553027

Sandia National Laboratories

Waste Isolation Pilot Plant

Analysis Package for CCDFGF: CRA-2009 Performance Assessment Baseline Calculation

Revision 0

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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 (U.S. EPA 1993). The DOE demonstrates compliance with the containment requirements according to the Certification Criteria in Title 40 CFR Part 194 (U.S. EPA 1996) 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 are maintained and updated with new information as part of a recertification process that occurs at five-year intervals after the first waste is received at the site.

PA calculations were included in the 1996 Compliance Certification Application (CCA) (U.S. DOE 1996), and in a subsequent Performance Assessment Verification Test (PAVT) (MacKinnon and Freeze 1997a, 1997b and 1997c). Based in part on the CCA and PAVT PA calculations, the EPA certified that the WIPP met the containment criteria in the regulations and was approved for disposal of transuranic waste in May 1998 (U.S. EPA 1998) with the first shipment of TRU waste being received in 1999. PA calculations were also an integral part of the 2004 Compliance Recertification Application (CRA-2004) (U.S. DOE 2004). During their review of the CRA-2004, the EPA requested an additional PA calculation, referred to as the CRA-2004 Performance Assessment Baseline Calculation (PABC) (Leigh et al. 2005), be conducted with modified assumptions and parameter values (Cotsworth 2005).

Since the CRA-2004 PABC, additional PA calculations were completed for and documented in the 2009 Compliance Recertification Application (CRA-2009). The CRA-2009 PA resulted from continued review of the CRA-2004 PABC, including a number of technical changes and corrections, as well as updates to parameters and improvements to the PA computer codes (Clayton et al. 2008). The EPA has requested that additional information, which was received between the commencement of the CRA-2009 PA (December 2007) and the submittal of the CRA-2009 (March 2009), be included in an additional PA calculation (Cotsworth 2009), referred to as the CRA-2009 Performance Assessment Baseline Calculation (PABC-2009). The PABC-2009 analysis is guided by AP-145 (Clayton 2009). This report documents the calculations performed by the code CCDFGF for the AP-145 PA and compares results with those obtained in the CRA-2009 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.

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 release exceeds R. The curve defined by the mean probabilities for each value of R is the mean CCDF. The 10^{th} and 90^{th} 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 can not 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 cd containing the data loaded into this utility resulting from PABC-2009 CCDFGF calculations, and subsequent Excel plots, are included as an attachment to this document.

2.1 Code Version

No modifications have been made to the codes PRECCDFGF and CCDFGF since completion of the CRA 2004 PABC. PRECCDFGF version 1.01 and CCDFGF version 5.02 were used for the PABC-2009 and the CRA-2009 PA.

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 PABC-2009 and the CRA-2009 PA, the same random seeds for CCDFGF were used as in the CRA 2004 PABC. This was done to allow a vector by vector comparison of the results of the PABC-2009 to those obtained in the CRA-2009 PA. As the random seeds used to initialize the sampling of the epistemic parameters were unchanged in PABC-2009 and CRA-2009, any differences between the analyses can be attributed solely to the changes in the parameters used in those calculations. Random seeds used in the PABC-2009 calculations are specified in the files CCGF_PABC09_CONTROLRr.inp, where r = 1,2,3. These files are located in class PABC09-0 in CMS library LIBPABC09_CCGF.

2.3 Run Control

Run control for this analysis is documented in Long (2010).

3 Analysis and Results

Results obtained from PABC-2009 calculations are broken out in subsections for each component of release. At the conclusion of the subsection for each release component, results obtained for PABC-2009 are compared to those found in the CRA-2009 PA. 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. Normalized transport releases are presented in Subsection 3.4. Finally, total normalized releases are shown in Subsection 3.5.

3.1 Cuttings and Cavings Normalized Releases

PABC-2009 cuttings and cavings releases are presented in this section and subsequently compared to results obtained in the CRA-2009 PA. Figure 3-1, Figure 3-2, and Figure

3-3 contain PABC-2009 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.

To facilitate comparisons of cuttings and cavings releases calculated in PABC-2009 to those obtained in the CRA-2009 PA, overall mean and volume CCDFs obtained in these two analyses are plotted simultaneously in Figure 3-6 and Figure 3-7. Overall, cuttings and cavings normalized releases obtained in PABC-2009 were slightly less than those obtained in the CRA-2009 PA. The activities for the waste inventories (in EPA units) used in both analyses started at similar levels. However, the PABC-2009 inventory became lower after roughly 350 years and remained lower for the rest of the 10,000-year regulatory period (Fox and Clayton 2010). As a result, direct solids releases for the PABC-2009 decreased as most repository intrusions occur at later times. Release volumes obtained for both analyses were identical as no changes were made to the underlying models or parameters used in the calculation of cuttings and cavings areas (Ismail 2010).

Figure 3-1: PABC-2009 Replicate 1 Cuttings and Cavings Normalized Releases

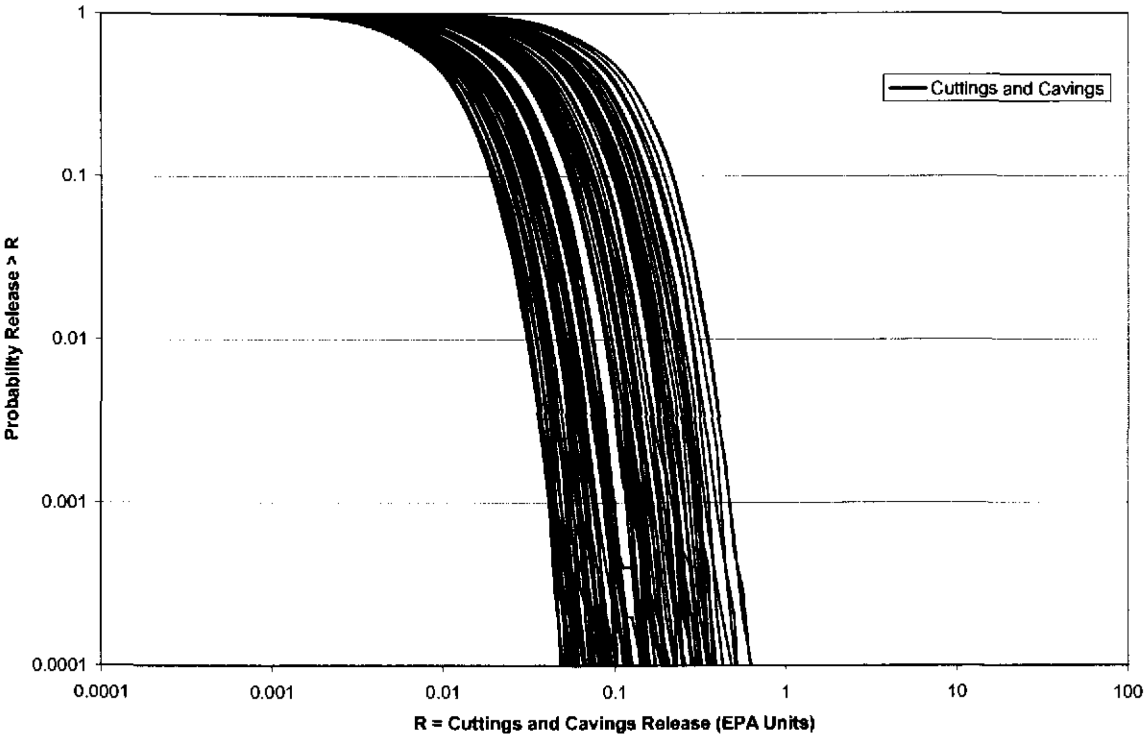

Figure 3-2: PABC-2009 Replicate 2 Cuttings and Cavings Normalized Releases

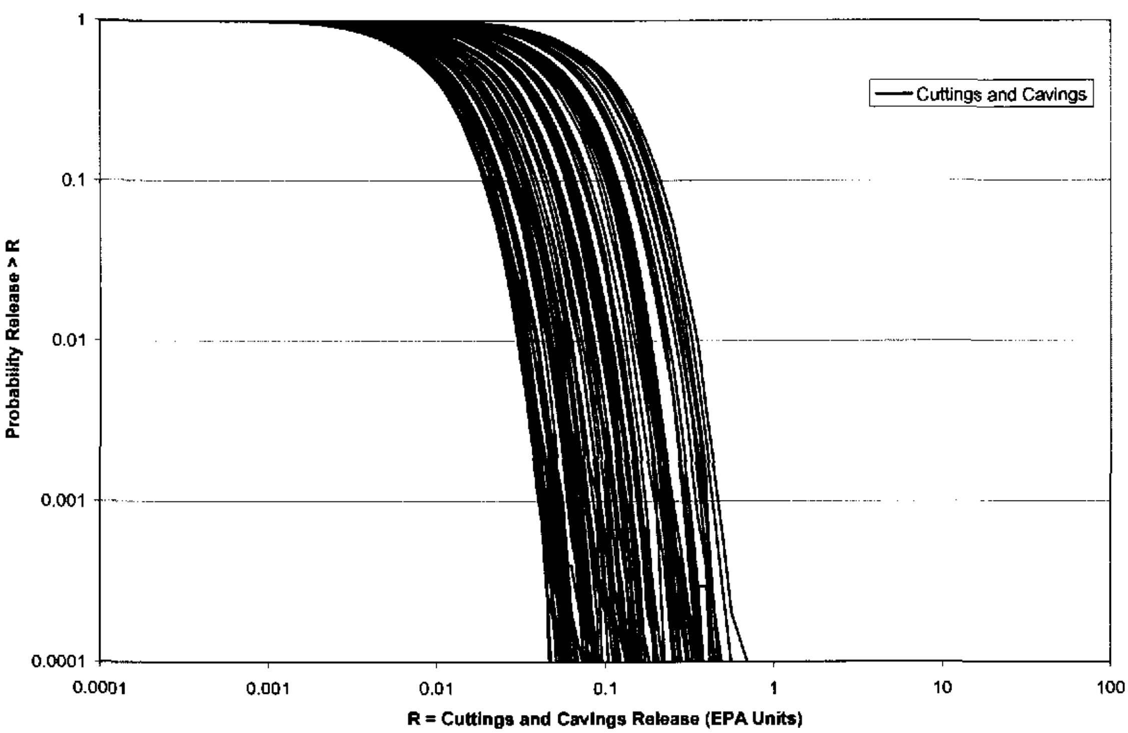

Figure 3-3: PABC-2009 Replicate 3 Cuttings and Cavings Normalized Releases

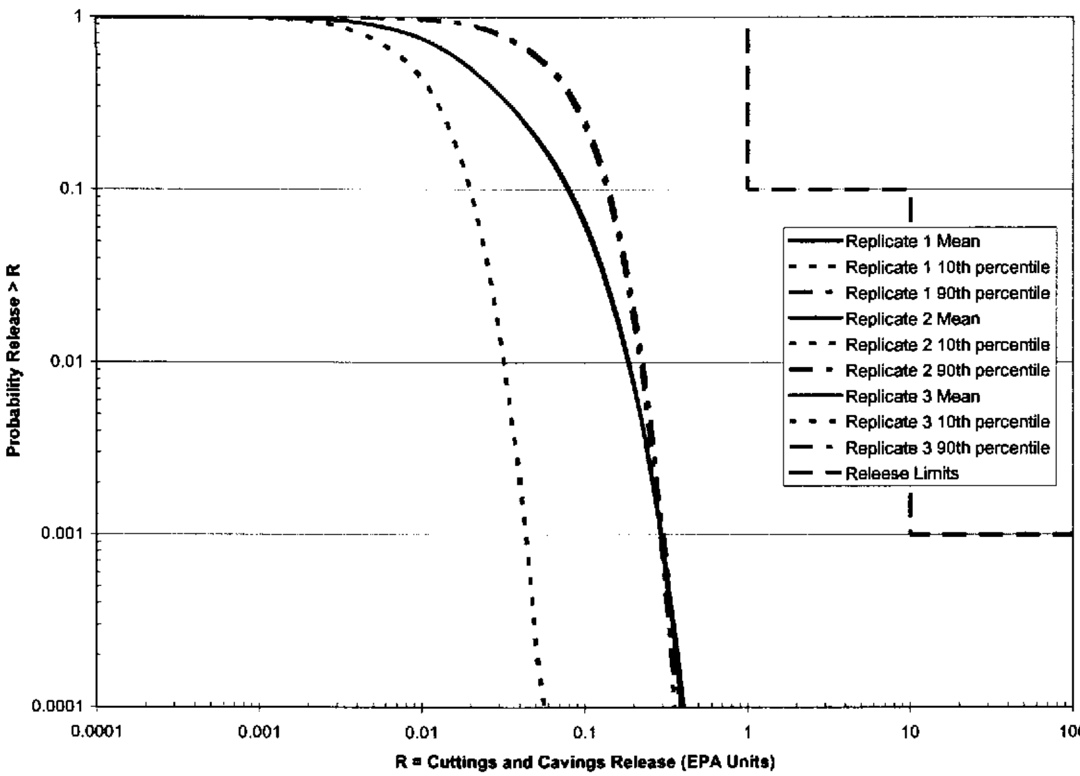

Figure 3-4: PABC-2009 Mean and Quantile CCDFs for Cuttings and Cavings Normalized Releases, Replicates 1-3

