Savannah River Remediation
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INTEROFFICE MEMORANDUM

SRR-CWDA-2018-00009

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Recommended Sampling Distribution for SDF Performance Assessment Inventory

This document outlines the approach and methodology used to recommend an input distribution for a sampling multiplier for various radionuclides in the SDF Performance Assessment (PA) model. The objective of this approach is to apply a statistical method to process historical Tank Farm inventory data and develop a best-fitting sampling distribution that reasonably emulates the ranges and behaviors of real-world data. MATLAB's Distribution Fitter Analysis Tool Pack will be used to process and fit data. MATLAB uses a fit function to recommend a mean and standard deviation based on the desired distribution to be fitted.

Table 1 shows a list of radionuclides that were selected as the most important relative to dose contributions in recent SDF modeling (SRR-CWDA-2014-00006; SRR-CWDA-2016-00072). The focus of this report is to develop an appropriate recommended distribution that can be applied to multiple radionuclides for future SDF PA modeling.

Table 1: Top Contributors for Dose

I-129
Tc-99
K-40
Cl-36
Ra-226 (and parent products Th-230, U-234, and Pu238)
Np-237 (and parent products Am-241, Pu-241, and Cm-245)
Se-79
Pu-239 (and parent products Cm-243 and Am-243)
Al-26
C-14

I-129 and Tc-99

Recommended input distributions for the two most significant dose contributors (I-129 and Tc-99) are provided in separate documents: reference SRR-CWDA-2015-00077 (I-129) and SRR-CWDA-2015-00123 (Tc-99).

Research and Selection Process

Data was gathered from 10 years of historical Tank Farm inventory report data, dating back to 2008, searching for concentration values for the radionuclides in Table 1. Table 2 displays the number of samples found for each radionuclide, as well as the number of samples that were less than their applicable detection limits. Of the 16 radionuclides listed, 10 had an adequate sample size to analyze the data. K-40, Cl-36, Th-230, Se-79, Cm-243, and Al-26 were not included in the rest of this analysis because of limited sample data available. Additionally, many of the available sample values were identified as detection limit values. For some radionuclides (Ra-226, Cm-245, and Am-243), all the available sample data was below the detection limits; therefore, these radionuclides are also excluded from the rest of this inventory analysis. Samples that are reported as being below the applicable detection limits are not accurate indications of concentration values, and are not appropriate for data analysis.

The remaining radionuclides were U-234, Pu-238, Np-237, Am-241, Pu-239, Pu-241, and C-14, all of which had an adequate sample size of data to work with. Because only seven of the original 16 radionuclides have enough historical data to test, the best approach is to develop a sampling distribution for each of the seven radionuclides with historical data, and then develop a single universal distribution based on the behavior from the seven developed distributions.

Table 2: Radionuclide Sample Count

Radionuclide	Total Samples	Samples Less than detection limit	Adequate Samples for Analysis
K-40	0	0	0
Cl-36	0	0	0
Ra-226	12	12	0
Th-230	1	1	0
U-234	23	13	10
Pu-238	29	2	27
Np-237	12	8	4
Am-241	14	8	6
Pu-241	28	16	12
Cm-245	11	11	0
Se-79	0	0	0
Pu-239	32	8	24
Cm-243	1	1	0
Am-243	11	11	0
Al-26	0	0	0
C-14	15	5	10

MATLAB Inputs

The 7 data sets for U-234, Pu-238, Np-237, Am-241, Pu-239, Pu-241, and C-14 were used as inputs for MATLAB's distribution fitter application. Because the distribution to be developed is designed as a sampling multiplier to a radionuclide inventory amount, each data point will be scaled to its respective set's mean. The inventory concentrations vary so widely between different tanks, that using an arithmetic mean is not ideal to get a best estimate of central tendency. Instead, a logarithmic scale and geometric mean will be used. Each sample point was decayed to an assumed SDF closure date (October 2032). The log of the decayed value was taken, and scaled to the respective mean of the set of log-scaled data. Tables 3 through 8 display all the data that was used for calculations and inputs. Concentration values were converted to picocuries per milliliter (pCi/mL) if presented in different units in the reference document. The columns titled "Log Scaled to Average" are the calculated data points used for distribution testing in MATLAB.

