

SOARCA Peach Bottom Atomic Power Station Long-Term Station Blackout Uncertainty Analysis: Convergence of the Uncertainty Results

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Abstract: This paper describes the convergence of MELCOR Accident Consequence Code System, Version 2 (MACCS2) probabilistic results of offsite consequences for the uncertainty analysis of the State-of-the-Art Reactor Consequence Analyses (SOARCA) unmitigated long-term station blackout scenario at the Peach Bottom Atomic Power Station. The consequence metrics evaluated are individual latent-cancer fatality (LCF) risk and individual early fatality risk. Consequence results are presented as conditional risk (i.e., assuming the accident occurs, risk per event) to individuals of the public as a result of the accident. In order to verify convergence for this uncertainty analysis, as recommended by the Nuclear Regulatory Commission's Advisory Committee on Reactor Safeguards, a 'high' source term from the original population of Monte Carlo runs has been selected to be used for: (1) a study of the distribution of consequence results stemming solely from epistemic uncertainty in the MACCS2 parameters (i.e., separating the effect from the source term uncertainty), and (2) a comparison between Simple Random Sampling (SRS) and Latin Hypercube Sampling (LHS) in order to validate the original results obtained with LHS. Three replicates (each using a different random seed) of size 1,000 each using LHS and another set of three replicates of size 1,000 using SRS are analyzed. The results show that the LCF risk results are well converged with either LHS or SRS sampling. The early fatality risk results are less well converged at radial distances beyond 2 miles, and this is expected due to the sparse data (predominance of "zero" results).

Keywords: SOARCA, MACCS, Uncertainty Analysis, Accident Consequence Analysis, Convergence

1. SOURCE TERM SELECTION

In order to test the influence of uncertain MACCS2 parameters by themselves for the SOARCA Uncertainty Analysis for the Peach Bottom unmitigated long-term station blackout scenario (documented in draft NUREG/CR-7155 [1]), three representative source terms were selected first, in order to rule out potential dependencies on a specific source term. Each of these was used as a reference source term in a Monte Carlo simulation in which only MACCS parameters were varied.

The selection of these source terms required an initial MACCS2 run in which all previously 865 source terms were used while all MACCS2 uncertain parameters were set to nominal values (SOARCA point estimates). This way it was possible to assess the influence of the source term when MACCS parameters are fixed. A set of 11 results were then used as metrics to select the three representative source terms:

- Latent Cancer Fatality (LCF) at 5 different locations (10, 20, 30, 40 and 50 miles)
- Fraction of inventory released for 5 radionuclides (Cs, I, Ba, Ce, Te)
- Release time

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The ensemble of possibility (prob=1) was decomposed into three equal groups ([0,1/3], [1/3,2/3] and [2/3,1]) and the mid-point quantile of each group was used as the ideal theoretical value (i.e., $q_1=1/6$, $q_2=1/2$ and $q_3=5/6$) to identify a representative (1) “low,” (2) “medium,” and (3) “high” source term. Amongst the 865 results generated, the following needed to be selected:

- One realization such as its position for all the metrics is close to $q_1=1/6$
- One realization such as its position for all the metrics is close to $q_2=1/2$
- One realization such as its position for all the metrics is close to $q_3=5/6$

One additional constraint added to the problem was that the metrics were not weighed to be equally important. For example, LCF results were considered more important (they are the final result of interest) than fractions of radionuclides released, and release time was considered the least important metric.

1.1 Methodology

Each of the 865 calculations generated a result for all the 11 metrics considered. For each realization the result for each metric was replaced by its quantile position, based on the 865 results. The value was ranked with respect to the 864 other values and normalized by 865. Therefore, each realization was associated with 11 quantile positions (one for each metric).

$$Q_i = \{q_{1,i}, q_{2,i}, \dots, q_{10,i}, q_{11,i}^*\} \quad (1)$$

Where i represents the realization number, Q_i the set of quantiles associated with realization i and $q_{j,i}$ the quantile associated with metric j for realization i . As release time influence is inverse from the other metrics (the earlier the release time, the worse it is), a reserve quantile ($q^*=1-q$) has been used for this metric. The importance of each metric is determined via a weight factor:

$$W = \{w_1, w_2, \dots, w_{11}\} \quad (2)$$

Where W represents the set of weights and w_j the weight associated with metric j .

Three normalized distances (based on the L^2 norm) are estimated for each realization, one for each of the theoretical quantiles, via the following formula:

$$d_{i,k} = \sqrt{\frac{\sum_{j=1}^{11} w_j (q_{j,i} - q_k)^2}{\sum_{j=1}^{11} w_j}} \quad (3)$$

Where k represents the theoretical quantile reference number, q_k the quantile for reference k . For each reference k the realization leading to the minimum of $d_{i,k}$ is selected as representative for the set. It will be the one that minimizes the difference between the theoretical quantile and actual quantile (in the L^2 norm sense) according to the weight of importance.

1.2 Selection of the Weight

The weights were selected for each metric to represent the importance of the metric relative to the others according to the analyst. One important point, when the weights are chosen, is to consider the eventual correlations amongst the results. LCF results will be correlated (and some more strongly than other). For strongly correlated results (beyond 0.9 for instance), the group can be considered as a single metric, and the weights associated to each member of the group will be added to the influence to the group. As an

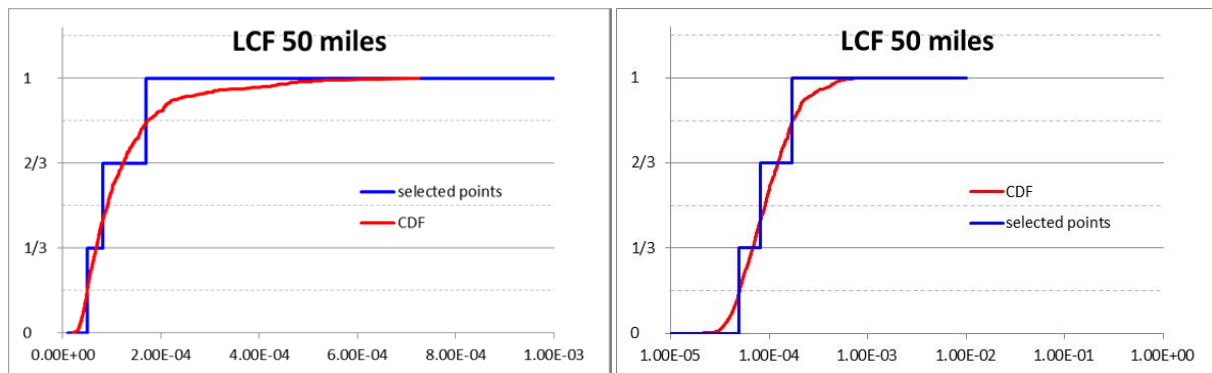
example, LCF at 50 miles and LCF at 40 miles results have a correlation of 0.999 (essentially correlation of 1). Associating a weight of 1 to both of these metrics will be equivalent to associating a weight of 2 for the group consisting of these two metrics.