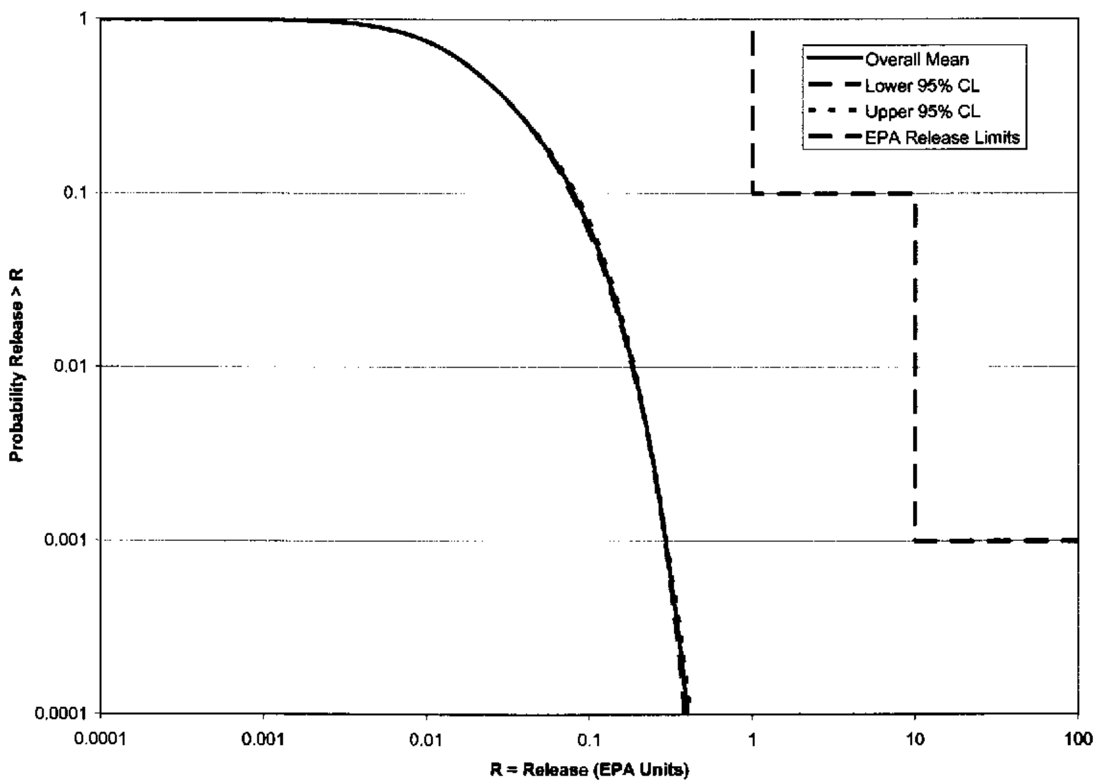

Figure 3-5: PABC-2009 Confidence Limits on Overall Mean for Cuttings and Cavings Normalized Releases

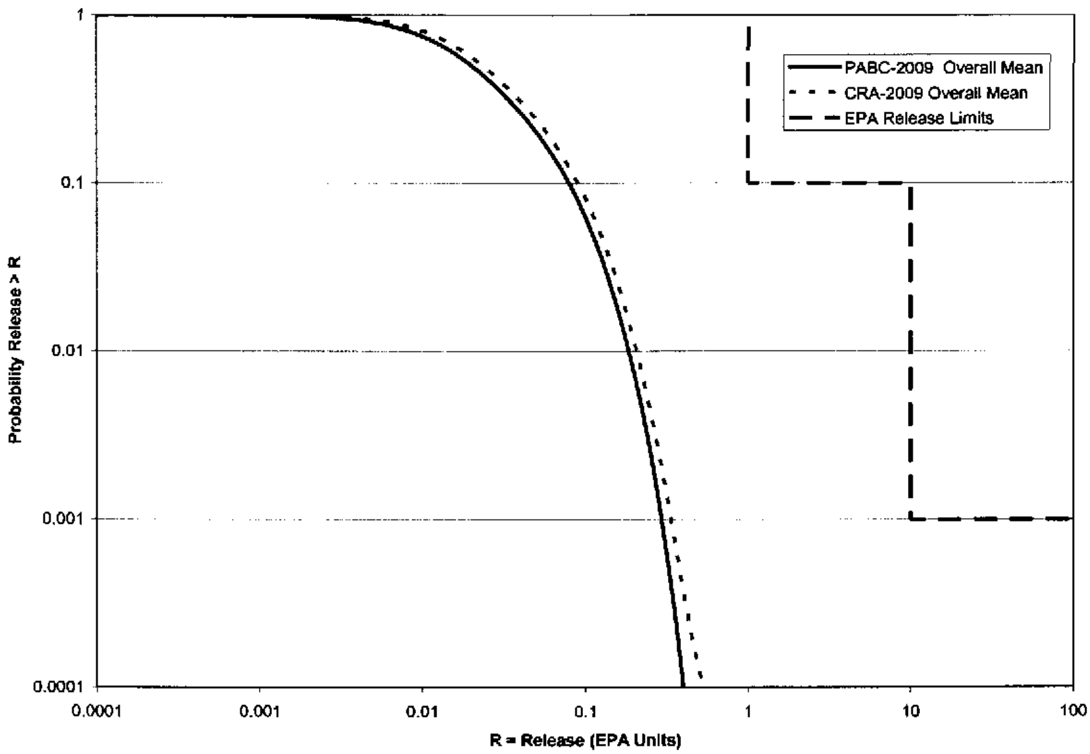

Figure 3-6: PABC-2009 and CRA-2009 Overall Mean CCDFs for Normalized Cuttings and Cavings Releases

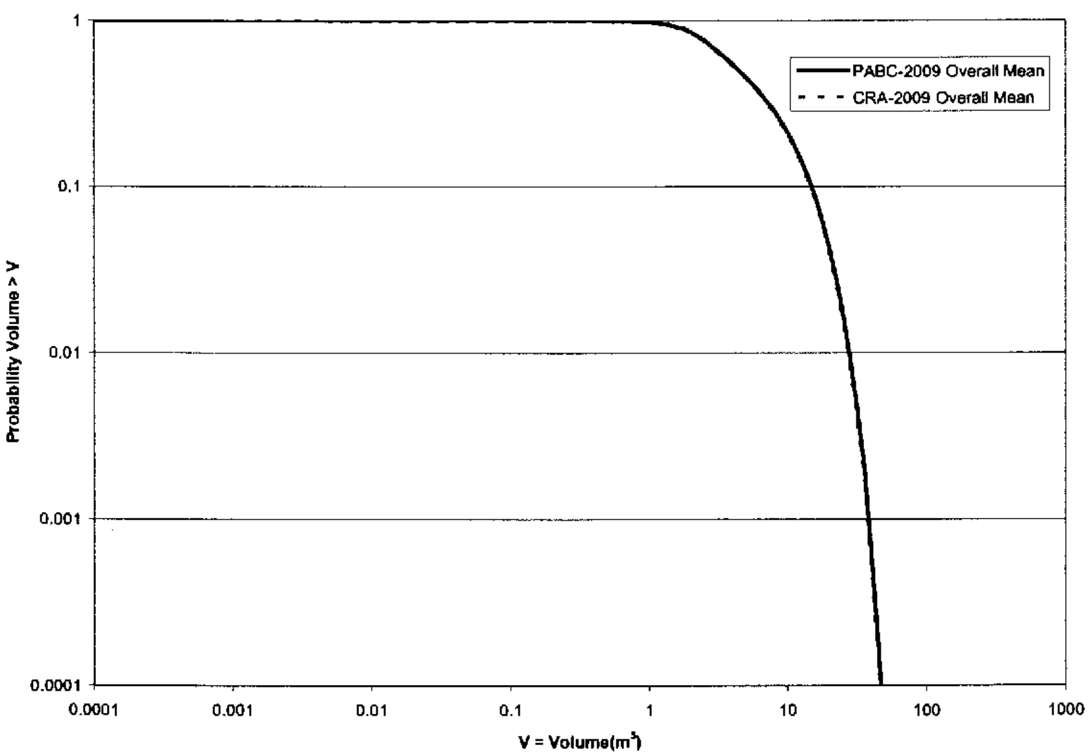

Figure 3-7: PABC-2009 and CRA-2009 Overall Mean CCDFs for Cuttings and Cavings Volumes

3.2 Spallings Normalized Releases

PABC-2009 spallings releases are presented in this section and subsequently compared to results obtained in the CRA-2009 PA. Figure 3-8, Figure 3-9, and Figure 3-10 contain PABC-2009 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. 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.

To facilitate comparisons of spallings releases calculated in PABC-2009 to those obtained in the CRA-2009 PA, 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, there is a reduction in the PABC-2009 spallings overall mean and volume CCDFs as compared to those obtained in the CRA-2009 PA. Ismail (2010) attributes the reduction in spallings releases to the slightly lower repository pressures in the undisturbed scenario observed in the PABC-2009 calculations. A reduction in repository pressure translates into smaller spallings volumes as these volumes depend directly on repository pressure. The decrease in the activity in the PABC-2009 waste inventory (in EPA units) at later times, compared with the inventory used for the CRA-2009 PA also contributed to the reduction in spallings releases.

