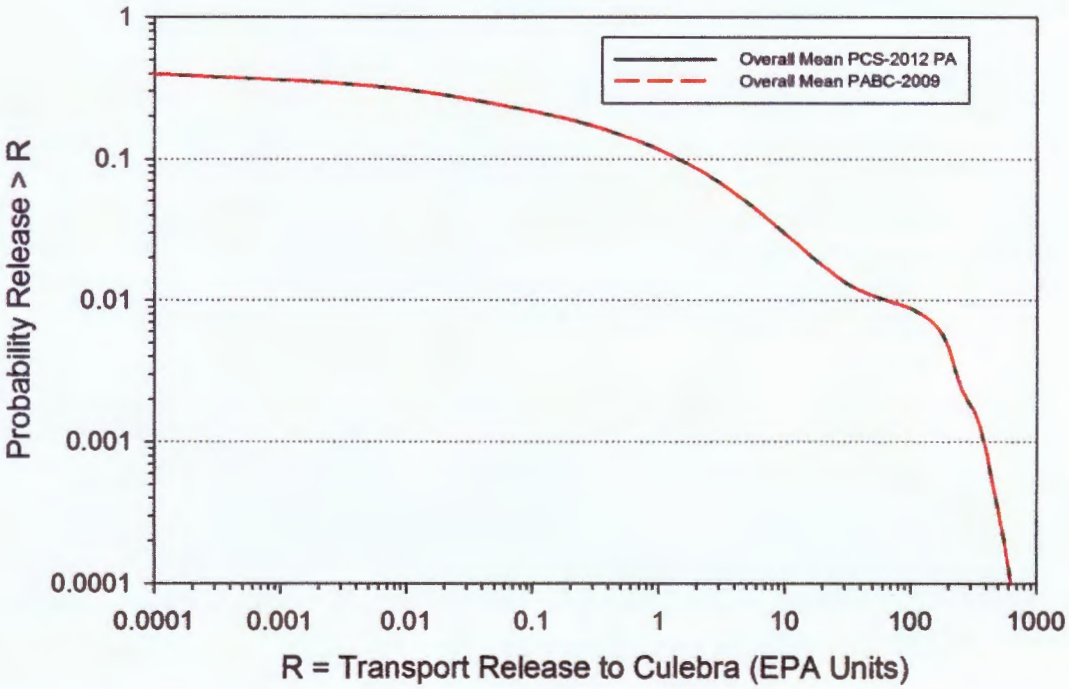

Figure 3-23: PCS-2012 PA and PABC-2009 Overall Mean CCDFs for Transport Releases to the Culebra

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3.5 Total Normalized Releases

Total normalized releases for PCS-2012 PA are presented in this section and subsequently compared to results obtained in the PABC-2009. Total releases are calculated by forming the summation of releases across each potential release pathway, namely cuttings and cavings releases, spallings releases, direct brine releases, and transport releases. PCS-2012 PA CCDFs for total releases are presented in Figure 3-24, Figure 3-25, and Figure 3-26 for replicates 1, 2, and 3, respectively. Mean and quantile CCDF distributions for the three replicates are shown together in Figure 3-27. Figure 3-28 contains the 95 percent confidence limits about the overall mean of total releases. As seen in Figure 3-28, the overall mean for normalized total releases and its lower/upper 95% confidence limits are well below acceptable release limits. As a result, the panel closure design and repository configuration changes investigated in the PCS-2012 PA do no result in WIPP non-compliance with the containment requirements of 40 CFR Part 191.