1.3 Checking of Results

Once the realizations are selected, one can check how good the selection is, with the selected set of weights, for example, using two graphical methods.

The first one is a cumulative distribution function (CDF) comparison for each metric. The CDF resulting from the 865 values is plotted for each metric. On top, a CDF consisting of the three selected realizations is displayed. The analyst can then check how good the fit is between the two CDFs. A good fit will be obtained if the distance between the two CDFs is small. Another point of reference to evaluate the goodness of fit is to check whether the CDFs cross at or close to the selected quantiles (1/6, 1/2 and 5/6). An example for LCF for a 50 miles radius is displayed in Figure 1.

Figure 1: Example of CDFs Comparison in Linear Scale (left) and Semi-log Scale (right)



The second one uses a Cobweb to represent how far the selected realizations are from the theoretical quantiles (see Figure 2). The three selected realizations' quantile curves are in color thick blue, green, and red lines, the theoretical quantiles in dot-dashed dark lines and a set of 150 realizations are displayed in thin gray lines as reference.

1.4 Cobweb Results

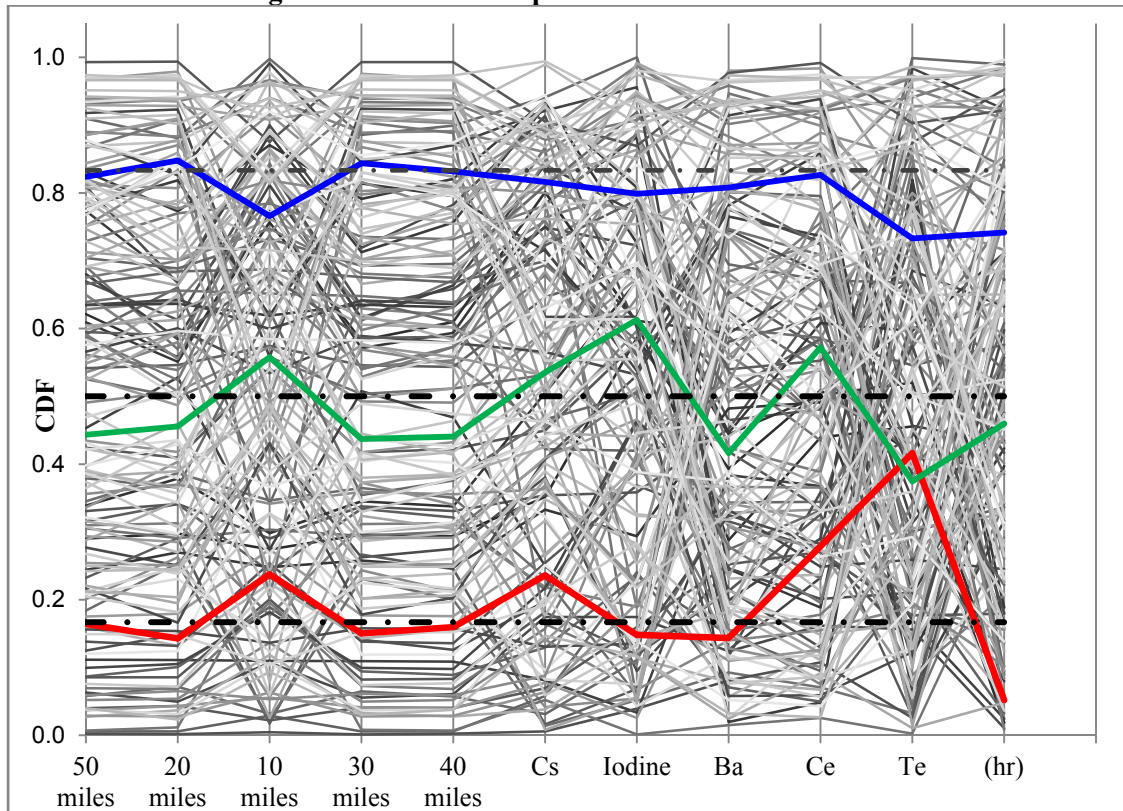
The selection of these three source terms are based on the results for 11 input and output parameters. Each of these 11 parameters is assigned an importance factor based on their respective CDFs (i.e., conditional LCF risk, radionuclides, and release timing). The 11 parameters are shown in Table 1 with their respective weighting factor.

The source terms selected try to best represent 1/3 of the total CDF's considered, by trying to best correspond to the 17th, 50th, and 83rd percentiles for each of the 11 parameters considered. Figure 2 shows a cobweb graph for the low (red line), medium (green line), and high (blue line) source terms selected. In Figure 2, each of the source terms shows their respective representation to the parameters considered and their corresponding CDF information.

Table 1: Parameters and Weighting (0.0 to 1.0) for Source Term Selection

Conditional, Mean, Individual LCF Risk (per Event) at:				
50 miles	20 miles	10 miles	30 miles	40 miles
1	0.3	0.6	0.1	0.1
Radionuclide Group				
Cesium	Iodine	Barium	Cerium	Tellurium
0.6	0.3	0.3	0.1	0.1
Environmental Release Time (hour)				
0.1				

Figure 2: Cobweb Graph for Selected Source Terms



2. WEATHER UNCERTAINTY & CONVERGENCE

For the five source terms considered from NUREG/CR-7155 (highest early fatality risk source term, highest LCF risk source term, and three high/medium/low source terms selected by the methodology described in Section 1), three LHS runs of 1,000 samples using all 350 MACCS2 uncertain input variables were conducted. As part of this analysis, the distribution across the sampled weather is considered. Table 2 provides the average percent difference in results across the weather distribution for each of the source terms considered. The largest deviation between the three LHS runs is observed for the 0-10 mile radial distance to be the ‘low’ source term (4.5%) at the 99th percentile, and for the 0-50 mile radial distance it is observed for the ‘medium’ source term (8.5%) at the 99th percentile. Considering that these largest variations occur at the extreme percentiles and are still relatively low, and that the average differences in spread of results are low (on the order of 1%), it is judged that the MACCS2 model is well converged for LCF risk with respect to weather uncertainty.

Table 2: Average difference between the three separate LHS runs over all Aleatory Weather Distributions (1st to 99th percentile)

Source Term	Conditional LCF Risk 0-10 miles	Conditional LCF Risk 0-50 miles
Highest Early Fatality Risk	0.8%	0.8%
Highest LCF Risk	0.8%	0.9%
Low (17 th percentile)	0.9%	0.8%
Medium (50 th percentile)	0.8%	0.9%
High (83 rd percentile)	1.0%	0.6%
Overall Average	0.9%	0.8%

3. STABILITY ANALYSIS USING BOOTSTRAP APPROACH

The ‘high’ source term was used for a comparison between SRS and LHS in order to validate the use of LHS. In addition to the three MACCS2 replicates of size 1000 each using LHS (called CAP 34, CAP 35, and CAP 36), another set of three replicates were run using the same sample size and same random seed, but using SRS (called CAP 37, CAP 38, and CAP 39).