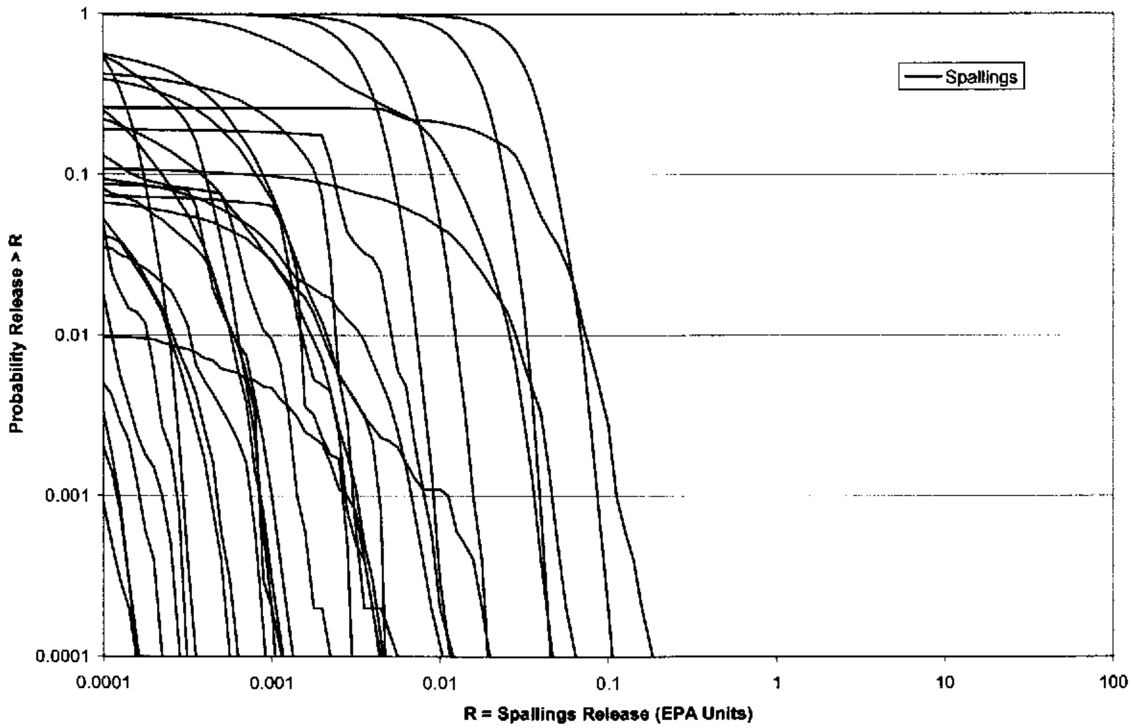

Figure 3-8: PABC-2009 Replicate 1 Spallings Normalized Releases

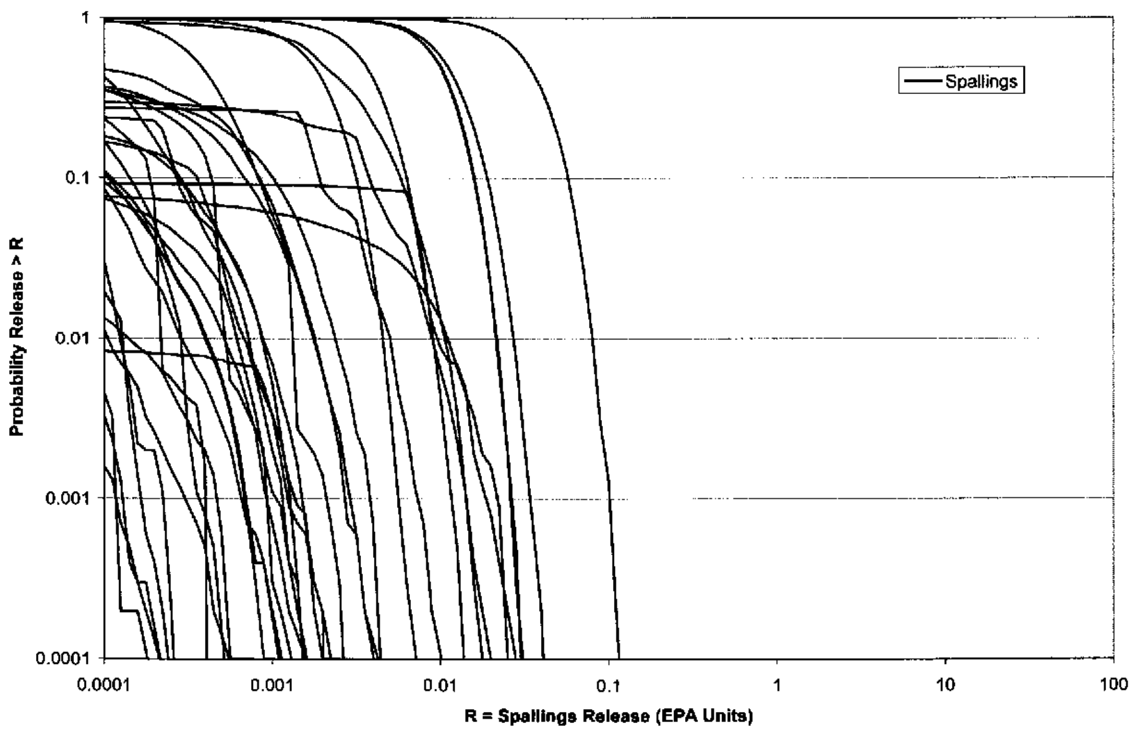

Figure 3-9: PABC-2009 Replicate 2 Spallings Normalized Releases

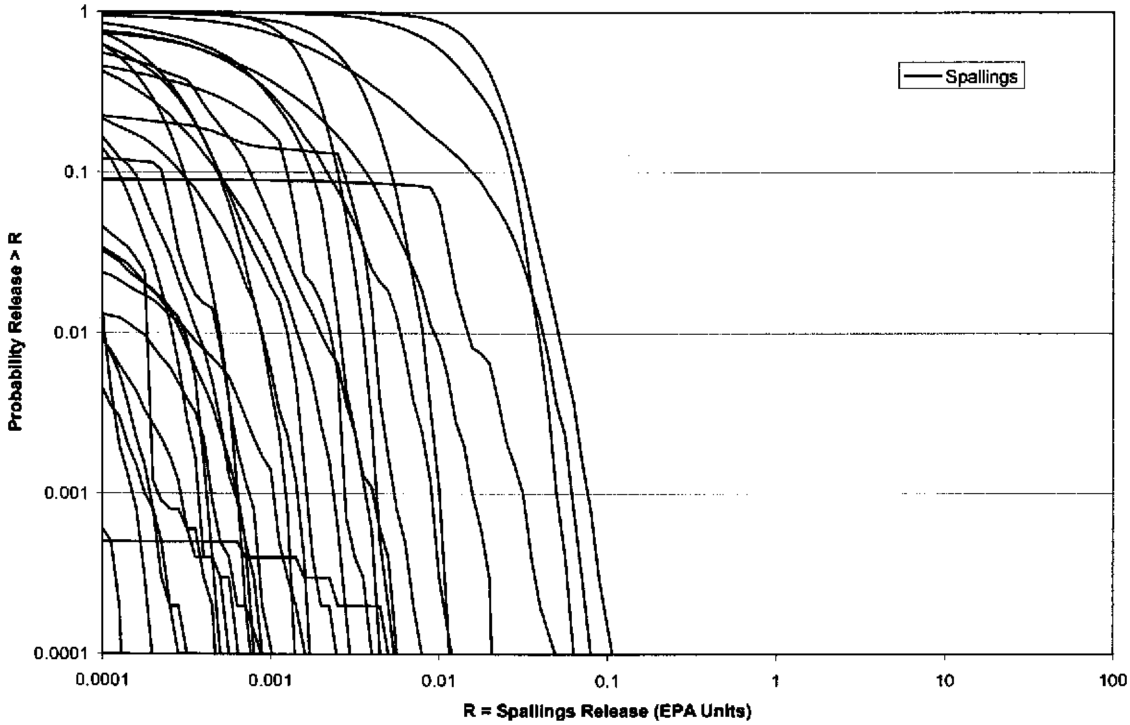

Figure 3-10: PABC-2009 Replicate 3 Spallings Normalized Releases

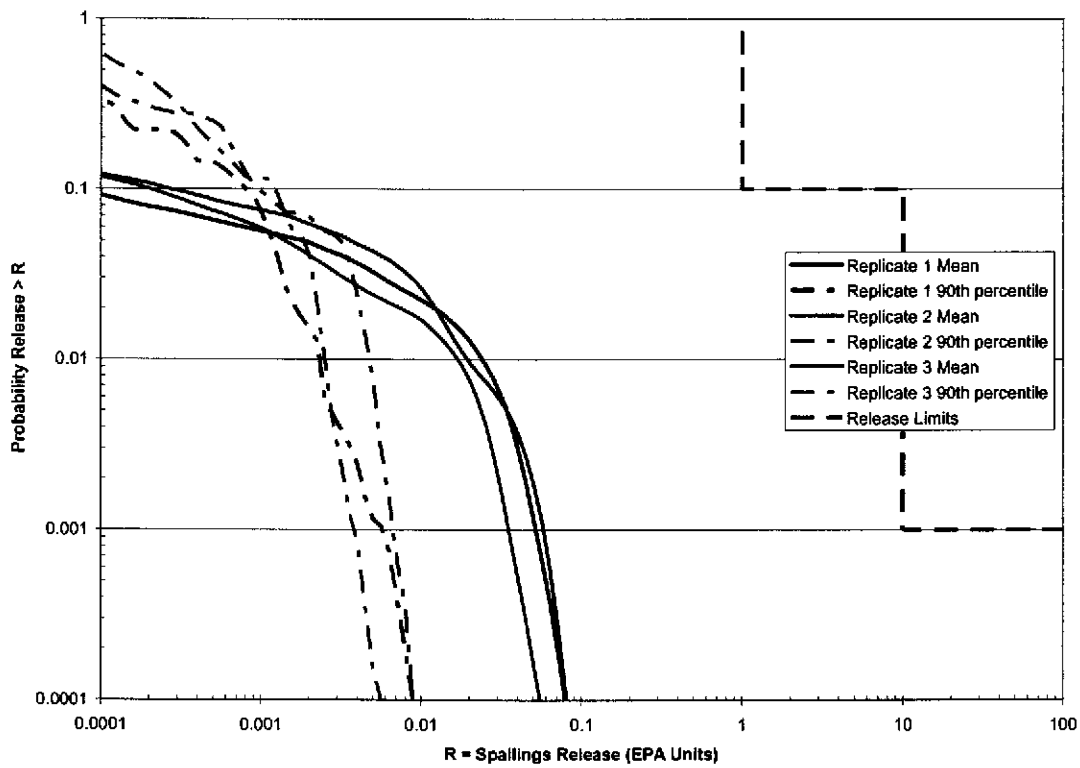

Figure 3-11: PABC-2009 Mean and Quantile CCDFs for Spallings Normalized Releases, Replicates 1-3

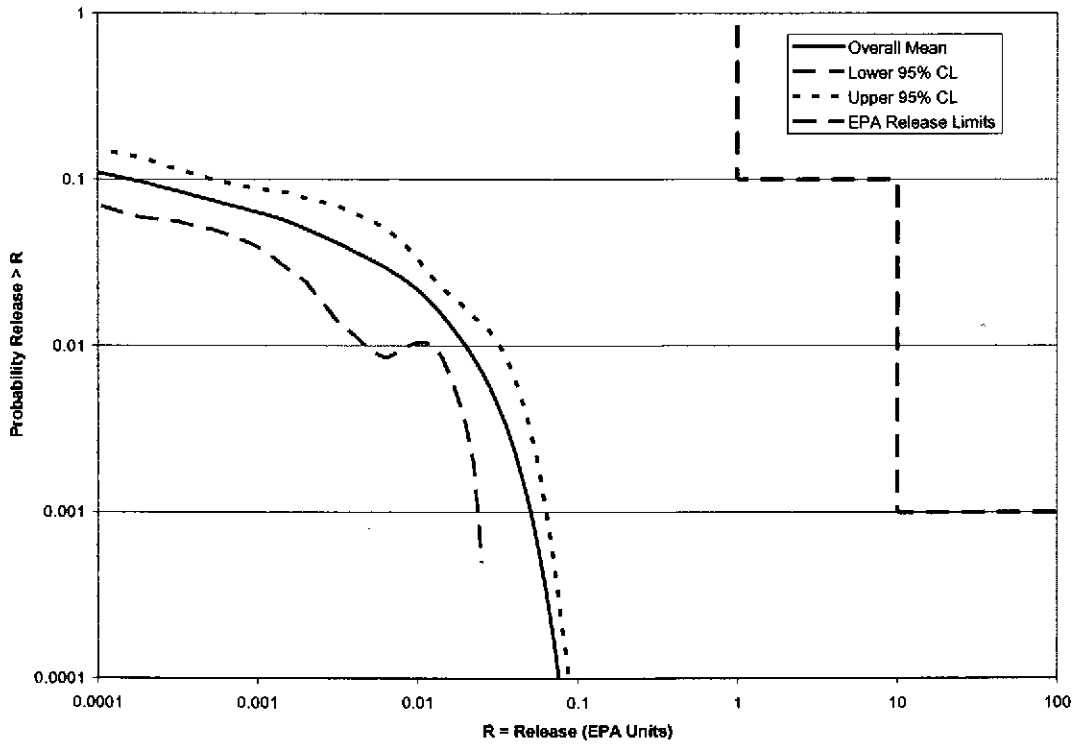

Figure 3-12: PABC-2009 Confidence Limits on Overall Mean for Spallings Normalized Releases

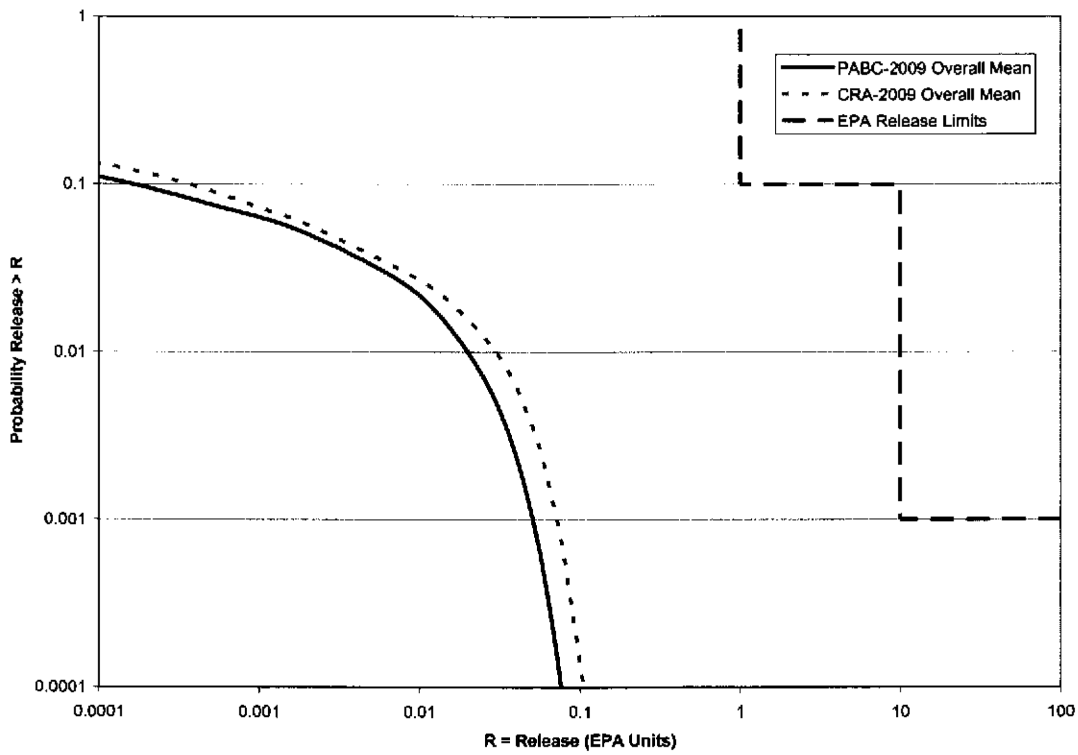

Figure 3-13: PABC-2009 and CRA-2009 Overall Mean CCDFs for Normalized Spallings Releases

