ENHANCED UNCERTAINTY ANALYSIS FOR SRS COMPOSITE ANALYSIS

F. G. Smith, III
M. A. Phifer

JUNE, 2011

Savannah River National Laboratory
Savannah River Nuclear Solutions
Savannah River Site
Aiken, SC 29808

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LIST OF ACRONYMS

ACP	Area Completion Projects
BCF	Bioaccumulation Factor
CA	Composite Analysis
CIG	Components in Grout
DOE	Department of Energy
DWPF	Defense Waste Processing Facility
ET	Engineered Trench
FAMS	F-Area Material Storage
FMB	Fourmile Branch
FTF	F-Area Tank Farm
GOU	Groundwater Operable Unit
GSA	General Separations Area
HANM	H-Area New Manufacturing
HAOM	H-Area Old Manufacturing
HTF	H-Area Tank Farm
HWMF	Hazardous Waste Management Facility
ILV	Intermediate Level Vault
IOU	Integrator Operable Unit
IPSL	Inoperative Process Sewer Line
KAC	K-Area Complex
LAC	L-Area Complex
LAWV	Low Activity Waste Vault
LFRG	Low Level Waste Disposal Facility Federal Review Group
LLRWDF	Low Level Radioactive Waste Disposal Facility
LLWF	Low Level Waste Facility
LPPP	Low Point Pump Pit
LTR	Lower Three Runs
MWMF	Mixed Waste Management Facility
NR	Naval Reactor
NRCDA	Naval Reactor Components Disposal Area
ORWBG	Old Radioactive Waste Burial Ground
PB	Pen Branch
POA	Point of Assessment
SC	Steel Creek
SDF	Saltstone Disposal Facility
SR	Savannah River
SRS	Savannah River Site
SS	Stainless Steel
SWPF	Salt Waste Processing Facility
TEF	Tritium Extraction Facility
TPBAR	Tritium Producing Burnable Absorber Rods
TRU	Transuranic
UTR	Upper Three Runs

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1.0 Executive Summary

The Composite Analysis (CA) performed for the Savannah River Site (SRS) in 2009 (SRS CA 2009) included a simplified uncertainty analysis. The uncertainty analysis in the CA (Smith et al. 2009b) was limited to considering at most five sources in a separate uncertainty calculation performed for each POA. To perform the uncertainty calculations in a reasonable amount of time, the analysis was limited to using 400 realizations, 2,000 years of simulated transport time, and the time steps used for the uncertainty analysis were increased from what was used in the CA base case analysis. As part of the CA maintenance plan, the Savannah River National Laboratory (SRNL) committed to improving the CA uncertainty/sensitivity analysis.

The previous uncertainty analysis was constrained by the standard GoldSim licensing which limits the user to running at most four Monte Carlo uncertainty calculations (also called realizations) simultaneously. Some of the limitations on the number of realizations that could be practically run and the simulation time steps were removed by building a cluster of three HP Proliant windows servers with a total of 36 64-bit processors and by licensing the GoldSim DP-Plus distributed processing software. This allowed running as many as 35 realizations simultaneously (one processor is reserved as a master process that controls running the realizations). These enhancements to SRNL computing capabilities[1] made uncertainty analysis: using 1000 realizations, using the time steps employed in the base case CA calculations, with more sources, and simulating radionuclide transport for 10,000 years feasible[2].

In addition, an importance screening analysis was performed to identify the class of stochastic variables that have the most significant impact on model uncertainty. This analysis ran the uncertainty model separately testing the response to variations in the following five sets of model parameters:

a. K_d values (72 parameters for the 36 CA elements in sand and clay),
b. Dose Parameters (34 parameters),
c. Material Properties (20 parameters),
d. Surface Water Flows (6 parameters),
e. Vadose and Aquifer Flow (4 parameters).

Results provided an assessment of which group of parameters is most significant in the dose uncertainty[3]. It was found that K_d and the vadose/aquifer flow parameters, both of which impact transport timing, had the greatest impact on dose uncertainty. Dose parameters had an intermediate level of impact while material properties and surface water flows had little impact on dose uncertainty. Results of the importance analysis are discussed further in Section 7 of this report.

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[1] This addresses Item 15 in SRS CA Table 11-2 and partially addresses LFRG Review Team Observation 21 in SRS CA Appendix H.

[2] This partially addresses Item 14 in SRS CA Table 11-3 and the review comment in Appendix G Section 3.3.8.1.

[3] This more structured uncertainty analysis partially addresses Items 16 and 17 in SRS CA Table 11-2; review comments in Appendix G Section 3.3.8.1; Appendix G "General Comments from Bruce Crowe" 1.d; and LFRG Review Team Observation 21 in Appendix H. However this uncertainty analysis did not include inventory and bioaccumulation factor (transfer factor) distributions, which will need to be included in the next CA revision.

The objectives of this work were to address comments received during the CA review on the uncertainty analysis and to demonstrate an improved methodology for CA uncertainty calculations as part of CA maintenance. This report partially addresses the LFRG Review Team issue of producing an enhanced CA sensitivity and uncertainty analysis. This is described in Table 1-1 which provides specific responses to pertinent CA maintenance items extracted from Section 11 of the SRS CA (2009). As noted above, the original uncertainty analysis looked at each POA separately and only included the effects from at most five sources giving the highest peak doses at each POA. Only 17 of the 152 CA sources were used in the original uncertainty analysis and the simulation time was reduced from 10,000 to 2,000 years. A major constraint on the original uncertainty analysis was the limitation of only being able to use at most four distributed processes. This work expanded the analysis to 10,000 years using 39 of the CA sources, included cumulative dose effects at downstream POAs, with more realizations (1,000) and finer time steps. This was accomplished by using the GoldSim DP-Plus module and the 36 processors available on a new windows cluster. The last part of the work looked at the contribution to overall uncertainty from the main categories of uncertainty variables: K_ds, dose parameters, flow parameters, and material properties. This was not intended to be a detailed sensitivity analysis but only to see in very general terms what broad category of parameters contributes most significantly to overall uncertainty in the CA dose. This analysis was not intended to be a final CA uncertainty calculation and there was no intent to revise the stochastic distributions as part of this work.

Table 1-1 Items in CA maintenance program addressed through this work.

Priority Future Work Category: SRS CA Sensitivity and Uncertainty Analysis (Table 11-2, SRS CA, 2009)		
Item	**Description**	**As Addressed by This Work**
15	GoldSim™ has a distributed processing (DP) capability that can be used when performing probabilistic calculations. Using this feature, individual realizations can be run on as many processors as the master GoldSim™ simulation can be linked to. The basic GoldSim™ software is limited to using four processors one of which is reserved for the master simulation that farms out realizations to the connected processors. This capability was utilized in performing the CA uncertainty calculations which reduced the simulation run time by a factor of three. However, by adding the GoldSim™ DP module, available from GoldSim Technology Group at a nominal cost, a probabilistic GoldSim™ simulation can be connected to as many processors as are available. This offers the possibility of dramatically decreasing probabilistic simulation run times and increasing the capability of performing uncertainty calculations including more sources with more realizations. Utilizing this approach is currently limited by our inability to access other computers through the SRS network primarily from computer security concerns. If a large cluster of Windows machines could be assembled off the SRS network, all of the processors could be accessed by GoldSim™ for probabilistic calculations. This item was specifically added to the 2010 SRNS PA/CA maintenance plan, and work on this item has been initiated. (Smith 2009b)	The computing capability proposed in Item 15 was created as a part of the work described in this report. A cluster of three HP Proliant windows servers having a total of 36 64-bit processors were purchased and the GoldSim DP-Plus distributed processing software was licensed. This gives SRNL the capability of running as many as 35 simultaneous GoldSim realizations which allowed uncertainty calculations to be run over 10,000 years including more sources and using finer time steps. Item 15 is therefore complete as a result of the work described in this report.
16	A systematic sensitivity analysis should be performed to identify the model parameters that have the greatest impact on CA results. This analysis should investigate the additive and multiplicative effects of parameters on the CA results. This analysis should investigate parameters in the transport model and in the dose model separately. This systematic sensitivity analysis along with a more structured uncertainty analysis (Item 17) will assist in future work prioritization. Expertise in the SRNL statistical group should be utilized to help structure this investigation and interpret the results.	Item 16 is partially addressed by the work described in this report. As part of the enhanced uncertainty analysis a limited sensitivity analysis was performed to determine what general categories of uncertainty parameters (K_d, material properties, water flow, and dose parameters) had the greatest impact on uncertainty in the calculated dose. Final sensitivity analysis work must await development of inventory uncertainty distributions from the remaining significant radionuclide source locations under CA maintenance.

Priority Future Work Category: SRS CA Sensitivity and Uncertainty Analysis (Table 11-2, SRS CA, 2009)		
Item	**Description**	**As Addressed by This Work**
17	A more structured uncertainty analysis should be performed to identify both those stochastic variables that have the greatest impact on model results and stochastic variables that have an insignificant impact on model results and can be eliminated from the uncertainty analysis. In particular inventory uncertainty distributions developed from Items 4, 5, 6, and 7 should be included in the uncertainty analysis. This structured uncertainty analysis along with a more systematic sensitivity analysis (Item 16) will assist in future work prioritization. Expertise in the SRNL statistical group should be utilized to help structure this investigation and interpret the results.	Item 17 is partially addressed by the work described in this report. A methodology to conduct a more structured uncertainty analysis was demonstrated and preliminary results obtained. However, this work did not include developing inventory uncertainty distributions or distributions for bioaccumulation factors which were not included in the dose module. Items 16 and 17 can be completed when these distributions are available.
Potential Future Work Category: SRS CA Model Improvements (Table 11-3, SRS CA, 2009)		
Item	**Description**	**As Addressed by This Work**
14	After Item 15 in **Error! Reference source not found.** is completed, a fully probabilistic analysis should be conducted over 10,000 years both at the base case POAs and at the Alternate Industrial POAs.	Item 14 is partially addressed by the work described in this report. A methodology capable of conducting a full probabilistic analysis over 10,000 years at the base case POAs was developed and demonstrated. Lack of inventory and bioaccumulation factor distributions prevented conducting a final CA uncertainty analysis. Alternative Industrial POAs were not considered in this work.

2.0 GoldSim Uncertainty Model

To further enhance CA uncertainty analysis capabilities, a new GoldSim model was created. Some basic features of this model are shown in Figures 2-1 through 2-4 which are graphic displays copied directly from the model. As indicated in Figure 2-1, the model can use as many as 32 individual sources in a single calculation. Each source models the release of radionuclides from the source material and transport through the waste zone, vadose zone and aquifer to the stream outfall. Figure 2-2 shows the contents of a single source model container. The basic transport calculations are unchanged from those in the original CA model as described by Smith, et al. (2009a). Each source is automatically linked to its corresponding Point of Assessment (POA) using the source stream number which is an input parameter to the model. The user can connect as many as 32 sources to a single POA or distribute the 32 sources among some or all of the POAs. As illustrated in Figure 2-3, the model automatically includes the impact from upstream POAs on downstream locations which adds a new capability to the CA uncertainty analysis.

The original CA deterministic calculations were performed for each source individually and composite results were collected and further analyzed in a series of Excel spreadsheets. A simplification realized in constructing the multi-source uncertainty model was that an Integrator Operable Unit (IOU), which represents a source of radionuclides released from stream bed sediment directly to the stream, can be modeled without using the full transport model shown in Figure 2-2. With a slight loss of generality, models for the IOU sources were embedded in the POA containers. This is illustrated in Figure 2-4 which shows the model for the Steel Creek/Pen Branch POA. Two IOU sources, one from each stream, contribute to the dose at this POA. Therefore, two sediment release models are included with this POA. In this way, the multi-source model also included seven specific IOU sources along with the 32 surface sources for a total of 39 sources. Figure 2-4 also shows that each POA has a separate dose calculation.

The original CA uncertainty calculations considered a total of only 17 sources. Therefore, it is possible to duplicate the full extent of the previous CA uncertainty calculations with a single run of the multi-source, multi-POA model which also includes the impact from upstream POAs on downstream locations. However, the 32 source, multiple POA model is about 226 Mb in size versus the 13 Mb size of the original CA model. Run time scales linearly with the number of sources so that, whereas the original CA model typically ran one source calculation in about one minute, the multi-source, multi-POA model runs using 32 sources typically take about 30 minutes. When using the full multi-source, multi-POA model for Monte-Carlo uncertainty analysis, saving the data from all realizations creates very large GoldSim files from 10 to 20 Gb in size. To reduce the file size as much as possible, output provided by the original CA model to trace the dose results to individual sources, radionuclides, and pathways is not saved in the multi-source, multi-POA model.

GoldSim run settings used in the uncertainty analysis were: 1,000 realizations, a 10,100 year simulation (running from 1950 to 12050), and 2,600 time steps. The uncertainty calculations used the same time period and time steps used for in the original CA deterministic calculations. The uncertainty runs were made on the GoldSim servers typically using 30 slave processes. Each calculation took about 20 hours to complete.

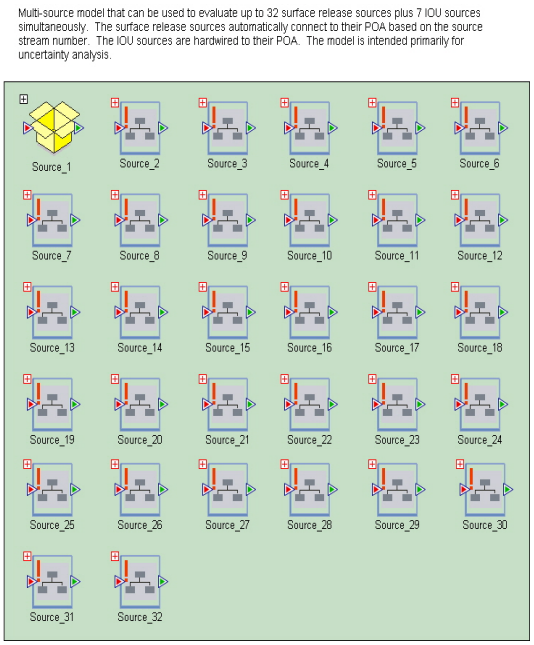

Figure 2-1. View of sources in GoldSim model used for enhanced CA uncertainty analysis.

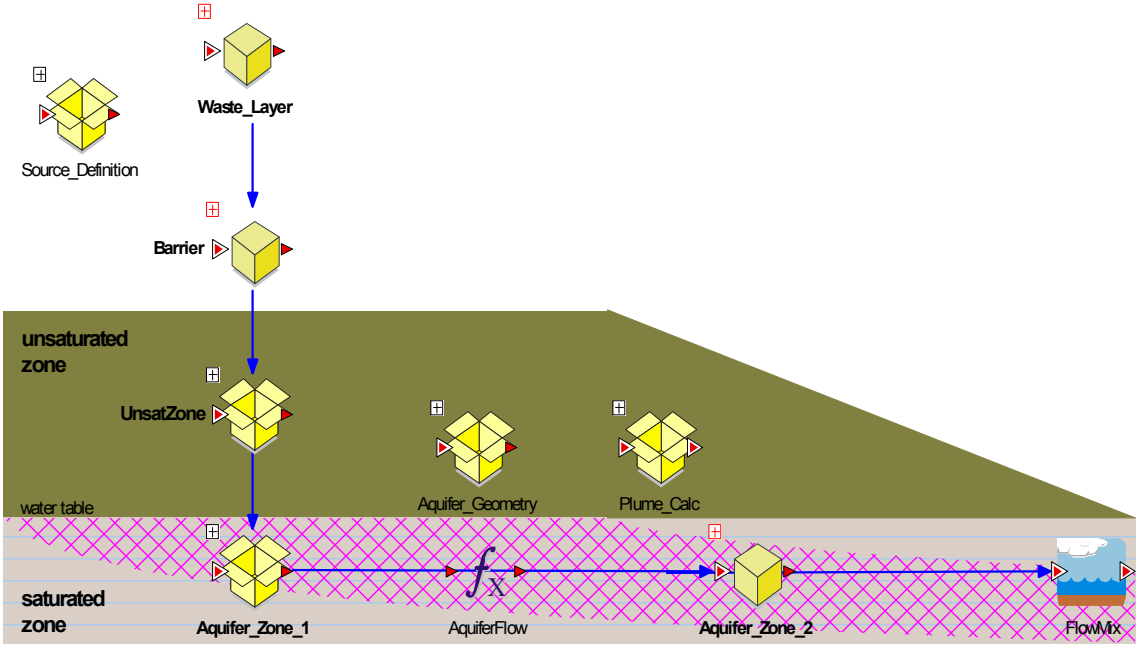

Figure 2-2. GoldSim transport model used for each of the 32 sources.

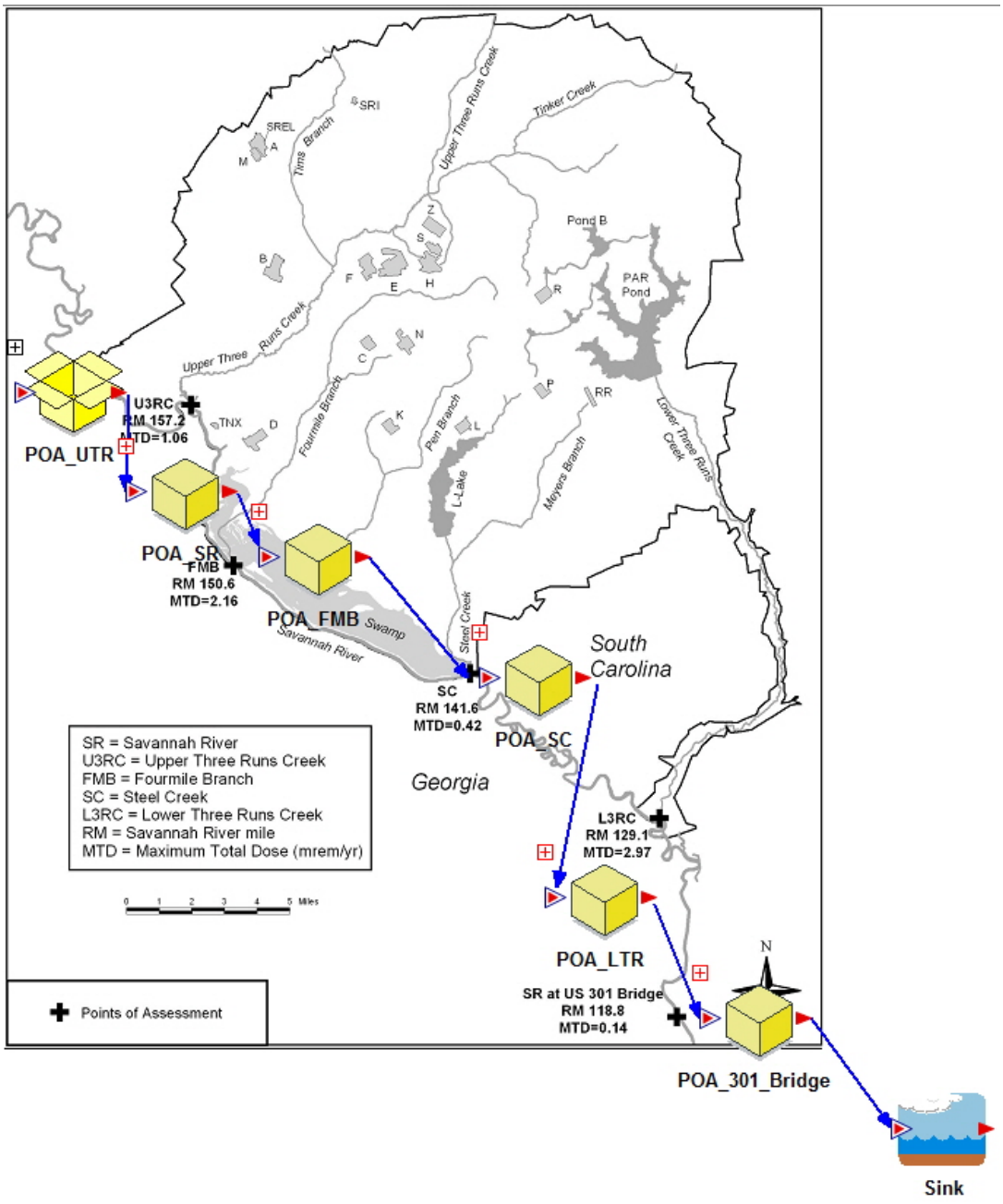

Figure 2-3. View of POAs in GoldSim model used for enhanced CA uncertainty analysis.

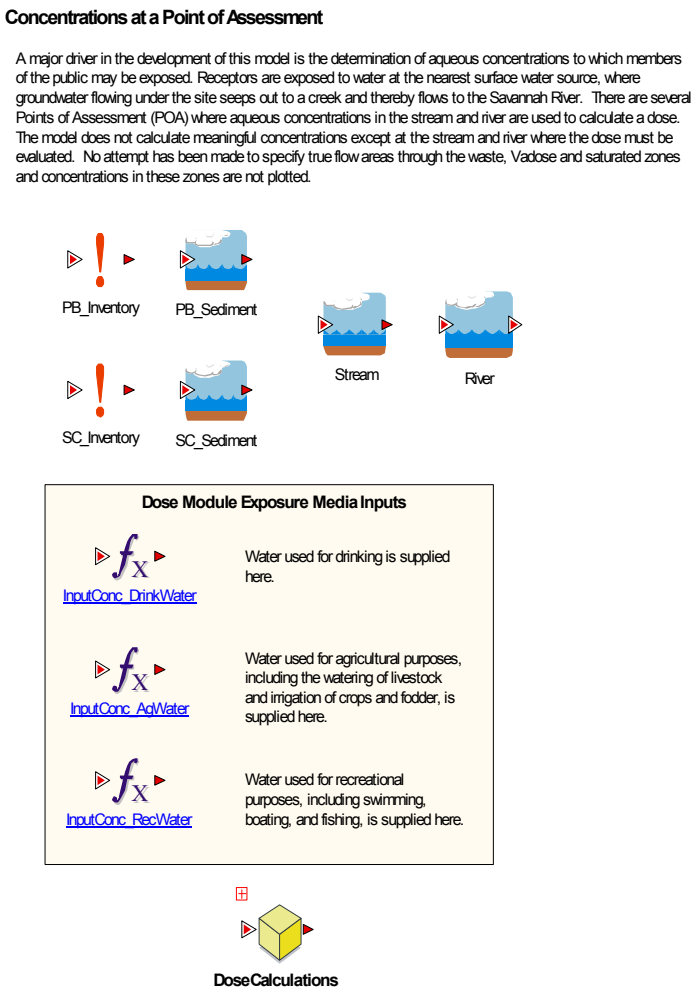

Figure 2-4. GoldSim model of Steel Creek/Pen Branch POA.

2.1 Model Development

The multi-source, multi-POA uncertainty model was developed in several stages. Initially a 16 source model was created and tested. In the second stage of development, the model was expanded to 24 sources and retested. Finally, in the last stage, the model with 32 surface sources and 7 IOU sources that was used for the final uncertainty analysis was created. The staged approach was useful in that it allowed testing and the correction of coding errors as development progressed. Initially, there was some concern that the overhead associated with the GoldSim master process managing as many as 30 slave processes would decrease model performance as the model was enlarged. The large size of the output files was also of concern. However, in practice, it was found that GoldSim using the DP-Plus module performed very well on the Windows servers. Both run time and output file size scaled approximately linearly as sources were added to the model and no serious problems were encountered in running the final model.

During development of the enhanced uncertainty model, two relatively minor errors in the original CA uncertainty analysis were discovered and corrected. These errors were:

1. The original CA uncertainty model connected five sources to a single POA. Sandy soil K_d's used in the dose module in the original uncertainty analysis had CDP on or off depending on the setting used in the first of the five sources. In the new uncertainty analysis, sandy soil K_d's in the dose module always use CDP off values.
2. Saturations of clayey soil and sandy soil in the original CA uncertainty analysis were calculated for all sources using the Darcy velocity from the first source. In the new uncertainty analysis, soil saturation is calculated as a function of infiltration separately for each source.

Other modifications made in new uncertainty analysis are:

1. The Eta_{clay} and Eta_{sand} factors that determined aquifer flow distributions are the same for each source in the new uncertainty model. These factors varied for each source in the original CA uncertainty model. This approach was changed in the new model to reduce the number of uncertainty parameters. Aquifer flow velocities themselves are still source dependent.
2. The cap infiltration distribution factor is the same for each source. This factor varied for each source in the original CA uncertainty model and was changed in the new model to reduce the number of uncertainty parameters. The infiltration flow itself is still source dependent.

These corrections and modifications mean that the new uncertainty analysis model will not give exactly the same results as the original five-source, single-POA CA uncertainty model used for uncertainty analysis in the CA. However, the changes are relatively minor and the results should be comparable to those obtained previously.

The output file for a 1,000 realization uncertainty analysis with 39 sources is about 16 Gb in size. Not only is this a significant amount of storage space but the GoldSim model file takes about 2.5 hours to save. GoldSim has the option to save a limited number of realization results to reduce the output file size. However, when this option was tested, it was found that different results were obtained than when all realizations were saved. Therefore, all realizations were saved for the uncertainty runs made in this study. With results from all of the realizations available, it is possible to extract more information from the results. For example, the uncertainty results show that the most extreme case produces high doses. When all realizations are saved, it is possible to scan through the results and identify the realization producing the maximum dose. GoldSim has the option of running a specific realization. Rerunning the extreme realization would identify the parameter settings producing this result.

3.0 Sources

The 39 sources used in the new uncertainty analysis are listed in Table 3-1. Sources added to the original CA uncertainty analysis are highlighted in the table. These 39 sources were chosen such that 99% of the sum of the peak doses found at each POA during the years 2025 to 3025 was included in the analysis. This time period was used because it is the 1,000 year CA compliance period. To achieve this, the sources used in the uncertainty analysis include all sources that produced peak doses during the years 2025 to 3025 greater than 0.005 mrem/yr.