Conditional, mean, individual LCF risks (per event) for the 10-mile the 50-mile radial distance were considered for this analysis. Each CDF was estimated three times using a different random seed. Bootstrapping was used on each of the three replicated CDFs, and for each radial distance considered, to generate a distribution of 1000 possible CDFs. This set of CDFs was used to estimate a 95% confidence interval (i.e., the confidence interval is centered, so using the 2.5th and 97.5th percentiles) for each replicate.

In order to estimate the stability of results, one replicate’s CDF is displayed along with the confidence intervals for the two other replicates. Having the replicate CDF within the confidence interval defined by two other replicates (i.e., the other two replicates used a different random seed) can be considered a good test of stability. Furthermore, the distribution of mean value based on bootstrap has been displayed for all three replicates, with the density estimated via binning for one of the replicates. This is presented in Figure 3 and Figure 4 for the 10-mile and 50-mile radial distances, respectively. This comparison provides information on the stability of the mean result for a sample of size 1000. Two things are considered at this level: (1) How close are the means, and (2) How close to a normal distribution is the density function.

Figure 3: 10-mile Conditional, Mean, Individual LCF Risk (per Event) CDFs for the ‘High’ Source Term with All Three Random Seeds with SRS and the Density Function for Random Seed 1 with SRS

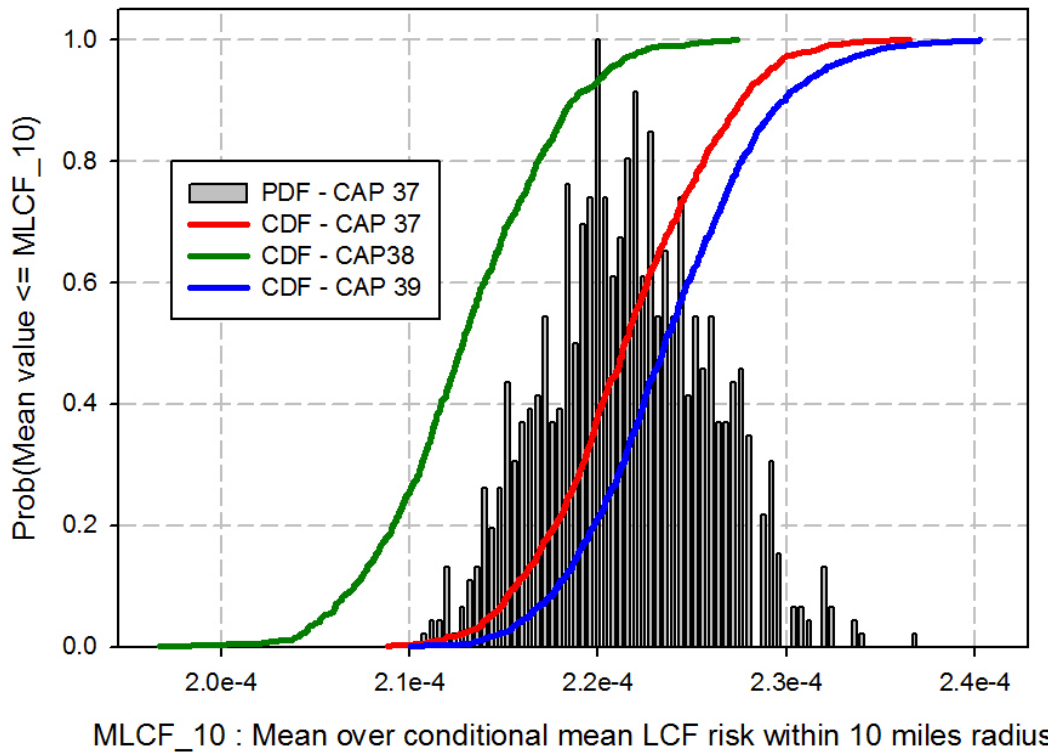
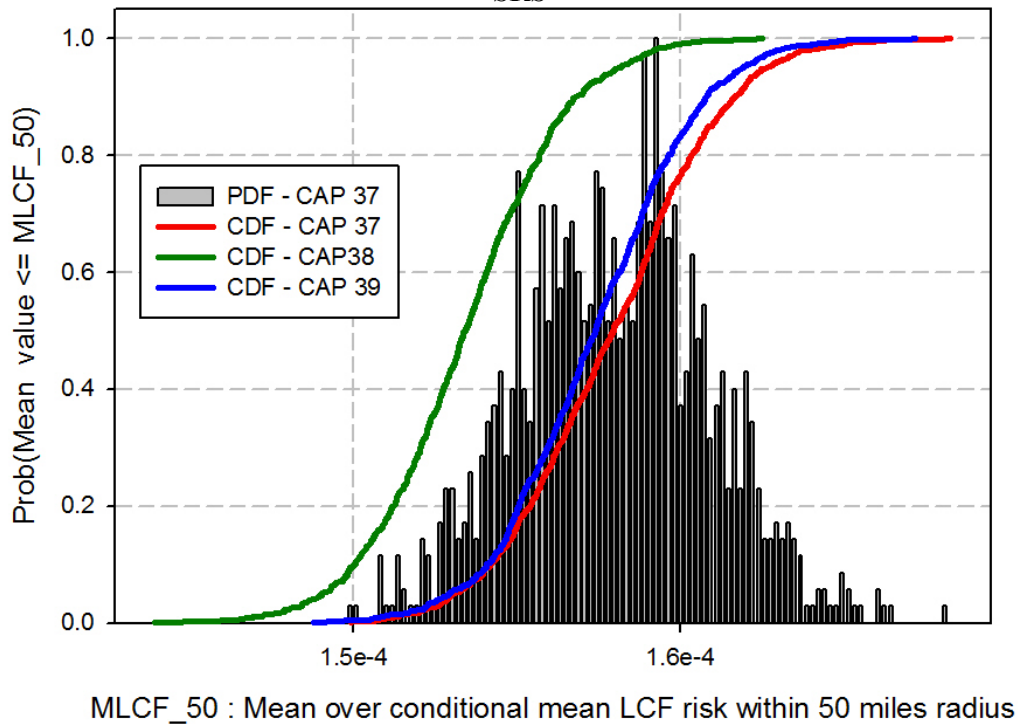


Figure 4: 50-mile Conditional, Mean, Individual LCF Risk (per Event) CDFs for the ‘High’ Source Term with all Three Random Seeds with SRS and the Density Function for Random Seed 1 with SRS



Several analyses have demonstrated the faster convergence of LHS results compared to SRS (i.e., see Reference [2] for an example). One of the limitations of LHS compared to SRS is, however, with respect to the use of bootstrapping to estimate confidence intervals over estimators. Bootstrapping assumes that the set of observations used is from an independent and identically distributed population. While the LHS stratification enforces the identical distribution, it violates the independency statement; as each stratum is only used once. This means that each stratum already used cannot be used again and such action creates dependency in the sampling.