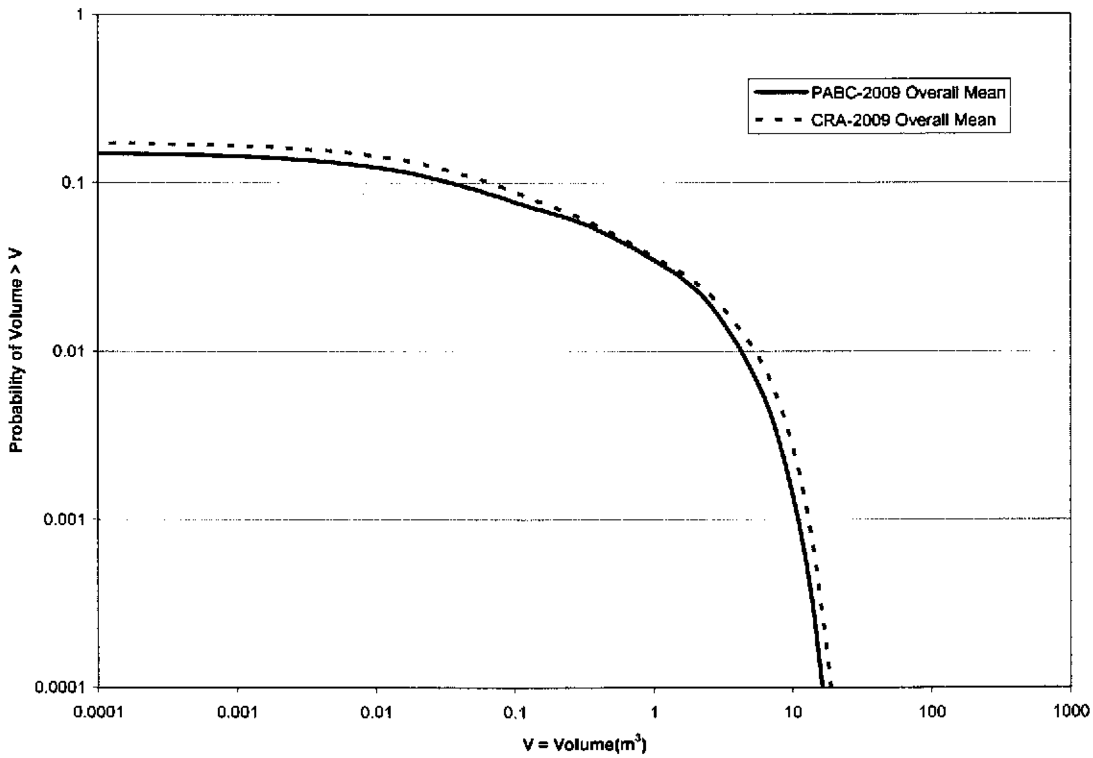

Figure 3-14: PABC-2009 and CRA-2009 Overall Mean CCDFs for Spallings Volumes

3.3 Normalized Direct Brine Releases

PABC-2009 normalized direct brine releases are presented in this section and subsequently compared to results obtained in the CRA-2009 PA. Figure 3-15, Figure 3-16, and Figure 3-17 contain PABC-2009 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 the plot of normalized direct brine releases for Replicate 2, one vector generated a CCDF considerably different than the other 299. In particular, it resulted in a CCDF that exceeds one of the limits specified for acceptable releases. However, this does not result in the WIPP being out of compliance. As set forth in the Certification Criteria in Title 40 CFR Part 194, compliance is specified on the overall mean and its lower/upper 95% confidence limits, not the individual vectors. 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 PABC-2009 to those obtained in the CRA-2009 PA, overall mean and volume CCDFs obtained in these two analyses are plotted simultaneously in Figure 3-20 and Figure 3-21. As seen in Figure 3-20, there is an increase in the PABC-2009 DBR overall mean CCDF as compared to that obtained in the CRA-2009 PA. Garner (2010) attributes the increase in direct brine releases to increased radionuclide solubilities used in the PABC-2009 DBR calculation. Higher radionuclide solubilities resulted in an increase in total mobilized concentration, increasing the release associated with a given brine volume. DBR volumes to the surface were very similar in both analyses (Clayton 2010), resulting in overall volume CCDFs that were nearly identical.

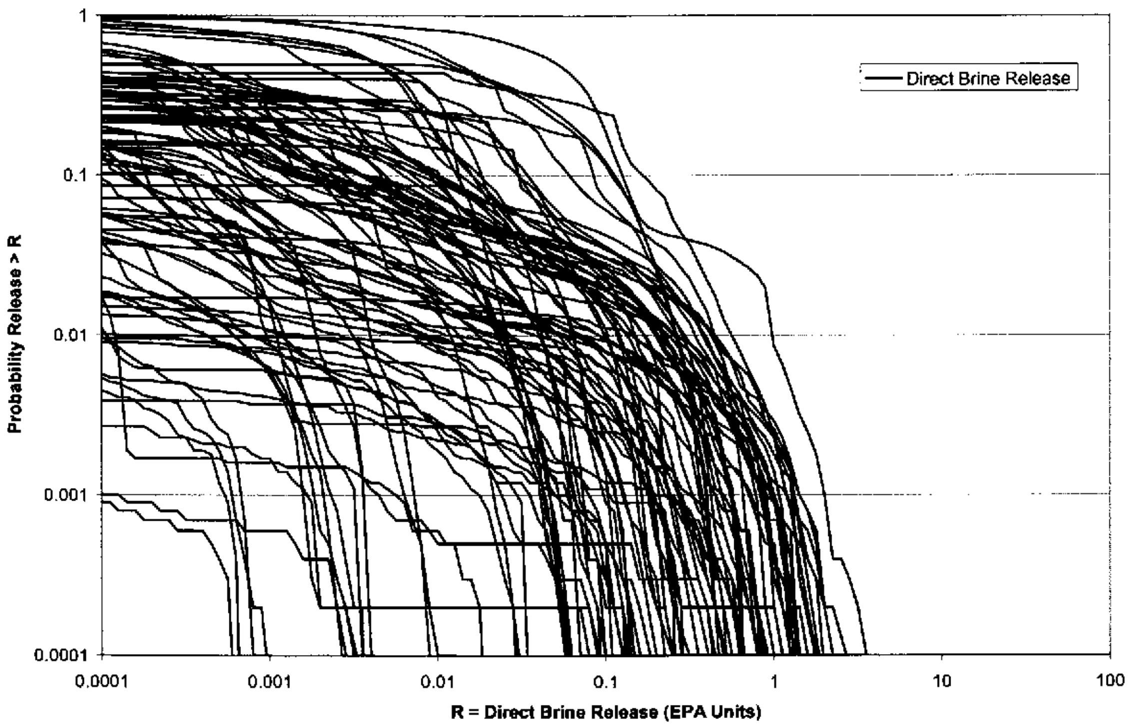

Figure 3-15: PABC-2009 Replicate 1 Normalized Direct Brine Releases

Figure 3-16: PABC-2009 Replicate 2 Normalized Direct Brine Releases

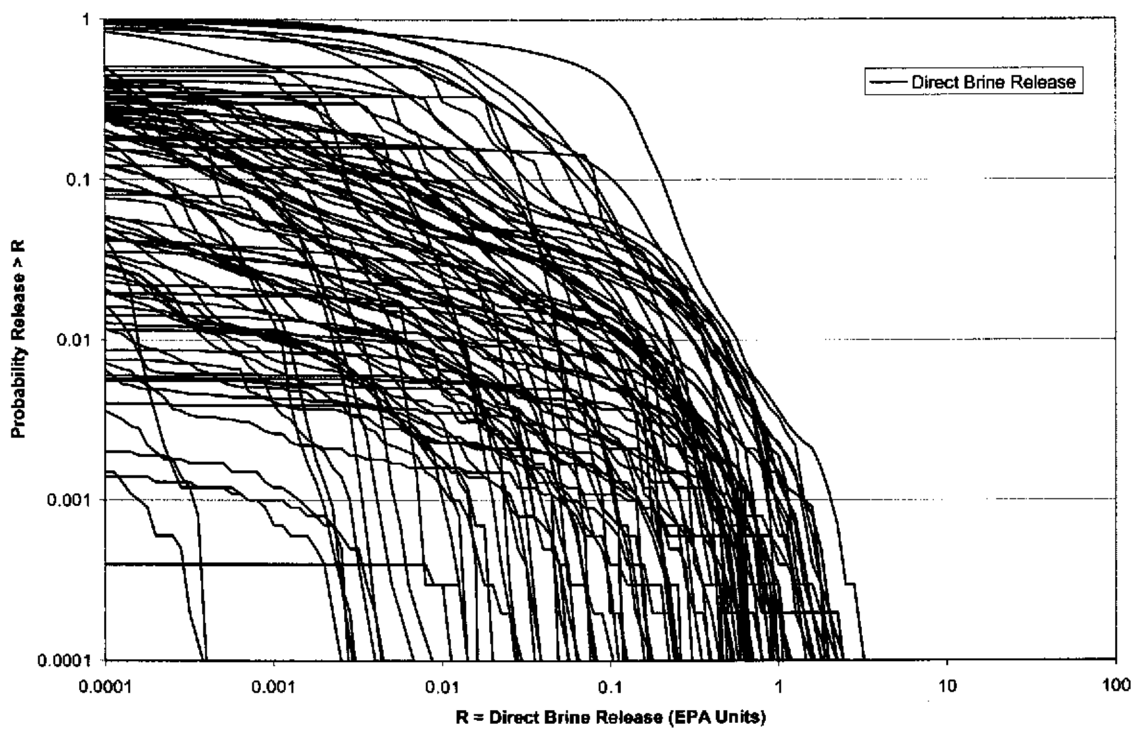

Figure 3-17: PABC-2009 Replicate 3 Normalized Direct Brine Releases

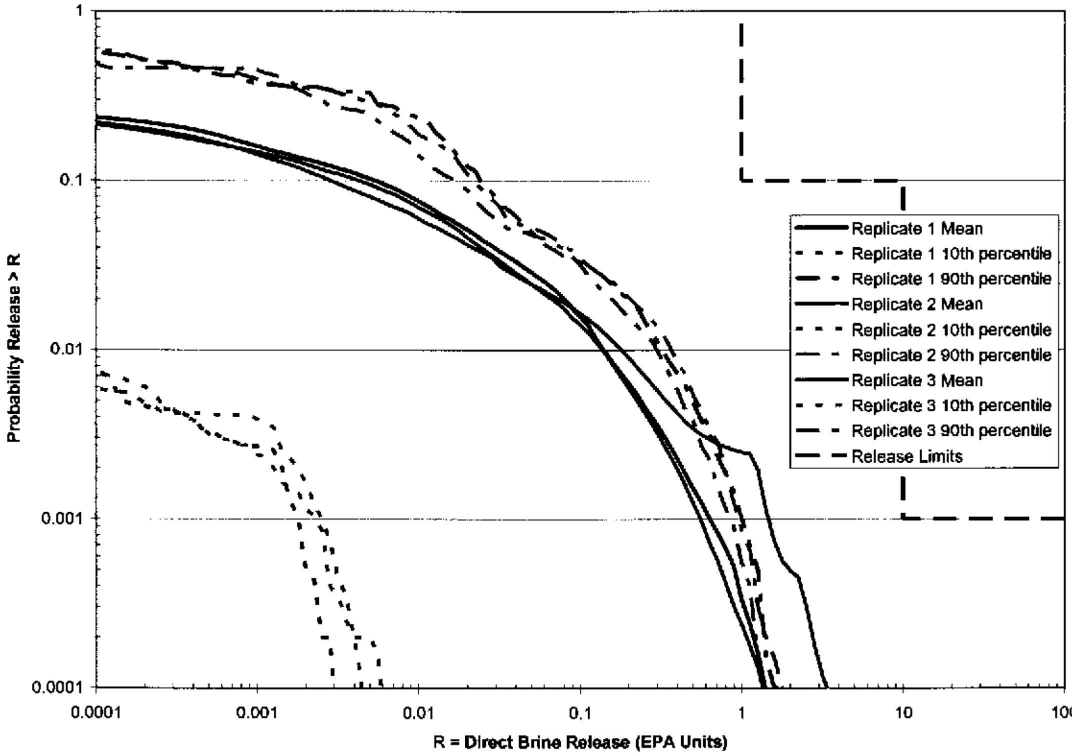

Figure 3-18: PABC-2009 Mean and Quantile CCDFs for Normalized Direct Brine Releases, Replicates 1-3