Table 3: Am-241 Data Inputs for MATLAB

Reference	Date of Sample or Reference	Tank	Am-241 (pCi/mL)	Am-241 pCi/mL at Closure	Log Am-241 pCi/mL at Closure	Log Scaled to Average
SRNL-STI-2017-00698	7/31/2017	21	6.21E+00	6.06E+00	0.78	0.58
SRNL-L3100-2017-00033	1/16/2017	50	4.52E+00	4.41E+00	0.64	0.48
SRNL-STI-2017-00055	11/21/2016	21	1.32E+00	1.29E+00	0.11	0.08
SRNL-STI-2012-00707	10/3/2012	21	6.17E+01	5.98E+01	1.78	1.33
SRNL-STI-2012-00420	2/28/2012	48	2.48E+03	2.40E+03	3.38	2.52
SRNL-STI-2010-00017	11/16/2009	23	2.29E+01	2.21E+01	1.34	1.00

Table 4: U-234 Data Inputs for MATLAB

Reference	Date of Sample or Reference	Tank	U-234 (pCi/mL)	U-234 pCi/mL at Closure	Log U-234 pCi/mL at Closure	Log Scaled to Average
SRNL-STI-2017-00698	7/31/2017	21	1.13E+02	1.13E+02	2.05E+00	1.04
SRNL-STI-2017-00055	11/21/2016	21	8.75E+01	8.75E+01	1.94E+00	0.99
SRNL-STI-2015-00662	10/21/2015	43	6.84E+01	6.84E+01	1.84E+00	0.93
SRNL-STI-2015-00622	9/1/2015	21	9.25E+01	9.25E+01	1.97E+00	1.00
SRNL-STI-2015-00336	5/11/2015	38	1.06E+02	1.06E+02	2.03E+00	1.03
SRNL-STI-2015-00336	5/11/2015	43	6.62E+01	6.62E+01	1.82E+00	0.93
SRNL-STI-2014-00561	9/18/2014	21	1.18E+02	1.18E+02	2.07E+00	1.05
SRNL-STI-2013-00437	5/16/2013	21	9.66E+01	9.66E+01	1.98E+00	1.01
SRNL-STI-2012-00076	10/13/2011	21	9.00E+01	9.00E+01	1.95E+00	0.99
SRNL-STI-2010-00017	11/16/2009	23	9.84E+01	9.84E+01	1.99E+00	1.01

Table 5: Np-237 Data Inputs for MATLAB

Reference	Date of Sample or Reference	Tank	Np-237 (pCi/mL)	Np-237 pCi/mL at Closure	Log Np-237 pCi/mL at Closure	Log Scaled to Average
SRNL-STI-2017-00698	7/31/2017	21	3.65E+00	3.65E+00	5.62E-01	0.78
SRNL-STI-2017-00055	11/21/2016	21	4.34E+00	4.34E+00	6.37E-01	0.88
SRNL-STI-2012-00076	10/13/2011	21	3.39E+00	3.39E+00	5.30E-01	0.73
SRNL-STI-2011-00061	9/23/2010	21	1.45E+01	1.45E+01	1.16E+00	1.61