Table 3-1. 39 Sources Included in Extended CA Uncertainty Analysis

Upper Three Runs (20)		**Fourmile Branch (7)**		**Steel Creek / Pen Branch (7)**	
Source	**MaxDose**	**Source**	**MaxDose**	**Source**	**MaxDose**
TEF	3.38E-03	FMB GOU	6.81E-03	LAC Con	8.24E-03
NR Pad 1 Part 6	3.66E-03	ORWBG	7.28E-03	105-P Con	1.54 E-02
H-Area IPSL UTR	3.69E-03	LLRWDF FMB	1.79E-02	KAC Surf	5.3E-02
234-7H	4.21E-03	105-C Surf	5.75E-02	PB IOU	6.00E-02
Z-Area Vault 1	7.71E-03	H_Area Seep	1.03E-01	LAC Surf	7.57E-02
281-3F	8.34E-03	ORWBG AgI	1.63E-01	105-P Surf	1.14E-01
232-H	1.11E-02	FMB IOU	1.97E+00	SC IOU	2.43E-01
F-Area Old Seep	1.16E-02				
E-Area ST Cent	1.33E-02	**Lower Three Runs (2)**		**Savannah River (3)**	
264-2H	1.48E-02	**Source**	**MaxDose**	**Source**	**MaxDose**
LLRWDF UTR	1.80E-02	105-R Surf S	4.68E-02	TNX Outfall	4.61E-04
HAOM	2.02E-02	LTR IOU	2.94E+00	SR-B IOU	1.38E-02
E-Area CIG	2.09E-02			SR-A IOU	1.76E-02
TPBAR	2.44E-02				
NR Pad 2	3.65E-02				
Z-Area Vault 4	4.93E-02				
HANM	6.07E-02				
UTR IOU	7.19E-02				
MWMF	1.35E-01				
H-Canyon	1.04E+00				

For reference, a histogram showing the distribution of peak doses in the years 2025 – 3025 calculated for all 152 CA sources is shown in Figure 3-1. The category for each bar is labeled with the log to the base 10 of the maximum peak dose for that category. The first bar then shows that there are three peak doses greater than 1.0 mrem/yr, the second bar shows there are five peak doses less than 1.0 and greater than 0.1 mrem/yr, and so forth. The 39 sources used in the uncertainty analysis represent the first three bars of the histogram and part of the fourth.

In fact, the 39 sources used in the uncertainty analysis are not exactly the same as those giving the highest 39 peak doses since the criterion of representing 99% of the sum of the peak does at each POA was also used in the selection. However, there are only two differences in these lists. The highest 39 peak doses include the H-Area IPSL FMB and HTF Type IIIA FMB sources while the uncertainty analysis list includes TEF and TNX Outfall instead.

If peak doses from all 152 CS sources are ranked for the 1,000 year period from the years 2025 to 3025 and for the 10,000 year period from the years 2025 to 12025, and these lists are compared to that used in the uncertainty analysis, the top 14 sources are the same in all cases. There are only

four differences between the lists of the 39 sources producing the highest peak doses in the 1,000 year and 10,000 year time periods. For the 1,000 year time period, the sources H-Area IPSL FMB, HTF Type IIIA FMB, 234-7H, and H-Area IPSL UTR appear while in the 10,000 year list the sources E-Area ILV, NR Pad 1 Part 5, 105-C SS, and KAC SS appear instead.

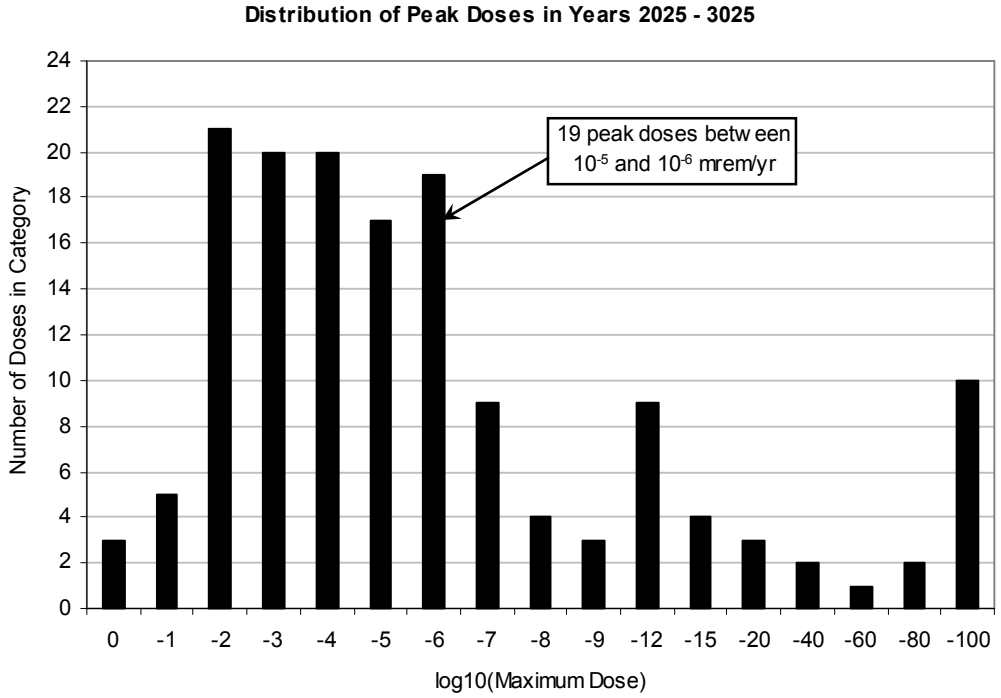

Figure 3-1. Distribution of peak doses during the years 2025 to 3025.

4.0 Deterministic Calculations

Deterministic results obtained with the multi-source, multi-POA uncertainty model were compared to those obtained with the original single-source CA deterministic model to verify that the multi-source, multi-POA model was functioning correctly. Simulations were performed using the uncertainty model with the stochastic variables set to their deterministic values. The majority of the deterministic value settings were set to the mean of the stochastic variable distribution. However, for some of the stochastic variables associated with the dose calculation, their deterministic (most likely) values were set to the minimum or maximum extreme values of their distributions. The original CA model calculations considered all 152 sources, whereas the multi-source, multi-POA model considers 39 sources as discussed in Section 3.0.

Figure 4-1 shows the cumulative doses calculated at each POA over 10,000 years from all 152 sources while Figure 4-2 shows the cumulative doses for the first 2,000 years from the original CA deterministic model. The original CA GoldSim calculations ran each source separately and cumulative doses were obtained from the results using an Excel spreadsheet. As described in Section 2.0, the multi-source, multi-POA model automatically calculates cumulative doses at each POA but only uses the 39 sources listed in Table 3-1. Figure 4-3 shows the cumulative doses calculated at each POA over 10,000 years using the multi-source, multi-POA model, while Figure 4-4 shows the cumulative doses for the first 2,000 years of the simulation. Comparison of Figure 4-3 with 4-1 and Figure 4-4 with 4-2 shows that the results obtained using the 39 sources having peak doses greater than 0.005 mrem/yr compare favorably to the results obtained using all 152 CA sources.

Direct comparisons of the two calculations of cumulative doses at each POA are shown in Figures 4-5 and 4-6 for 10,000 and 2,000 years, respectively. As expected, the results of the multi-source, multi-POA model (39 source) compare favorably with the 152 CA source model, particularly with respect to the peak values. Greater deviation between the 39 source model and the 152 CA source model is seen in the valleys and after 1,000 years. In all cases, doses greater than 0.1 mrem/yr are reproduced accurately with the new model. As noted in Section 3, the 39 sources used for the uncertainty analysis were based on peak doses during the years 2025 to 3025 and the additional criterion that at least 99% of the sum of the peak doses at each POA be represented. This choice of sources based upon peak values explains why there is greater deviation in the valleys. Additionally, if the 39 sources were chosen based on peak doses over the entire 10,000 year simulation four different sources would have been used. This choice of sources based upon peaks and to best represent the CA period of performance explains why the 39 source deterministic results deviate from the results obtained using all 152 sources beyond 1,000 years.

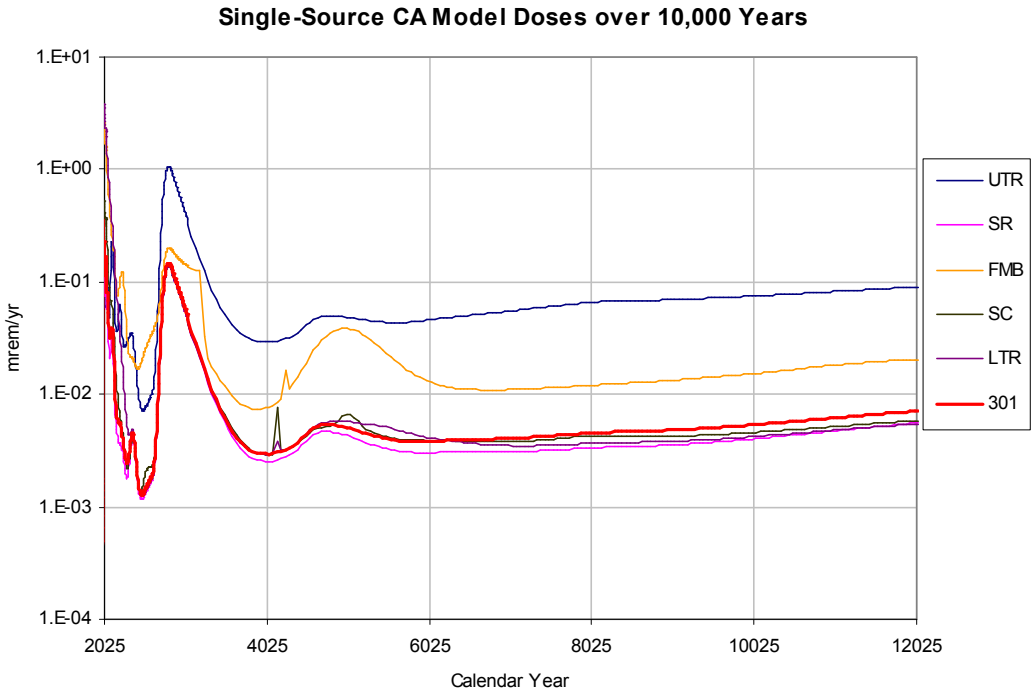

Figure 4-1. Original CA deterministic calculation of cumulative doses at each POA from all sources over 10,000 year time period.

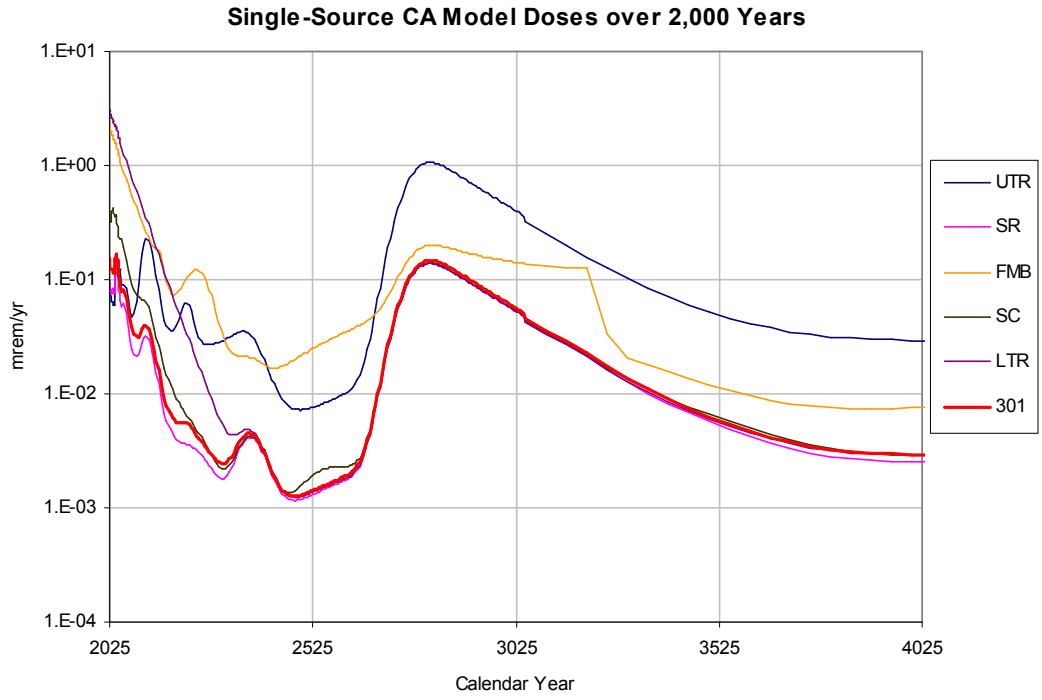

Figure 4-2. Original CA deterministic calculation of cumulative doses at each POA from all sources over 2,000 year time period.

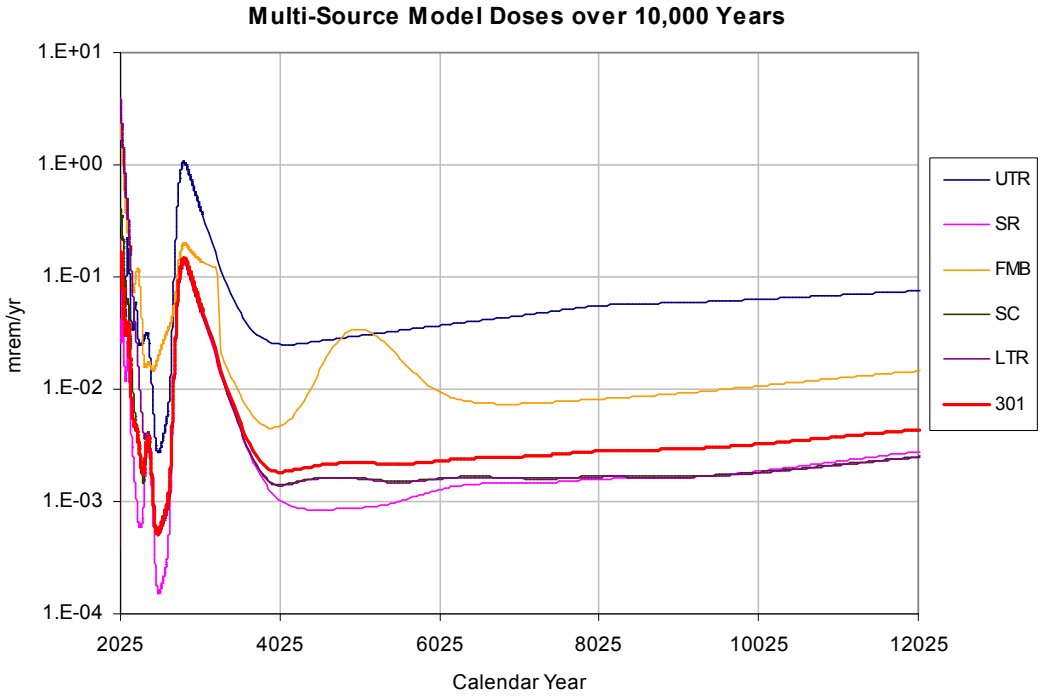

Figure 4-3. Deterministic calculation of cumulative doses at each POA over 10,000 year time period using multi-source, multi-POA model with 39 sources.

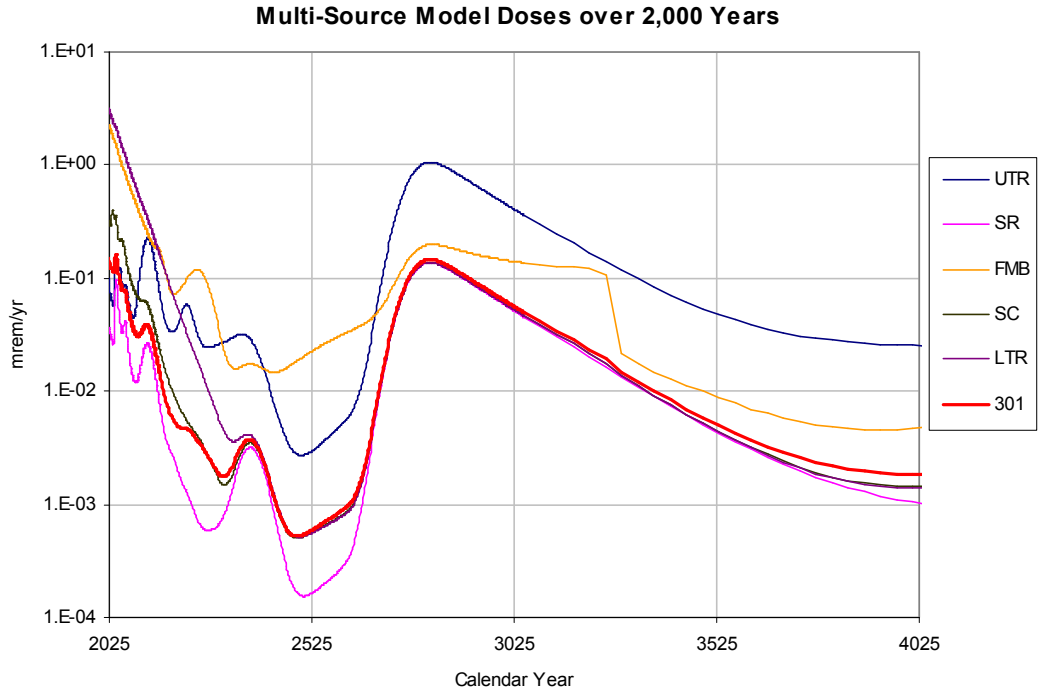

Figure 4-4. Deterministic calculation of cumulative doses at each POA over 2,000 year time period using multi-source, multi-POA model with 39 sources.

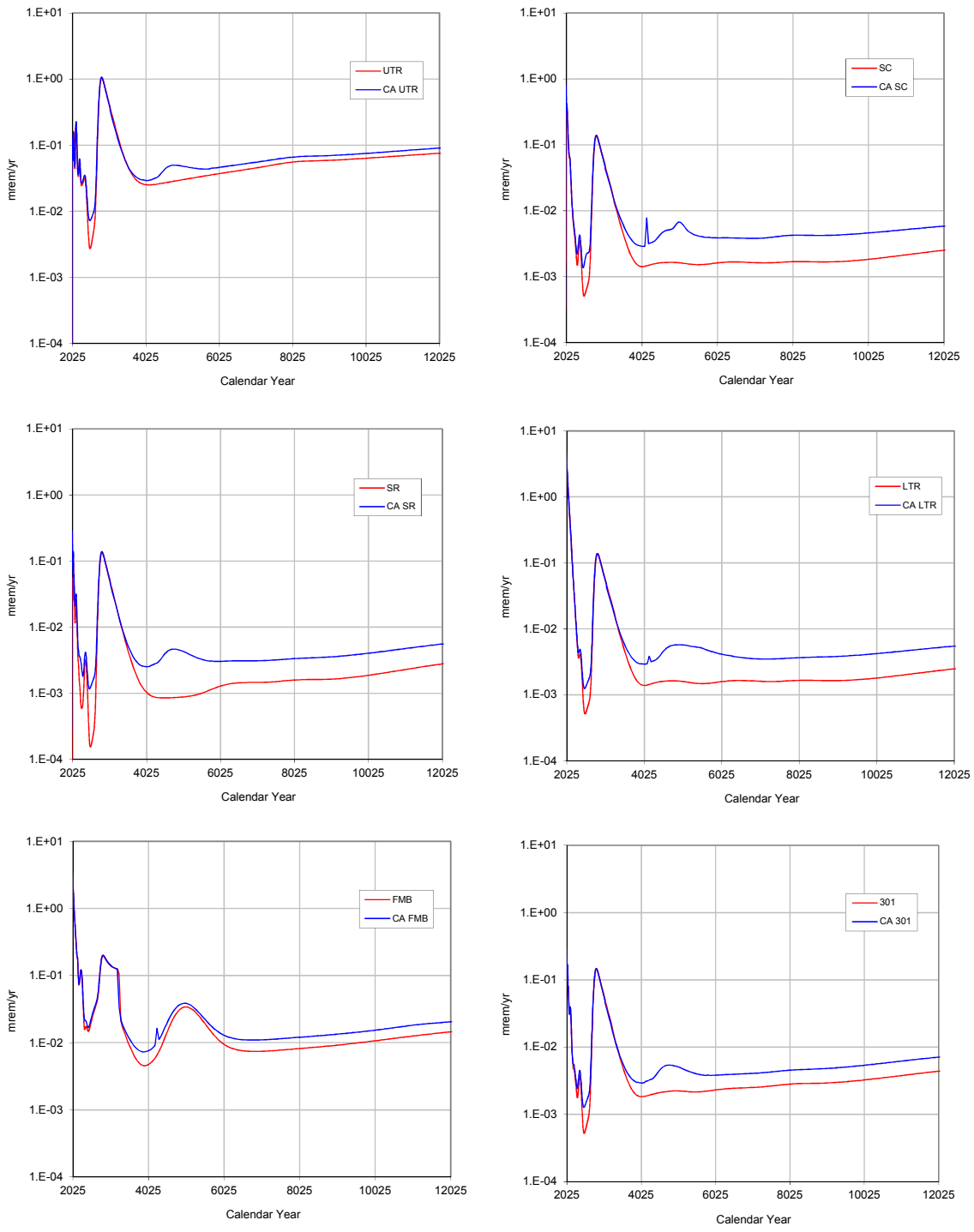

Figure 4-5. Comparison of deterministic doses calculated at each POA over 10,000 years using the original CA model with all 152 sources and the multi-source, multi-POA model with 39 sources.

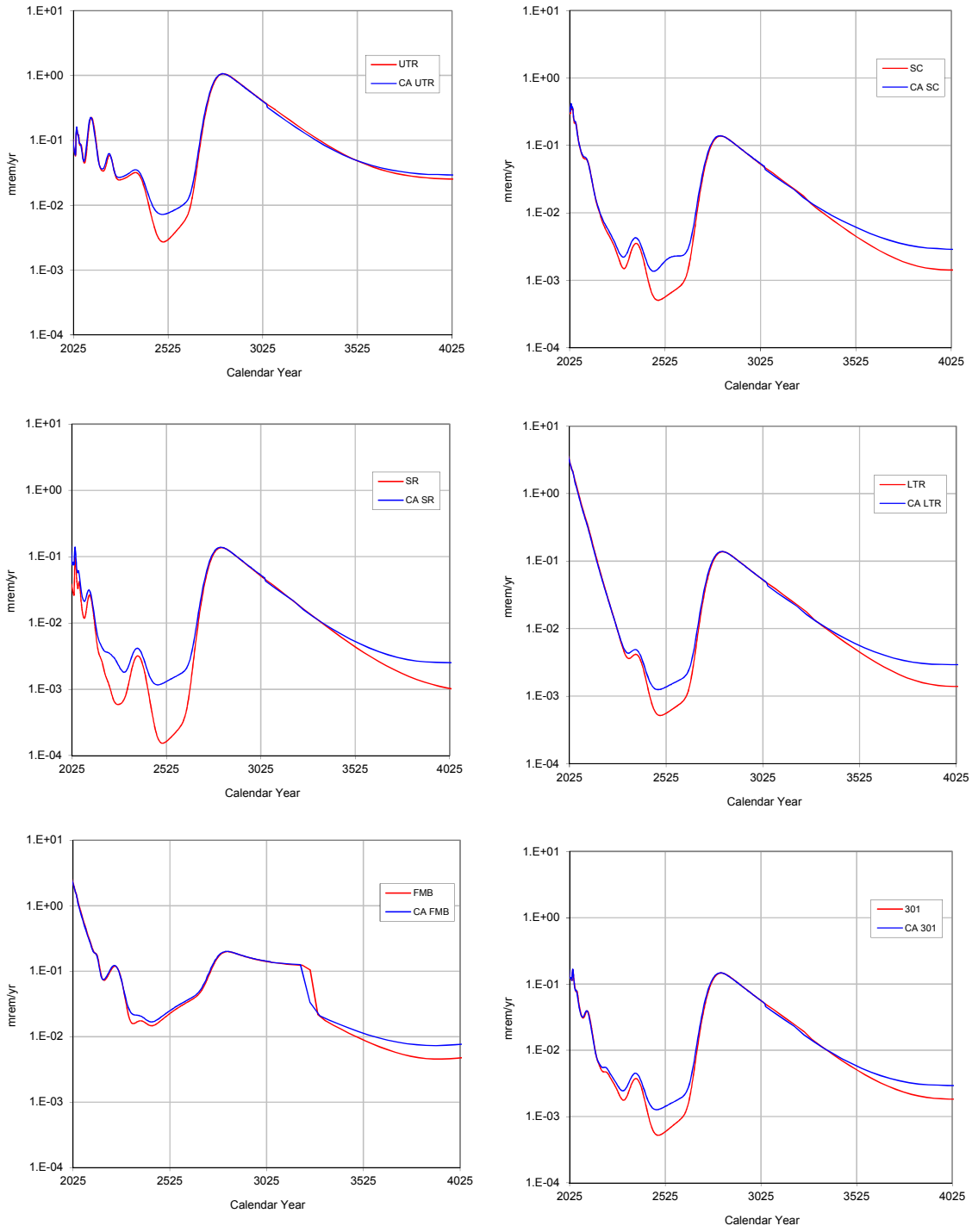

Figure 4-6. Comparison of deterministic doses calculated at each POA over 2,000 years using the original CA model with all 152 sources and the multi-source, multi-POA model with 39 sources.

5.0 Uncertainty Distributions

Parameters in the CA model that were assigned stochastic distributions are listed in Tables 5-1 through 5-4. For probabilistic Monte-Carlo calculations, GoldSim randomly chooses a value for each of these parameters from the associated distribution. Stochastic distributions that appear in the dose module (Phifer et al. 2009) are given in Table 5-1, distributions for material property values (Phifer and Dixon 2009) are listed in Table 5-2, and distributions for flow parameters (Phifer and Dixon 2009, Shine 2009, and Hamm et al. 2009) are listed in Table 5-3 and Table 5-4. In all cases, the mean or, for triangular distributions, the most likely value was the value used for base case deterministic calculations (Smith et al. 2009a). The cap infiltration distributions listed in Table 5-4 are applied as multipliers to the nominal cap infiltration flow calculated as a function of time (Smith et al. 2009a). Similarly, the aquifer sand and clay velocity distributions shown in Table 5-4 are factors applied to the nominal Darcy velocities. The nominal aquifer velocities are divided by these flow factors to obtain a revised estimate of the velocity (Hamm et al. 2009). The only other distributions used in the CA model were applied to K_d values. Following McDowell-Boyer and Kaplan (2009), it was assumed that K_d values have log-normal distributions and that for sandy soil and cement the standard deviation is 75% of the mean value and for clayey soil the standard deviation is 50% of the mean value. Neither the original CA model nor this multi-source, multi-POA uncertainty model included inventory and bioaccumulation factor (transfer factor) distributions. Inventory and bioaccumulation factor (transfer factor) distributions will need to be included in the next CA revision.

Table 5-1. Dose module parameter distributions (34).