PCS-2012 PA and PABC-2009 overall mean CCDFs for total releases are shown together in Figure 3-29. As seen in that figure, the overall mean CCDFs obtained in the two analyses are nearly identical for release values less than approximately 0.1 EPA units. For releases greater than 0.1 EPA units, the CCDF curve obtained in the PCS-2012 PA is higher than that found in the PABC-2009. This increase corresponds primarily to the differences found for direct brine releases between the two analyses as discussed in Section 3.3 and illustrated in Figure 3-20. The differences found for spallings may slightly affect the total CCDF curve as well (Section 3.2, Figure 3-13). PCS-2012 PA cuttings and cavings results are unchanged from those found in the PABC-2009. The panel closure design change investigated in the PCS-2012 PA has an impact on the overall mean of total releases from the PABC-2009 to the PCS-2012 PA due to the changes in direct brine releases calculated in those analyses (Figure 3-30).

A comparison of the statistics on the overall mean for total normalized releases obtained in the PCS-2012 PA and the PABC-2009 can be seen in Table 1. At a probability of 0.1, values obtained for mean total releases has increased from 0.09 to 0.10 for the PCS-2012 PA. At a probability of 0.001, the increase in DBRs seen at that probability in the PCS-2012 PA results in an increase in the mean total release by approximately 0.41 EPA units. An increase is seen in the 95% confidence limit when compared to the PABC-2009 results, while the 90th percentile remains the same. An increase in the mean total release accompanied by no change to the 90th percentile value is additional evidence that only a few vectors have significantly increased releases.

Probability	Analysis	Mean Total Release	90th Percentile	Lower 95% CL	Upper 95% CL	Release Limit
0.1	PCS-2012 PA	0.10	0.17	0.10	0.10	1
	PABC-2009	0.09	0.16	0.09	0.10	1
0.001	PCS-2012 PA	1.51	1.00	0.33	2.81	10
	PABC-2009	1.10	1.00	0.37	1.77	10

Table 1: PCS-2012 PA and PABC-2009 Statistics on the Overall Mean for Total Normalized Releases in EPA Units at Probabilities of 0.1 and 0.001

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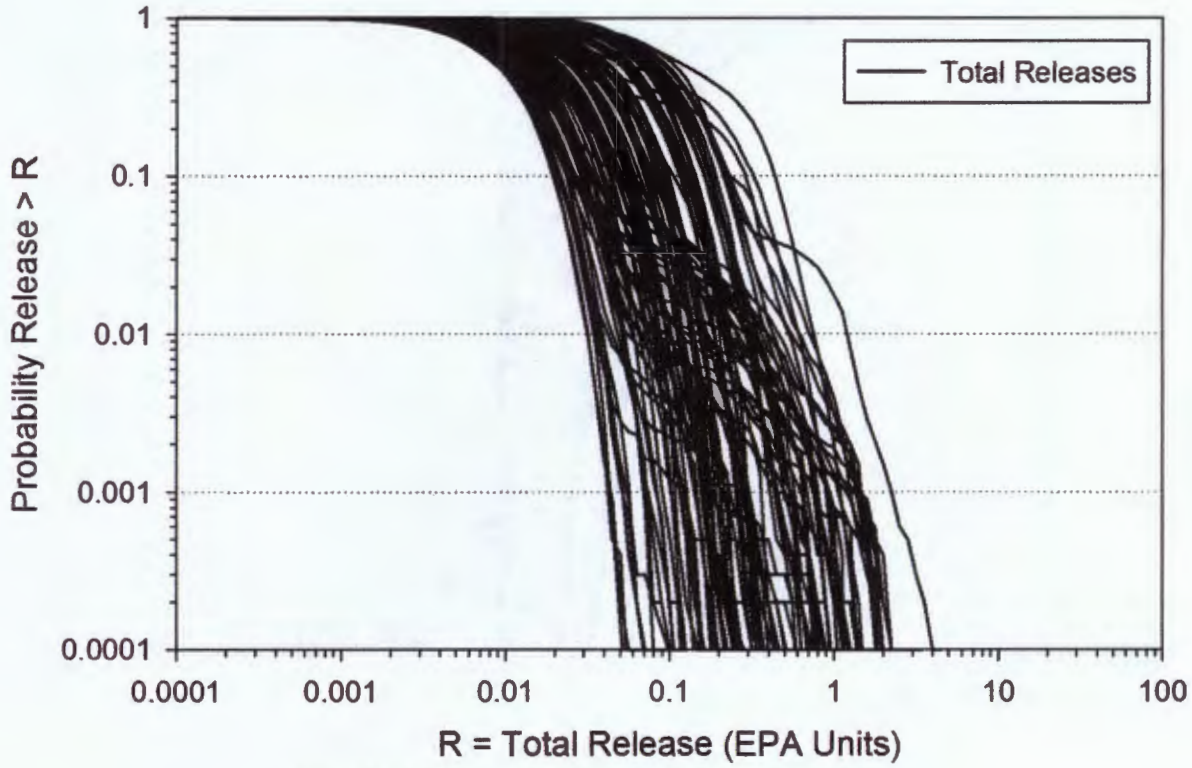