Table 6: Pu-238 Data Inputs for MATLAB

Reference	Date of Sample or Reference	Tank	Pu-238 (pCi/mL)	Pu-238 pCi/mL at Closure	Log Pu-238 pCi/mL at Closure	Log Scaled to Average
SRNL-L3100-2017-00141	7/21/2017	25	5.27E+04	4.67E+04	4.67E+00	1.22
SRNL-L3100-2017-00141	8/21/2017	36	1.87E+03	1.66E+03	3.22E+00	0.84
SRNL-L3100-2017-00141	8/14/2017	42	2.00E+03	1.77E+03	3.25E+00	0.85
SRNL-L3100-2017-00033	1/16/2017	50	2.80E+04	2.47E+04	4.39E+00	1.15
SRNL-STI-2017-00055	11/21/2016	21	1.83E+04	1.61E+04	4.21E+00	1.10
SRNL-STI-2015-00662	10/8/2015	38	2.58E+03	2.26E+03	3.35E+00	0.87
SRNL-STI-2015-00662	10/21/2015	43	4.69E+03	4.10E+03	3.61E+00	0.94
SRNL-STI-2015-00622	9/1/2015	21	4.16E+04	3.64E+04	4.56E+00	1.19
SRNL-STI-2015-00456	8/19/2015	4	1.36E+02	1.19E+02	2.07E+00	0.54
SRNL-STI-2015-00369	6/8/2015	23	7.13E+03	6.22E+03	3.79E+00	0.99
SRNL-STI-2015-00336	5/11/2015	38	7.61E+03	6.64E+03	3.82E+00	1.00
SRNL-STI-2015-00336	5/11/2015	43	4.53E+03	3.95E+03	3.60E+00	0.94
SRNL-STI-2015-00064	12/4/2014	13	1.55E+03	1.34E+03	3.13E+00	0.82
SRNL-STI-2014-00561	9/18/2014	21	5.63E+04	4.88E+04	4.69E+00	1.22
SRNL-TR-2014-00141	6/2/2014	43	5.50E+03	4.76E+03	3.68E+00	0.96
SRNL-TR-2014-00141	6/2/2014	38	7.41E+03	6.41E+03	3.81E+00	0.99
SRNL-STI-2013-00730	8/28/2013	35	1.43E+05	1.23E+05	5.09E+00	1.33
SRNL-STI-2013-00437	5/16/2013	21	1.20E+04	1.03E+04	4.01E+00	1.05
SRNL-STI-2012-00707	10/3/2012	21	1.08E+04	9.22E+03	3.96E+00	1.03
SRNL-STI-2012-00420	2/28/2012	48	1.41E+05	1.20E+05	5.08E+00	1.32
SRNL-STI-2012-00076	10/13/2011	21	1.49E+04	1.26E+04	4.10E+00	1.07
SRNL-STI-2011-00061	9/23/2010	21	1.26E+04	1.06E+04	4.02E+00	1.05
SRNL-STI-2010-00017	11/16/2009	23	9.65E+03	8.06E+03	3.91E+00	1.02
SRNL-STI-2009-00805	8/17/2009	21	1.01E+01	8.42E+00	9.25E-01	0.24
SRNL-STI-2009-00805	7/28/2009	24	1.18E+04	9.83E+03	3.99E+00	1.04
SRNS-TR-2008-00103	7/2/2008	23	1.26E+04	1.04E+04	4.02E+00	1.05
WSRC-STI-2008-00227	2/15/2008	11	4.57E+04	3.76E+04	4.58E+00	1.19

Table 7: Pu-239 Data Inputs for MATLAB

Reference	Date of Sample or Reference	Tank	Pu-239 (pCi/mL)	Pu-239 pCi/mL at Closure	Log Pu-239 pCi/mL at Closure	Log Scaled to Average
SRNL-L3100-2017-00141	7/21/2017	25	1.59E+03	1.59E+03	3.20E+00	1.17
SRNL-L3100-2017-00141	8/14/2017	42	5.09E+02	5.09E+02	2.71E+00	0.99
SRNL-STI-2017-00698	7/31/2017	21	8.55E+02	8.55E+02	2.93E+00	1.07
SRNL-L3100-2017-00033	1/16/2017	50	6.80E+02	6.80E+02	2.83E+00	1.03
SRNL-STI-2017-00055	11/21/2016	21	7.81E+02	7.81E+02	2.89E+00	1.06
SRNL-STI-2015-00662	10/8/2015	38	7.12E+01	7.12E+01	1.85E+00	0.68
SRNL-STI-2015-00622	9/1/2015	21	6.97E+02	6.97E+02	2.84E+00	1.04
SRNL-STI-2015-00456	8/19/2015	4	7.03E+01	7.03E+01	1.85E+00	0.67
SRNL-STI-2015-00369	6/8/2015	23	1.89E+02	1.89E+02	2.28E+00	0.83
SRNL-STI-2015-00336	5/11/2015	38	2.71E+02	2.71E+02	2.43E+00	0.89
SRNL-STI-2015-00336	5/11/2015	43	1.33E+02	1.33E+02	2.12E+00	0.78
SRNL-STI-2015-00008	12/1/2014	38	3.15E+02	3.15E+02	2.50E+00	0.91
SRNL-STI-2015-00008	11/25/2014	43	3.95E+02	3.95E+02	2.60E+00	0.95
SRNL-STI-2014-00561	9/18/2014	21	9.89E+02	9.89E+02	3.00E+00	1.09
SRNL-TR-2014-00141	6/2/2014	43	2.92E+02	2.92E+02	2.47E+00	0.90
SRNL-TR-2014-00141	6/2/2014	38	5.53E+02	5.53E+02	2.74E+00	1.00
SRNL-STI-2013-00730	8/28/2013	35	2.98E+03	2.98E+03	3.47E+00	1.27
SRNL-STI-2013-00437	5/16/2013	21	1.57E+03	1.57E+03	3.20E+00	1.17
SRNL-STI-2012-00707	10/3/2012	21	9.90E+02	9.90E+02	3.00E+00	1.09
SRNL-STI-2012-00076	10/13/2011	21	1.49E+03	1.49E+03	3.17E+00	1.16
SRNL-STI-2011-00061	9/23/2010	21	2.74E+03	2.74E+03	3.44E+00	1.26
SRNL-STI-2010-00017	11/16/2009	23	1.47E+02	1.47E+02	2.17E+00	0.79
SRNL-STI-2009-00805	7/28/2009	24	6.03E+02	6.03E+02	2.78E+00	1.02
WSRC-STI-2008-00227	2/15/2008	11	1.88E+03	1.88E+03	3.27E+00	1.20