Parameter	Units	Distribution	Mean or Most Likely Value	Standard Deviation	Minimum	Maximum
Exposures						
Irrigation_rate	$L/d/m^2$	Triangular	3.6		2.08	5.5
retention_leaf		Triangular	0.25		0.2	0.25
soil_depth	m	Triangular	0.15		0.15	0.61
holdup_vegetable[1]	hr	Normal	8.7	1	1	1.0E+40
Irrigation_time_garden	d	Normal	70	7		
Weathering_loss	1/d	Triangular	0.0495		0.03	0.0495
Vegetable_Yield	kg/m^2	Triangular	0.7		0.2	4
Buildup_Time_Soil	d	Triangular	183		60	365
Irrigation_time_pasture[1]	d	Normal	70	7		
Fodder_intake_beef	kg/d	Normal	36	8		
Fodder_intake_milk	kg/d	Normal	52	11		
Frac_Pasture_beef		Triangular	0.75		0.5	1
Frac_Pasture_milk		Triangular	0.56		0.5	1
Water_intake_beef	L/d	Triangular	28		28	50
Water_intake_milk	L/d	Triangular	50		50	60
holdup_beef	d	Triangular	6		6	20
holdup_milk	d	Triangular	3		1	4
Behaviors						
Soil_Ing_Rate	kg/yr	Triangular	0.0365		0.0008	0.05
Inhalation_Rate	m^3/yr	Triangular	5,548		1,267	11,600
Dust_Loading_Garden	kg/m^3	Triangular	1.0E-07		1.0E-08	3.0E-07
Water_Ing_Rate	L/yr	Triangular	337		184	730
Garden_Time_frac		Triangular	0.01		0.01	0.08
Veg_Ing_Rate _nonleafy	kg/yr	Triangular	163		90	276
Veg_Ing_Rate_leafy	kg/yr	Triangular	21		18	43
Meat_Ing_Rate	kg/yr	Triangular	43		26	81
Milk_Ing_Rate	L/yr	Triangular	120		73.7	230
Frac_Local_Veg _leafy		Triangular	0.173		0	0.5
Frac_Local_Veg _nonleafy		Triangular	0.173		0	0.5
Frac_Local_Meat		Triangular	0.306		0	0.5
Frac_Local_Milk		Triangular	0.207		0	0.5
Fish_Ing_Rate	kg/yr	Triangular	9		2.2	19
Shoreline_Time	hr/yr	Triangular	23		11	35
Swimming_Time	hr/yr	Triangular	8.9		8.9	13
Boating_Time	hr/yr	Triangular	21		9.1	31.5

[1]For the following two parameters the deterministic value was not equal to the mean or most likely value: the deterministic value for holdup_vegetable was 6 hr, and
the deterministic value for Irrigation_time_pasture was 30 d.

Table 5-2. Material property distributions (20).

Parameter	Units	Distribution	Mean or Most Likely	Standard Deviation	Minimum (-3σ)	Maximum (+3σ)
Sandy Soil						
Dry Bulk Density	g/cm^3	Normal	1.650	0.022	1.590	1.710
Porosity		Normal	0.380	0.008	0.360	0.400
Water Saturation[1]		Triangular	1.000		0.968	1.032
Tortuosity		Triangular	0.500		0.227	1.000
Clayey Soil						
Dry Bulk Density	g/cm^3	Normal	1.680	0.028	1.600	1.760
Porosity		Normal	0.370	0.011	0.340	0.400
Water Saturation[1]		Triangular	1.000		0.982	1.018
Tortuosity		Triangular	0.331		0.202	0.557
Intact Concrete						
Dry Bulk Density	g/cm^3	Normal	2.060	0.100	1.760	2.360
Porosity		Normal	0.221	0.013	0.172	0.250
Tortuosity		Triangular	0.050		0.011	0.217
Saturated Sandy Soil						
Dry Bulk Density	g/cm^3	Normal	1.040	0.024	0.968	1.112
Porosity		Normal	0.250	0.009	0.225	0.276
Tortuosity		Triangular	0.331		0.202	0.557
Saturated Clayey Soil						
Dry Bulk Density	g/cm^3	Normal	1.040	0.024	0.968	1.112
Porosity		Normal	0.250	0.009	0.225	0.276
Tortuosity		Triangular	0.250		0.176	0.368
Concrete Aging Pore Volume Flushes						
1^{st} Flush		Triangular	50		1	100
2^{nd} Flush		Triangular	500		100	1000
3^{rd} Flush		Triangular	7000		1000	10000

[1]Variation in water saturation is calculated as the deviation about the nominal value.

The evaluation of concrete aging using the pore flush distributions, listed in the bottom of Table 5-2 requires some explanation. The first flush (nominally 50 pore volumes) sets the point of transition from applying young to middle-age concrete K_d values. The second flush sets the point of transition from using middle-age to old concrete K_d values. The third flush sets the point of transition from using old concrete K_d values to using K_d values for sandy soil. When uncertainty in material properties alone was tested, the distributions shown in Table 5-2 were applied using nominal K_d values for each element for the concrete age indicated. When uncertainty in K_d alone was tested, nominal flush volumes were used and the K_d values varied as described above.

Table 5-3. Stream and river flow distributions (6).

Parameter	Units	Distribution	Mean or Most Likely	Standard Deviation	Minimum (-3σ)	Maximum (+3σ)
Upper Three Runs Flow	cfs	Normal	237	1.35	232.94	241.06
Fourmile Branch Flow	cfs	Normal	32	0.41	30.78	33.22
Pen Branch / Steel Creek Flow	cfs	Normal	89	1.32	85.04	92.96
Lower Three Runs Flow	cfs	Normal	164	1.91	158.28	169.72
Savannah River Augusta Flow	cfs	Normal	9198	86.00	8940.00	9456.00
Savannah River U.S. 301 Bridge Flow	cfs	Normal	10175	102.63	9867.11	10482.89

Table 5-4. Infiltration and aquifer flow distributions (4).

Parameter	Units	Distribution	Mean or Most Likely	Standard Deviation	Minimum (-3σ)	Maximum (+3σ)
Natural Infiltration Flow	in/yr	Normal	15	0.17	14.48	15.52
Cap Infiltration		Normal	1	0.01133	0.966	1.034
Aquifer Sand Velocity		Log-normal	1	0.869	0.1	10
Aquifer Clay Velocity		Log-normal	1	1.31	0.1	10

6.0 Uncertainty Calculations

Probabilistic simulations were performed with GoldSim using the codes Monte-Carlo algorithm with the following options:

- Stochastic variables were chosen using a Latin Hypercube sampling algorithm.
- Sampling sequences are repeatable with the initial random seed set to one.

Results from this new uncertainty analysis are presented graphically in the following subsections. Section 6.1 shows plots of dose uncertainty at each POA over the entire 10,000 year simulation (Figures 6.1-1 through 6.1-6). To better see details during the 1,000 year CA period of compliance from 2025 to 3025, Section 6.2 presents the same plots for the first 2,000 years of the simulation (Figures 6.2-1 through 6.2-6). The plots are extended over 2,000 years to be certain that nothing unusual happens just beyond the assessment period.

Section 6.3 plots mean and median doses from this new multi-source, multi-POA stochastic analysis against the new deterministic value obtained with the multi-source, multi-POA model and the deterministic value obtained previously with the original CA deterministic model considering all 152 CA sources for the first 2,000 years of the simulation. There are significant differences between the mean and median results from the uncertainty analysis and the deterministic result, although the magnitude of the peaks are similar. As shown in Section 7.0, this is a result of sampling from the K_d, infiltration, and aquifer flow distributions. Different values for these parameters change the timing of dose peaks and thereby introduce some distortion into the dose profile. The abbreviated legends on the figures in Section 6.3 can be read more explicitly as, for example on Figure 6.3-1:

- UTR = Multi-source, multi-POA deterministic result
- CA UTR = Original CA deterministic result
- Mean = Multi-source, multi-POA stochastic analysis mean
- Median = Multi-source, multi-POA stochastic analysis median

Table 6-1 summarizes the results by listing the peak value of each statistic over the CA assessment period from 2025 to 3025. These results compare very closely to those obtained in the original limited CA uncertainty analysis shown in Table 6-2 (Smith et al. 2009b) with the single exception of the peak upper bound for the Upper Three Runs POA, which is much higher in this study. The origin of this high upper bound value, which, as shown in Figure 6.2-1, occurs in the year 2110, has not been traced. GoldSim offers some ability to determine the origin of this upper bound. Graphical results from all 1,000 realizations can be scanned to identify the one producing the upper bound. GoldSim then allows calculation of a specific realization. Running the realization that produced the upper bound result would allow identification of the stochastic parameters used and possibly identify the cause of the high dose. At each POA, the upper bound is much larger than the 95th percentile value which would typically be used as a 95% confidence bound on the median. None of the 95th percentile values challenge the 30 mrem/yr dose constraint. All other results in Table 6-2, including the deterministic values obtained from the multi-source, multi-POA model, are comparable to those obtained previously.

Table 6-1. Peak values of statistical parameters for total dose at each POA over the CA assessment period from 2025 to 3025 produced from the multi-source, multi-POA model.

Dose (mrem/yr)	Upper Three Runs	Savannah River	Fourmile Branch	Steel Creek/Pen Branch	Lower Three Runs	301 Bridge
Deterministic[2]	1.06	0.14	2.19	0.40	3.01	0.16
Mean	0.73	0.11	3.48	0.59	4.95	0.23
Lower Bound[1]	0.02	0.02	0.38	0.07	0.50	0.06
5th Percentile	0.06	0.03	0.87	0.17	1.24	0.10
25th Percentile	0.15	0.06	1.80	0.32	2.51	0.15
Median	0.53	0.10	2.73	0.50	3.88	0.20
75th Percentile	1.14	0.16	4.35	0.74	6.26	0.28
95th Percentile	4.44	0.63	8.71	1.40	12.49	0.65
Upper Bound[1]	60.20	11.01	22.33	11.05	30.99	10.61

Table 6-2. Peak values of statistical parameters for total dose at each POA over the CA assessment period from 2025 to 3025 produced from the original CA uncertainty analysis.

Dose (mrem/yr)	Upper Three Runs	Savannah River	Fourmile Branch	Steel Creek/Pen Branch	Lower Three Runs	301 Bridge[4]
Deterministic[2]	1.04	0.03	2.14	0.46	2.95	
Cumulative[3]	1.06	0.14	2.16	0.42	2.97	
Mean	0.60	0.05	3.25	0.72	4.64	
Lower Bound[1]	0.01	0.01	0.33	0.06	0.43	
5th Percentile	0.04	0.02	0.78	0.17	1.08	
25th Percentile	0.08	0.03	1.62	0.35	2.33	
Median	0.37	0.04	2.48	0.56	3.58	
75th Percentile	0.92	0.06	4.14	0.91	6.02	
95th Percentile	2.43	0.10	8.16	1.75	11.55	
Upper Bound[1]	5.59	0.20	17.99	3.71	24.78	

[1]The upper bound is the envelope of maximum values at each point in time that bounds all of the 1,000 realizations. Similarly, the lower bound is the envelope of minimum values at each point in time that bounds all of the 1,000 realizations. All of the doses calculated in the uncertainty analysis fall within the upper and lower bounds.

[2]Deterministic doses calculated using the uncertainty model. In the original CA these were not cumulative doses at each POA but only considered direct discharges to the POA.

[3]Cumulative doses calculated from the original CA deterministic results. These agree very well with the cumulative deterministic doses calculated with the multi-source multi-POA uncertainty model.

[4]The dose at the 301 Bridge could not be assessed with the original CA uncertainty model.

6.1 Dose Uncertainty over 10,000 Year Simulation

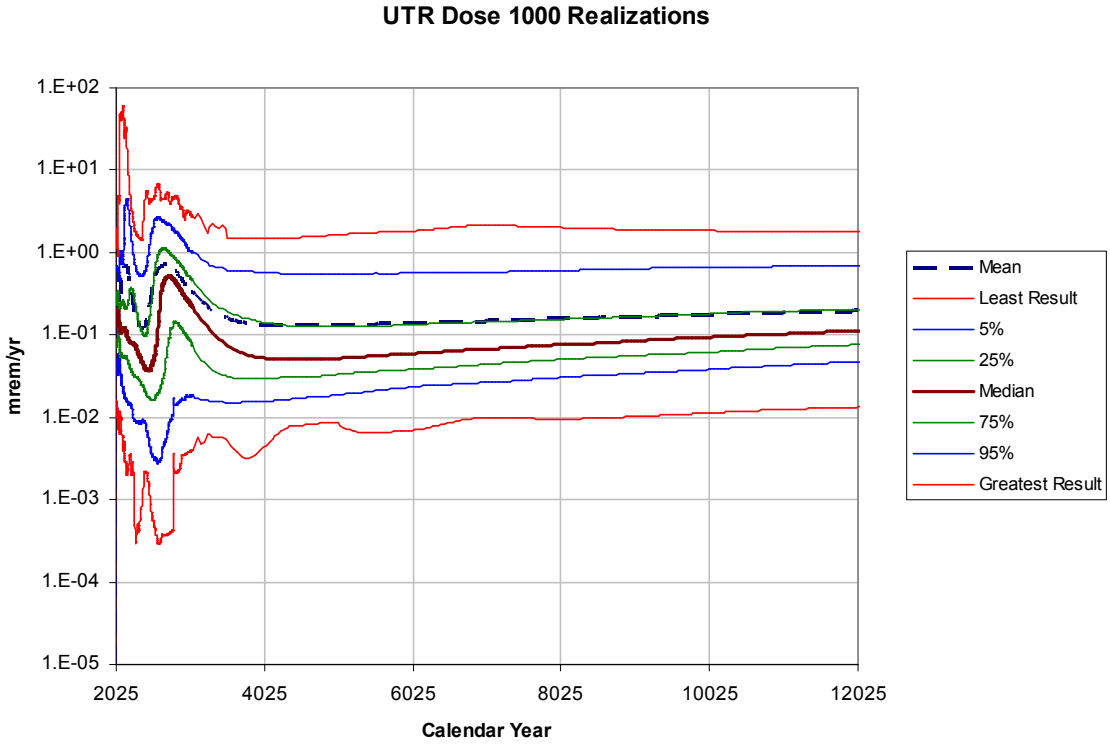

Figure 6.1-1. Uncertainty in dose at Upper Three Runs POA over 10,000 years.

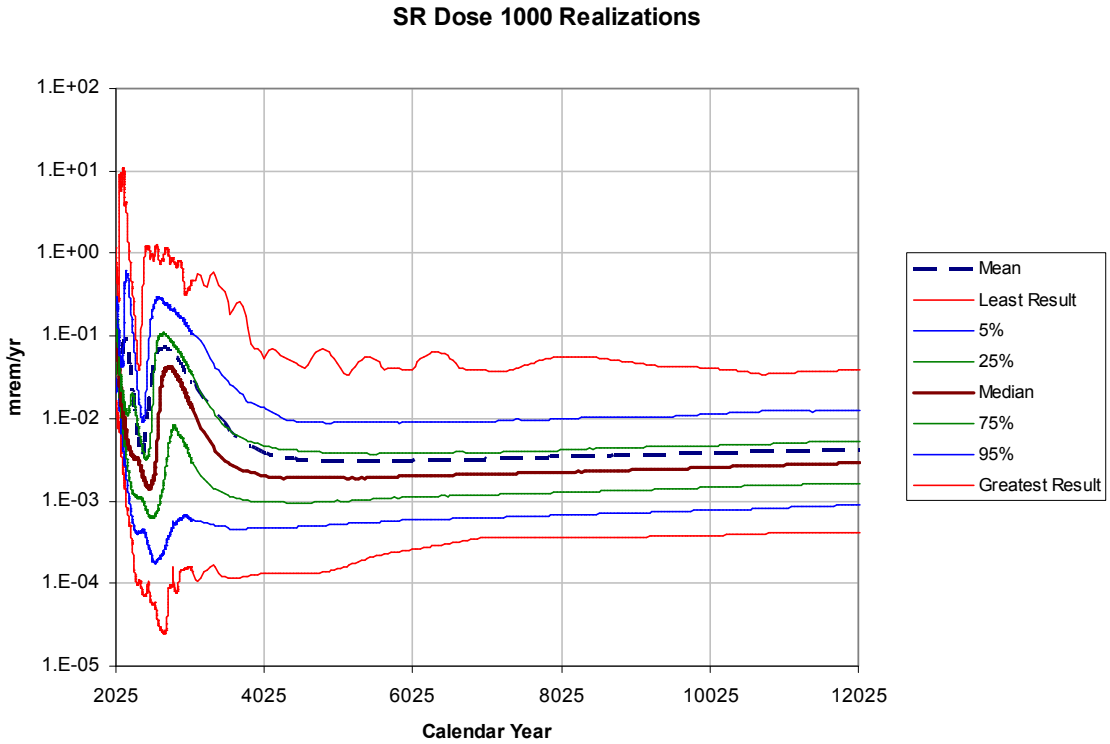

Figure 6.1-2. Uncertainty in cumulative dose at Savannah River POA over 10,000 years.

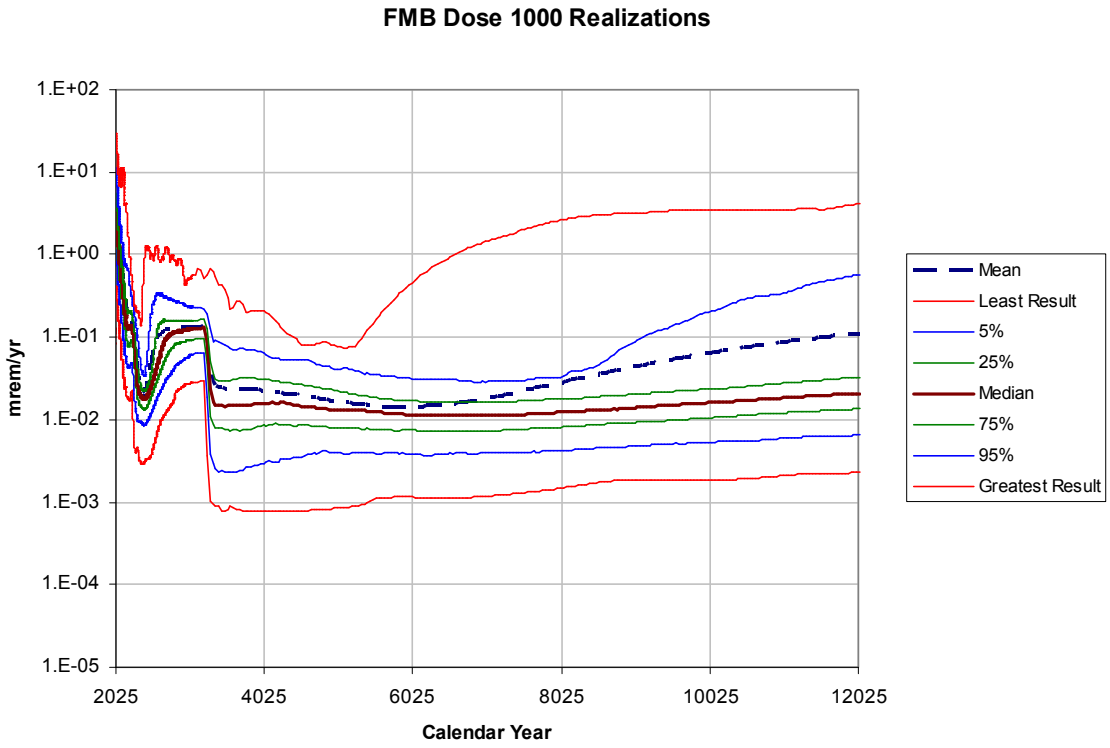

Figure 6.1-3. Uncertainty in cumulative dose at Fourmile Branch POA over 10,000 years.

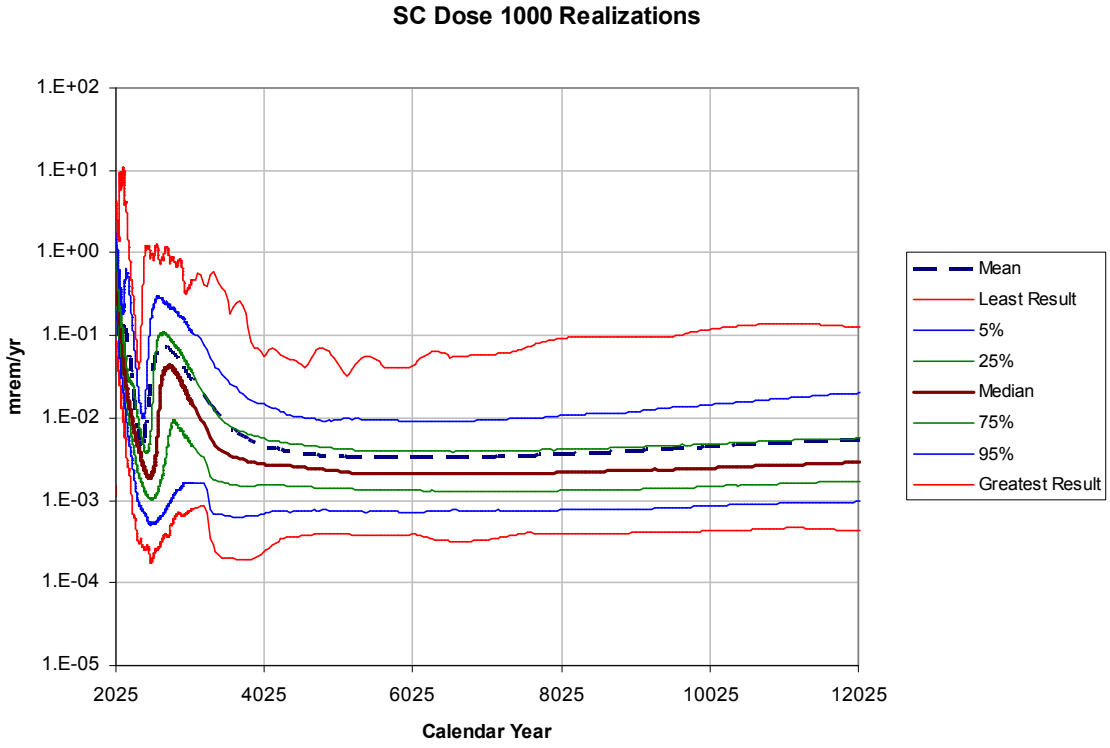

Figure 6.1-4. Uncertainty in cumulative dose at Steel Creek/Pen Branch POA over 10,000 years.

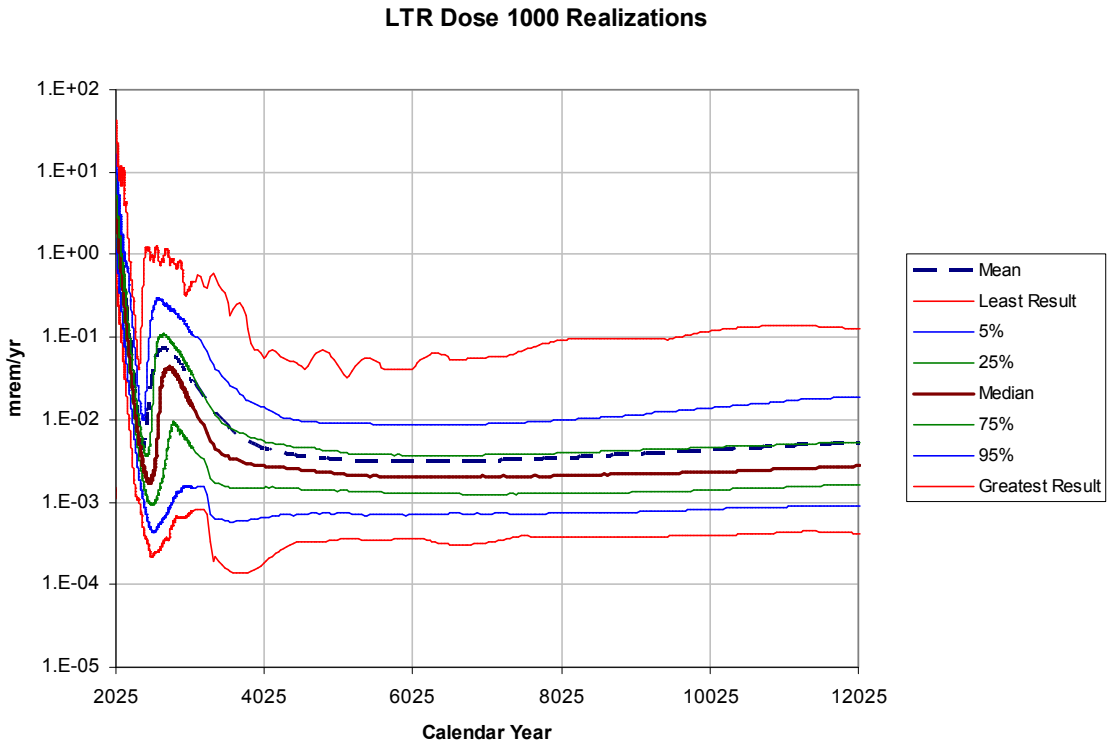

Figure 6.1-5. Uncertainty in cumulative dose at Lower Three Runs POA over 10,000 years.

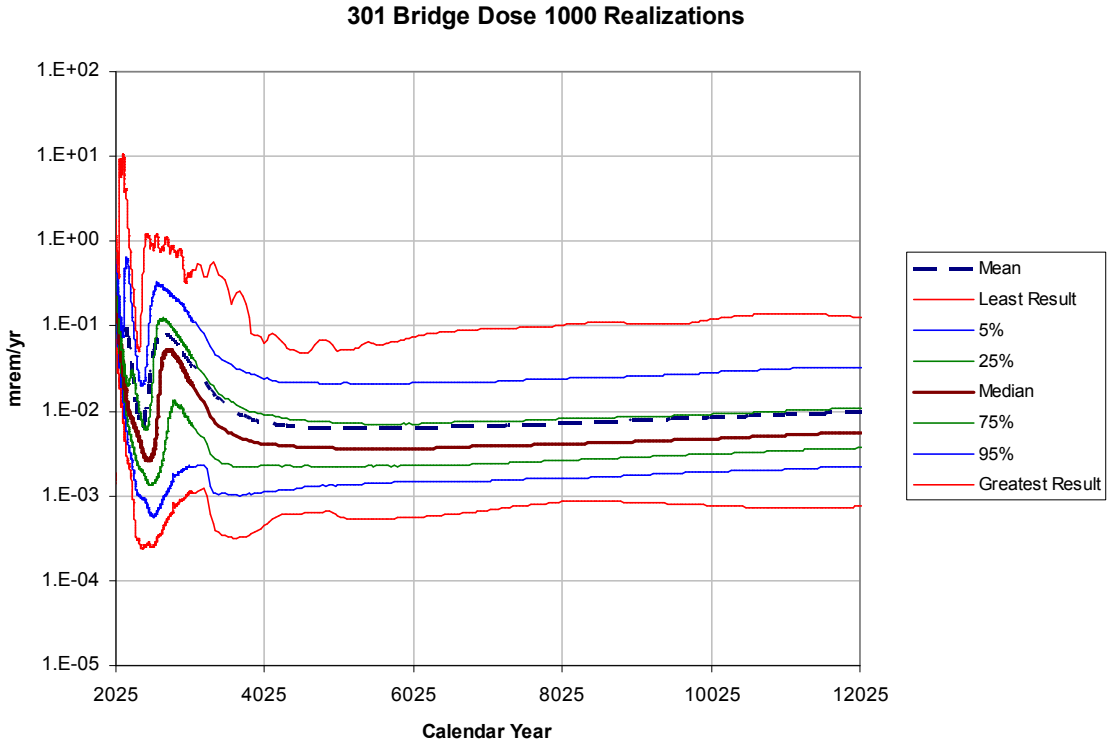

Figure 6.1-6. Uncertainty in cumulative dose at 301 Bridge POA over 10,000 years.