Figure 3-24: PCS-2012 PA Replicate 1 Total Normalized Releases

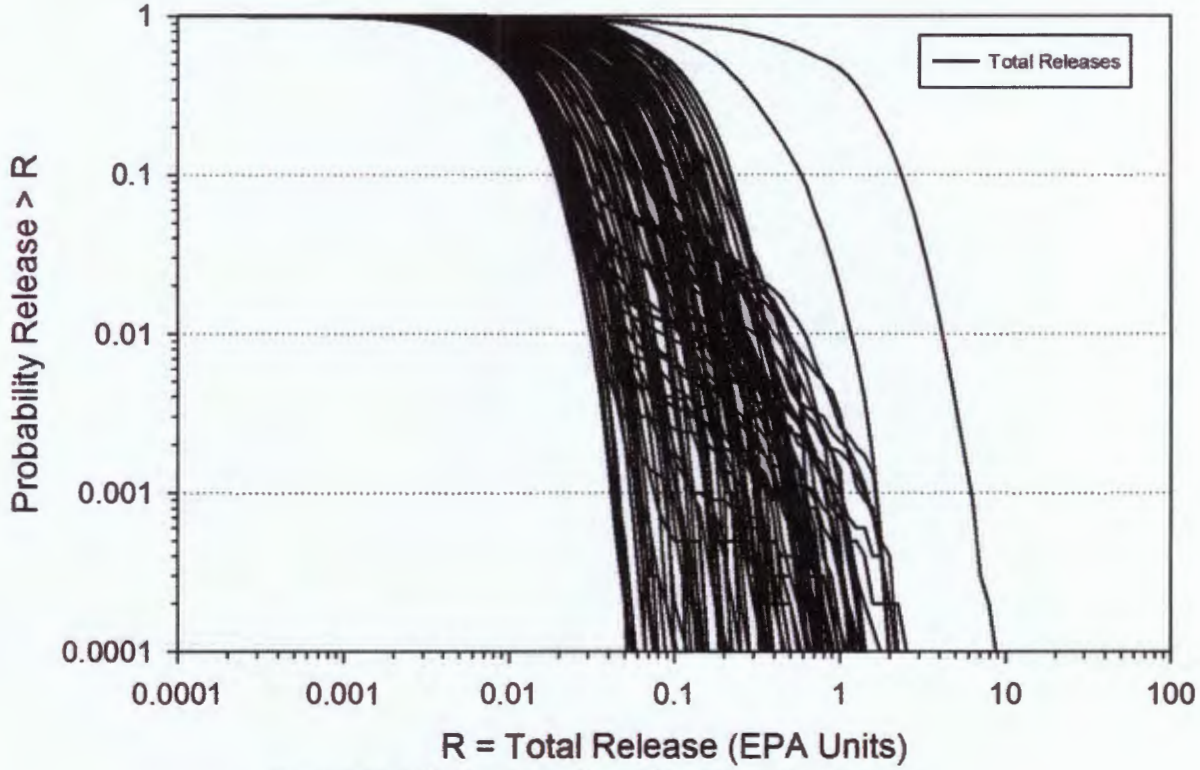

Figure 3-25: PCS-2012 PA