While it is theoretically not appropriate to use bootstrapping on LHS results, an original sample size of 1000 can be considered large enough so that a selection of values (with replacement) will still lead to a good representation of the uncertainty in the CDF. Thus, bootstrapping has been used on the LHS results in the same way it was used on SRS results in order to compare the stability and check if indeed the LHS results look more stable than conditional, mean, individual, LCF risk (per event) results when the same sample size is used. The distribution of mean value based on bootstrap has been displayed for all three replicates, with the density estimated via binning for one of the replicates. This is presented in Figure 5 and Figure 6 for the 10-mile and 50-mile radial distances, respectively.

Figure 5: 10-mile Conditional, Mean, Individual LCF Risk (per Event) CDFs for the ‘High’ Source Term with All Three Random Seeds with LHS and the Density Function for Random Seed 1 with LHS

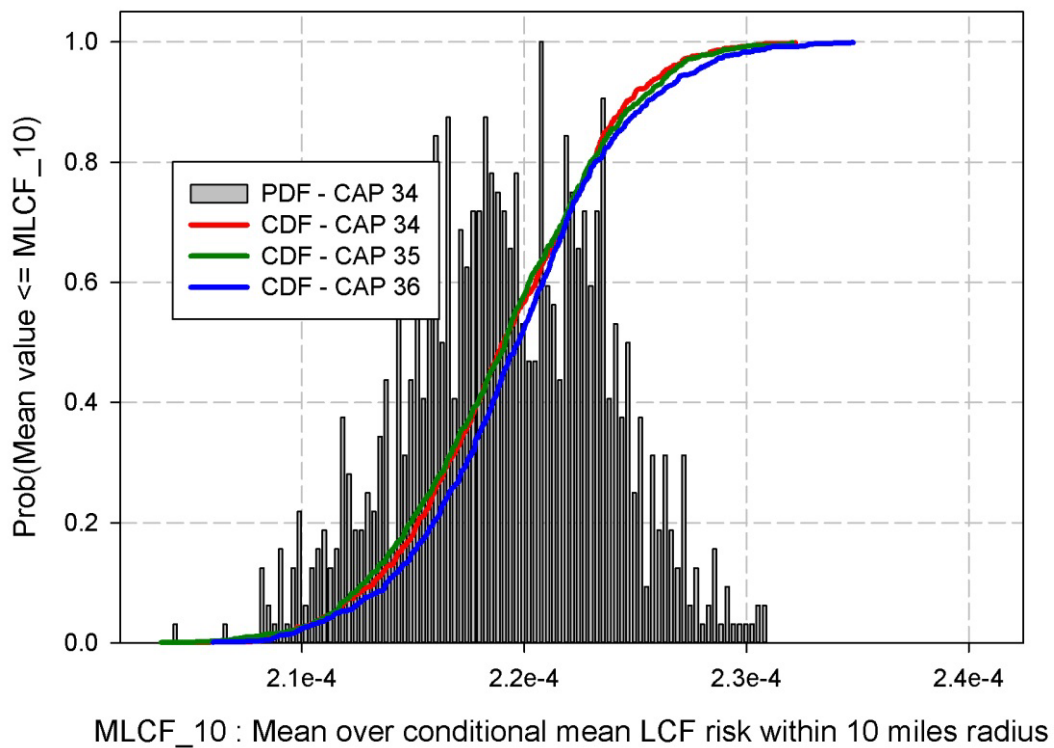
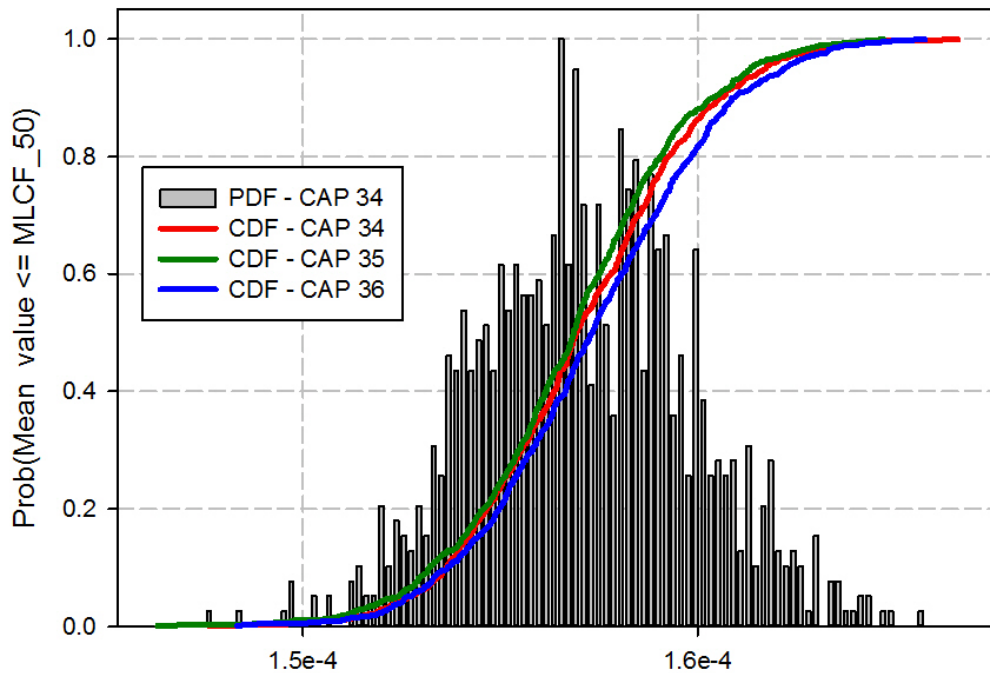


Figure 6: 50-mile Conditional, Mean, Individual LCF Risk (per Event) CDFs for the ‘High’ Source Term with All Three Random Seeds with LHS and the Density Function for Random Seed 1 with LHS



MLCF_50 : Mean over conditional mean LCF risk within 50 miles radius

3.1 Low, Medium, & High Source Term Combined Analysis

Three source terms were selected (as described in section 1) to test the influence of uncertain MACCS2 parameters by themselves in the uncertainty analysis. A representative overall CDF for these three source terms’ conditional, mean, individual LCF risk results was constructed by weighting the three source terms’ LCF risk CDFs by 1/3 (i.e., each represents 1/3 of the source term uncertainty). This result was then compared to the uncertainty analysis (documented in draft NUREG/CR-7155 [1]) LCF risk. Figure 7 and Figure 8 show the comparison for the ‘low’ source term (CAP29), ‘medium’ source term (CAP32), and ‘high’ source term (CAP35) with the draft NUREG/CR-7155 results (CAP17) at the 10- and 50-mile radial distances, respectively. As seen in these figures, the source terms selected are a good representation of the 10-mile radial distance and a good representation of the 50-mile radial distance to ~80th percentile; the difference between the original CAP17 result and the ‘averaged’ estimate is miniscule up to about the 80th percentile. After the 80th percentile, the ‘averaged’ estimate slightly under predicts the LCF risk when compared to draft NUREG/CR-7155. Overall, the comparison between the original CAP17 result and the ‘averaged’ estimate indicates that the 11 metrics chosen to pick the three representative “low,” “medium,” and “high” source terms were indeed good indicators of LCF risk, given the very good agreement up to the 80th percentile and only a small deviation above the 80th percentile.