6.2 Dose Uncertainty over First 2,000 Years of Simulation

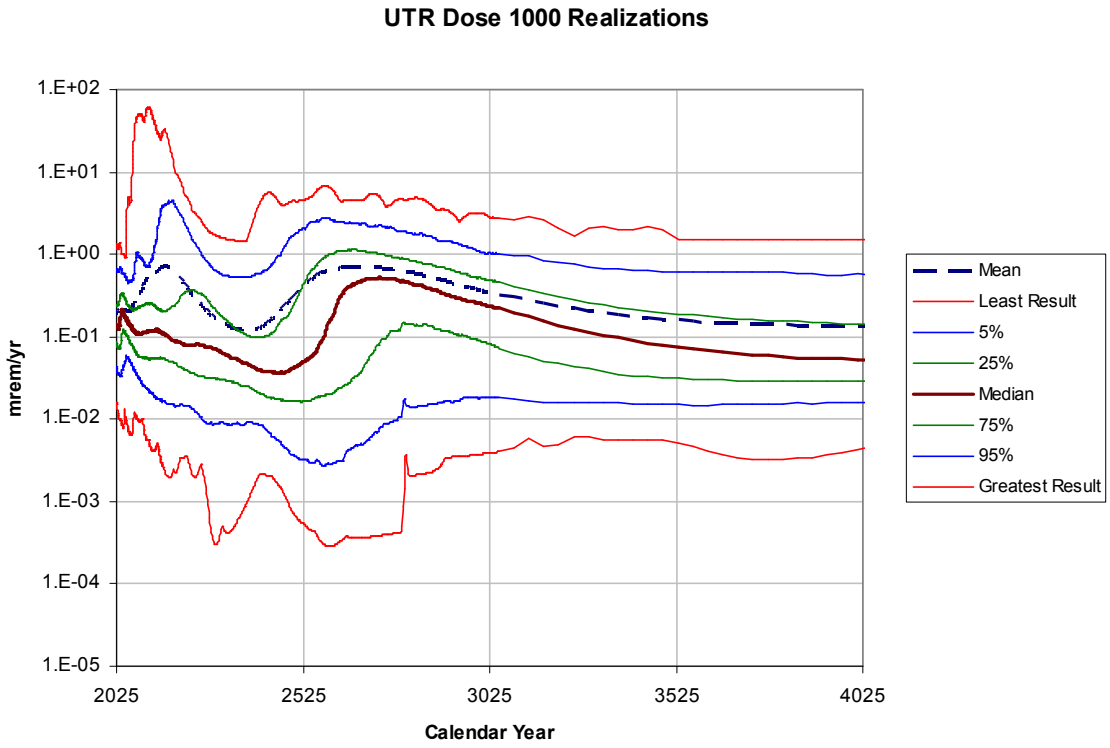

Figure 6.2-1. Uncertainty in dose at Upper Three Runs POA over 2,000 years.

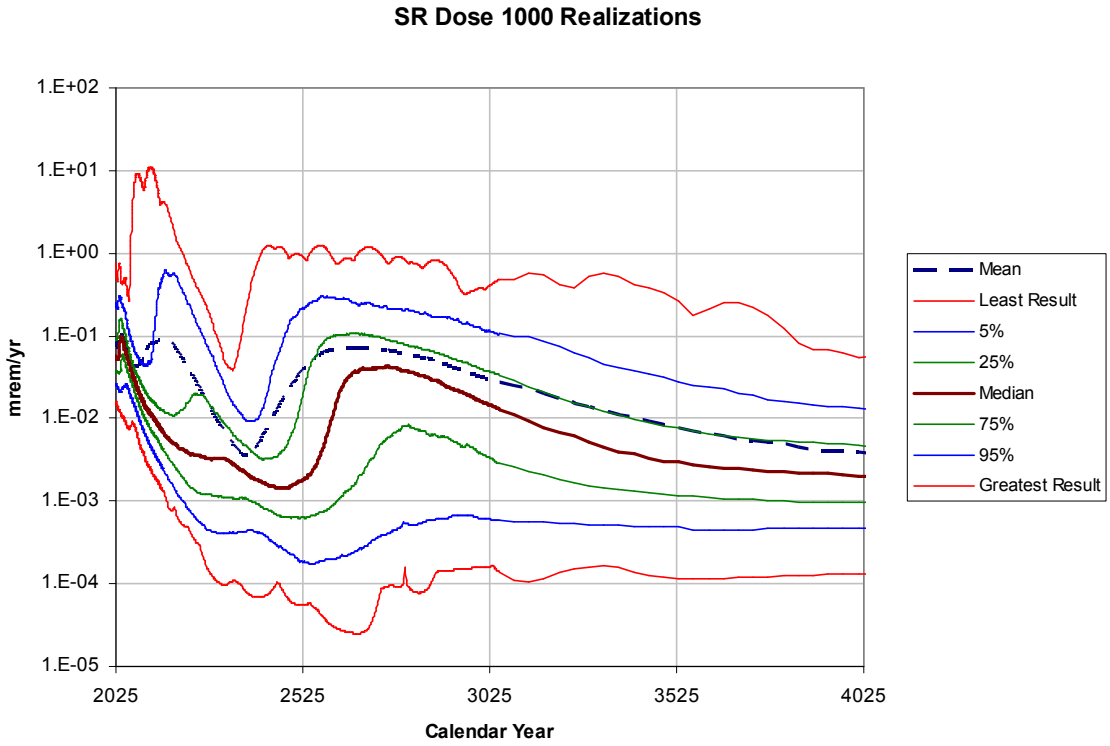

Figure 6.2-2. Uncertainty in cumulative dose at Savannah River POA over 2,000 years.

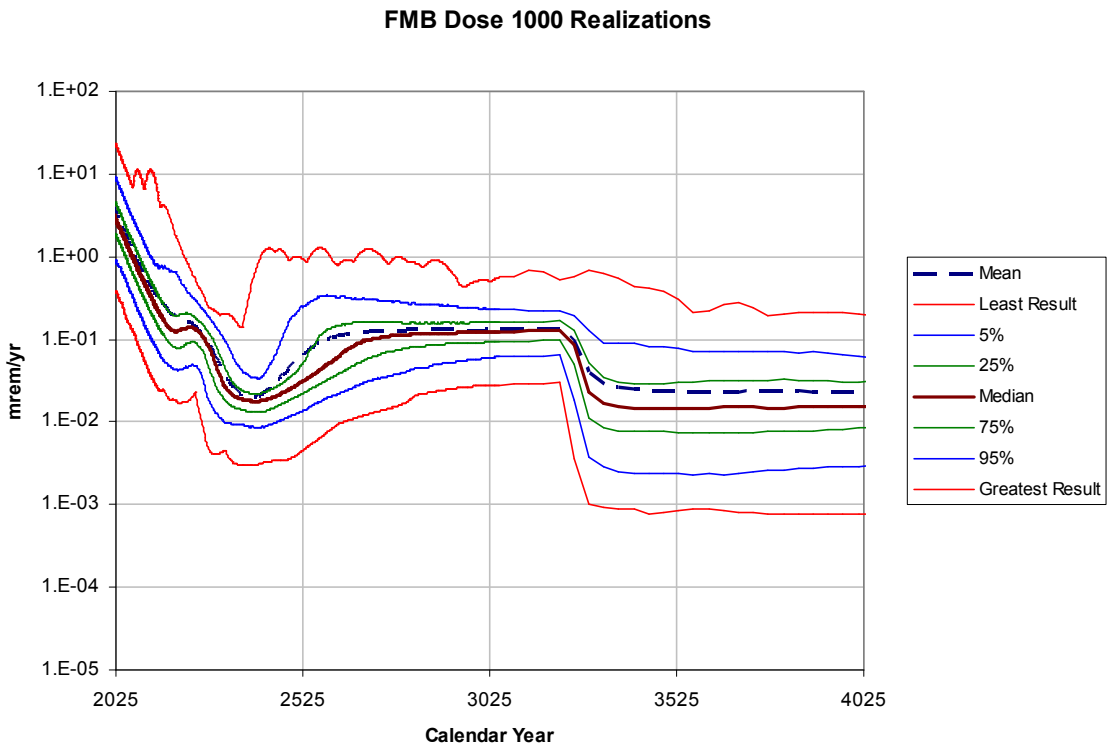

Figure 6.2-3. Uncertainty in cumulative dose at Fourmile Branch POA over 2,000 years.

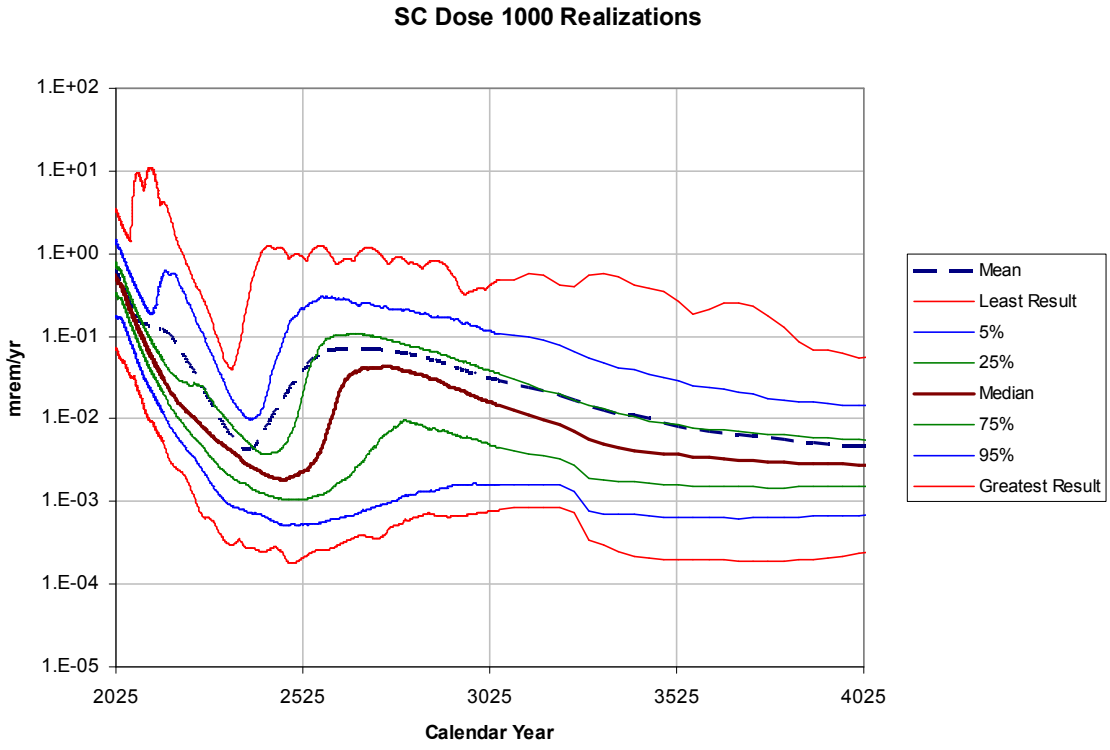

Figure 6.2-4. Uncertainty in cumulative dose at Steel Creek/Pen Branch POA over 2,000 years.

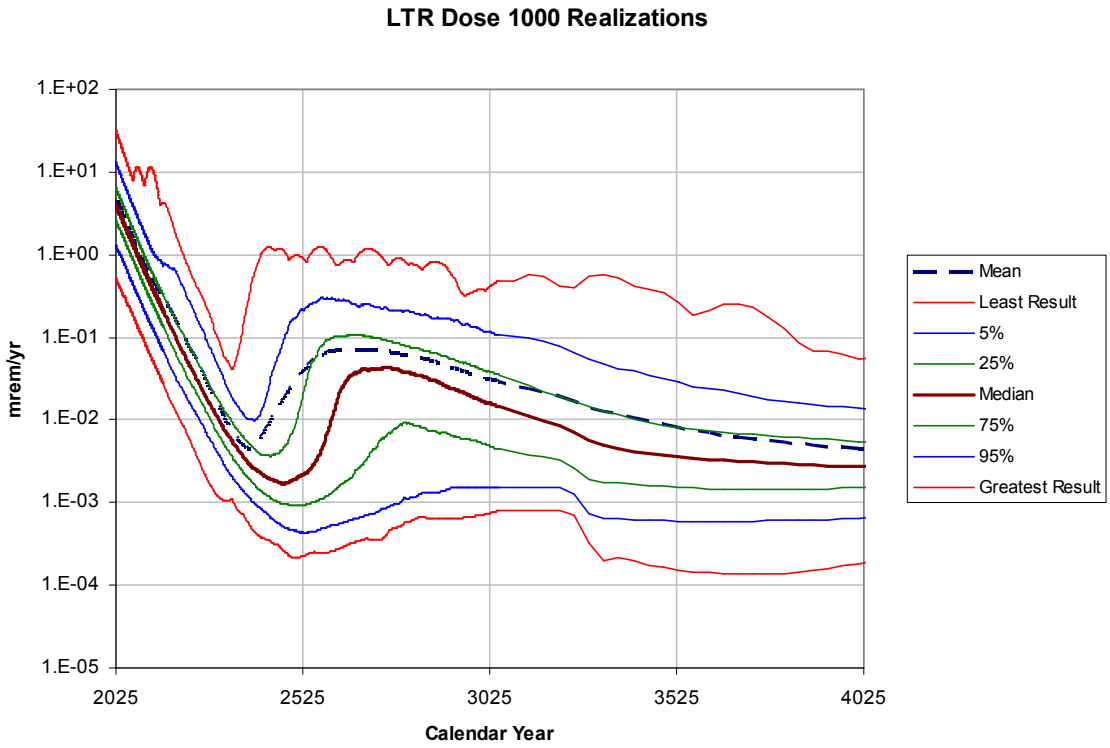

Figure 6.2-5. Uncertainty in cumulative dose at Lower Three Runs POA over 2,000 years.

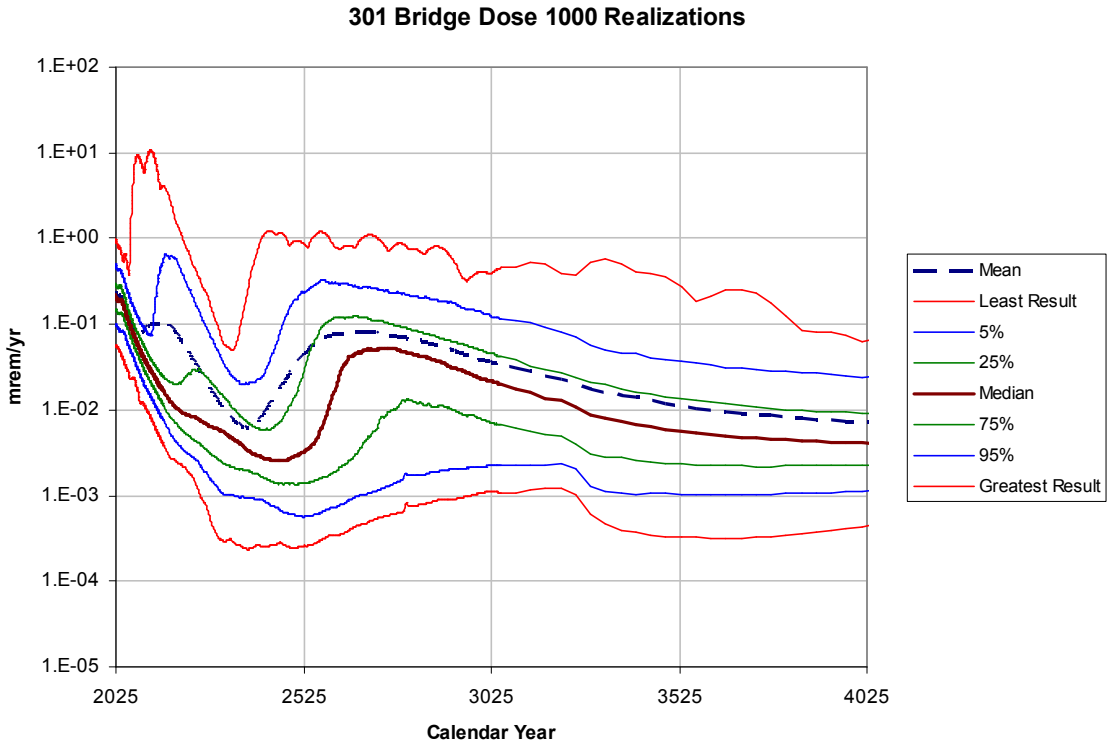

Figure 6.2-6. Uncertainty in cumulative dose at 301 Bridge POA over 2,000 years.

6.3 Mean, Median and Deterministic Doses

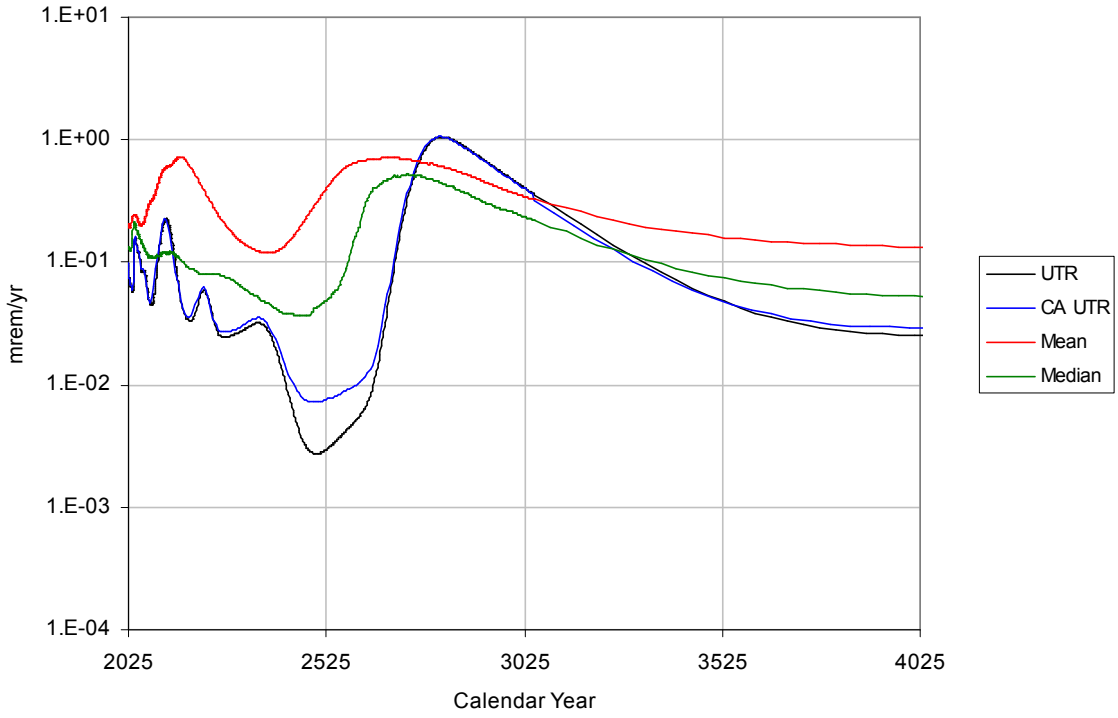

Figure 6.3-1. Mean, median and deterministic doses at Upper Three Runs POA.

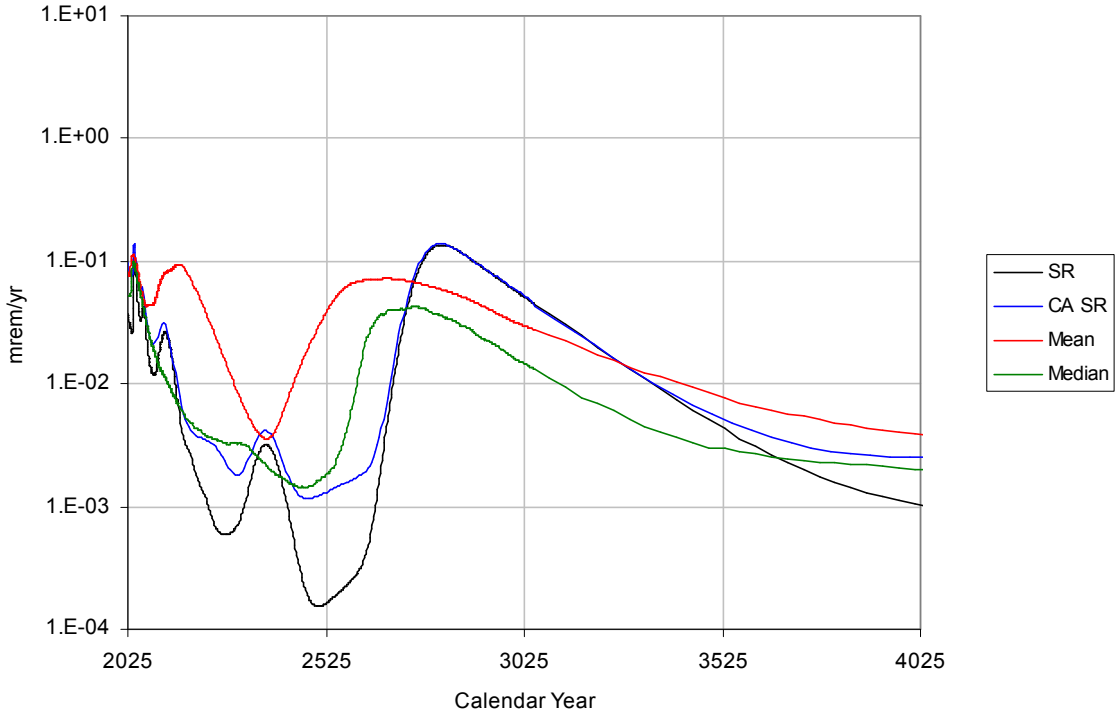

Figure 6.3-2. Mean, median and deterministic doses at Savannah River POA.

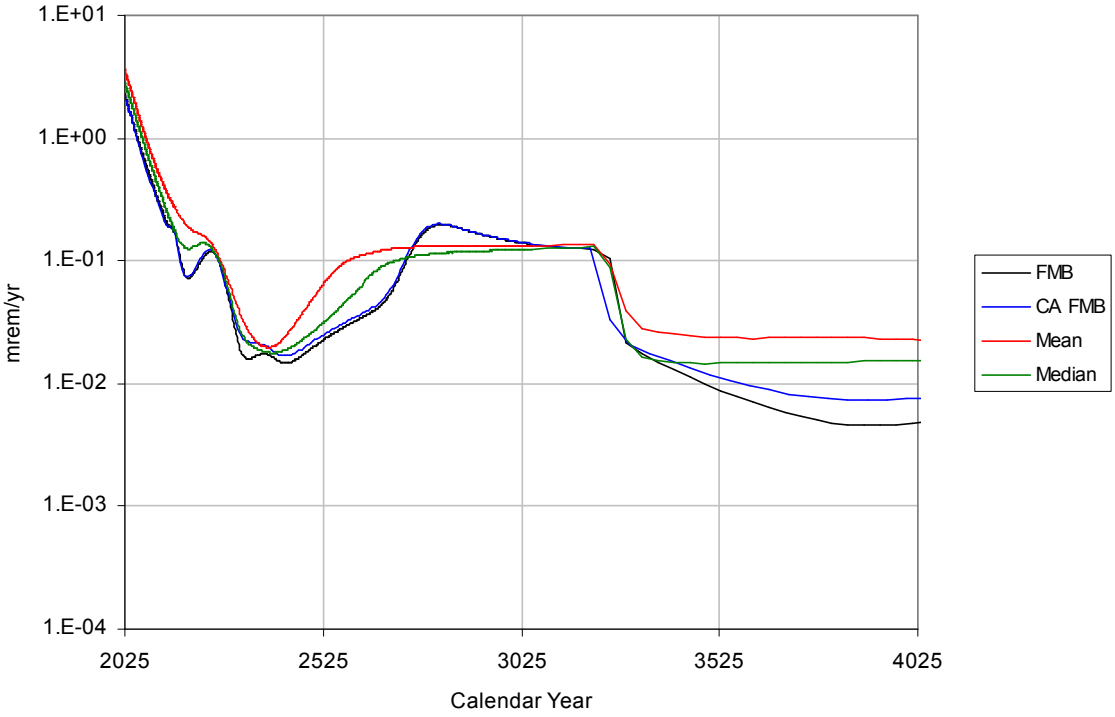

Figure 6.3-3. Mean, median and deterministic doses at Fourmile Branch POA.

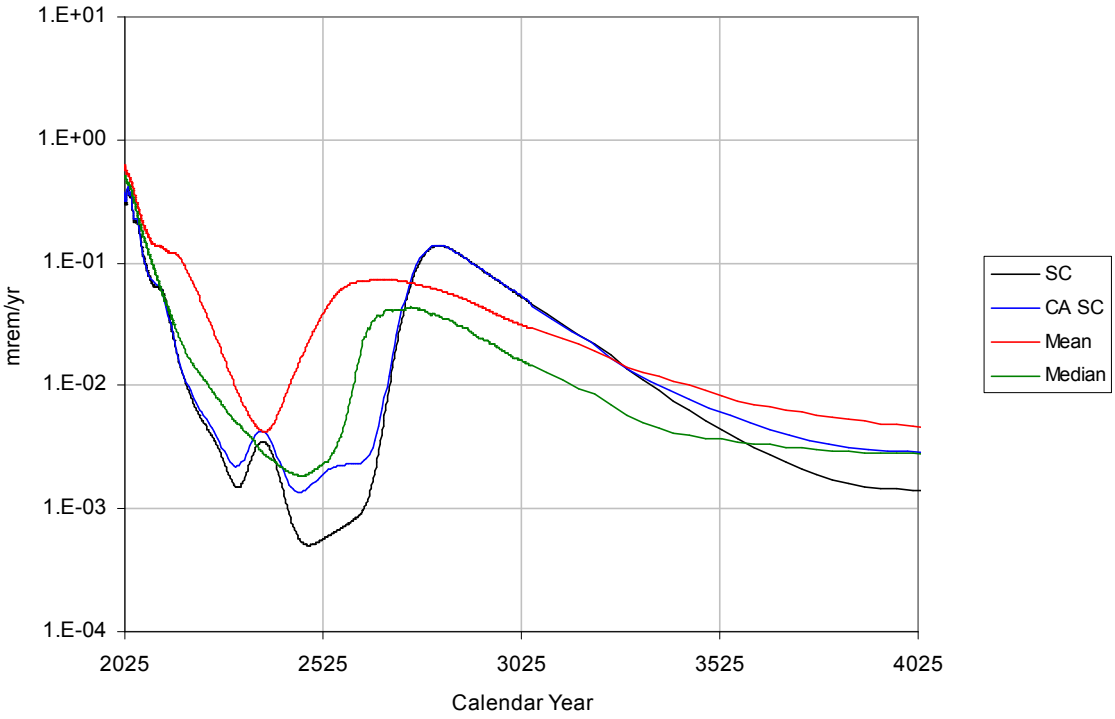

Figure 6.3-4. Mean, median and deterministic doses at Steel Creek/Pen Branch POA.