Replicate 2 Total Normalized Releases

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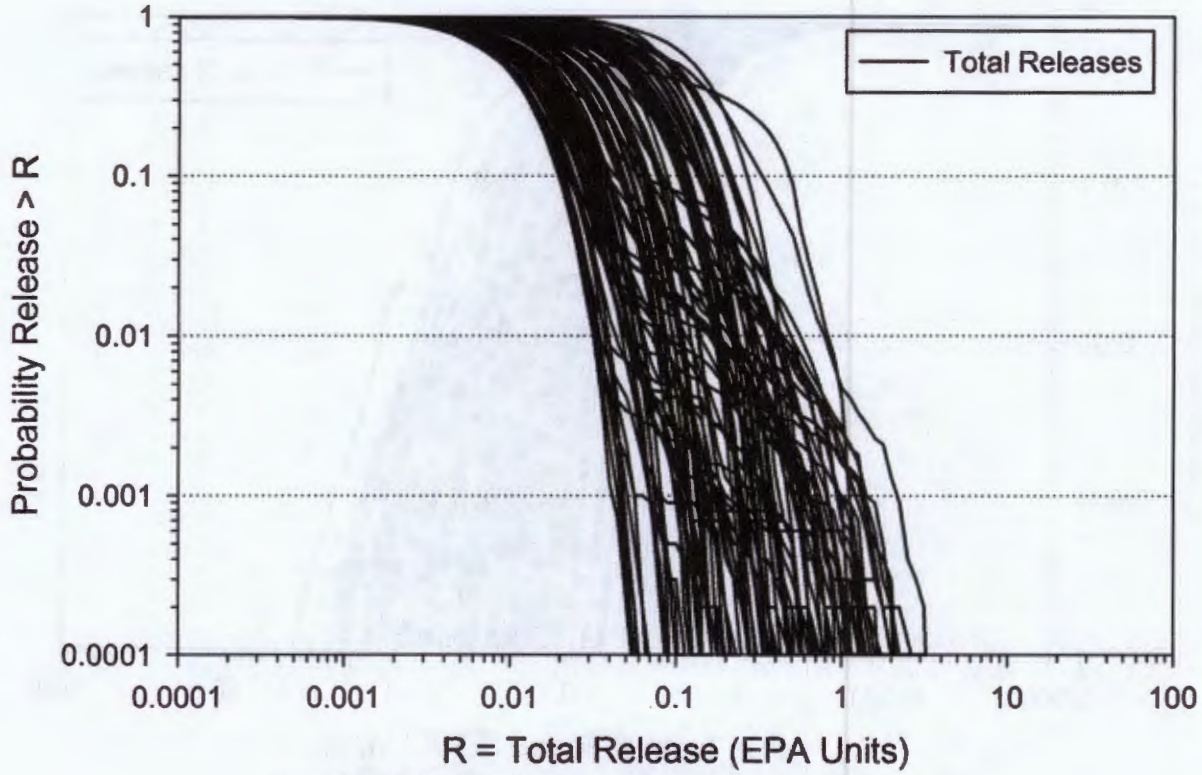