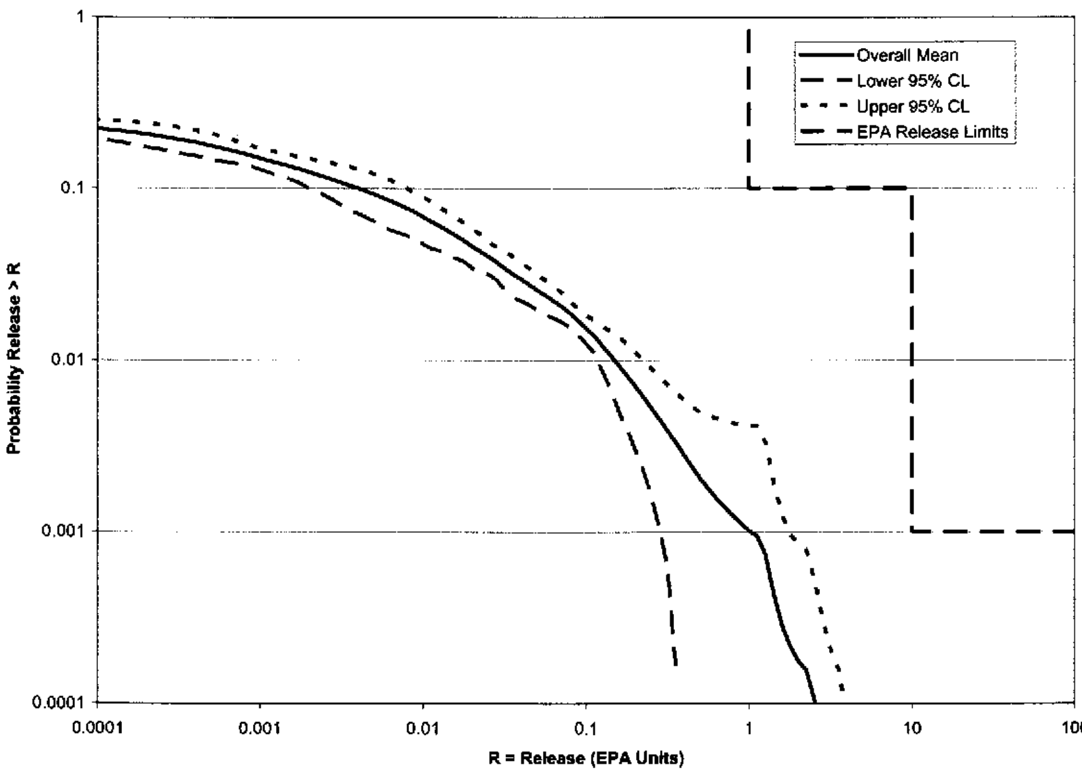

Figure 3-19: PABC-2009 Confidence Limits on Overall Mean for Normalized Direct Brine Releases

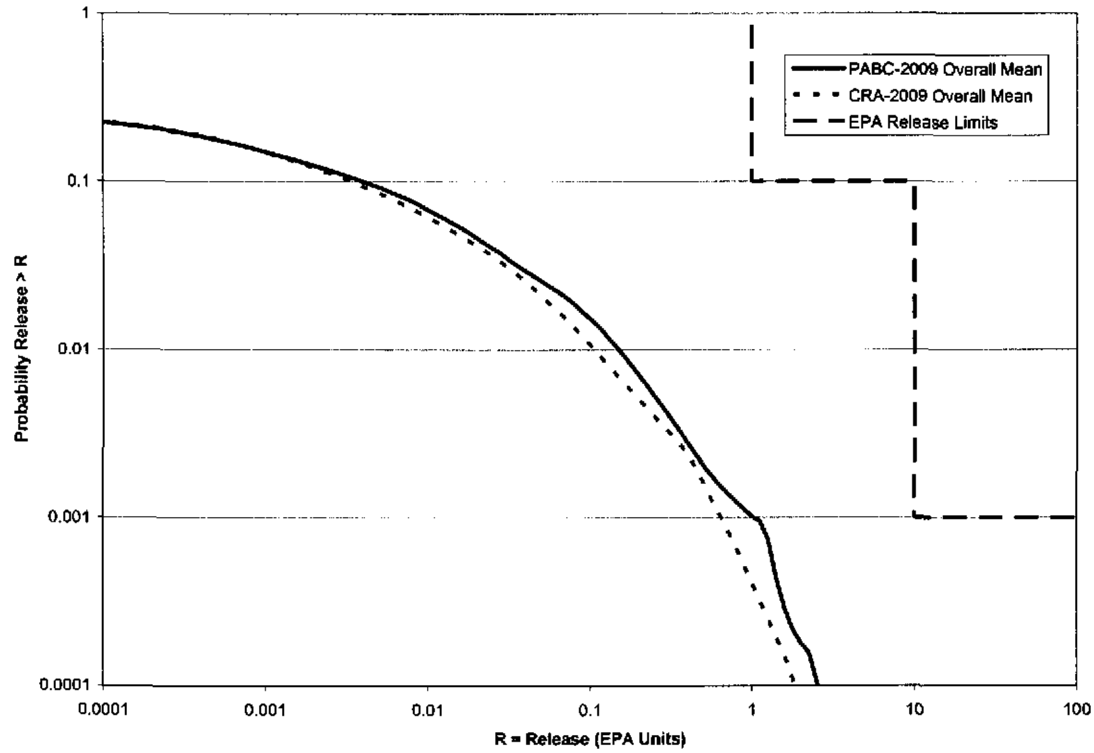

Figure 3-20: PABC-2009 and CRA-2009 Overall Mean CCDFs for Normalized Direct Brine Releases

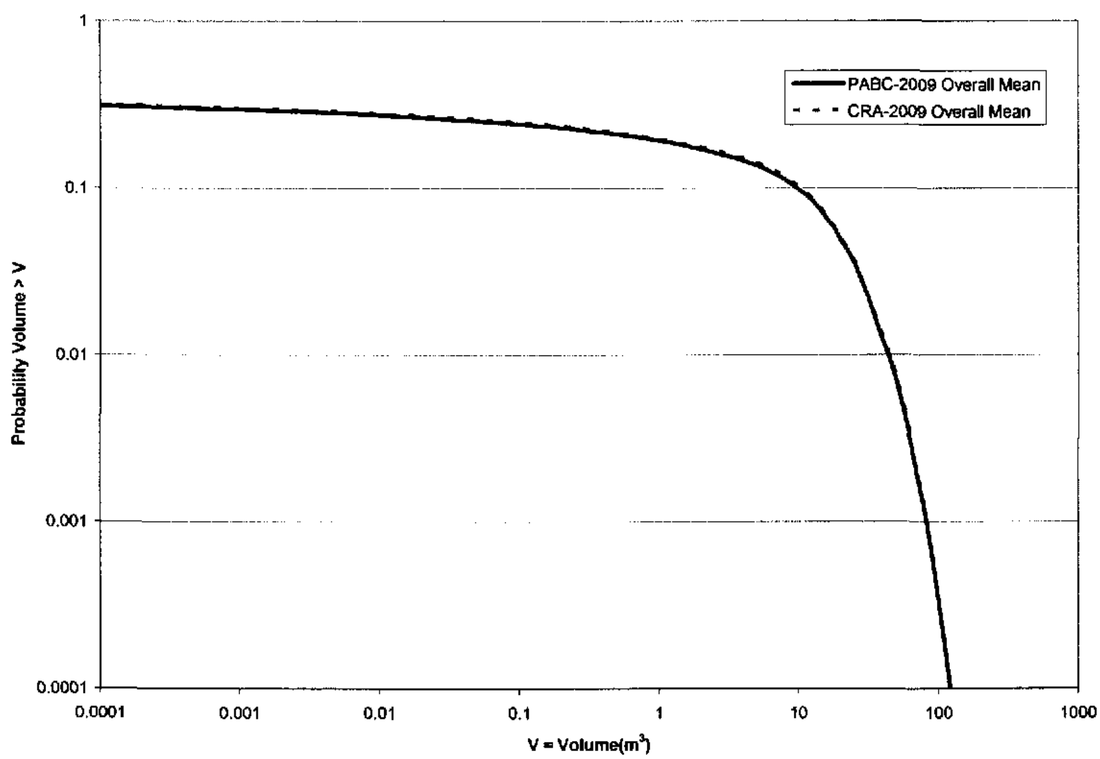

Figure 3-21: PABC-2009 and CRA-2009 Overall Mean CCDFs for Direct Brine Volumes

3.4 Normalized Transport Releases through the Culebra

PABC-2009 normalized transport releases through the Culebra are presented in this section and subsequently compared to results obtained in the CRA-2009 PA. Figure 3-22, Figure 3-23, and Figure 3-24 contain PABC-2009 CCDFs for Culebra releases to the LWB. Mean and quantile CCDF distributions for the three replicates are shown together in Figure 3-25. As seen in that figure, the 10^{th} percentiles for each replicate have releases sufficiently small as to not appear at all. The same is true of the 90^{th} percentile for replicate 3. Moreover, the mean CCDF for each replicate becomes larger than the 90^{th} percentile as releases increase. The large number of vectors with very small Culebra releases causes the distribution to be heavily right-skewed. This results in a mean that exceeds the 90^{th} percentile as releases increase. Figure 3-26 contains the 95 percent confidence limits about the overall Culebra transport mean.

None of the Culebra releases calculated in replicates 1 and 3 of the CRA-2009 PA were greater than the numerical uncertainty inherent in their calculation. Meaningful releases were only apparent in replicate 2. For the PABC-2009, however, Culebra releases were obtained for all three replicates. To facilitate comparisons of Culebra releases calculated in PABC-2009 to those obtained in the CRA-2009 PA, the CRA-2009 replicate 2 mean CCDF and the three replicate means obtained in the PABC-2009 are plotted simultaneously in Figure 3-27. For the sake of comparison, the overall Culebra transport mean CCDF obtained in PABC-2009 is also included in Figure 3-27. The overall Culebra transport mean CCDF obtained in the CRA-2009 PA is sufficiently small as to not appear in the plot at all for the chosen axis scale, and so is not included. As is evident, significantly more Culebra releases were realized in the results of PABC-2009 than were seen in the CRA-2009 PA.

There are several reasons for the increase in Culebra transport releases. As discussed in Ismail and Garner (2010), PABC-2009 maximum total releases to the Culebra are uniformly larger than those found in the CRA-2009 PA. The overall mean CCDFs of releases to the Culebra obtained in these two analyses are shown together in Figure 3-28. As is clear in that figure, the overall mean CCDF of releases to the Culebra increased in the PABC-2009. Larger releases to the Culebra seen in the PABC-2009 results are due to the higher solubilities of dissolved actinides used in their calculation.

In addition to increased releases to the Culebra, increased transport of radionuclides through the Culebra to the LWB were also obtained in the results of PABC-2009. Kuhlman (2010) attributes the increase in radionuclide transport releases to the LWB to three modifications that impact their calculation. These modifications all result in an increase in flow speed through the Culebra. First, the definition of minable potash was changed significantly in the PABC-2009, particularly inside the LWB. This resulted in minable potash ore being located in close proximity to the WIPP disposal panels. The increase in transmissivity due to mining increased the relative flow rate through the mining zones. Second, the lower limit of the matrix distribution coefficient was decreased by several orders of magnitude in the PABC-2009 calculations. This change resulted in smaller flow retardation and consequent increased flow speed. Third, a high transmissivity pathway out of the southeast portion of the LWB was present in all calibrated realizations of the MODFLOW model, creating a pathway for radionuclides to leave the LWB.