Figure 7: 10-mile Conditional, Mean, Individual LCF Risk (per Event) CDFs for Low, Medium, and High Source Terms with LHS and the Conditional, Mean, Individual LCF Risk (per Event) CDF for the SOARCA Peach Bottom Uncertainty Analysis with LHS Sampling

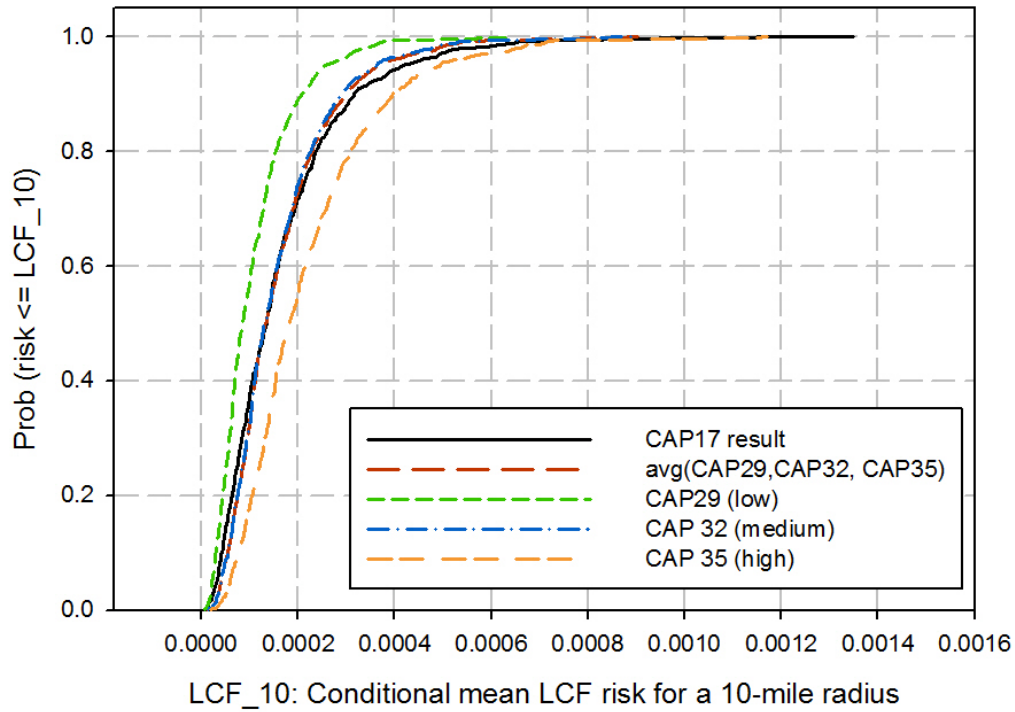
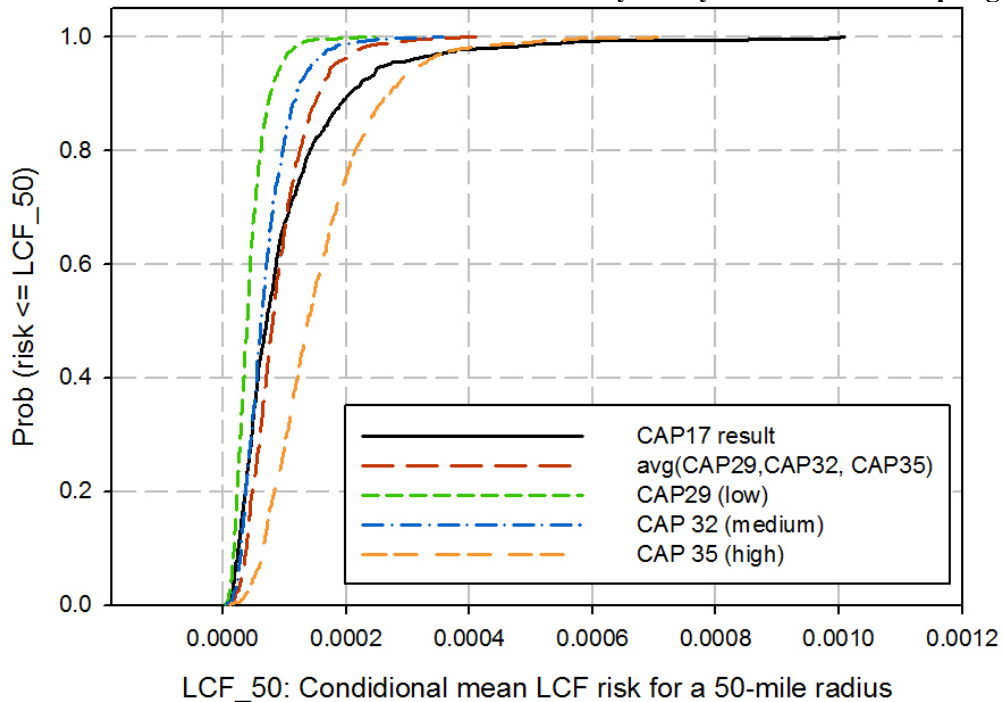


Figure 8: 50-mile Conditional, Mean, Individual LCF Risk (per Event) CDFs for Low, Medium, and High Source Terms with LHS and the Conditional, Mean, Individual LCF Risk (per Event) CDF for the SOARCA Peach Bottom Uncertainty Analysis with LHS Sampling



3.2 Bootstrap Comparison

In their review of the SOARCA Peach Bottom uncertainty analysis, some members of the U.S. Nuclear Regulatory Commission's (NRC) Advisory Committee on Reactor Safeguards (ACRS) asked why simple random/Monte-Carlo (MC) sampling was not used for the MACCS2 portion of the uncertainty analysis. NRC staff responded with an explanation of why an LHS is traditionally preferred (e.g., faster convergence of mean estimates). Additionally, the staff explained that the MACCS2 code did not have the capability to do a simple random/MC sampling (abbreviated as MC in the figure legends, same as SRS). Subsequent updates to the MACCS2 uncertainty code now allow SRS. Thus, a comparison of the draft NUREG/CR-7155 results (CAP17) to the CAP17 analysis using SRS/MC was conducted. Figure 9 shows the comparison of CAP17 CCDF conditional LCF risk for LHS and MC results for the 10- and 50-mile radial distances. As seen from this figure, the LHS and MC results are very similar and would be considered in good agreement for conditional LCF risk.