Figure 3-26: PCS-2012 PA Replicate 3 Total Normalized Releases

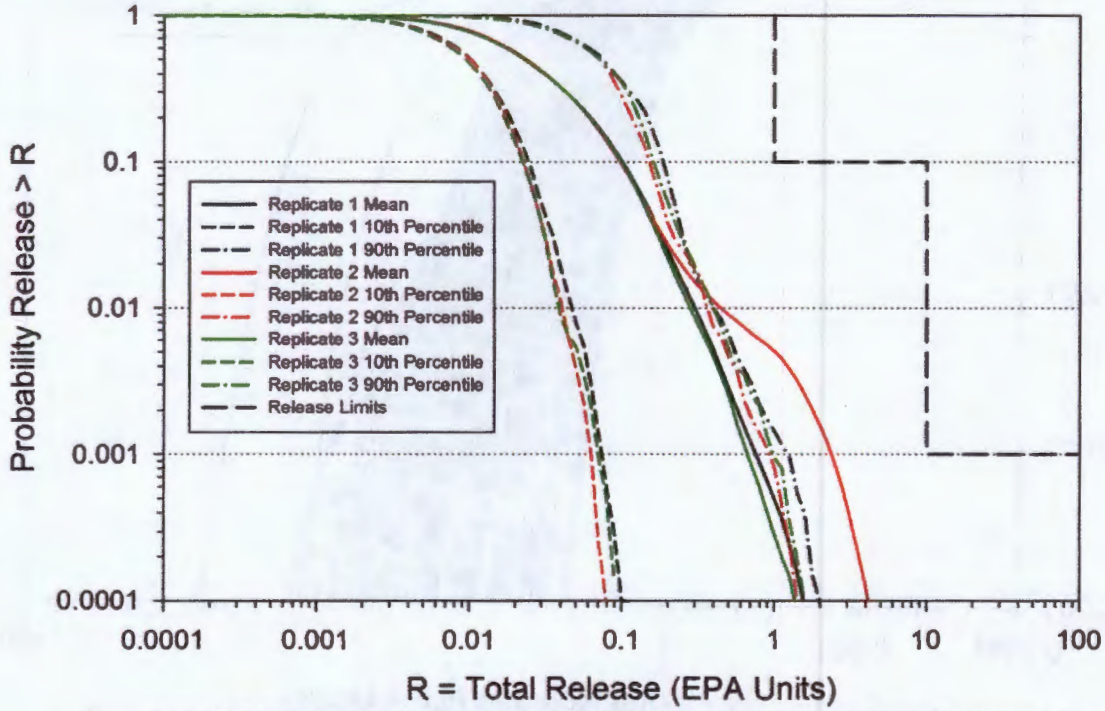

Figure 3-27: PCS-2012 PA Mean and Quantile CCDFs for Total Normalized Releases, Replicates 1-3

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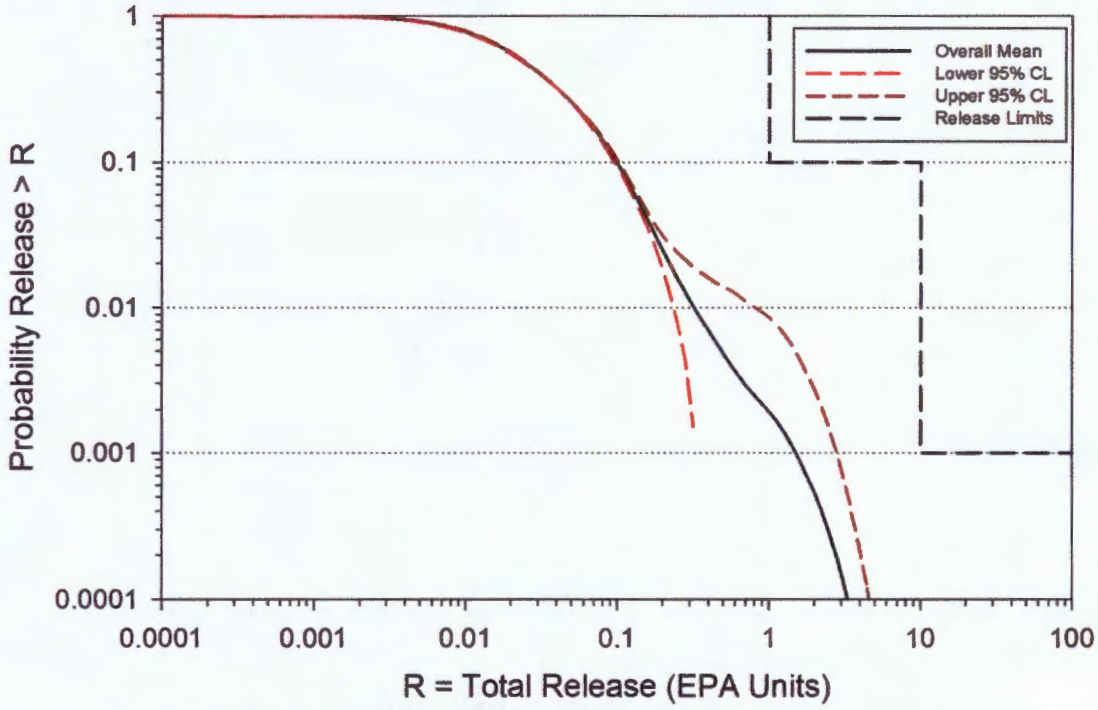