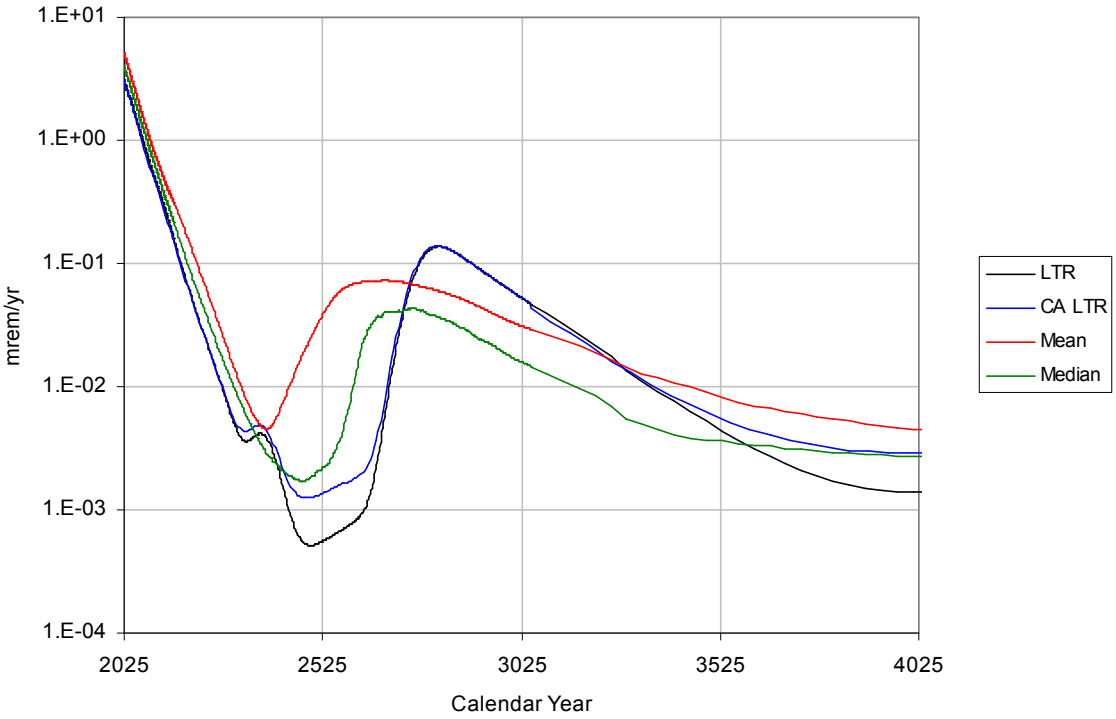

Figure 6.3-5. Mean, median and deterministic doses at Lower Three Runs POA.

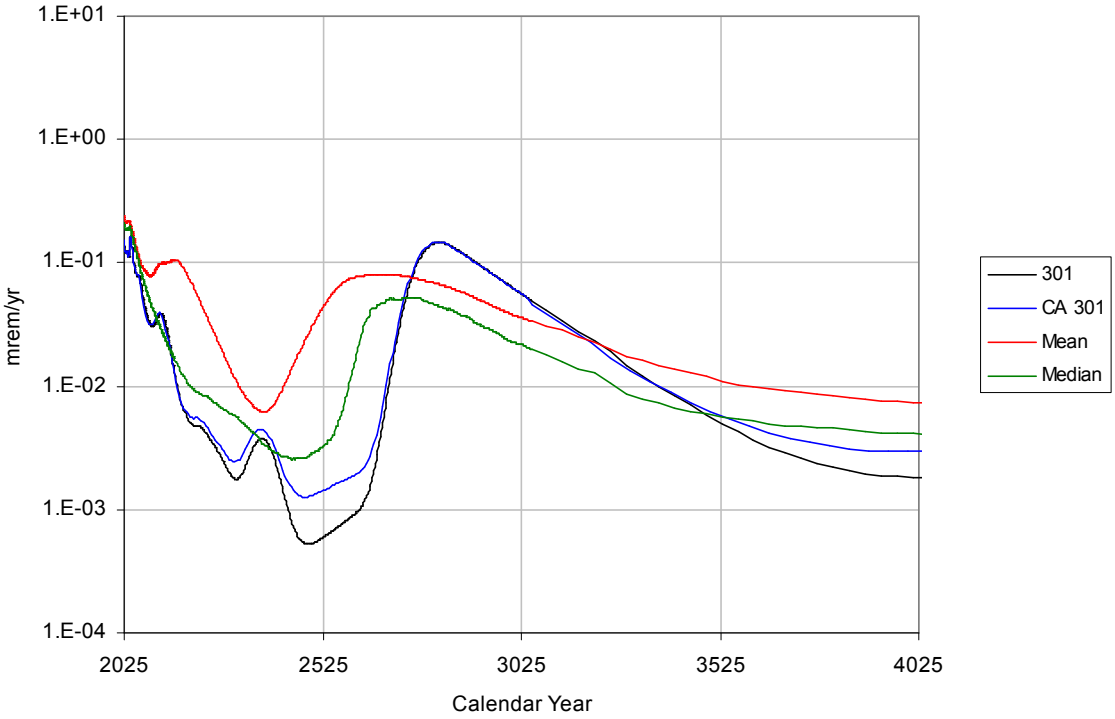

Figure 6.3-6. Mean, median and deterministic doses at 301 Bridge POA.

7.0 Separate Effects on Uncertainty

To further examine the important factors in CA uncertainty, the uncertainty in K_d and uncertainty in the four categories of stochastic parameters listed in Tables 5-1 through 5-4 were analyzed separately. Results from this analysis are presented for each POA in Sections 7.1 through 7.6. Figures in these subsections are limited to the time period 2025 to 4025. The first plot in each subsection shows the overall uncertainty when all stochastic parameters are allowed to vary and subsequent plots show the impact from varying each category of parameters alone.

Some general trends can be seen in the results of this separate effects analysis:

1. Results for uncertainty in dose parameters, material properties, and surface water flow follow the shape of the deterministic calculations for each POA as shown in Figure 4-4, whereas results for K_d and vadose and aquifer flow do not. This is because the K_d values and vadose and aquifer flow rates change the radionuclide transport times. Dose parameters and surface water flows (which are so large that they in effect instantaneously transport the radionuclides from the point of outcrop to the POA) have effectively no impact on the transport time to the POA and material properties have only a secondary effect on transport time. By altering the transport time, K_d and groundwater flow change the shape of the uncertainty response. If the transport time is not changed, uncertainty results spread about the deterministic calculation.

2. K_d values have a large impact on the uncertainty distributions. As noted in Section 5.0, relatively large standard deviations are assumed for these distributions.

3. Groundwater flow uncertainty also has a significant impact on the uncertainty distributions. This is likely caused by the relatively large standard deviations used for the aquifer flow parameters shown in Table 5-4.

4. Material properties do not have a significant impact on the uncertainty distributions.

5. Surface water flows have a small impact on the uncertainty distributions. However, the stochastic distribution assigned to the surface water flows represents an estimate of the distribution of 1,000 year average values as recommended by Shine 2009. These distributions are very narrow and the uncertainty results may not completely reflect the expected response to variations in surface water flow. Alternatively, using a distribution of yearly average flows is not appropriate for evaluating the impact on the CA dose over a 1,000 year period of assessment, since it is unreasonable to assume that the flow would remain at a value selected from this distribution throughout the entire time period. Another approach that could be considered in the next CA would be to use a yearly average flow distribution but to resample the distribution at each year or time step in the CA simulation. However, the representativeness of re-sampling at each time step would have to be evaluated closely due to the use of varying time steps. This approach would give a series of varying surface water flow rates that would simulate the expected yearly fluctuation in flow and give a better measure of uncertainty to flow during Monte Carlo runs. The feasibility of such an approach would have to be tested versus the potential increase in run times that might be incurred.

7.1 Dose Uncertainty at Upper Three Runs POA

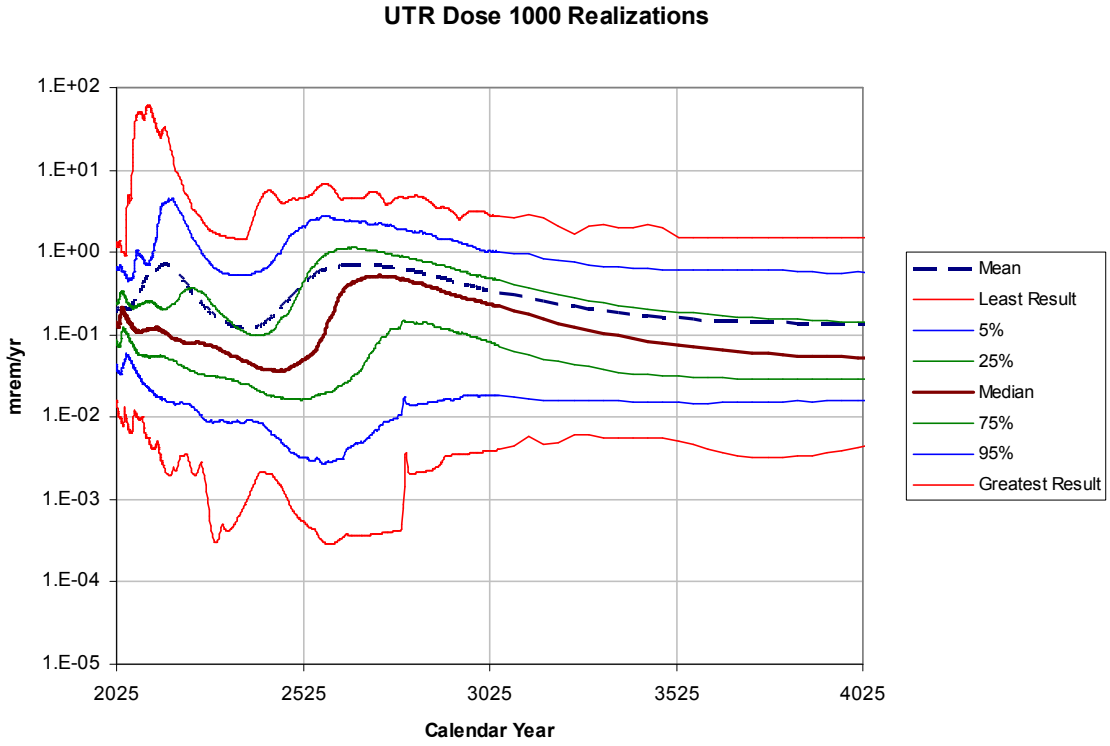

Figure 7.1-1. Overall uncertainty in dose at Upper Three Runs POA.

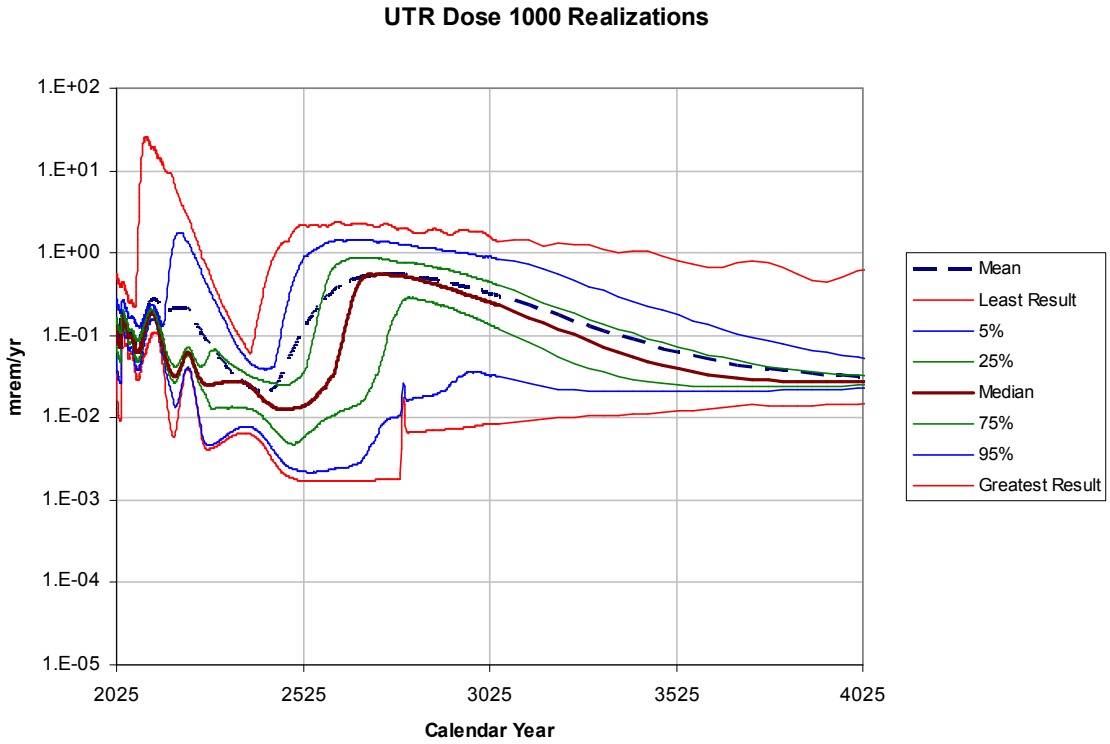

Figure 7.1-2. Uncertainty in dose at Upper Three Runs POA from variation in K_d.

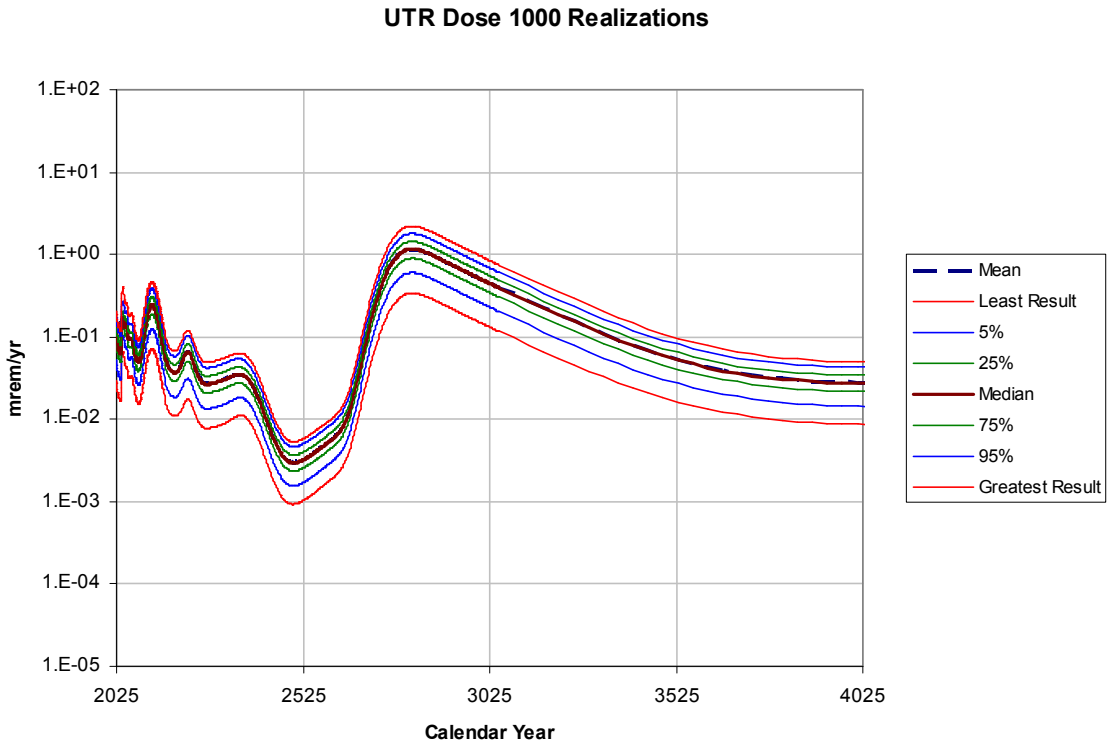

Figure 7.1-3. Uncertainty in dose at Upper Three Runs POA from variation in dose parameters.

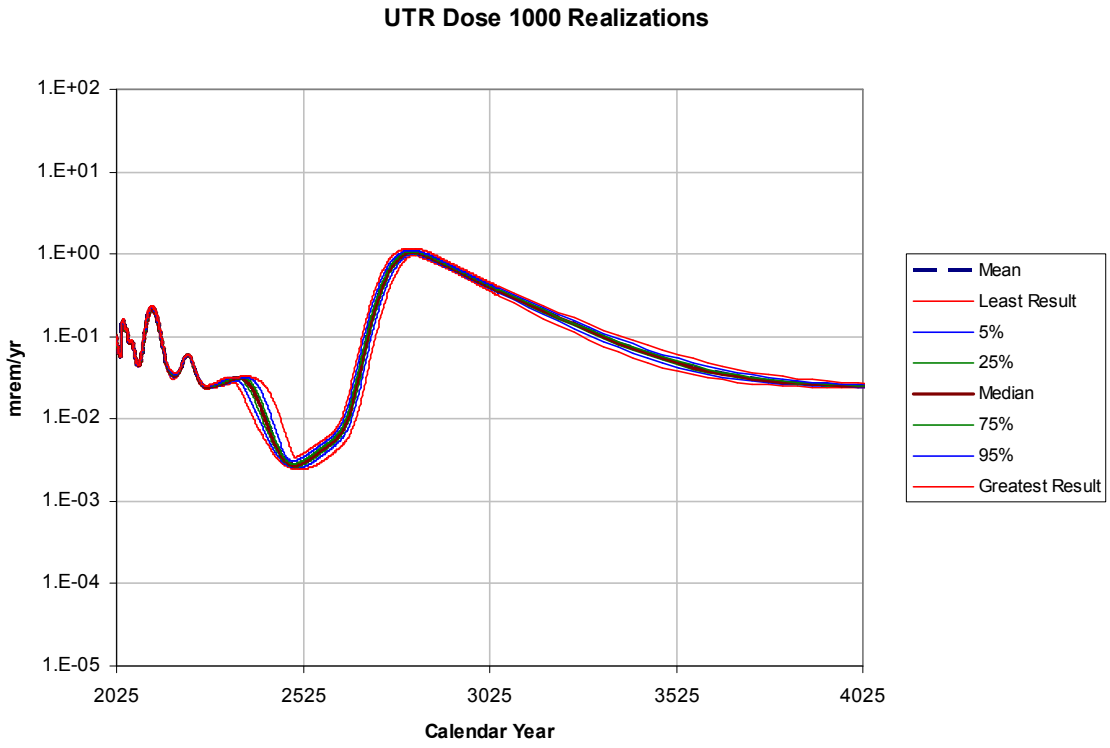

Figure 7.1-4. Uncertainty in dose at Upper Three Runs POA from variation in material properties.

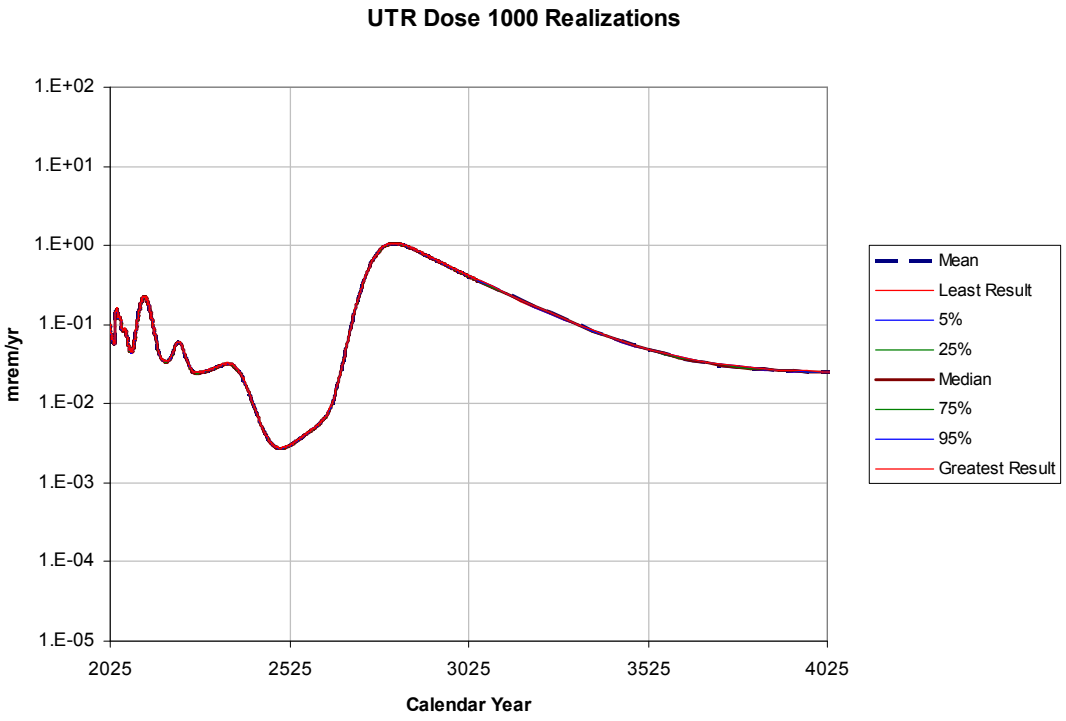

Figure 7.1-5. Uncertainty in dose at Upper Three Runs POA from variation in surface water flow.

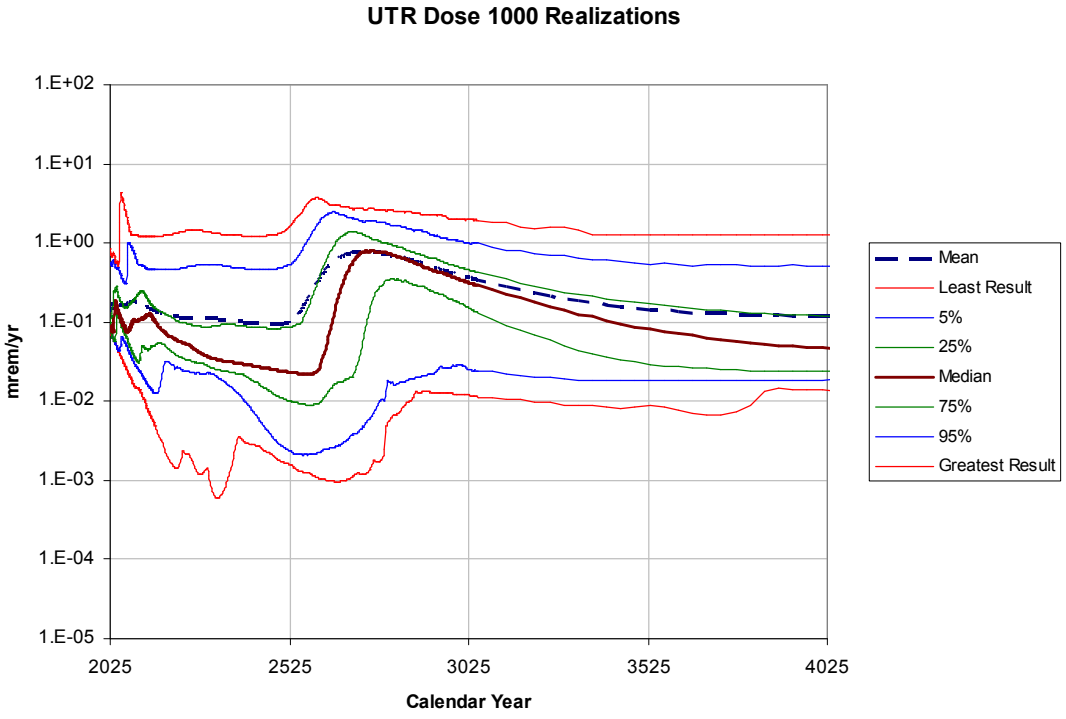

Figure 7.1-6. Uncertainty in dose at Upper Three Runs POA from variation in infiltration and aquifer flow.

7.2 Dose Uncertainty at Savannah River POA

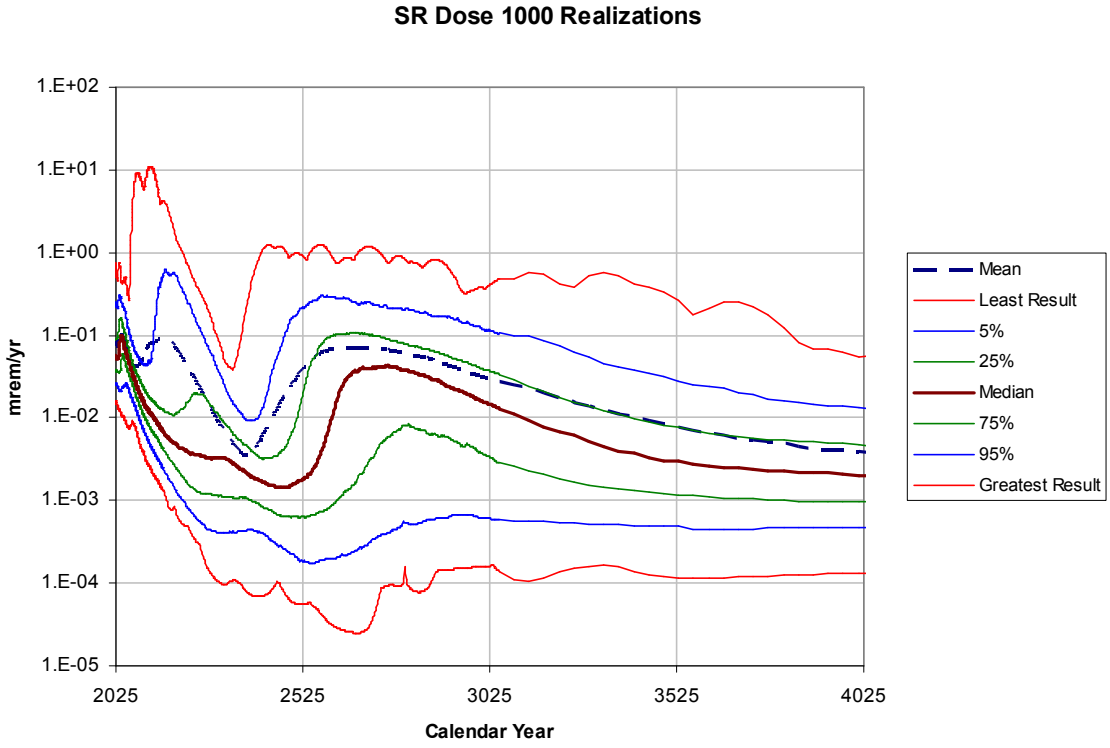

Figure 7.2-1. Overall uncertainty in dose at Savannah River POA.