Figure 9: CAP17 Conditional, Mean, Individual LCF Risk (per Event) CCDF with LHS and MC Sampling for the Radial Distances Considered

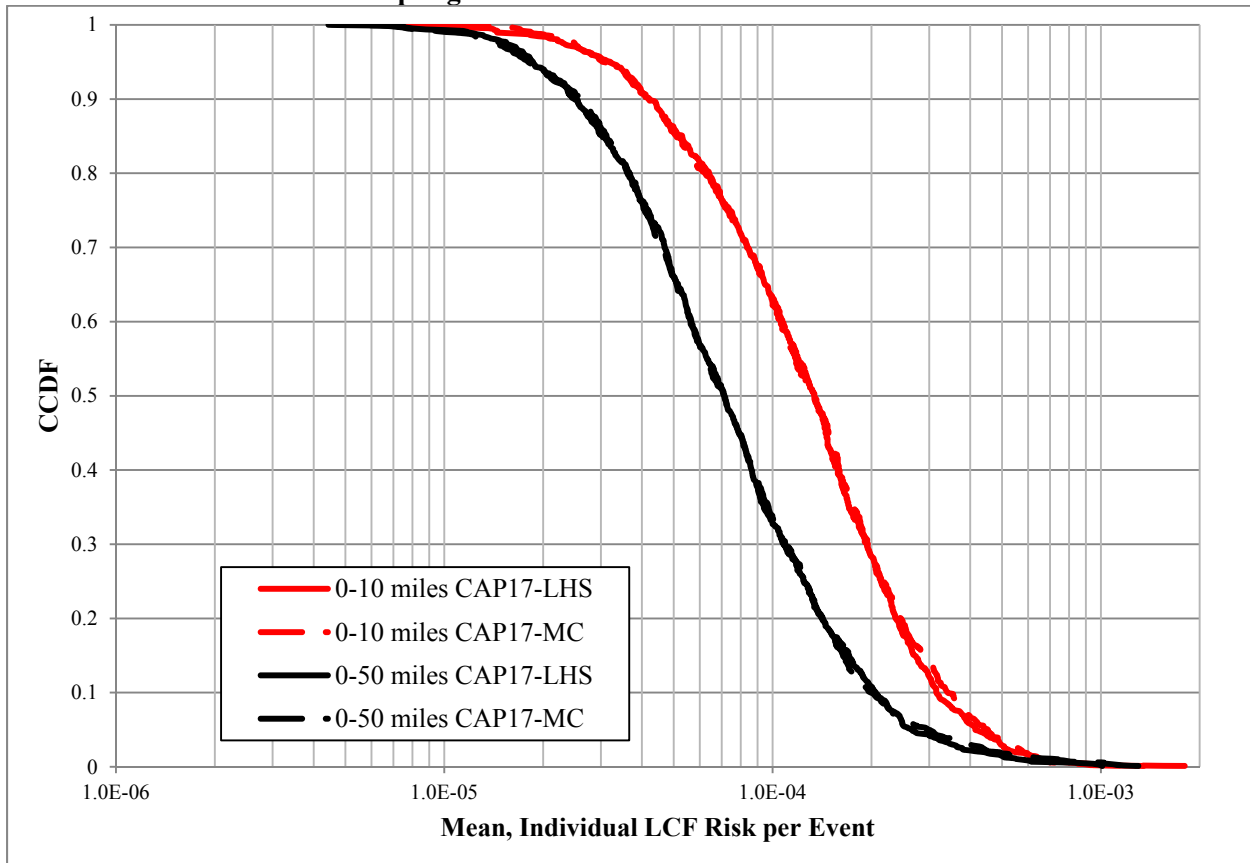
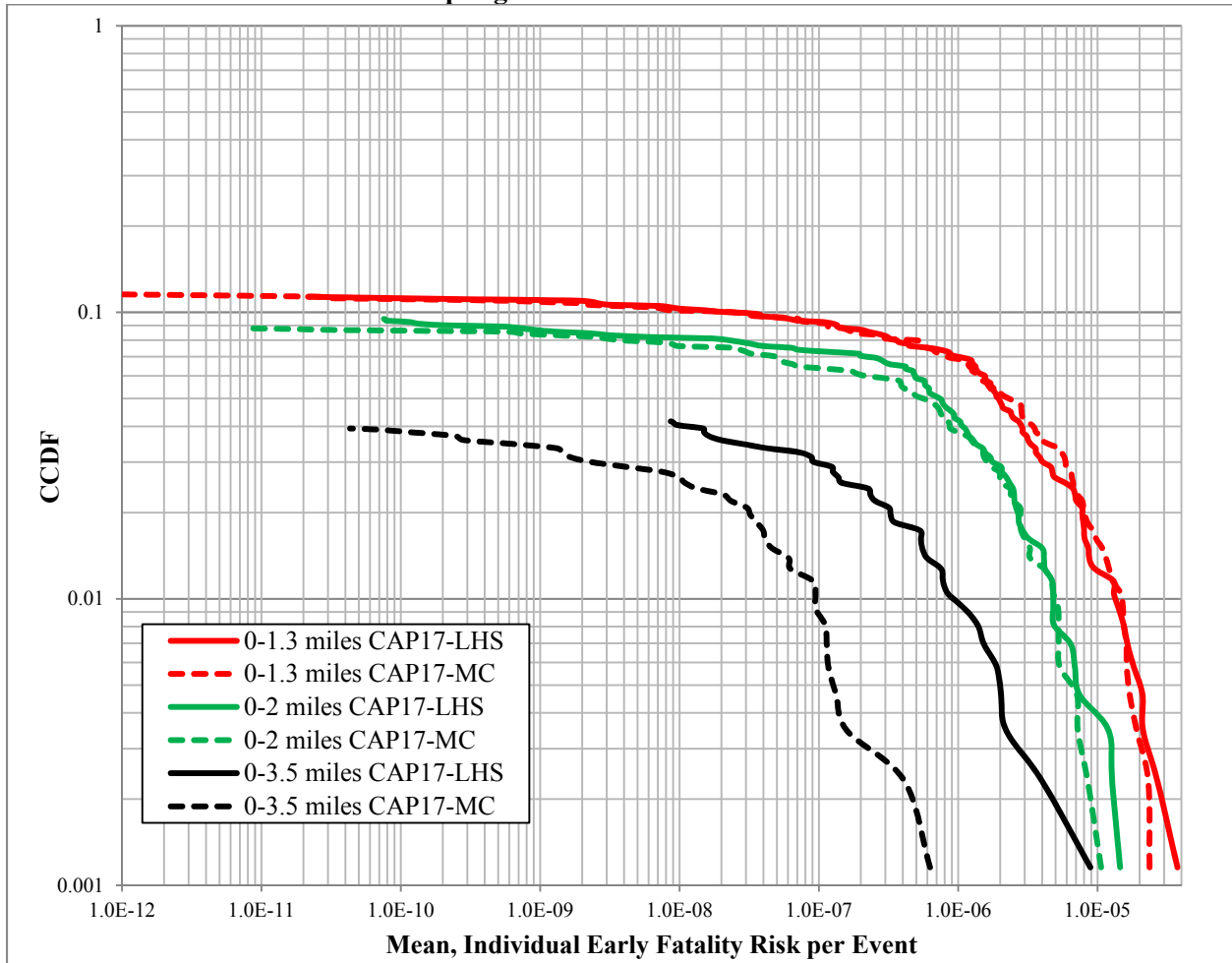


Figure 10 shows the comparison of CAP17 CCDF conditional early fatality risk for LHS and MC results for the 1.3-, 2-, and 3.5-mile radial distances. As seen from this figure, the LHS and MC results are very similar and would be considered in good agreement for conditional early fatality risk for the 1.3-mile and 2-mile radial distances. This is because there are a sufficient number of realizations that have a non-zero early fatality risk to provide a statistical comparison. Beyond 2 miles, there are few realizations that calculate a non-zero result and the statistics are less reliable.