Figure 3-28: PCS-2012 PA Confidence Limits on Overall Mean for Total Normalized Releases

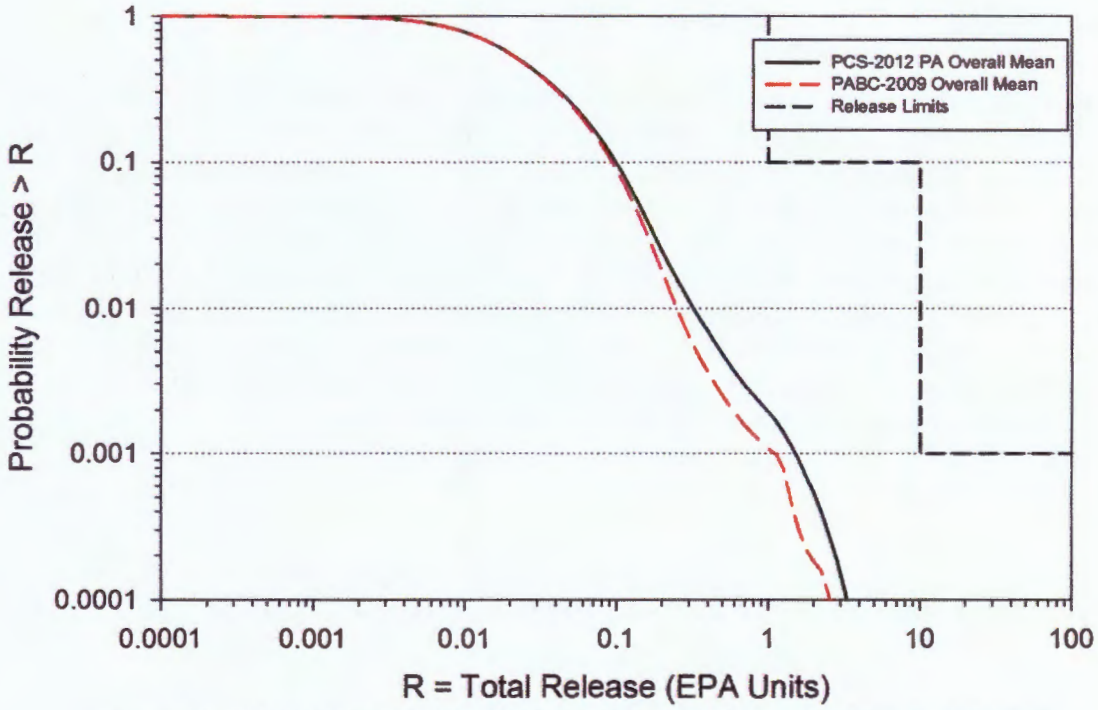

Figure 3-29: PCS-2012 PA and PABC-2009 Overall Mean CCDFs for Total Normalized Releases