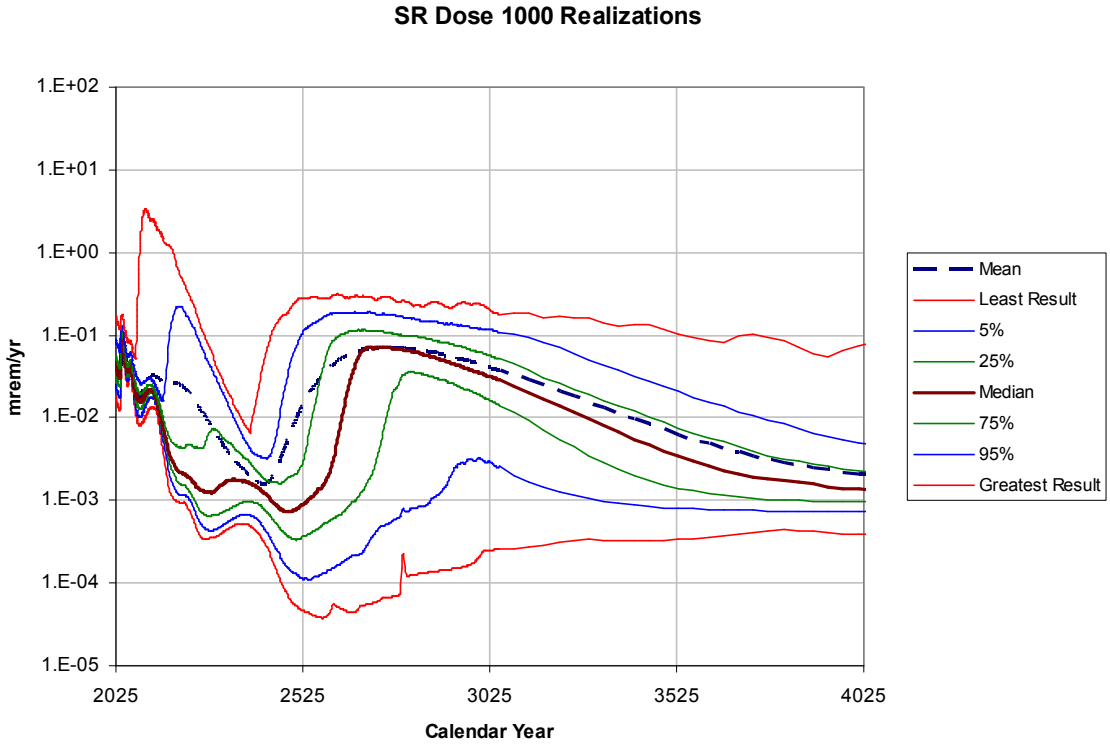

Figure 7.2-2. Uncertainty in dose at Savannah River POA from variation in K_d.

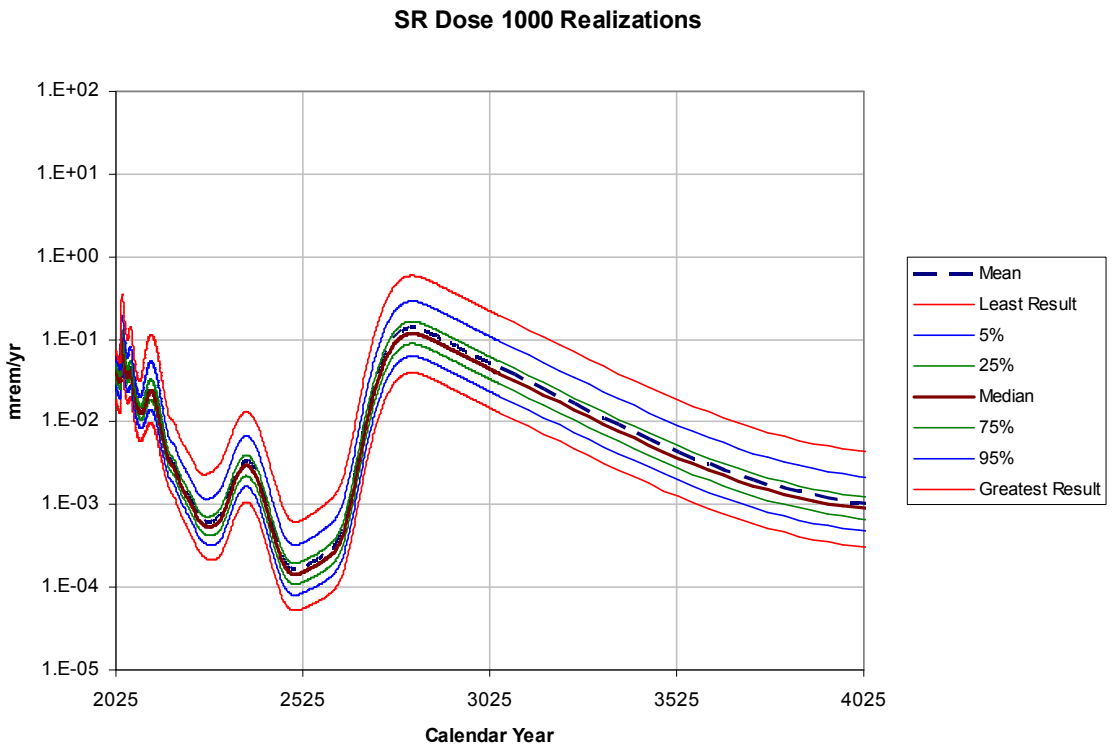

Figure 7.2-3. Uncertainty in dose at Savannah River POA from variation in dose parameters.

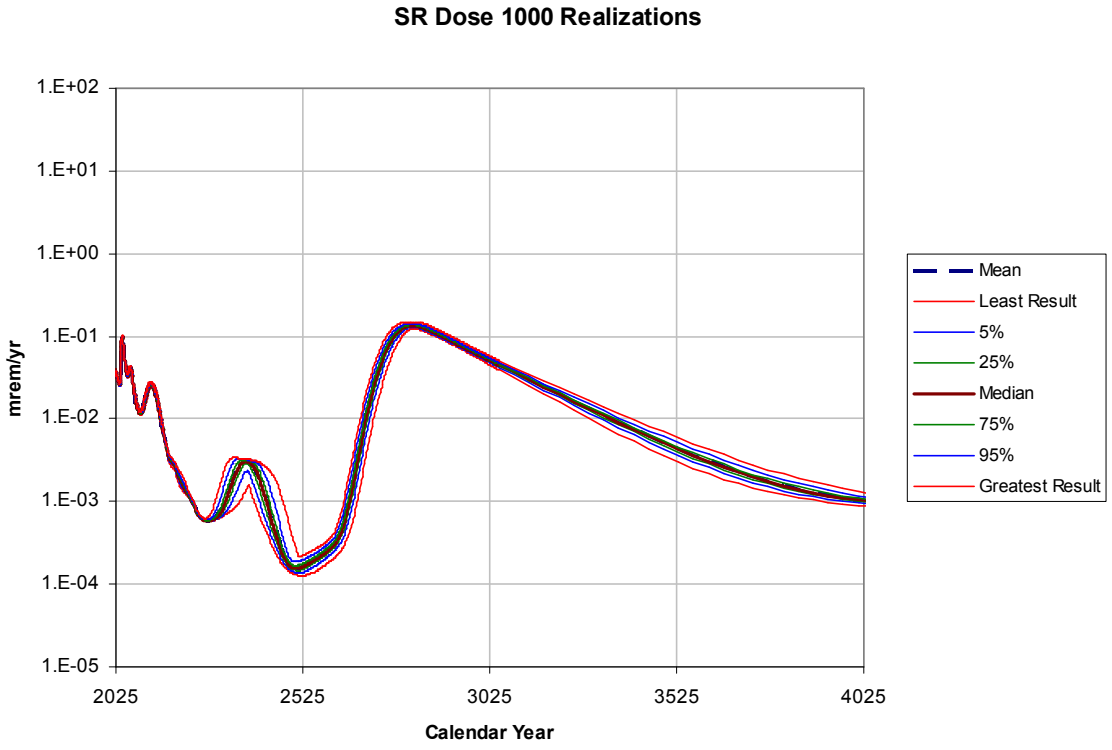

Figure 7.2-4. Uncertainty in dose at Savannah River POA from variation in material properties.

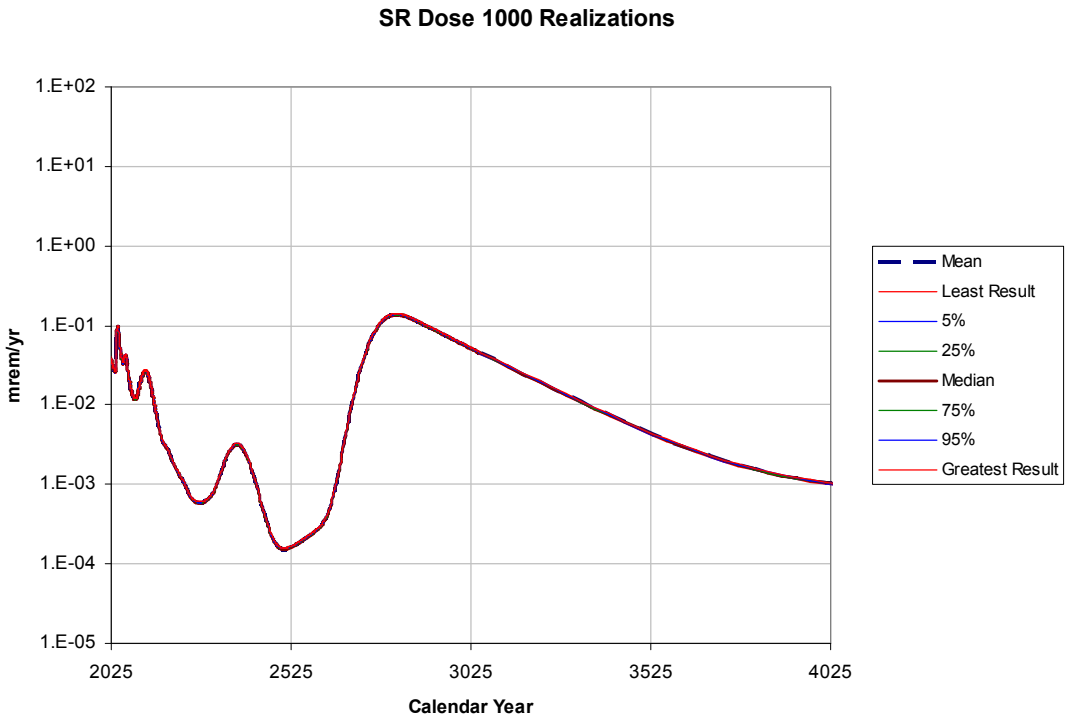

Figure 7.2-5. Uncertainty in dose at Savannah River POA from variation in surface water flow.

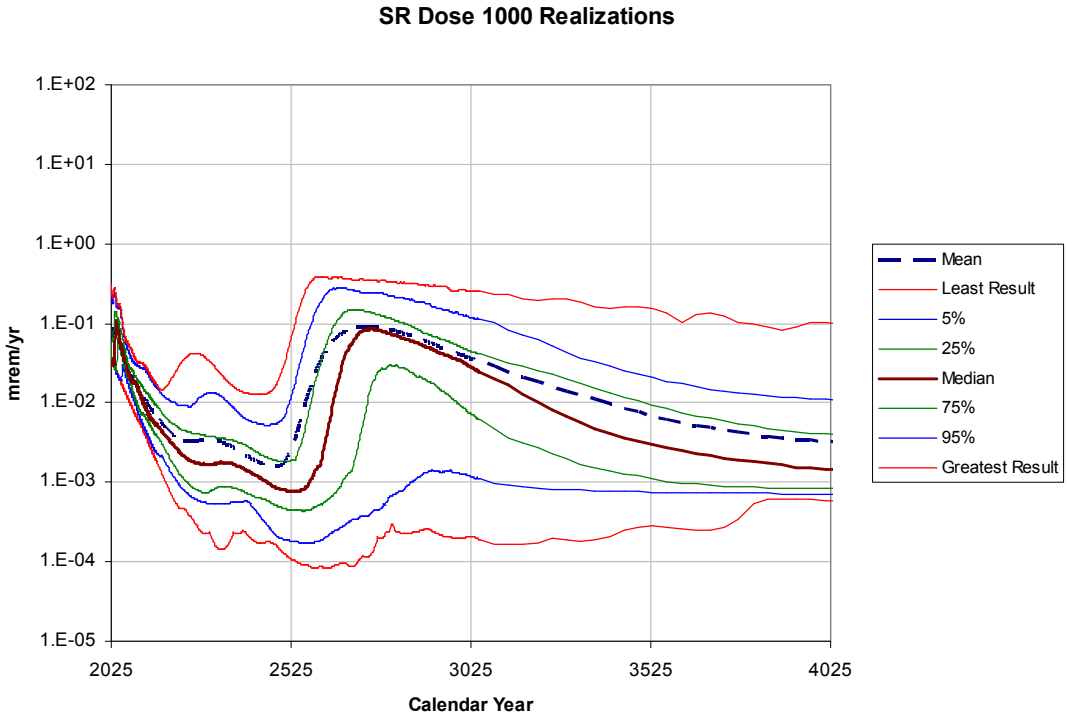

Figure 7.2-6. Uncertainty in dose at Savannah River POA from variation in infiltration and aquifer flow.

7.3 Dose Uncertainty at Fourmile Branch POA

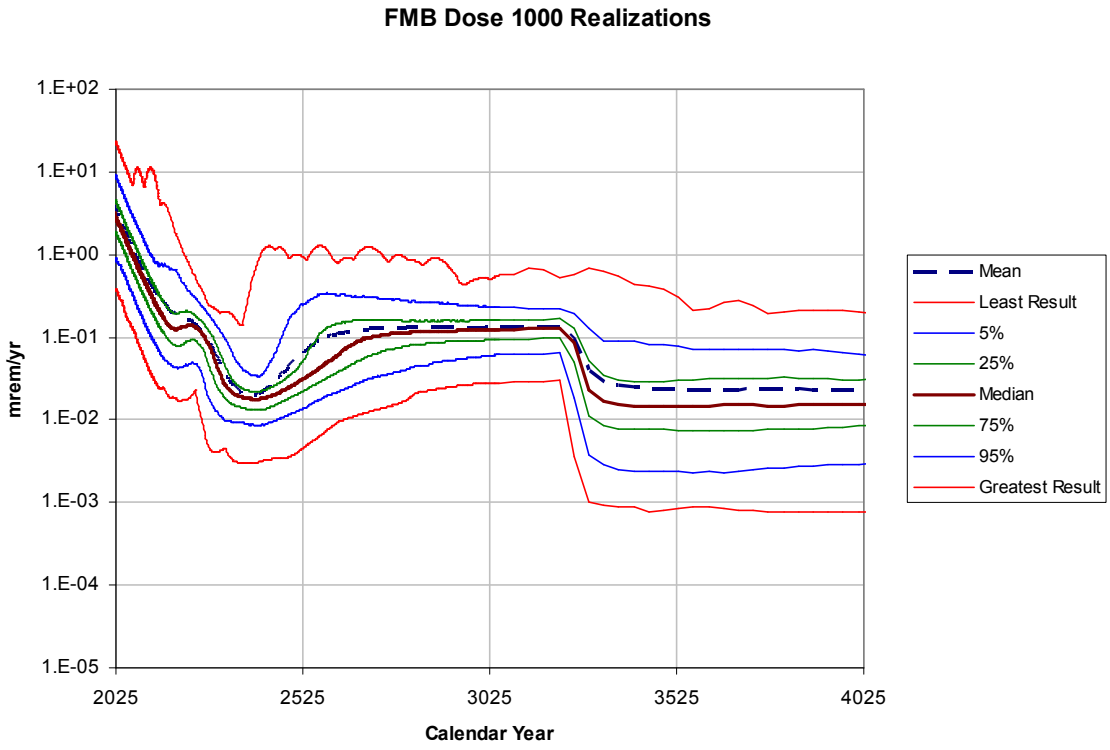

Figure 7.3-1. Overall uncertainty in dose at Fourmile Branch POA.

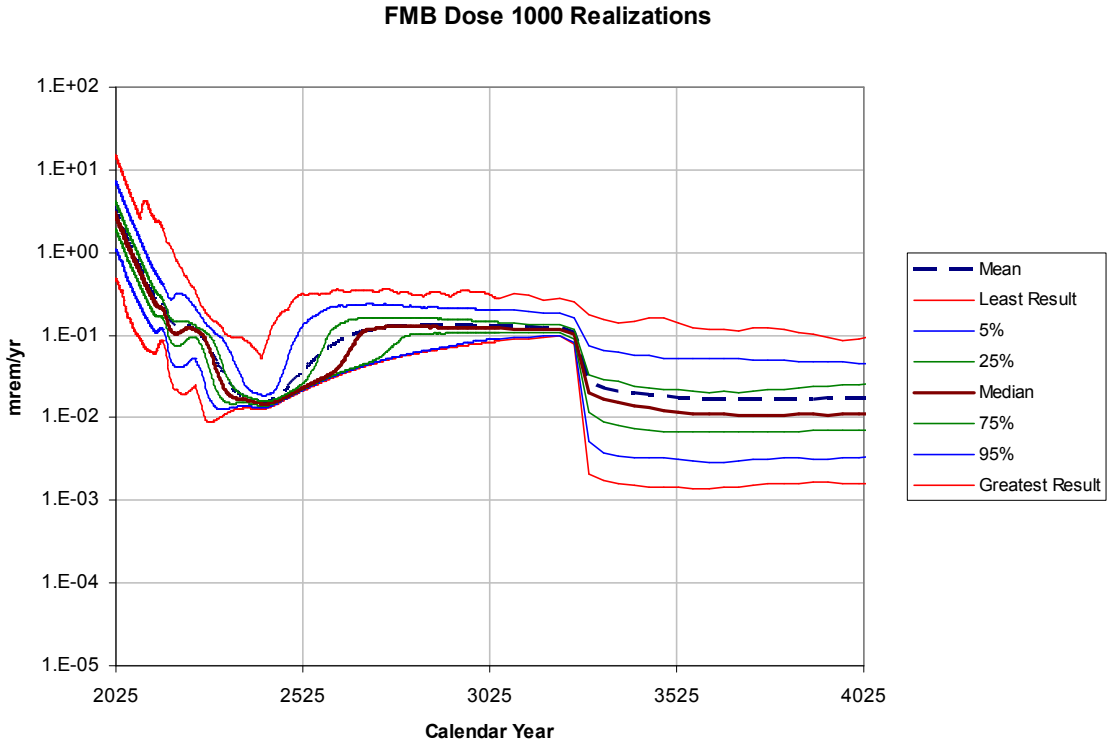

Figure 7.3-2. Uncertainty in dose at Fourmile Branch POA from variation in K_d.

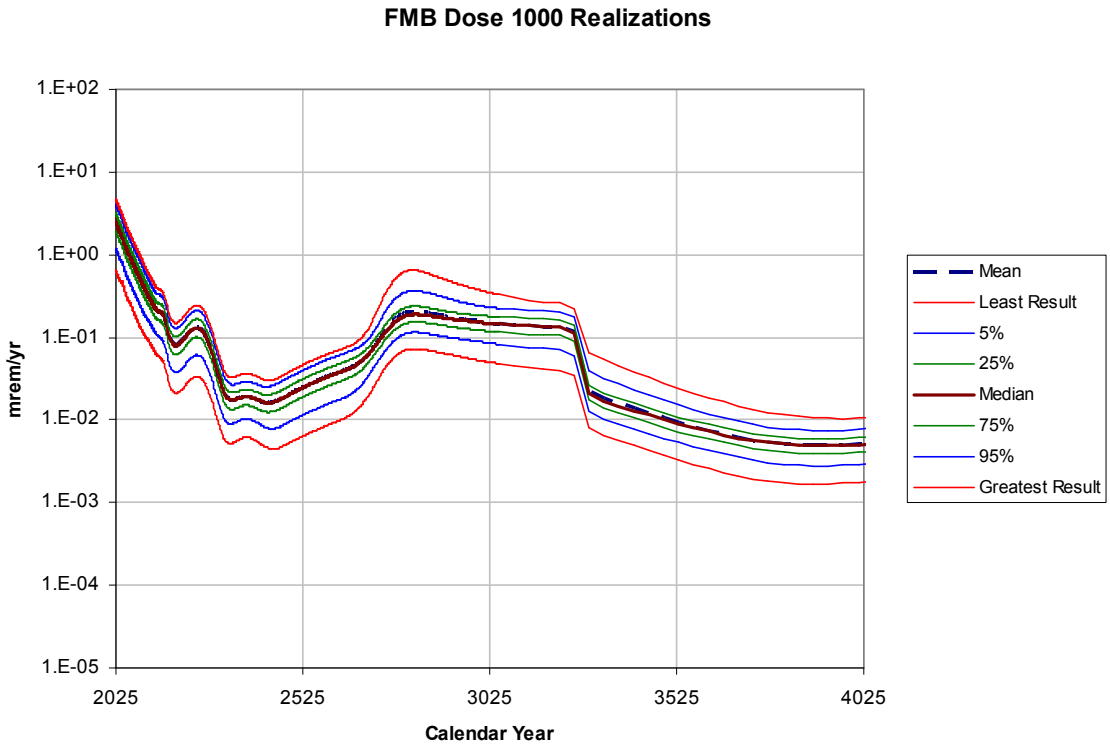

Figure 7.3-3. Uncertainty in dose at Fourmile Branch POA from variation in dose parameters.

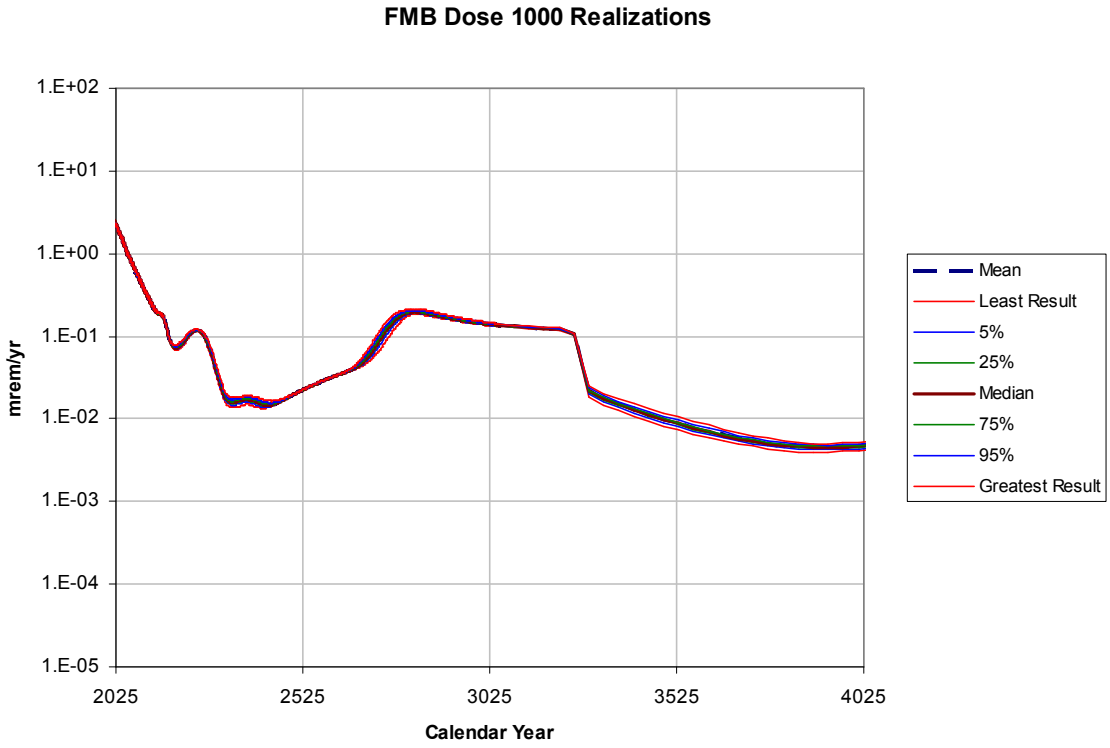

Figure 7.3-4. Uncertainty in dose at Fourmile Branch POA from variation in material properties.

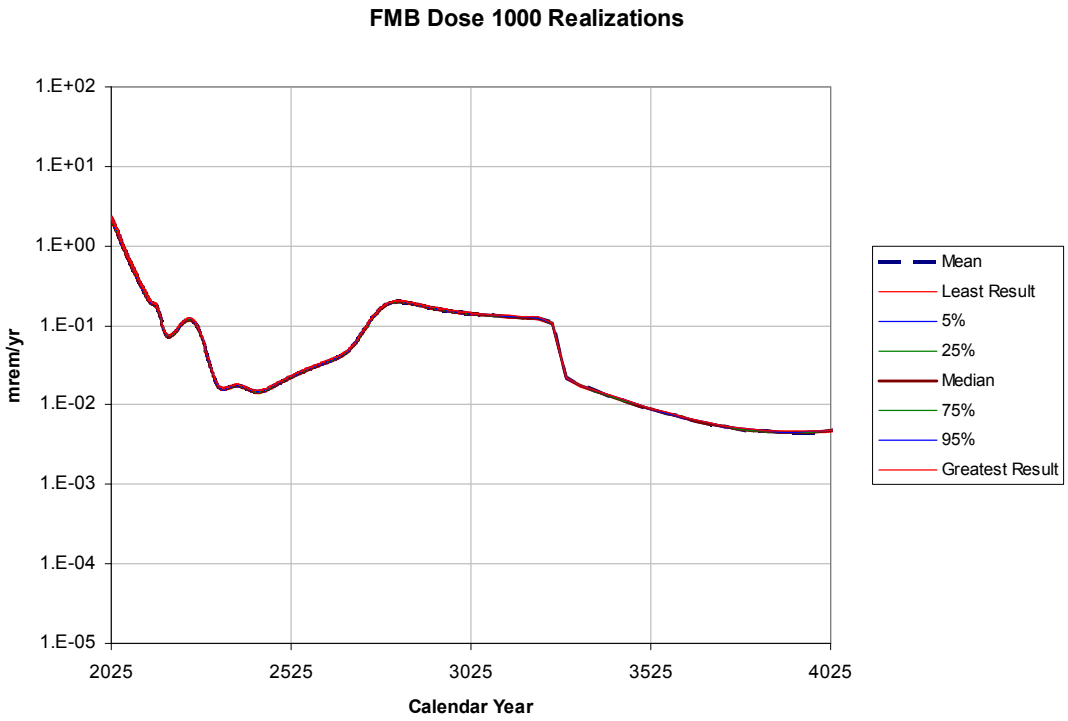

Figure 7.3-5. Uncertainty in dose at Fourmile Branch POA from variation in surface water flow.