Figure 10: CAP17 Conditional, Mean, Individual Early Fatality Risk (per Event) CCDF with LHS and MC Sampling for the Radial Distances Considered



For CAP17, the distribution of mean value based on bootstrap has been displayed for MC sampling (i.e., CAP40) and is presented in Figure 11 and Figure 12 for the 10-mile and 50-mile radial distances, respectively. Additionally, Figure 13 and Figure 14 show the distribution of the mean values based on bootstrap with the density estimated via binning for CAP40. This comparison provides information on the stability of the mean result for a sample of size 865. Two things are considered at this level: (1) how close are the means, and (2) how close to a normal distribution is the density function.

As noted above, while it is theoretically not appropriate to use bootstrapping on LHS results, an original sample size of 865 can be considered large enough so that a selection of values (with replacement) will still lead to a good representation of the uncertainty in the CDF. Thus, bootstrapping has been used on the LHS results for CAP17 in the same way it was used on SRS results in order to compare the stability and check if indeed the LHS results look more stable than conditional, mean, individual, LCF risk (per event) results when the same sample size is used. These results are presented in Figure 11 and Figure 12 for the 10-mile and 50-mile radial distances.

Figure 11: 10-mile Conditional, Mean, Individual LCF Risk (per Event) CDF for CAP17, CAP40, and 95% Confidence Interval Upper and Lower Bounds for CAP17 and CAP40

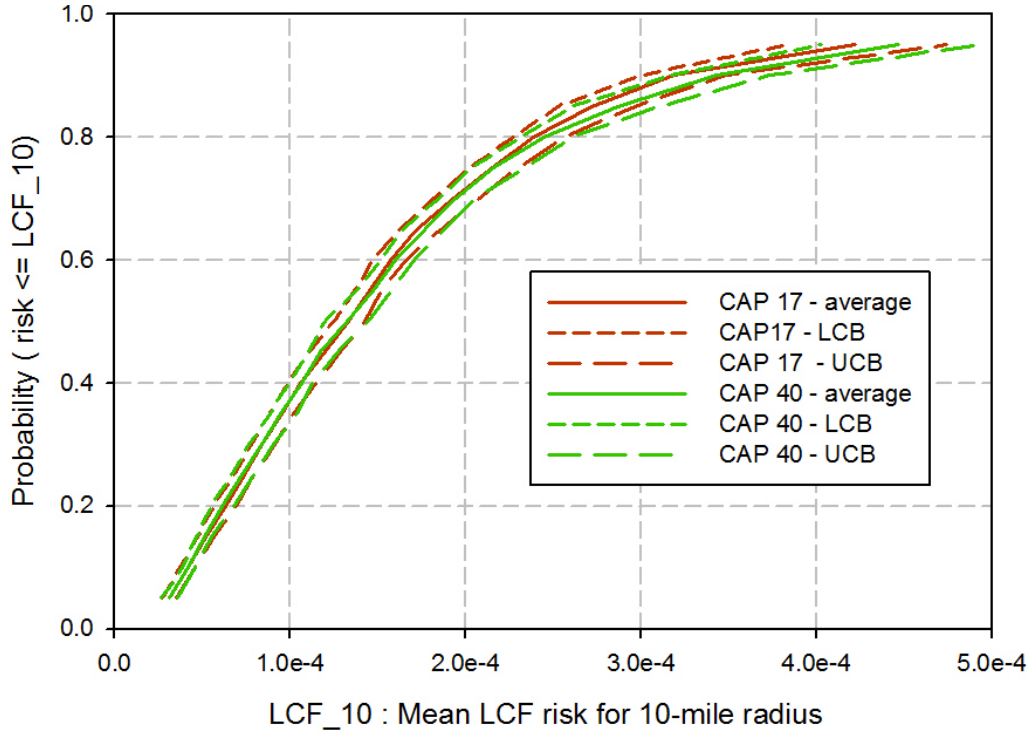
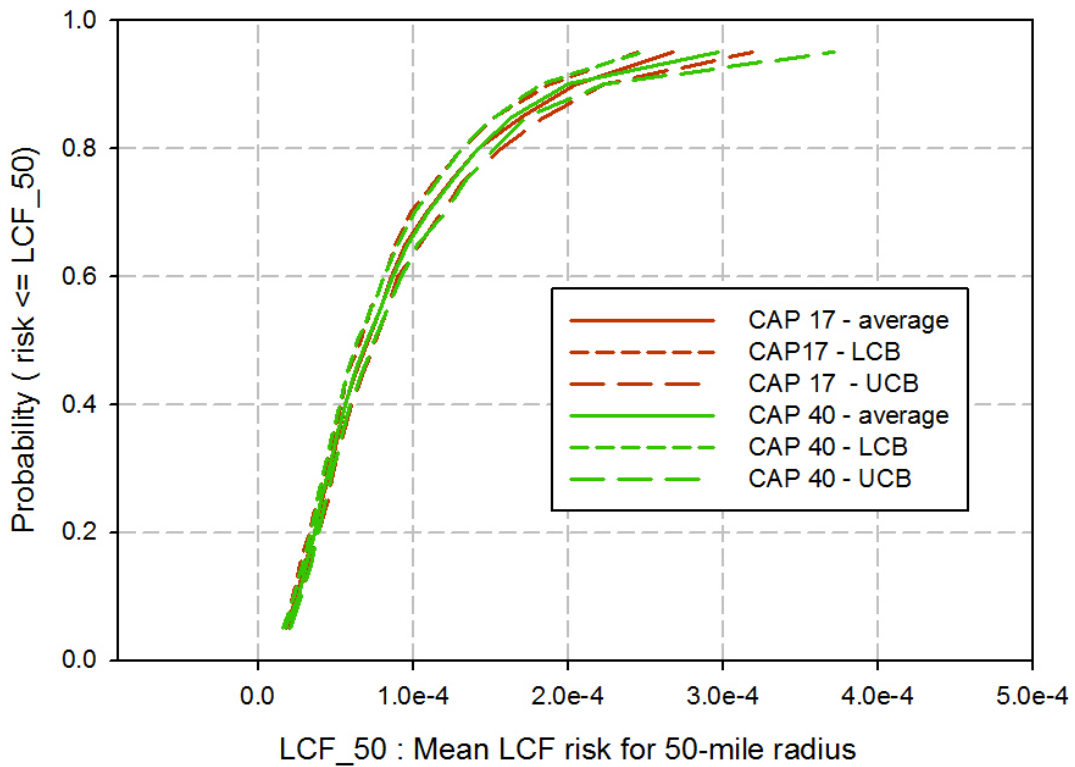


Figure 12: 50-mile Conditional, Mean, Individual LCF Risk (per Event) CDF for CAP17, CAP40, and 95% Confidence Interval Upper and Lower Bounds for CAP17 and CAP40



The distribution of mean value based on bootstrap has been displayed for CAP17 and CAP40, with the density estimated via binning for CAP40. This is presented in Figure 13 and Figure 14 for the 10-mile and 50-mile radial distances, respectively. As seen from Figure 11 through Figure 14, a reduction of variance in the mean for LHS sampling is seen (compared to SRS/MC); this is expected because LHS provides a faster convergence (per incremental Monte Carlo realization added) of summary metrics such as the mean of a distribution of results.