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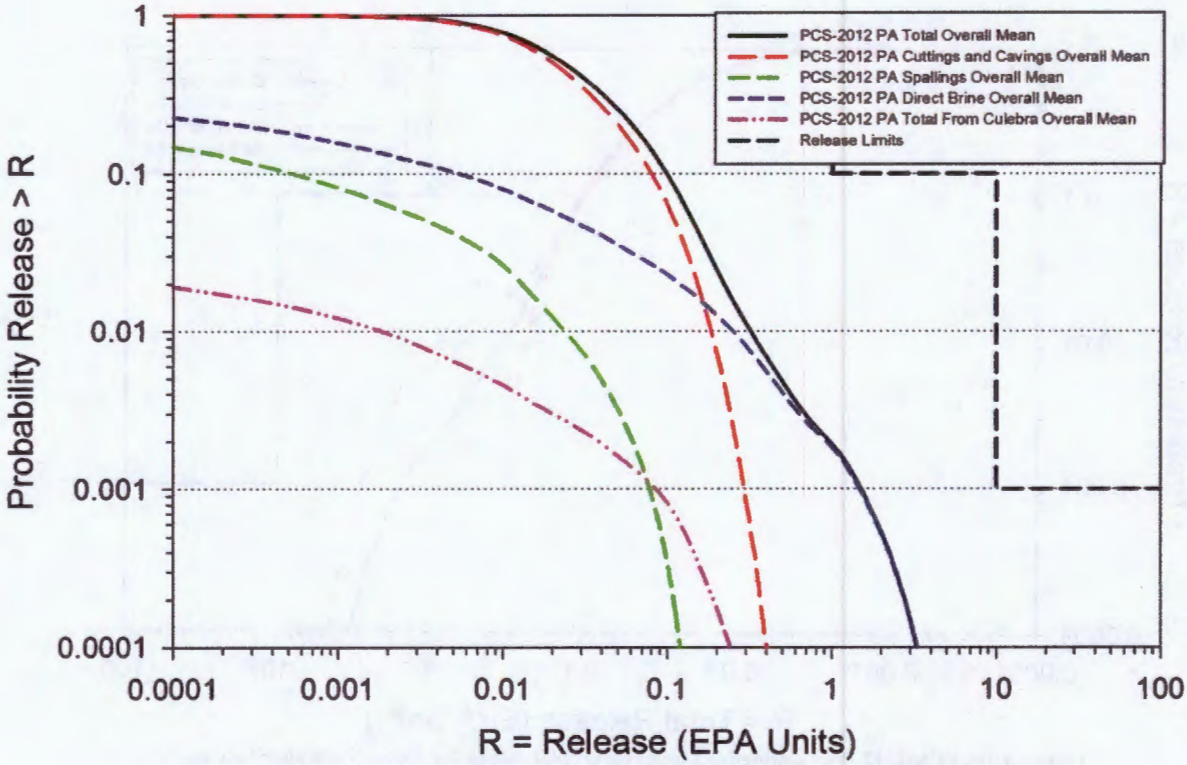

Figure 3-30: PCS-2012 PA Primary Components Contributing to Total Releases

4 SUMMARY

Total normalized releases calculated in the PCS-2012 PA remain below their regulatory limits. As a result, the panel closure design and repository configuration changes investigated in the PCS-2012 PA do not result in WIPP non-compliance with the containment requirements of 40 CFR Part 191. Cuttings and cavings releases and direct brine releases are the two primary release components contributing to total releases in the PCS-2012 PA. Cuttings and cavings releases are identical to those calculated in the PABC-2009. Changes in total releases are primarily attributed to changes calculated in direct brine releases from the PABC-2009 to the PCS-2012 PA. Increases are observed in PCS-2012 PA spallings releases as compared to the PABC-2009, but these differences are comparatively minor and do not have a significant impact on the overall total normalized releases found in the PCS-2012 PA.

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