Table 8: C-14 Data Inputs for MATLAB

Reference	Date of Sample or Reference	Tank	C-14 (pCi/mL)	C-14 pCi/mL at Closure	Log C-14 pCi/mL at Closure	Scaled to logarithmic mean
SRNL-STI-2017-00698	7/31/2017	21	5.47E+02	5.46E+02	2.74E+00	0.97
SRNL-L3100-2017-00033	1/16/2017	50	6.01E+02	6.00E+02	2.78E+00	0.98
SRNL-STI-2017-00055	11/21/2016	21	9.00E+02	8.98E+02	2.95E+00	1.04
SRNL-STI-2015-00622	9/1/2015	21	8.66E+02	8.64E+02	2.94E+00	1.04
SRNL-STI-2014-00561	9/18/2014	21	6.48E+02	6.47E+02	2.81E+00	0.99
SRNL-STI-2013-00437	5/16/2013	21	7.40E+02	7.38E+02	2.87E+00	1.01
SRNL-STI-2012-00076	10/13/2011	21	7.20E+02	7.18E+02	2.86E+00	1.01
SRNL-STI-2011-00061	9/23/2010	21	7.55E+02	7.53E+02	2.88E+00	1.02
SRNL-STI-2010-00017	11/16/2009	23	1.13E+03	1.13E+03	3.05E+00	1.08
SRNS-TR-2008-00103	7/2/2008	23	2.35E+03	2.34E+03	3.37E+00	1.19

Table 9: Pu-241 Data Inputs for MATLAB

Reference	Date of Sample or Reference	Tank	Pu-241 (pCi/mL)	Pu-241 pCi/mL at Closure	Log Pu-239 pCi/mL at Closure	Log Scaled to Average
SRNL-STI-2017-00698	7/31/2017	21	9.43E+03	4.53E+03	3.66E+00	1.14
SRNL-L3100-2017-00033	1/16/2017	50	1.05E+04	4.91E+03	3.69E+00	1.15
SRNL-STI-2017-00055	11/21/2016	21	5.63E+03	2.61E+03	3.42E+00	1.06
SRNL-STI-2015-00336	5/11/2015	38	1.21E+03	5.20E+02	2.72E+00	0.85
SRNL-STI-2015-00336	5/11/2015	43	6.93E+02	2.99E+02	2.48E+00	0.77
SRNL-STI-2015-00008	12/1/2014	38	1.18E+03	4.96E+02	2.70E+00	0.84
SRNL-STI-2015-00008	11/25/2014	43	2.99E+03	1.26E+03	3.10E+00	0.97
SRNL-STI-2014-00561	9/18/2014	21	2.23E+04	9.32E+03	3.97E+00	1.24
SRNL-TR-2014-00141	6/2/2014	43	9.17E+02	3.78E+02	2.58E+00	0.80
SRNL-TR-2014-00141	6/2/2014	38	1.90E+03	7.83E+02	2.89E+00	0.90
SRNL-STI-2013-00730	8/28/2013	35	6.03E+04	2.39E+04	4.38E+00	1.36
SRNL-STI-2013-00437	5/16/2013	21	2.21E+03	8.66E+02	2.94E+00	0.92