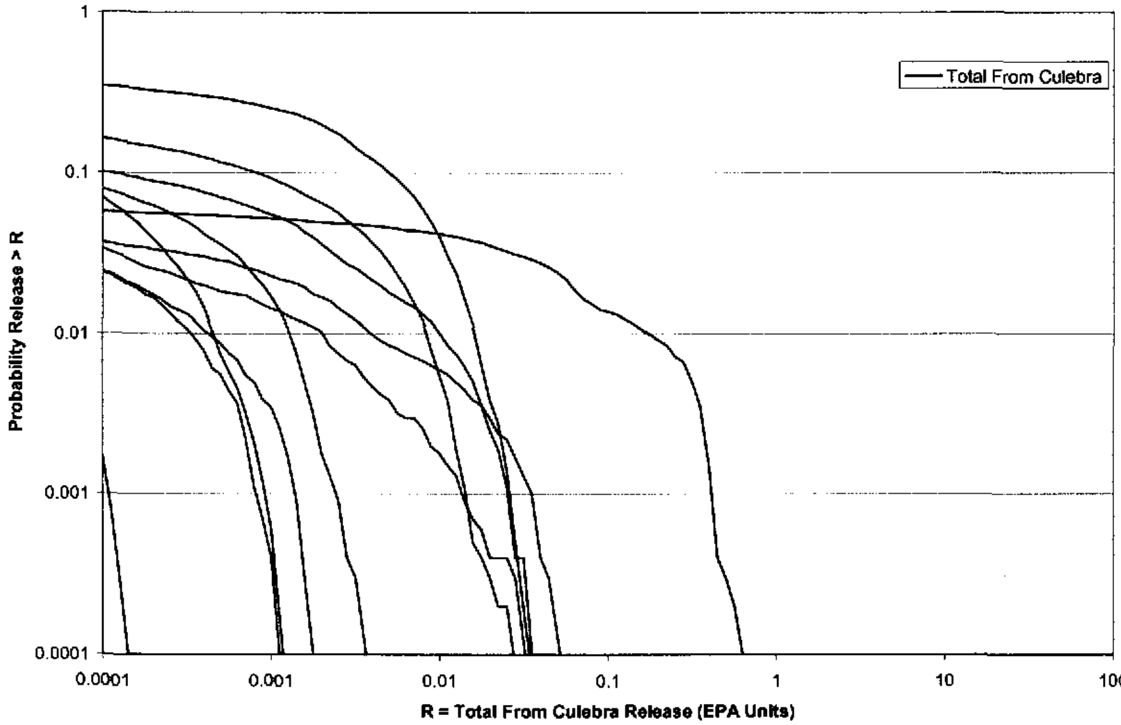

Figure 3-22: PABC-2009 Replicate 1 Normalized Culebra Transport Releases

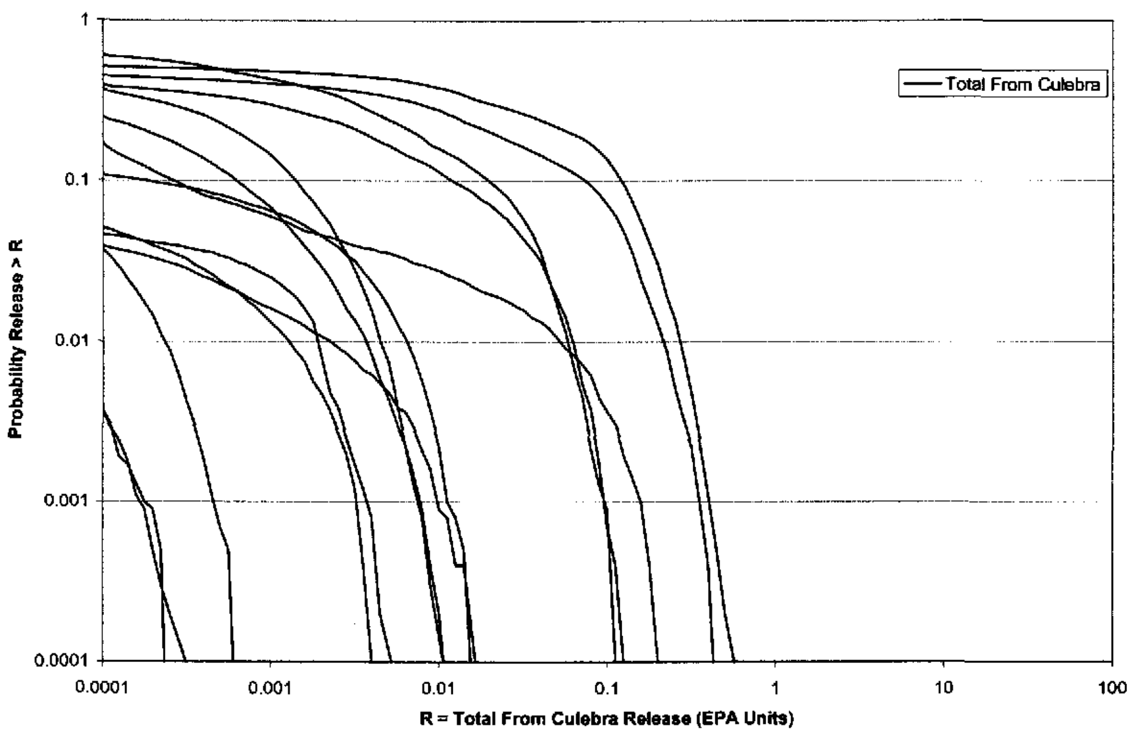

Figure 3-23: PABC-2009 Replicate 2 Normalized Culebra Transport Releases

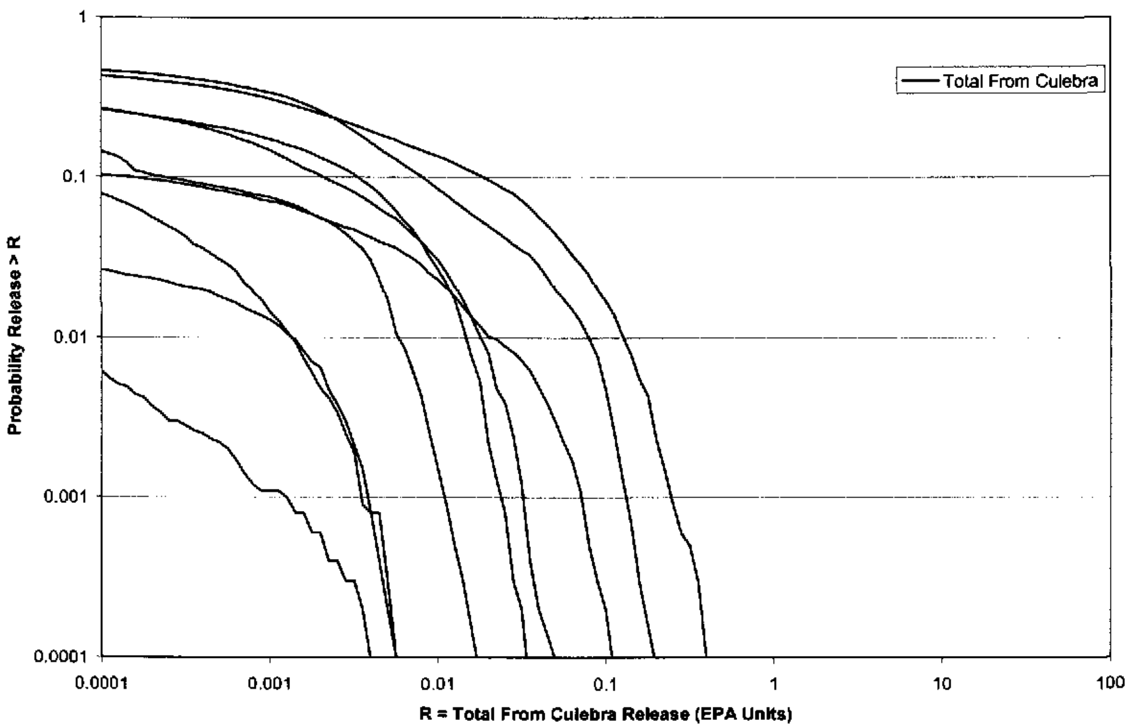

Figure 3-24: PABC-2009 Replicate 3 Normalized Culebra Transport Releases

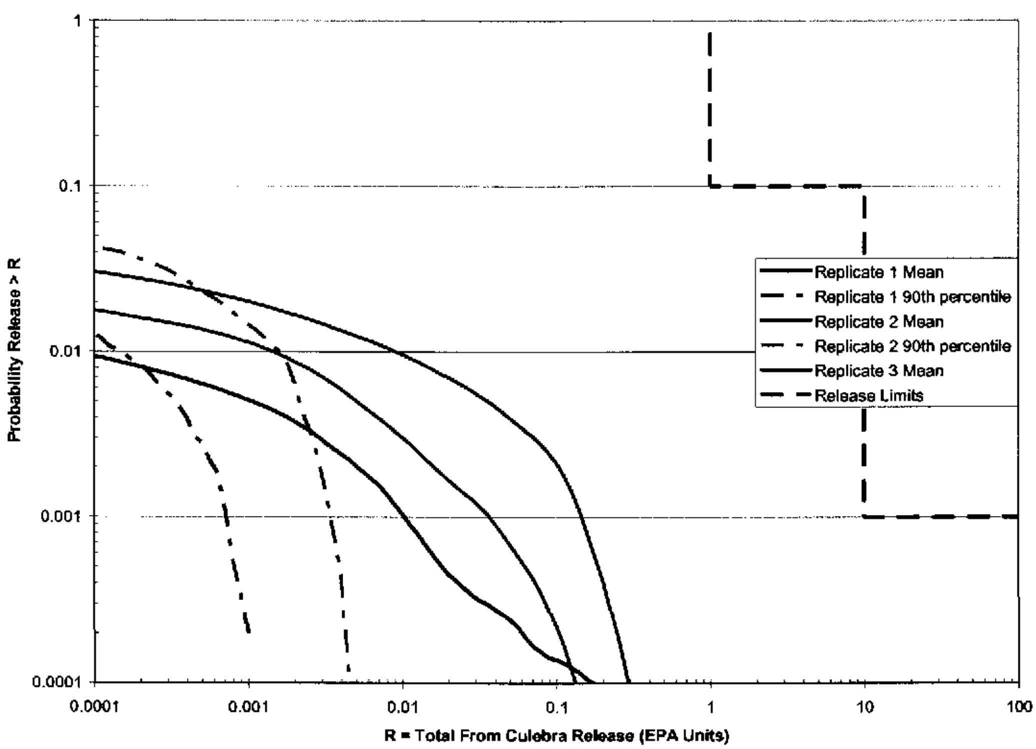

Figure 3-25: PABC-2009 Mean and Quantile CCDFs for Normalized Culebra Transport Releases, Replicates 1-3

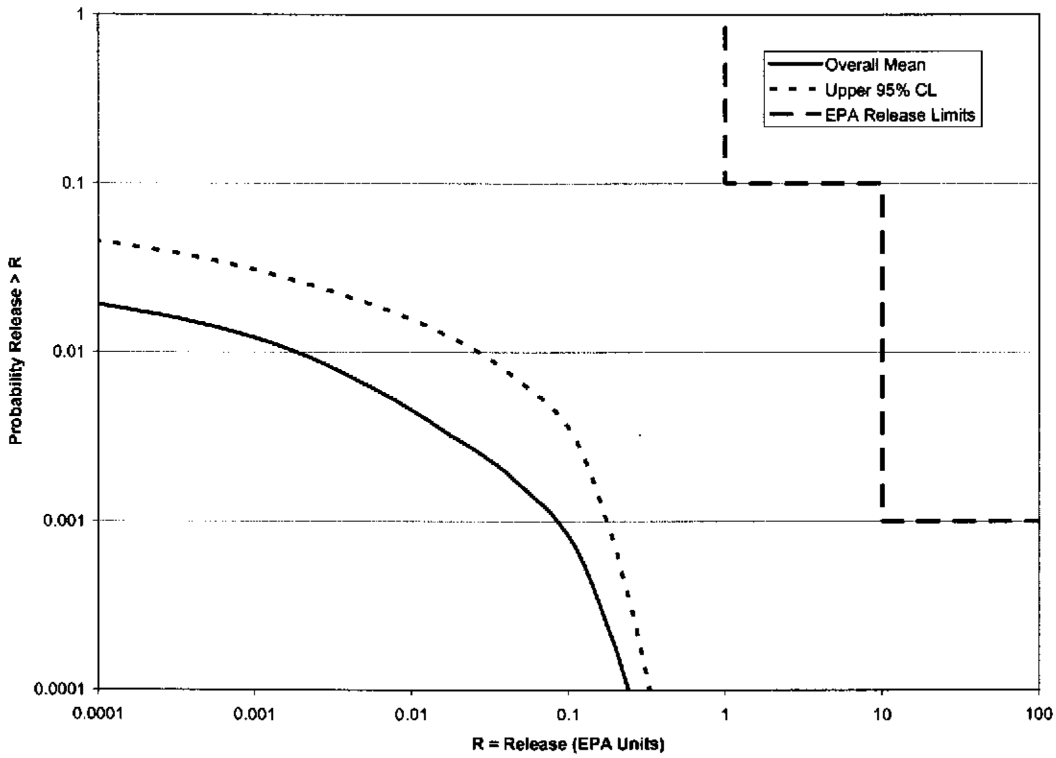

Figure 3-26: PABC-2009 Confidence Limits on Overall Mean for Normalized Culebra Transport Releases

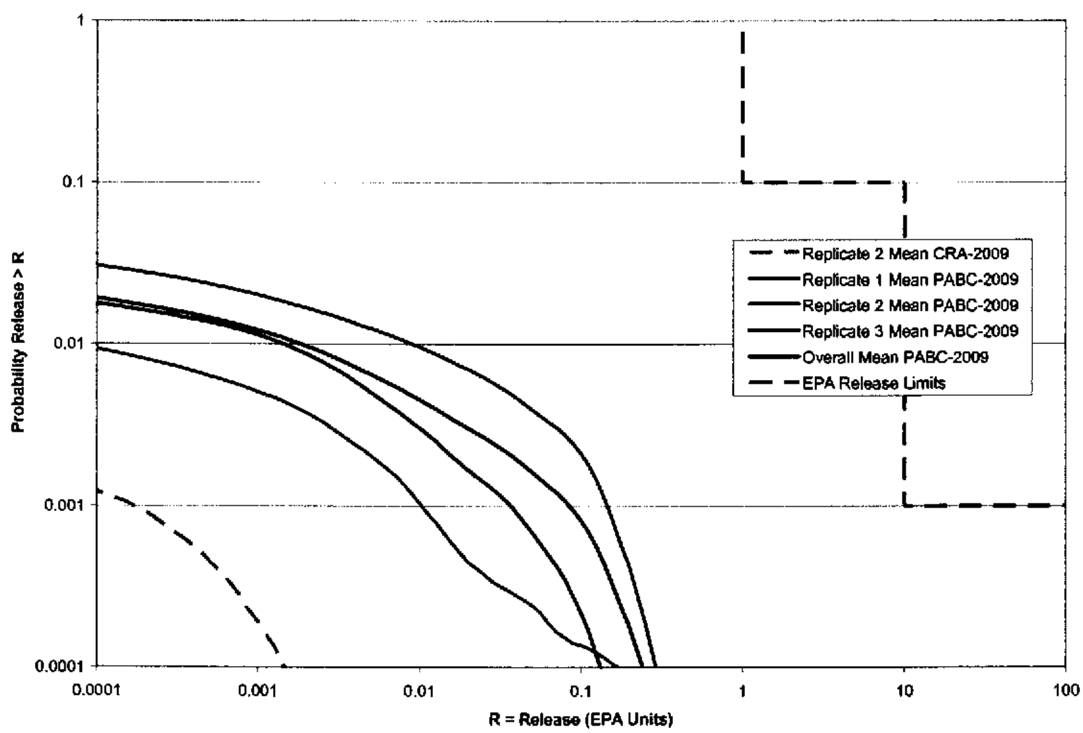

Figure 3-27: PABC-2009 and CRA-2009 Replicate Mean CCDFs for Normalized Culebra Transport Releases