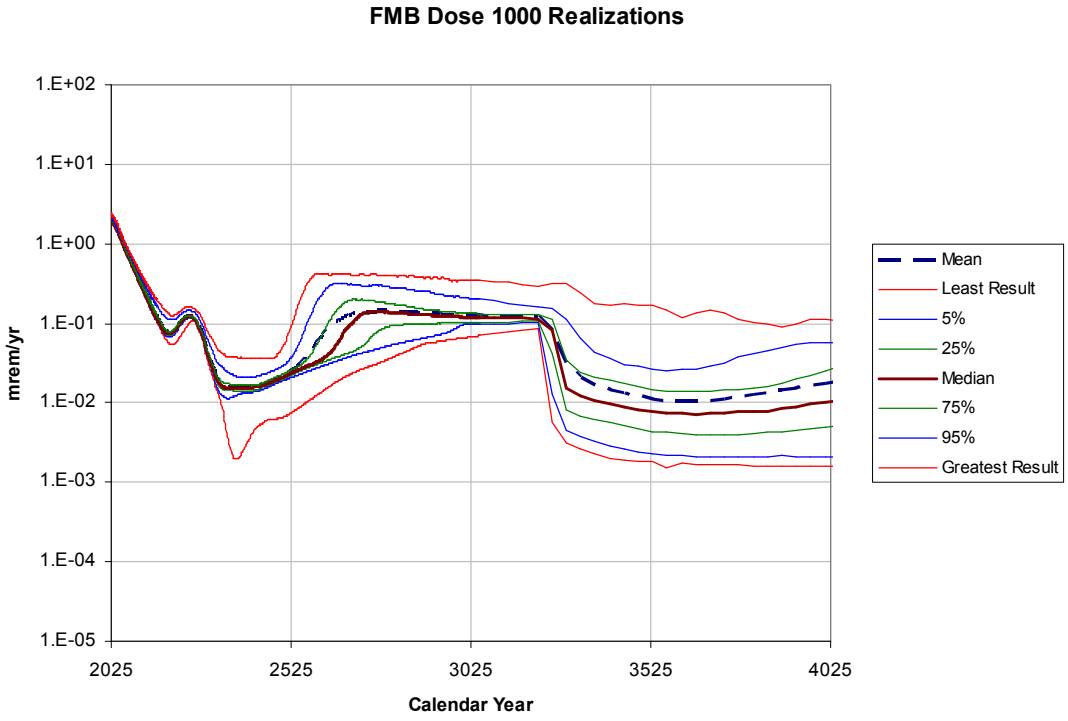

Figure 7.3-6. Uncertainty in dose at Fourmile Branch POA from variation in infiltration and aquifer flow.

7.4 Dose Uncertainty at Steel Creek/Pen Branch POA

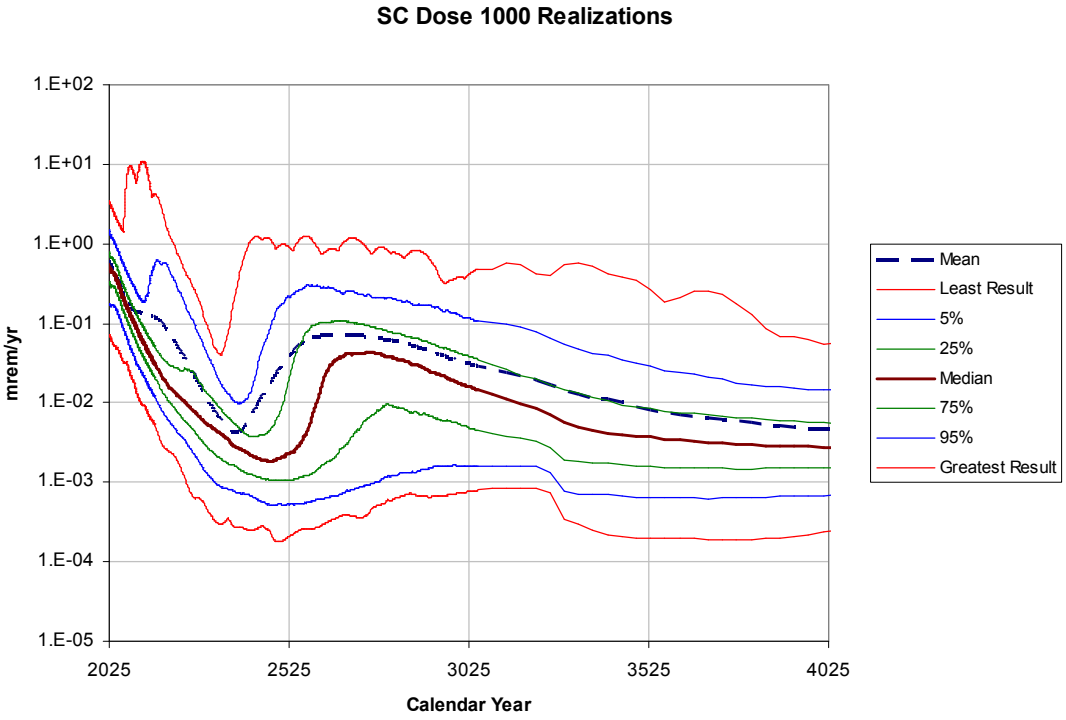

Figure 7.4-1. Overall uncertainty in dose at Steel Creek/Pen Branch POA.

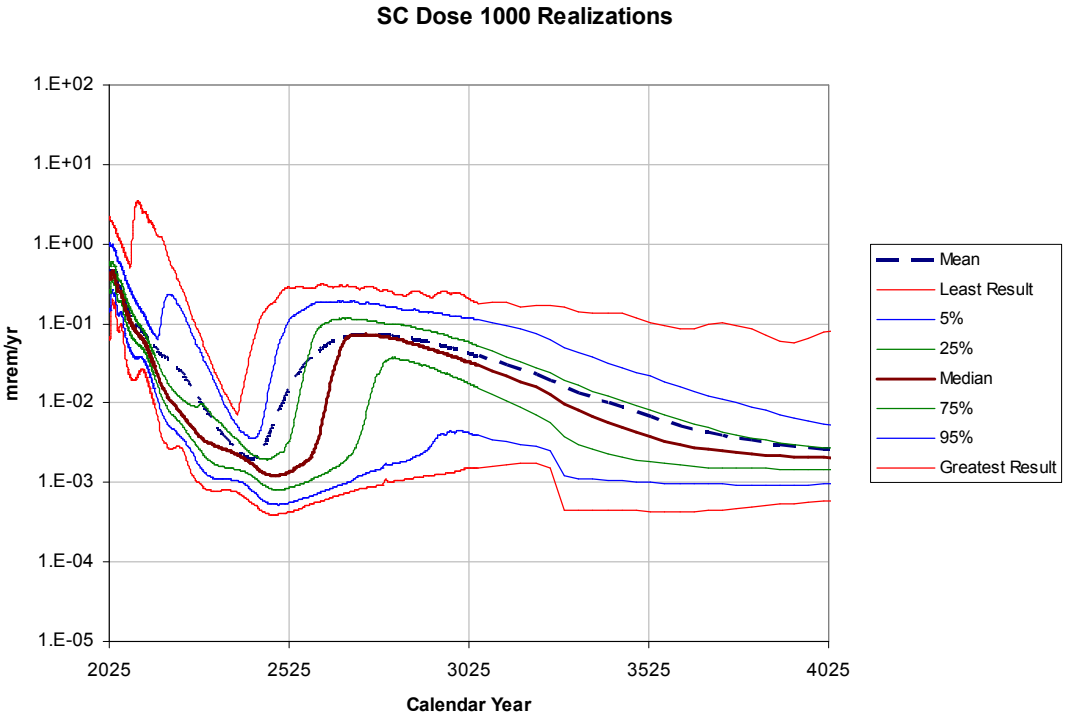

Figure 7.4-2. Uncertainty in dose at Steel Creek/Pen Branch POA from variation in K_d.

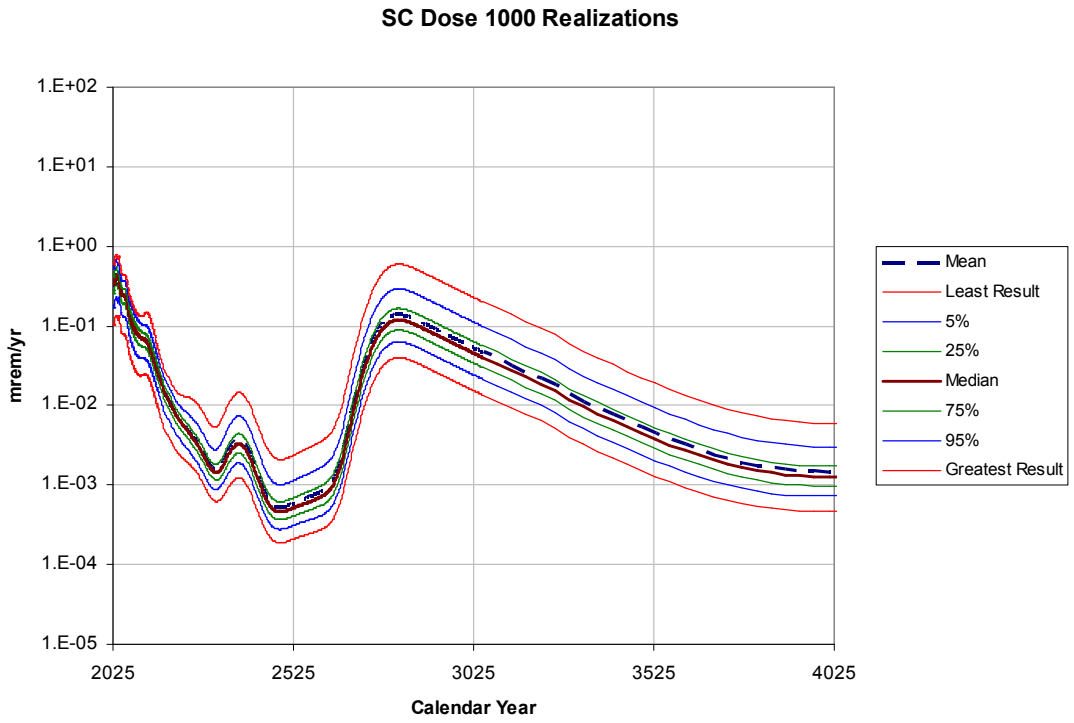

Figure 7.4-3. Uncertainty in dose at Steel Creek/Pen Branch POA from variation in dose parameters.

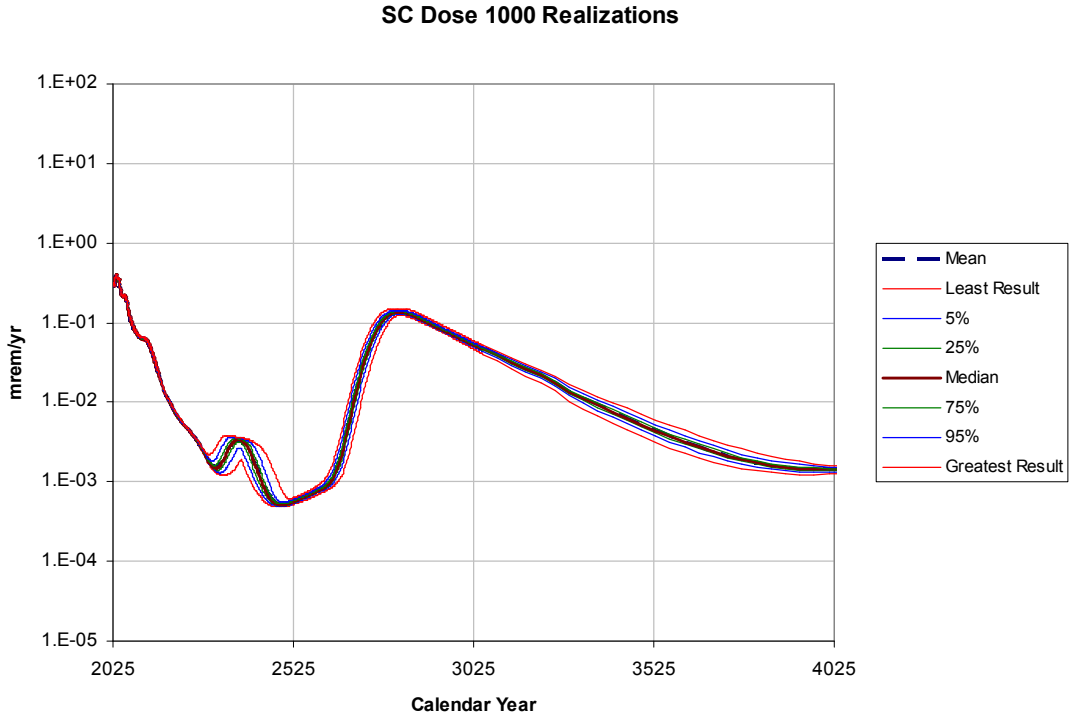

Figure 7.4-4. Uncertainty in dose at Steel Creek/Pen Branch POA from variation in material properties.

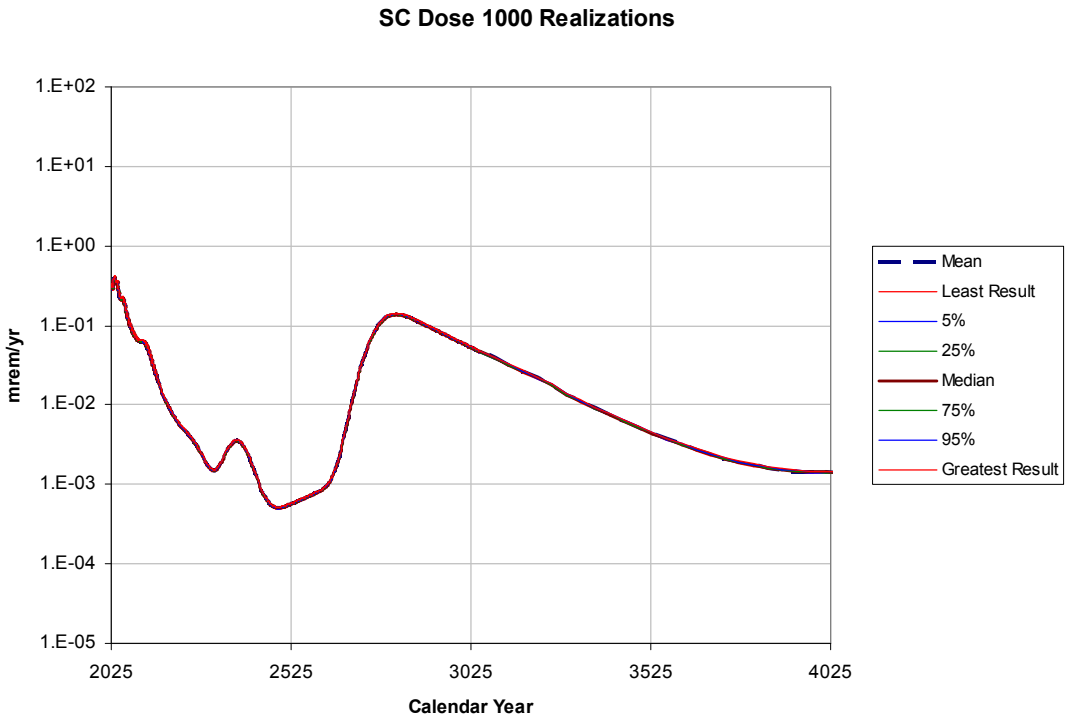

Figure 7.4-5. Uncertainty in dose at Steel Creek/Pen Branch POA from variation in surface water flow.

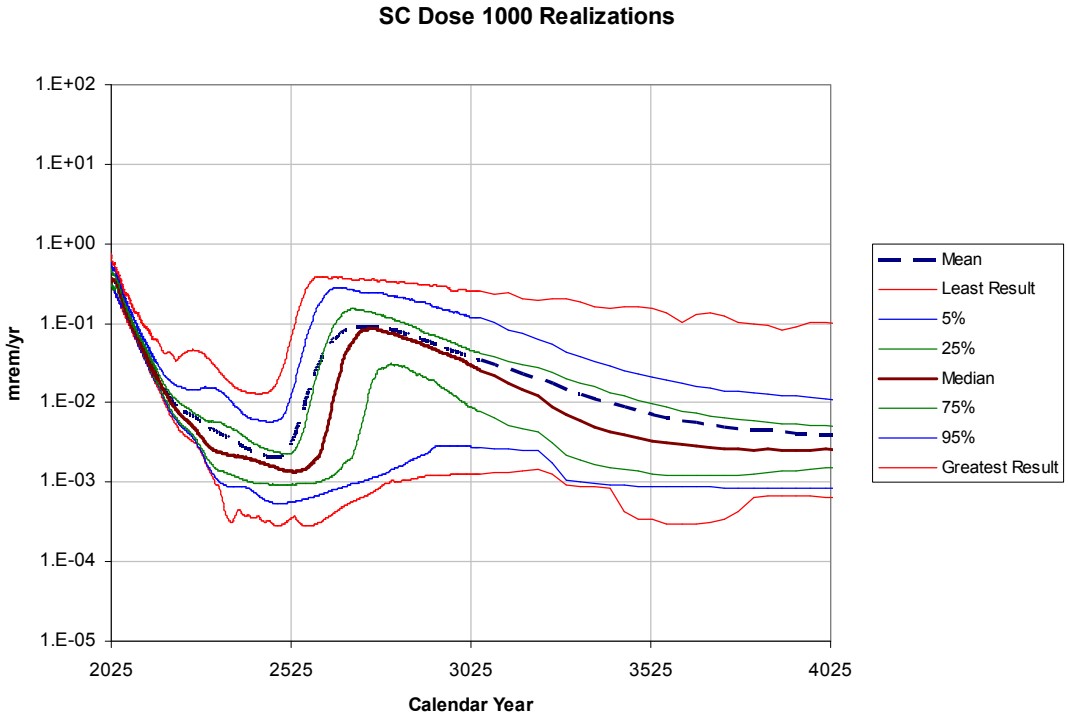

Figure 7.4-6. Uncertainty in dose at Steel Creek/Pen Branch POA from variation in infiltration and aquifer flow.

7.5 Dose Uncertainty at Lower Three Runs POA

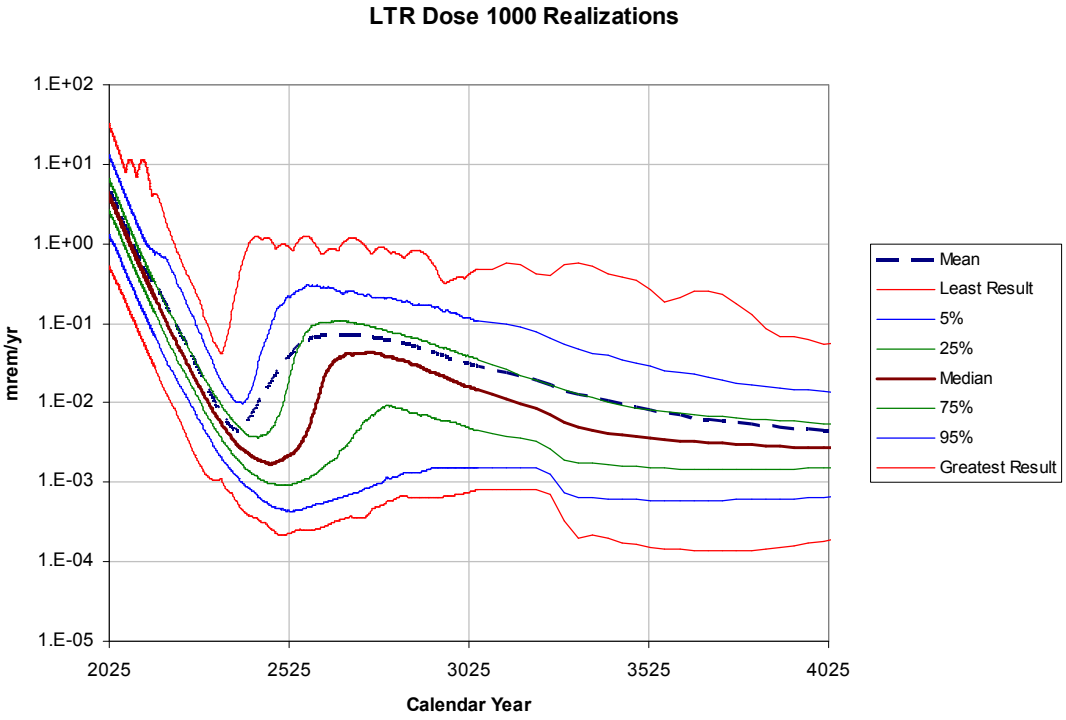

Figure 7.5-1. Overall uncertainty in dose at Lower Three Runs POA.

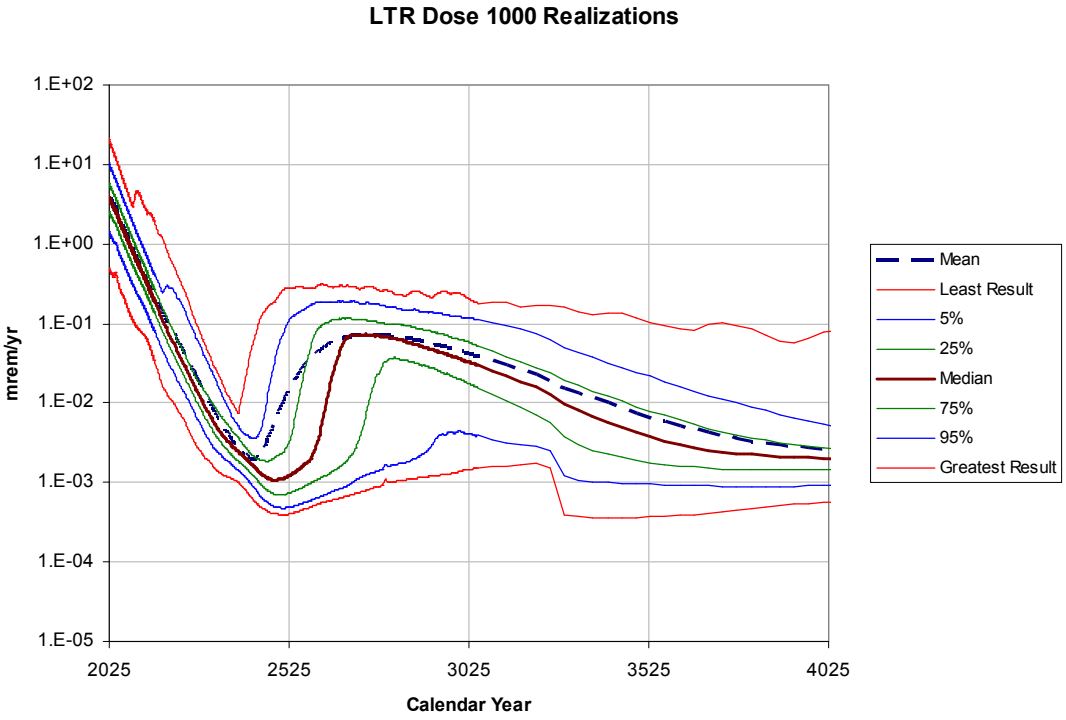

Figure 7.5-2. Uncertainty in dose at Lower Three Runs POA from variation in K_d.

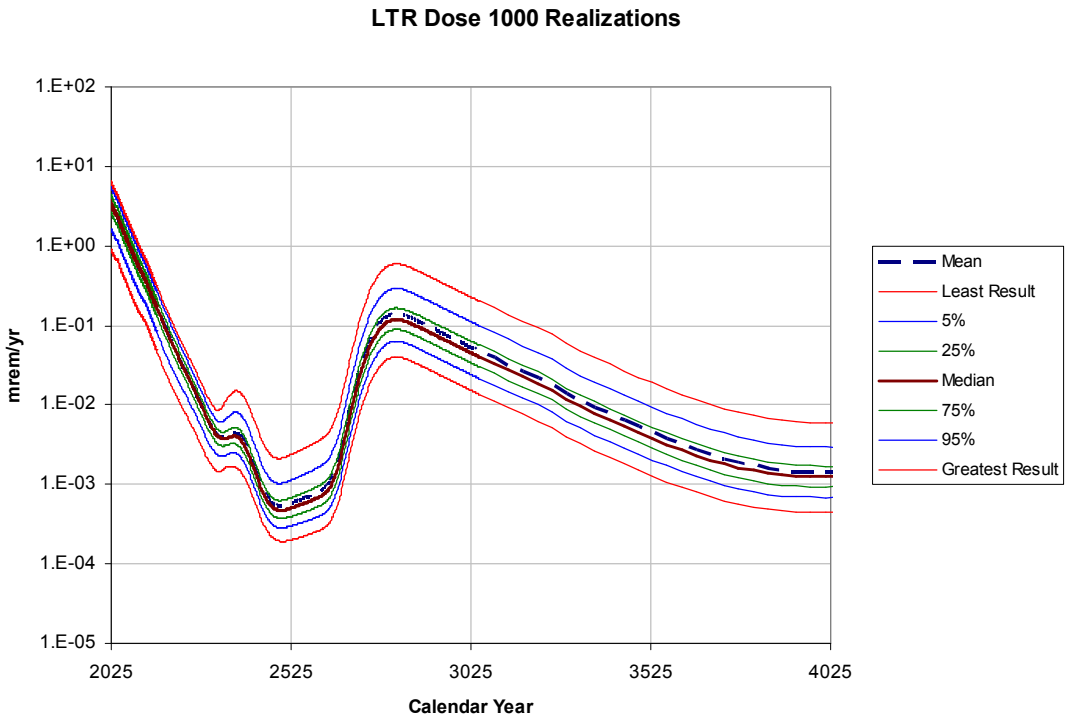

Figure 7.5-3. Uncertainty in dose at Lower Three Runs POA from variation in dose parameters.

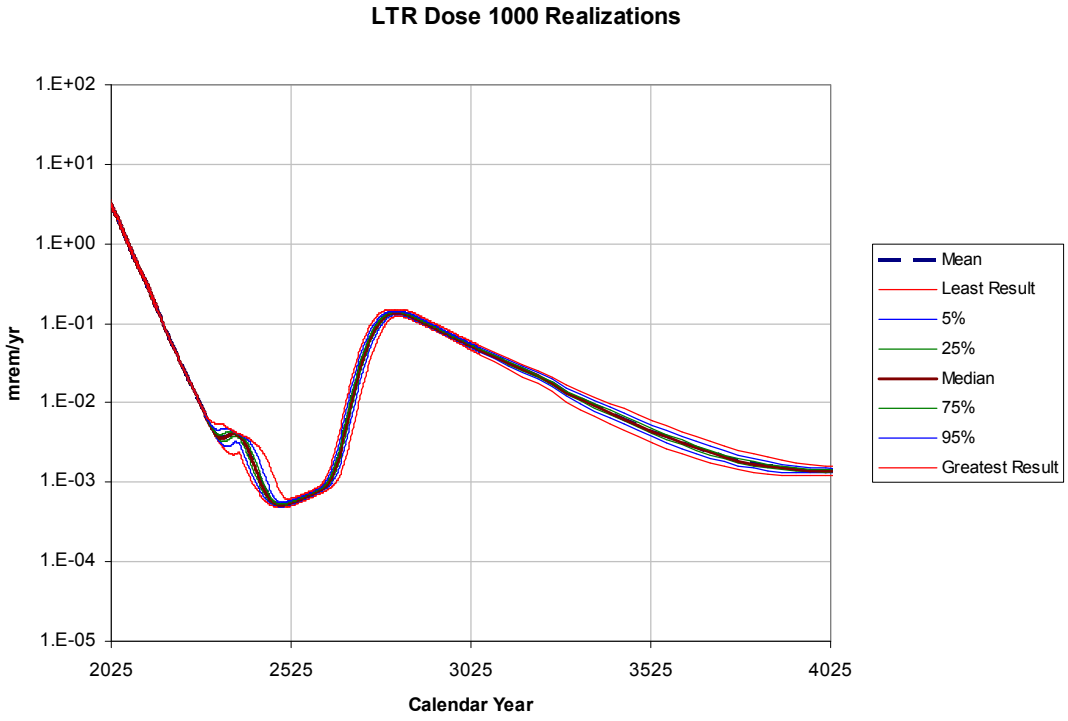

Figure 7.5-4. Uncertainty in dose at Lower Three Runs POA from variation in material properties.