Figure 13: 10-mile Conditional, Mean, Individual LCF Risk (per Event) CDFs for CAP17, CAP40 and the Density Function for CAP40

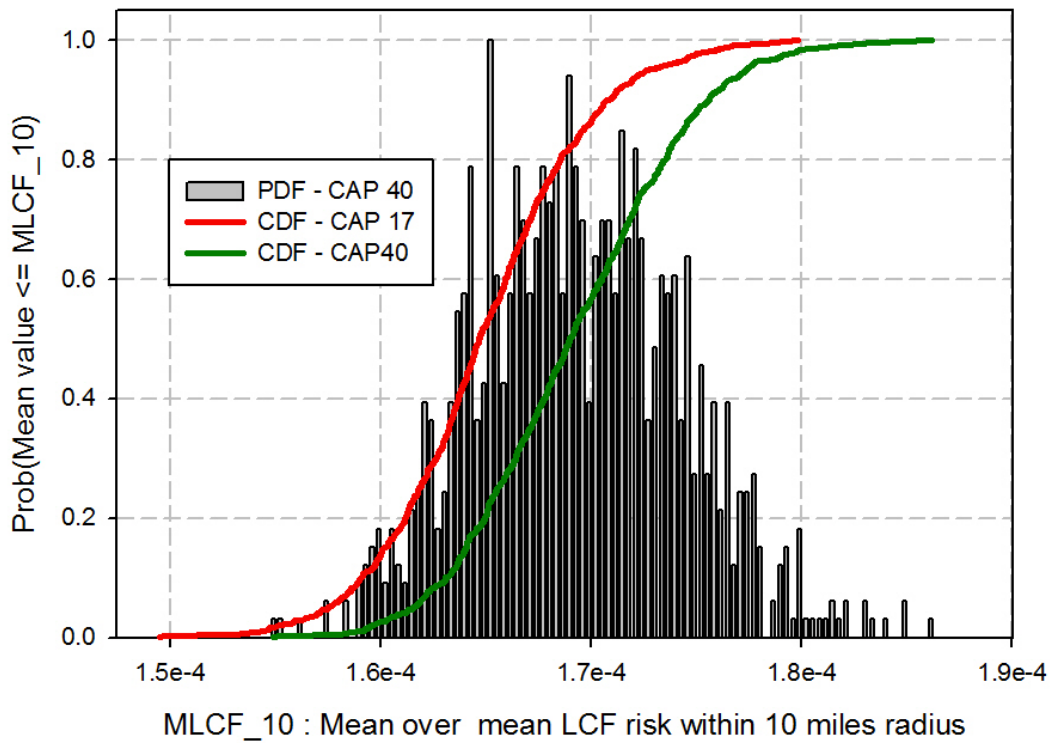
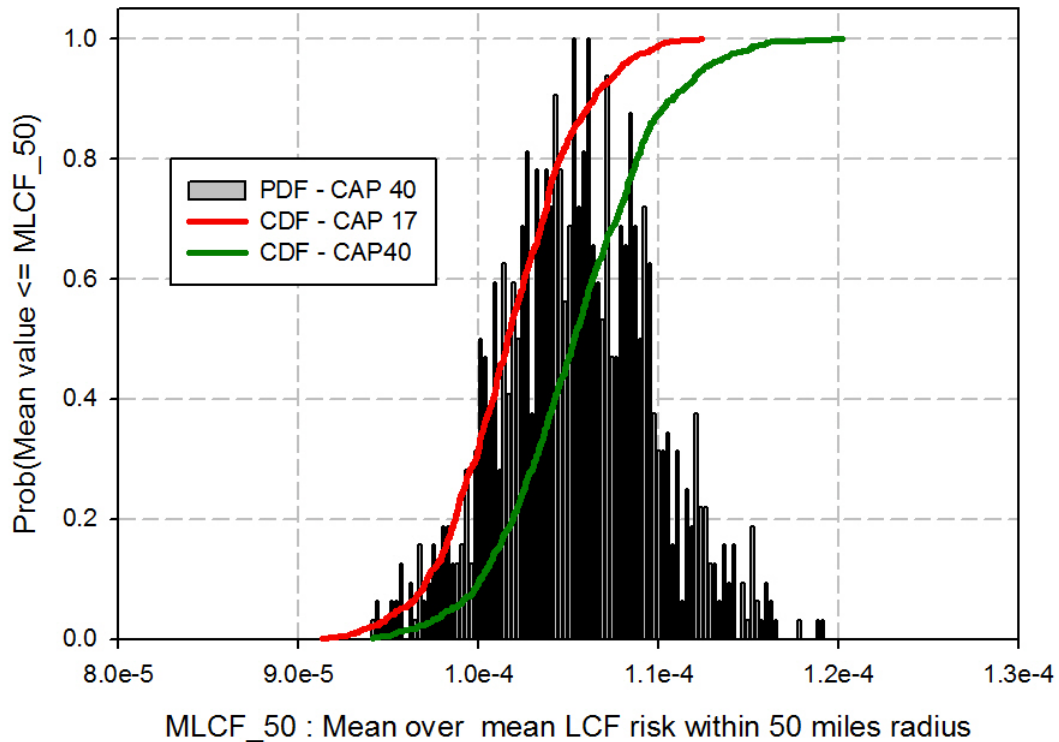


Figure 14: 50-mile Conditional, Mean, Individual LCF Risk (per Event) CDFs for CAP17, CAP40 and the Density Function for CAP40



4. CONCLUSIONS

LHS results for individual LCF and early fatality risks were compared with results using SRS. For the two radial distances considered (i.e., 10- and 50-mile), the LHS and SRS results are very similar and are considered in good agreement for conditional LCF risk. For the three radial distances considered (i.e., 1.3-, 2-, and 3.5-mile), the conditional early-fatality risk for LHS and SRS/MC results are very similar and are considered in good agreement for conditional early-fatality risk at the 1.3-mile and 2-mile radial distances. This is because there are a sufficient number of realizations that have a non-zero early-fatality risk to provide a good statistical comparison. Beyond 2 miles, there are fewer realizations (less than 10% of the total) that calculate a non-zero result and the statistics are less reliable.

This work shows that the results documented in draft NUREG/CR-7155 are well-converged. There was a question whether the integrated MELCOR-MACCS uncertainty analysis may have masked the true uncertainty in the MACCS portion of the analysis. This work shows that there were no surprises when removing the uncertainty due to source term and considering the uncertainty from only the uncertain MACCS2 parameters. This lends confidence to using the SOARCA Peach Bottom uncertainty analysis methodology and approach to future integrated uncertainty analyses for severe accident modeling. In addition, the results of this work will be studied further to assess whether future integrated uncertainty analyses could produce reliable results using fewer Monte Carlo realizations.

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