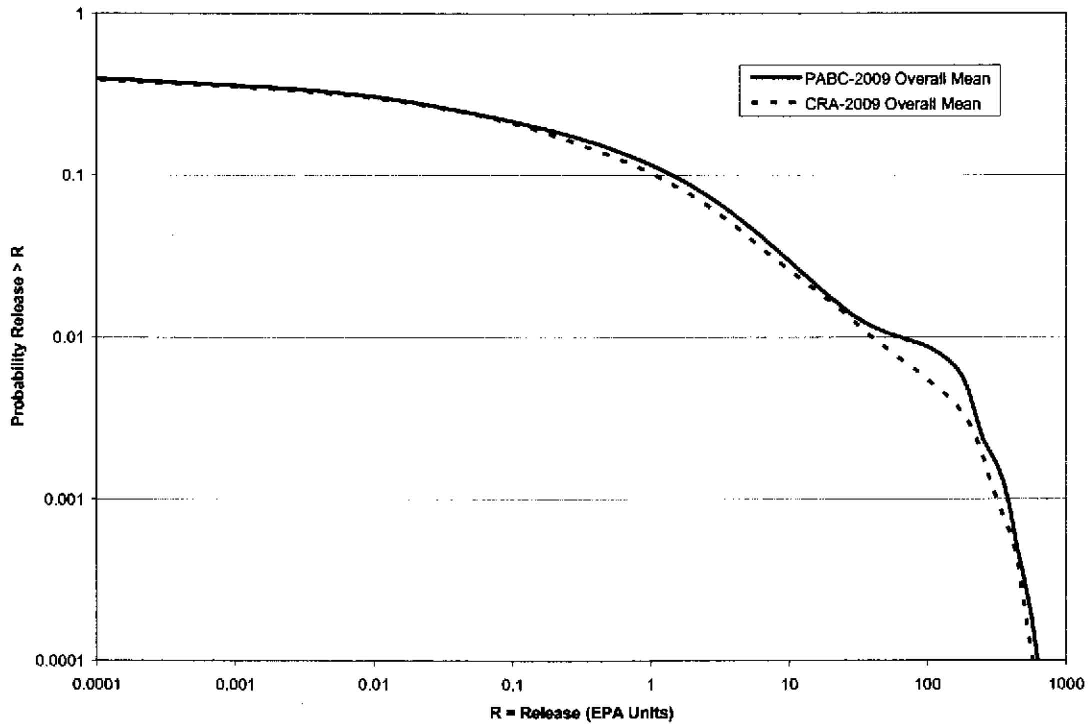

Figure 3-28: PABC-2009 and CRA-2009 Overall Mean CCDFs for Transport Releases to the Culebra

3.5 Total Normalized Releases

Total normalized releases for PABC-2009 are presented in this section and subsequently compared to results obtained in the CRA-2009 PA. 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. PABC-2009 CCDFs for total releases are presented in Figure 3-29, Figure 3-30, and Figure 3-31 for replicates 1, 2, and 3, respectively. Mean and quantile CCDF distributions for the three replicates are shown together in Figure 3-32. Figure 3-33 contains the 95 percent confidence limits about the overall transport mean.

As seen in the plot of normalized total releases for replicate 2, one vector generated a CCDF considerably different than the other 299. The outlier CCDF seen in replicate 2 for direct brine releases (see Figure 3-16) resulted in a total normalized release CCDF that exceeds one of the limits specified for acceptable releases. However, this does not result in the WIPP being out of compliance with the containment requirements. As set forth in the Certification Criteria in Title 40 CFR Part 194, compliance is specified on the overall mean and its lower/upper 95% confidence limits, not the individual vectors. As seen in Figure 3-33, the overall mean for normalized total releases and its lower/upper 95% confidence limits are well below acceptable release limits. Accordingly, the WIPP remains in compliance with the containment requirements of 40 CFR Part 191. The overall means of PABC-2009 components contributing to total releases are compared to their CRA-2009 counterparts in Figure 3-34. PABC-2009 and CRA-2009 overall mean CCDFs for total releases are compared in Figure 3-35. As seen in Figure 3-35, overall mean CCDFs obtained in PABC-2009 and the CRA-2009 PA are very similar for release values less than approximately 0.5 EPA units. For releases greater than 0.5 EPA units, the difference between the overall means obtained in the two analyses becomes more pronounced with PABC-2009 total releases being greater than those seen in the CRA-2009 PA. By examining the release components compared in Figure 3-34, the primary source of the difference is clear. For release values less than roughly 0.5 EPA units, PABC-2009 increases in overall mean CCDFs for DBRs and transport releases are effectively cancelled by reductions in the overall mean CCDFs for spallings as well as cuttings and cavings. Total releases greater than 0.5 EPA units are due to DBRs. The increase in the PABC-2009 overall mean for DBRs for releases greater than 0.5 EPA units results in a corresponding increase in the overall mean CCDF for total releases. A comparison of the statistics on the overall mean for total normalized releases obtained in the PABC-2009 and the CRA-2009 PA (Dunagan 2008) can be seen in Table 1. At a probability of 0.1, values obtained for the mean total release are very similar in both analyses with PABC-2009 values being slightly less. At a probability of 0.001, the increase in DBRs seen in the PABC-2009 calculations resulted in an increase in the mean total release of approximately 0.4 EPA units.

Probability	Analysis	Mean Total Release	90th Percentile	Lower 95% CL	Upper 95% CL	Release Limit
0.1	CRA-2009 PA	0.10	0.17	0.10	0.11	1
	PABC-2009	0.09	0.16	0.09	0.10	1
0.001	CRA-2009 PA	0.72	0.81	0.48	0.92	10
	PABC-2009	1.10	1.00	0.37	1.77	10