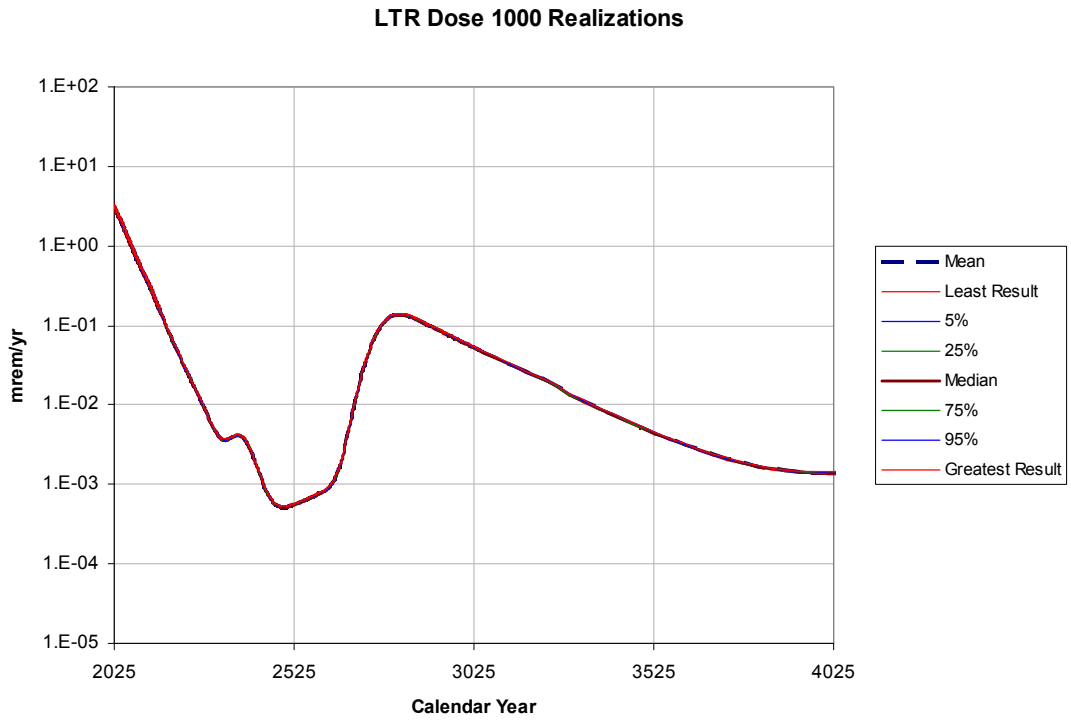

Figure 7.5-5. Uncertainty in dose at Lower Three Runs POA from variation in surface water flow.

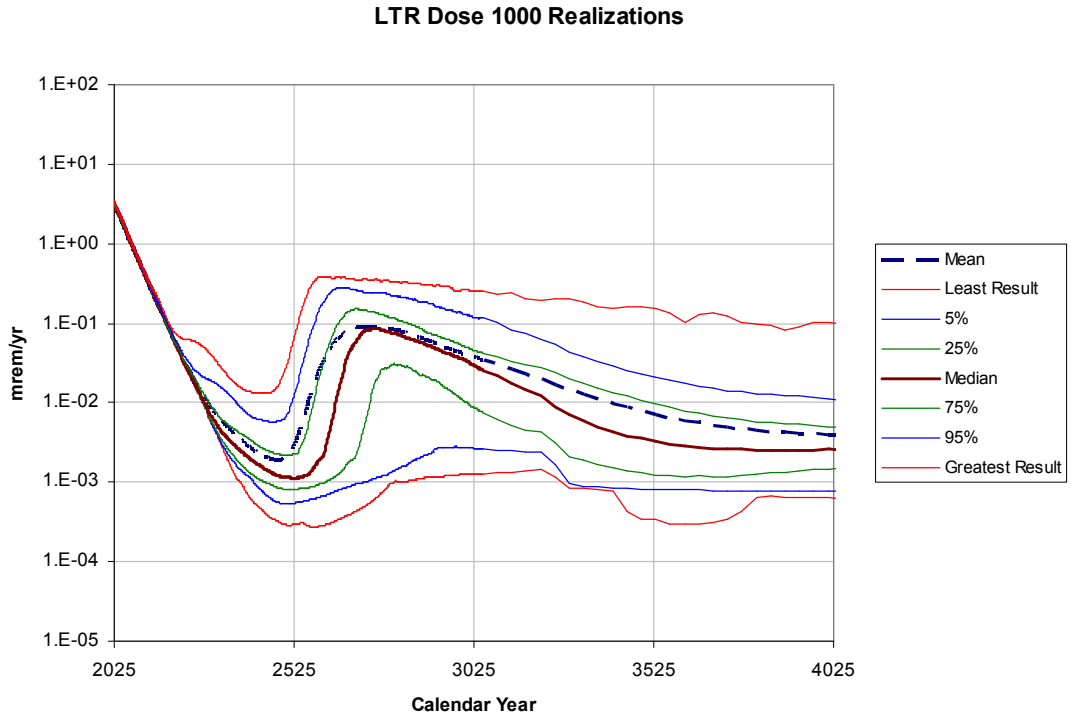

Figure 7.5-6. Uncertainty in dose at Lower Three Runs POA from variation in infiltration and aquifer flow.

7.6 Dose Uncertainty at 301 Bridge POA

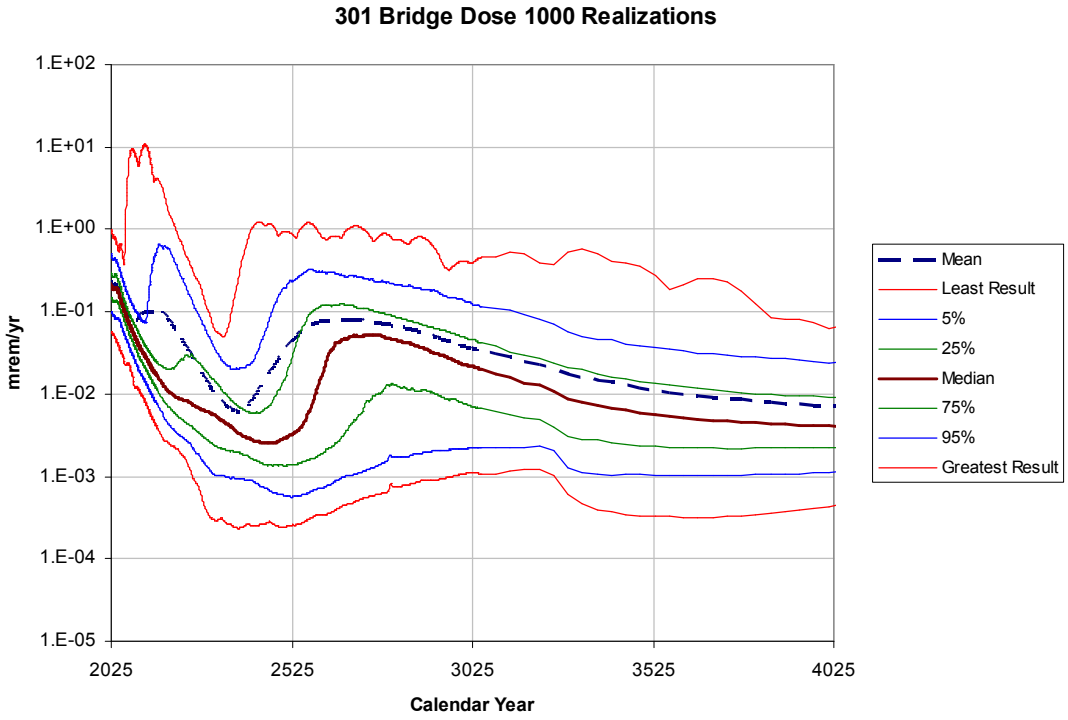

Figure 7.6-1. Overall uncertainty in dose at 301 Bridge POA.

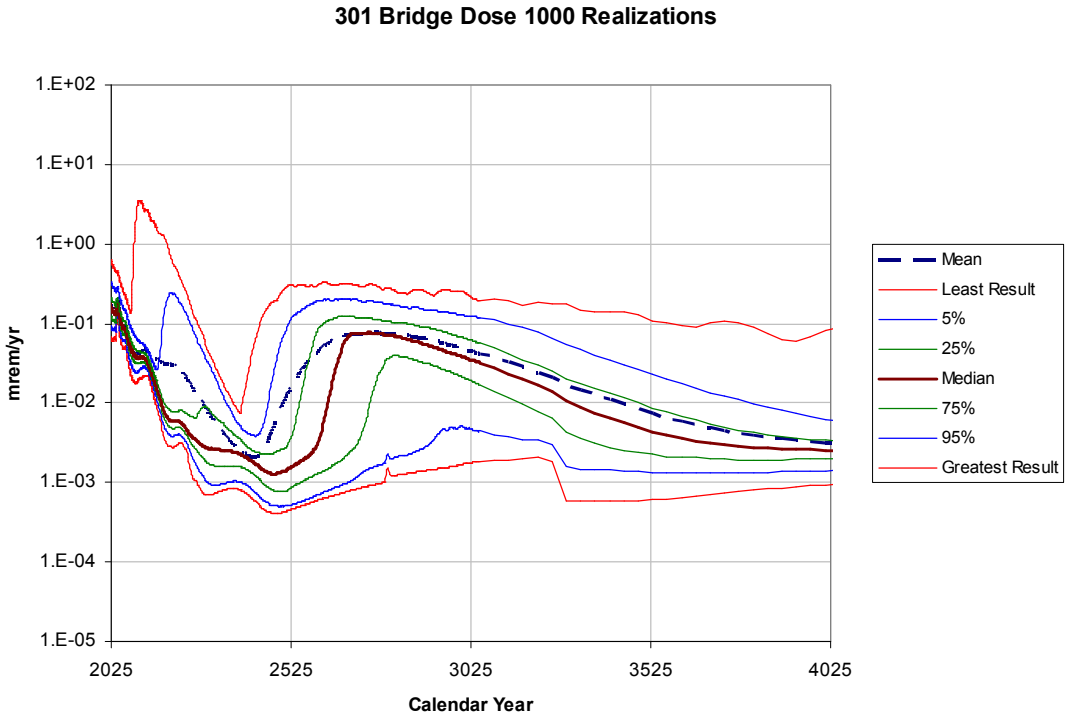

Figure 7.6-2. Uncertainty in dose at 301 Bridge POA from variation in K_d.

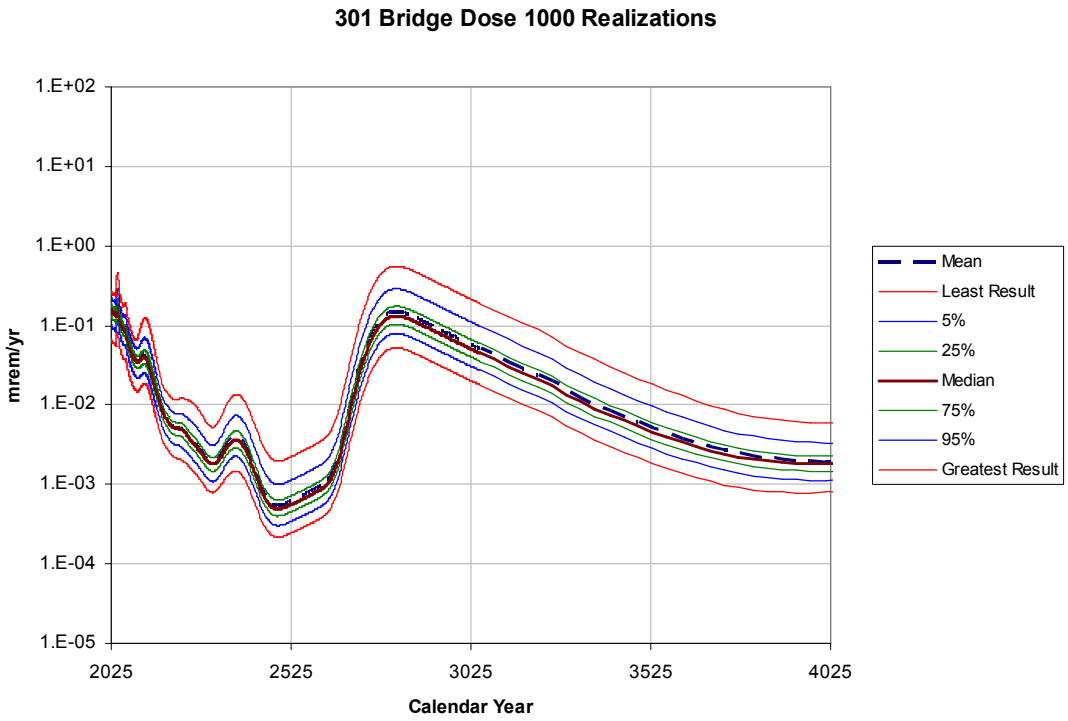

Figure 7.6-3. Uncertainty in dose at 301 Bridge POA from variation in dose parameters.

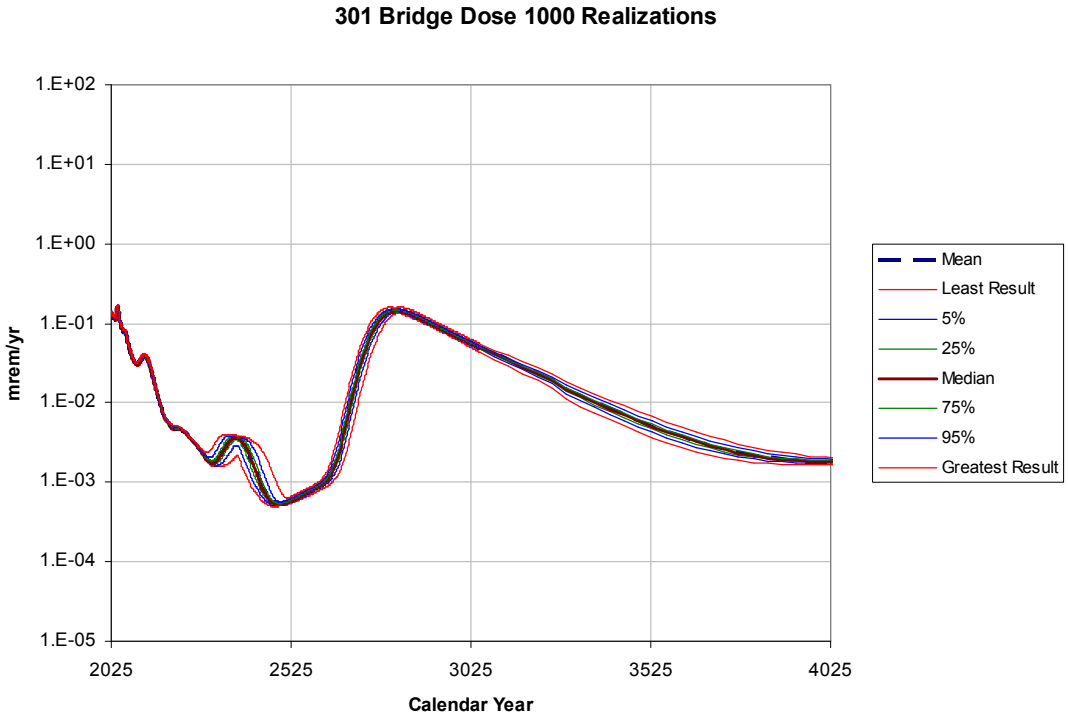

Figure 7.6-4. Uncertainty in dose at 301 Bridge POA from variation in material properties.

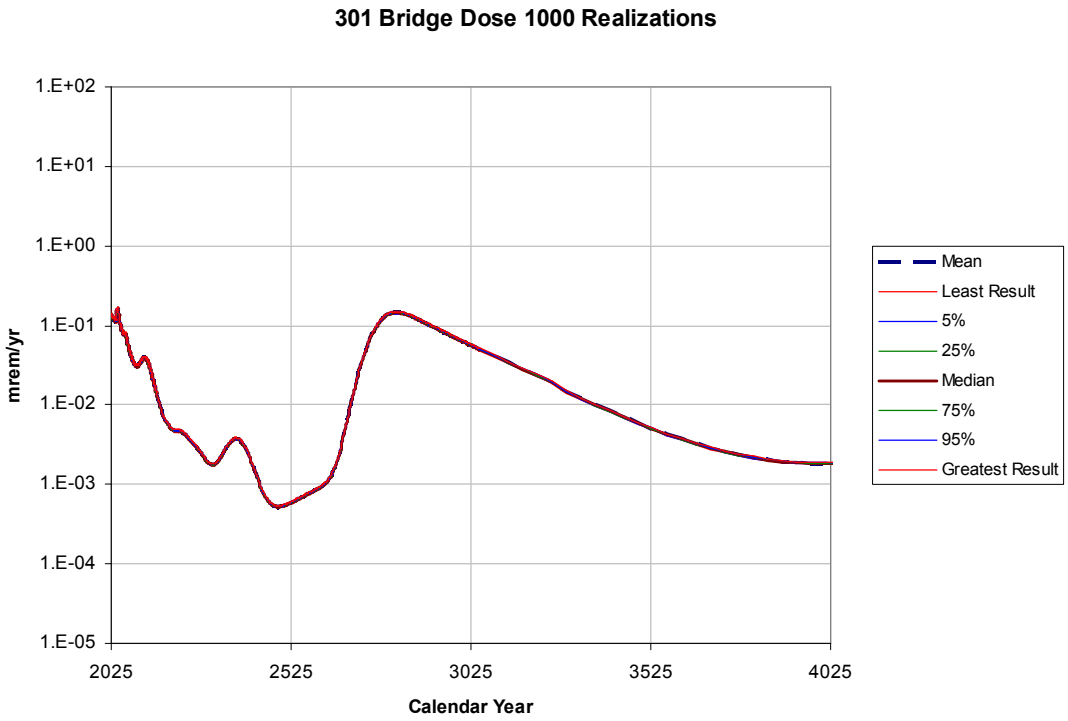

Figure 7.6-5. Uncertainty in dose at 301 Bridge POA from variation in surface water flow.

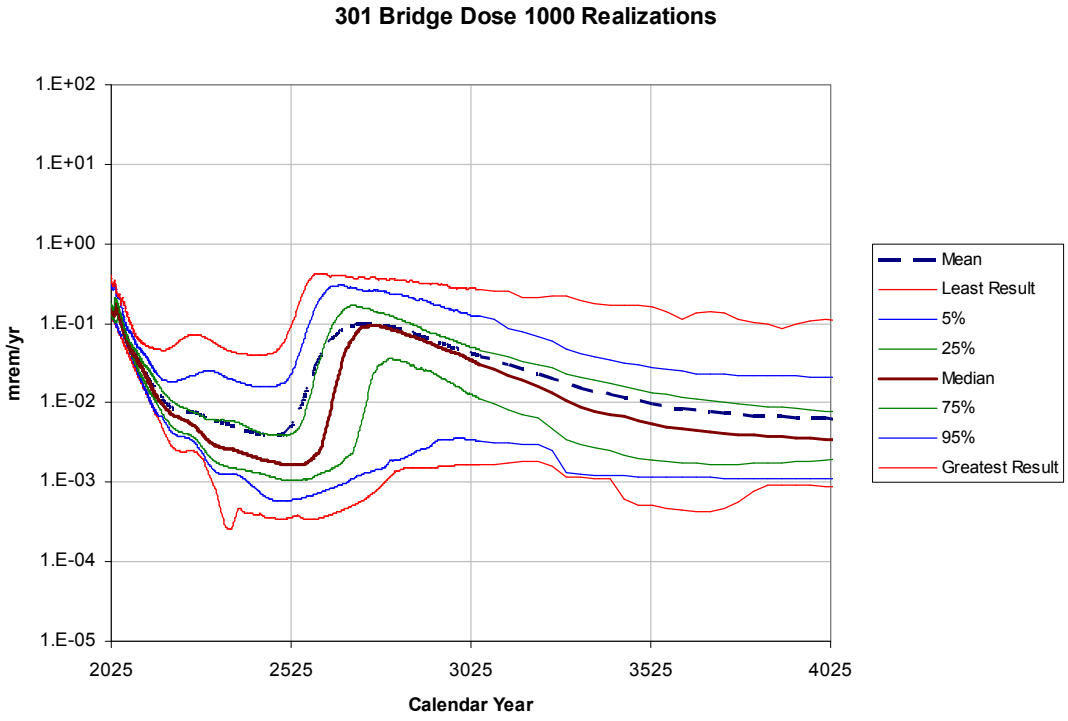

Figure 7.6-6. Uncertainty in dose at 301 Bridge POA from variation in infiltration and aquifer flow.

8.0 Conclusions and Recommendations

The GoldSim DP-Plus module in conjunction with dedicated servers providing up to 36 processors worked smoothly. A simulation modeling the performance of 32 surface and 7 IOU sources for 10,000 years using 1,000 realizations with reasonable time steps required about 20 hours to complete using 30 slave processes. This is a relatively convenient time in that a simulation started one work day would be completed before the end of the next work day allowing time to view the results and submit another job. The model appeared to run better on the servers than on a local workstation, which is likely caused by use of the GoldSim DP-Plus software on the servers.

Results from the expanded uncertainty analysis were in good agreement with those obtained in the original CA treatment. As shown in Table 6-1, the uncertainty analysis provided a high degree of confidence that peak doses at the POAs do not exceed the 30 mrem/yr dose constraint. The analysis found that variations in K_d values and in infiltration and aquifer flow rates had the greatest impact on dose uncertainty. Both of these factors influence the transport timing. In most cases, the peak dose at a POA occurred in the early part of the transient where the dose is predominantly from Cs-137 released from streambed sediments.

8.1 Future Work

As shown by the dose distribution plotted in Figure 8-1 (see also Figure 3-1), of the 152 CA sources, 49 (41 surface sources and 8 IOUs) have peak doses greater than 0.001 mrem/yr in the time period from 2025 to 3025. Based on the results obtained during this project, the GoldSim model could be expanded to include all of these sources in an uncertainty analysis. This model would scale up to about 280 Mb in size and require about 30 hours to complete a simulation with 30 slave processors. This expansion is feasible although the resulting GoldSim file size of 20 Gb will be difficult to work with. Another 47 CA sources had peak doses less than 1.0e-6 mrem/yr and could reasonably be excluded from the uncertainty analysis. Some of the remaining sources with similar source locations, release mechanisms, and vadose and aquifer path parameters could perhaps be lumped together to improve the model accuracy with a modest increase in computational burden.

Since the CA supports the PA facilities (E-Area low level waste disposal facilities, F and H-Area tank farms, and Z-Area saltstone) it would be desirable to include as many PA sources in the uncertainty analysis as possible. The PA facilities accounted for 46 of the 152 CA sources and ten of the 46 PA sources were included in the current uncertainty analysis. More PA sources could be included by lumping ones with similar transport paths into single composite sources. For example, source lumping could be applied to the eight H-Area tank farm sources that discharge to the Upper Three Runs POA which were not included in the present analysis.

Other modifications to the model that should be considered for future uncertainty analysis are:

- Bioaccumulation factors and source inventory were not included in the uncertainty analysis. Stochastic distributions need to be developed for these variables. Cook et al. (2011) reviewed two approaches for estimating inventory uncertainty.

- Surface water flow distributions used in the uncertainty analysis were based on estimates of the variability in the 1,000 year average flow which gave a very narrow distribution. Other methods of estimating the uncertainty in surface water flow should be evaluated.

- In the current model, stochastic parameters are the same in each source and each dose calculation. This approach significantly reduces the number of uncertainty parameters that must be analyzed; however, an argument could be made that each instance of a stochastic parameter should be allowed to vary independently.

- The model should be modified to output the stochastic parameter values used for each realization along with full results from each realization for a statistical analysis. A statistical analysis could be employed to identify the stochastic parameters having the most impact on peak doses with a single run of the uncertainty model.

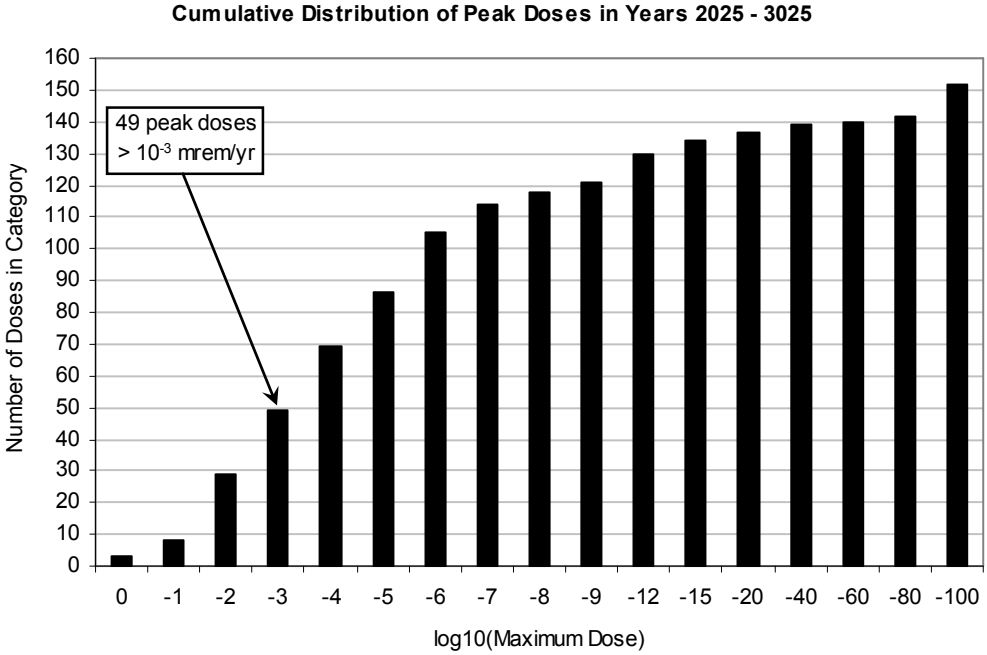

Figure 8-1. Cumulative distribution of peak doses from all CA sources during the years 2025 – 3025.

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