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

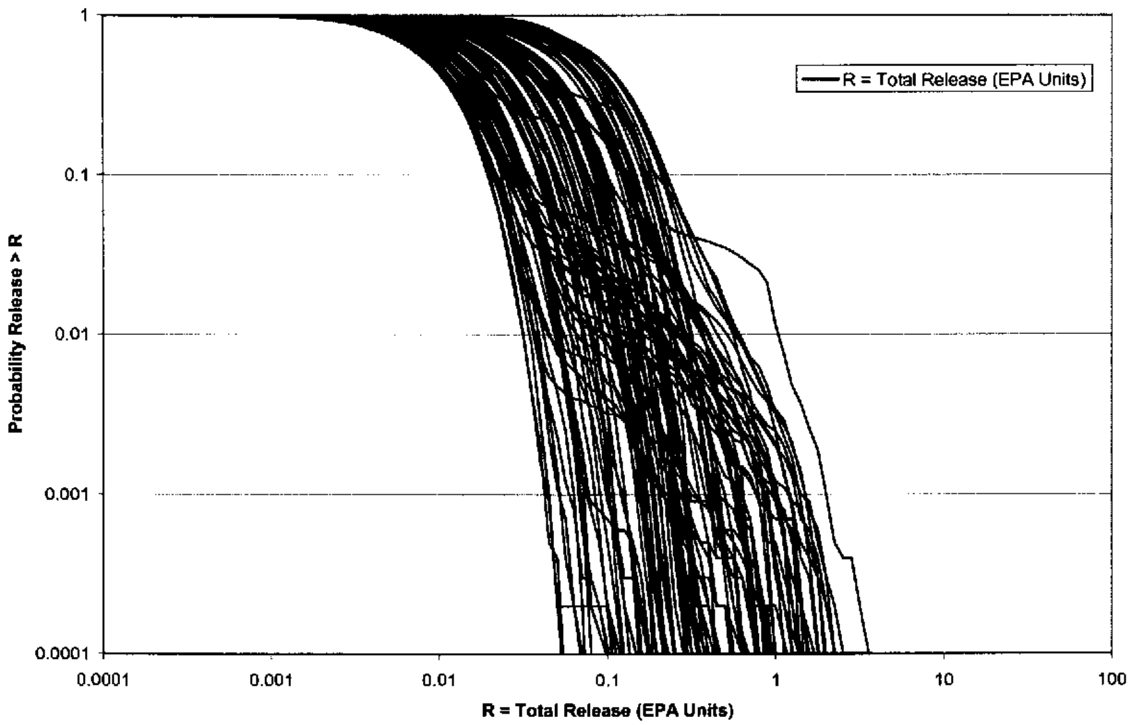

Figure 3-29: PABC-2009 Replicate 1 Total Normalized Releases

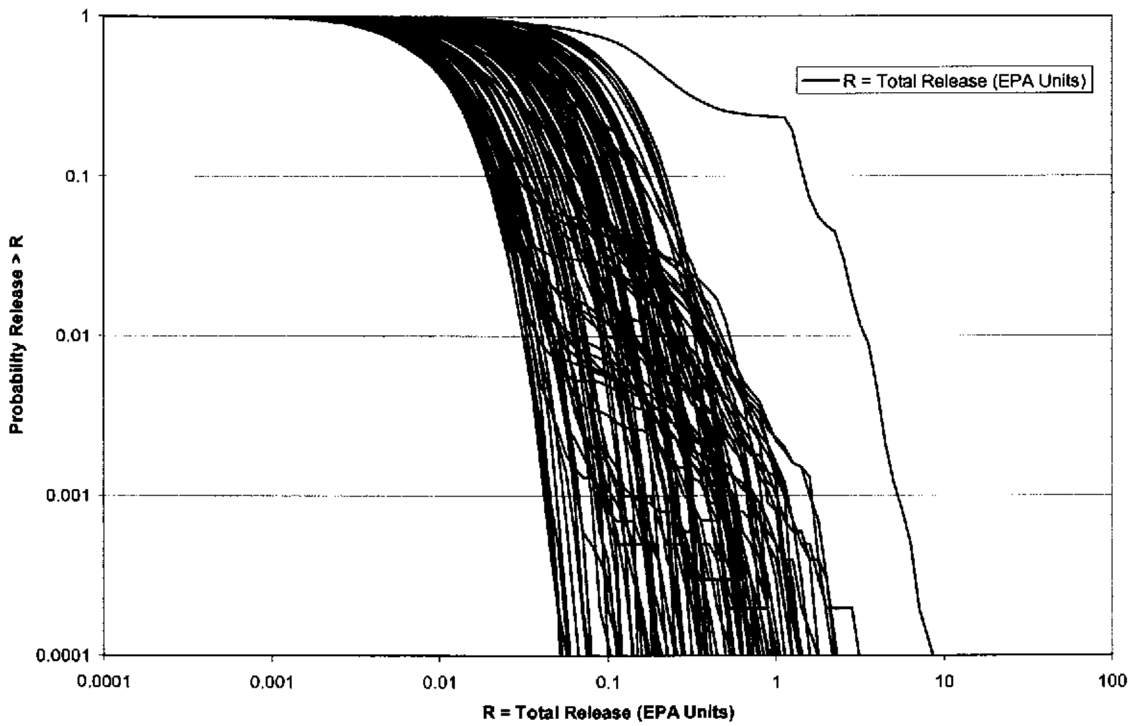

Figure 3-30: PABC-2009 Replicate 2 Total Normalized Releases

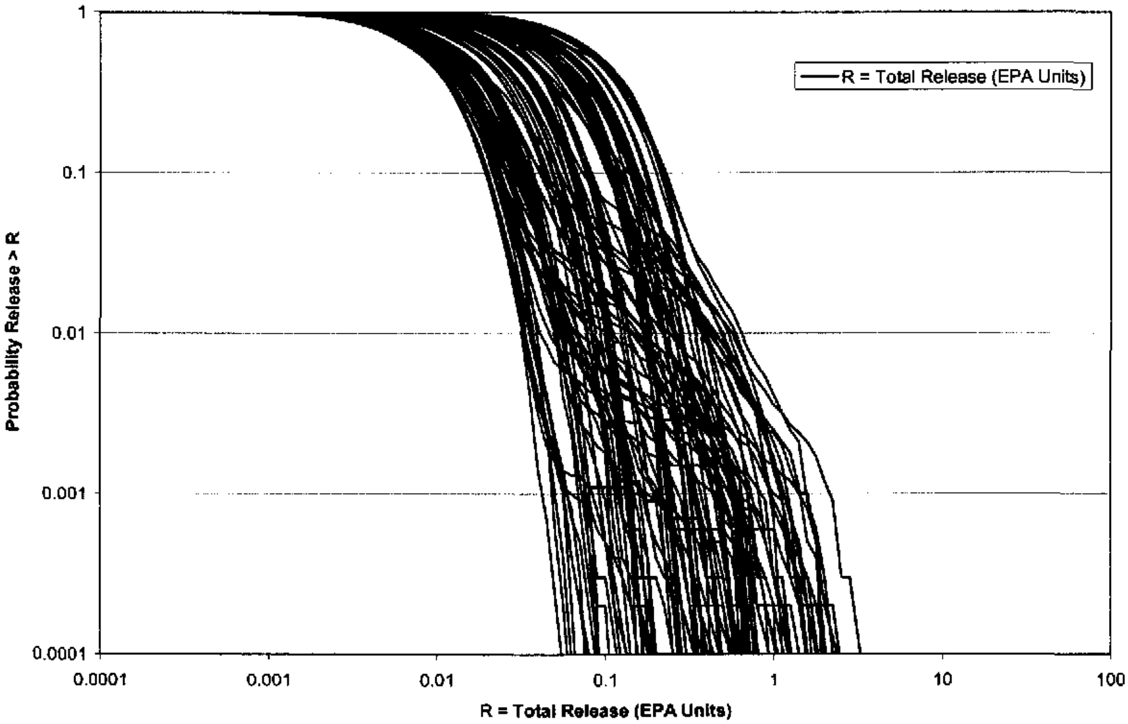

Figure 3-31: PABC-2009 Replicate 3 Total Normalized Releases

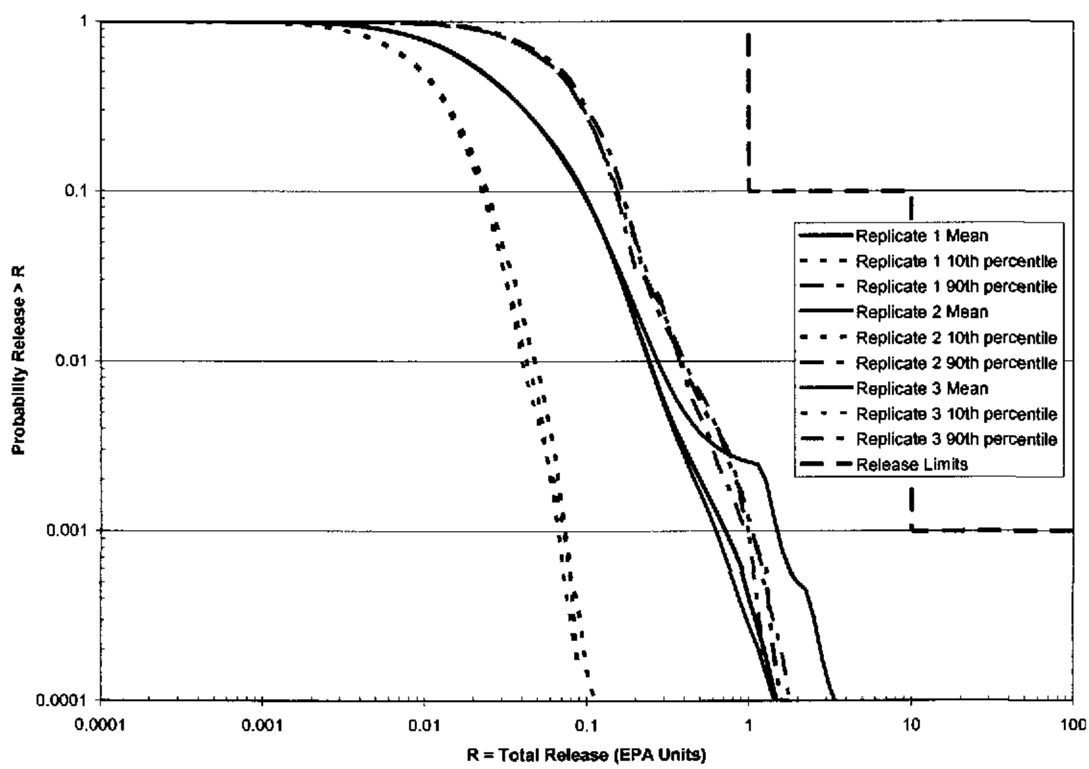

Figure 3-32: PABC-2009 Mean and Quantile CCDFs for Total Normalized Releases, Replicates 1-3

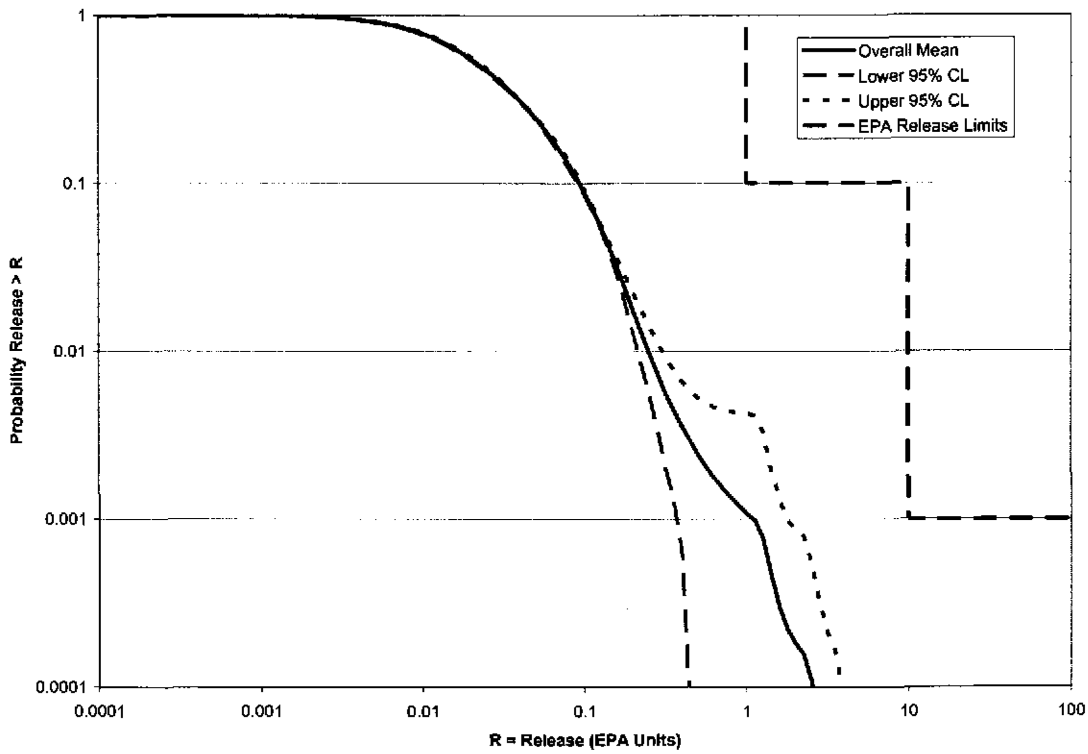

Figure 3-33: PABC-2009 Confidence Limits on Overall Mean for Total Normalized Releases

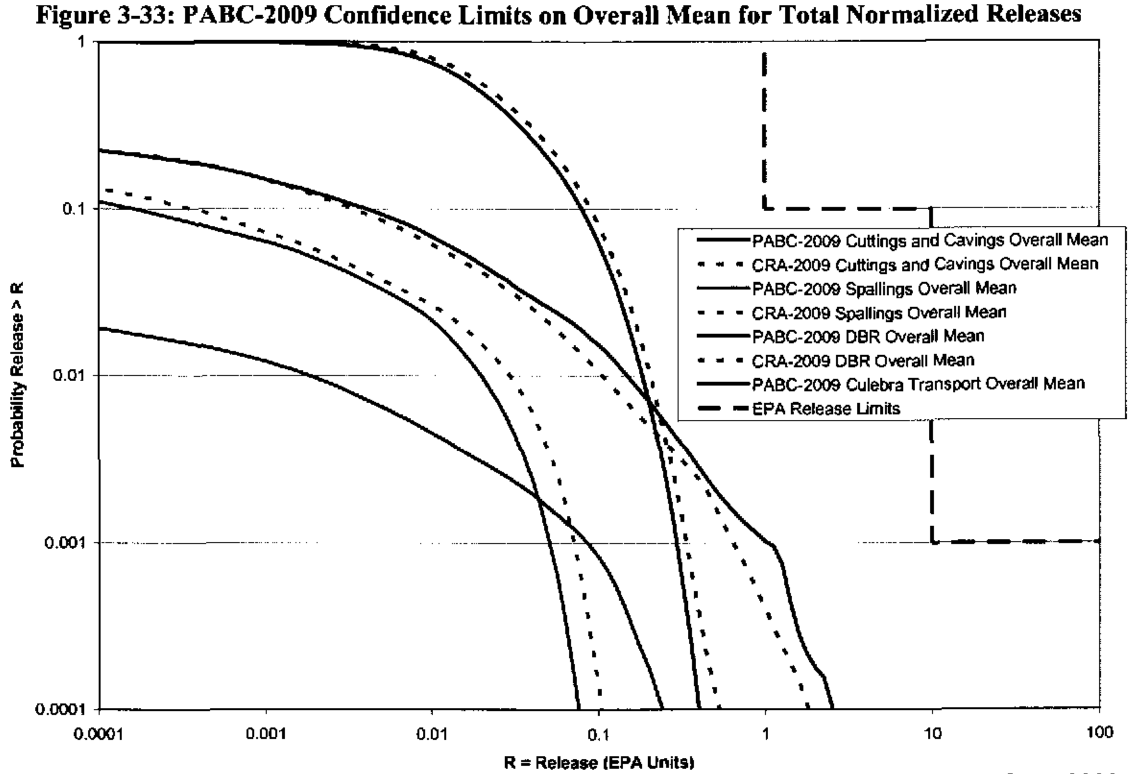

Figure 3-34: Comparison of Overall Means for Release Components of PABC-2009 and CRA-2009

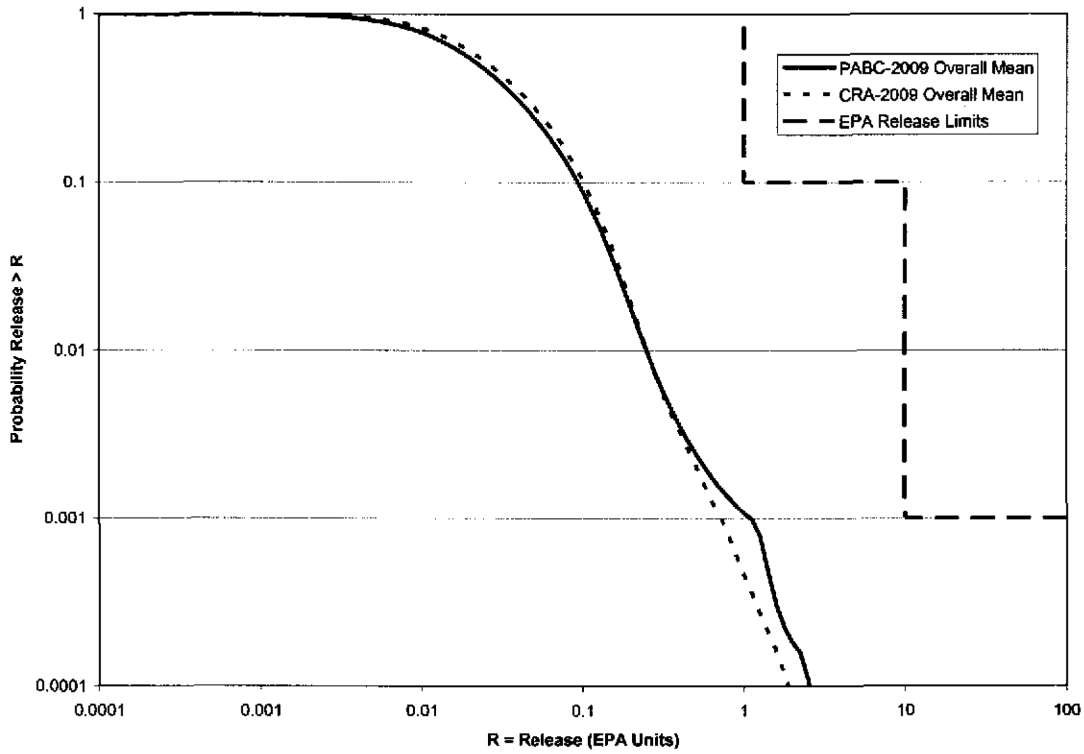

Figure 3-35: PABC-2009 and CRA-2009 Overall Mean CCDFs for Total Normalized Releases

4 Summary

Total normalized releases calculated in PABC-2009 remain below their regulatory limits. As a result, the WIPP remains in compliance with the containment requirements of 40 CFR Part 191. Cuttings and cavings, direct brine, and spallings releases continue to have the highest probability of release. Releases to the LWB resulting from subsurface transport of radionuclides through the Culebra increased in the PABC-2009 results because of an increase in releases to the Culebra as well as modifications in the transport calculations that resulted in increased flow speed through the Culebra. Direct brine releases increased in the PABC-2009 results due to an increase in actinide solubilities used in their calculation while DBR volumes were unchanged. PABC-2009 spallings volumes and releases were lower than those seen in the CRA-2009 PA because of slightly lower repository pressures in the undisturbed scenario observed in the PABC-2009 calculations. PABC-2009 cuttings and cavings releases and volumes are similar to those found in the CRA-2009 PA with slightly lower PABC-2009 releases being seen due to reduced waste levels in the updated repository inventory.

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