Distribution Development

Normal, gamma, and uniform distributions were created for U-234, Pu-238, Np-237, Am-241, Pu-239, Pu-241, and C-14. Tables 10 through 12 summarize the distribution values for all seven radionuclides as well as the resulting distribution when taking the average, and Figures 1 through 3 display all the distribution plots. The uniform distribution's slope and intercept values were derived by assigning equal probabilities to each data point of the log-scaled data, then sorting the data (from low to high values) and truncating the resulting data sets to between the 10^{th} and 90^{th} percentiles. It is expected that batch

preparations to support disposal at the SDF will consider concentrations in the feed such that operators will mix lower concentration material with higher concentration material; as such, truncating the concentrations to ignore the extreme values provides a more reasonable data set for reflecting future uncertainty in the SDF disposal inventory. The normal and gamma distribution values were derived using MATLAB's Distribution Fitter application tool pack.

Table 10: Summary of Recommended Normal Distributions

Radionuclide	Mean	Standard Deviation
C-14	1.001	0.123
U-234	0.998	0.041
Np-237	1.000	0.411
Pu-238	1.000	0.226
Pu-239	1.001	0.169
Pu-241	1.000	0.189
Am-241	0.998	0.862
Average	1.000	0.289

Figure 1: Normal Distribution Plot

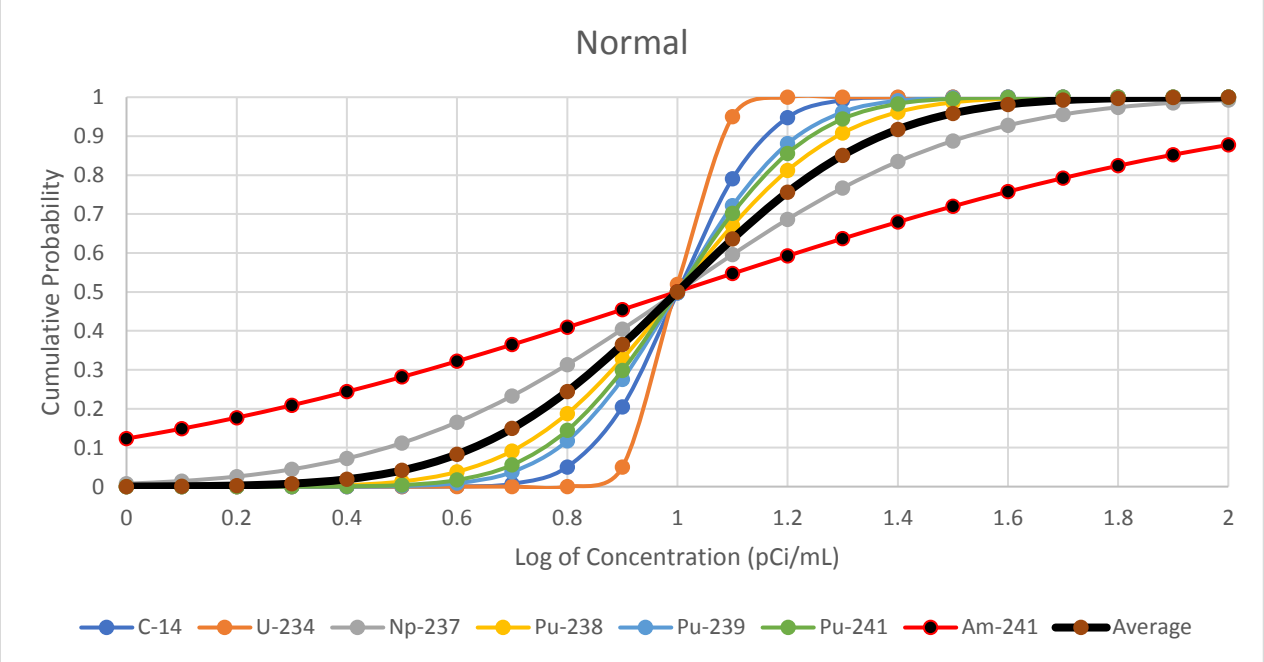


Table 11: Summary of Recommended Gamma Distributions

Radionuclide	A	B
C-14	63.159	0.016
U-234	645.187	0.002
Np-237	9.476	0.106
Pu-238	12.823	0.078
Pu-239	34.213	0.029
Pu-241	31.924	0.031
Am-241	1.302	0.767
Average	44.767	0.022

Figure 2: Gamma Distribution Plot

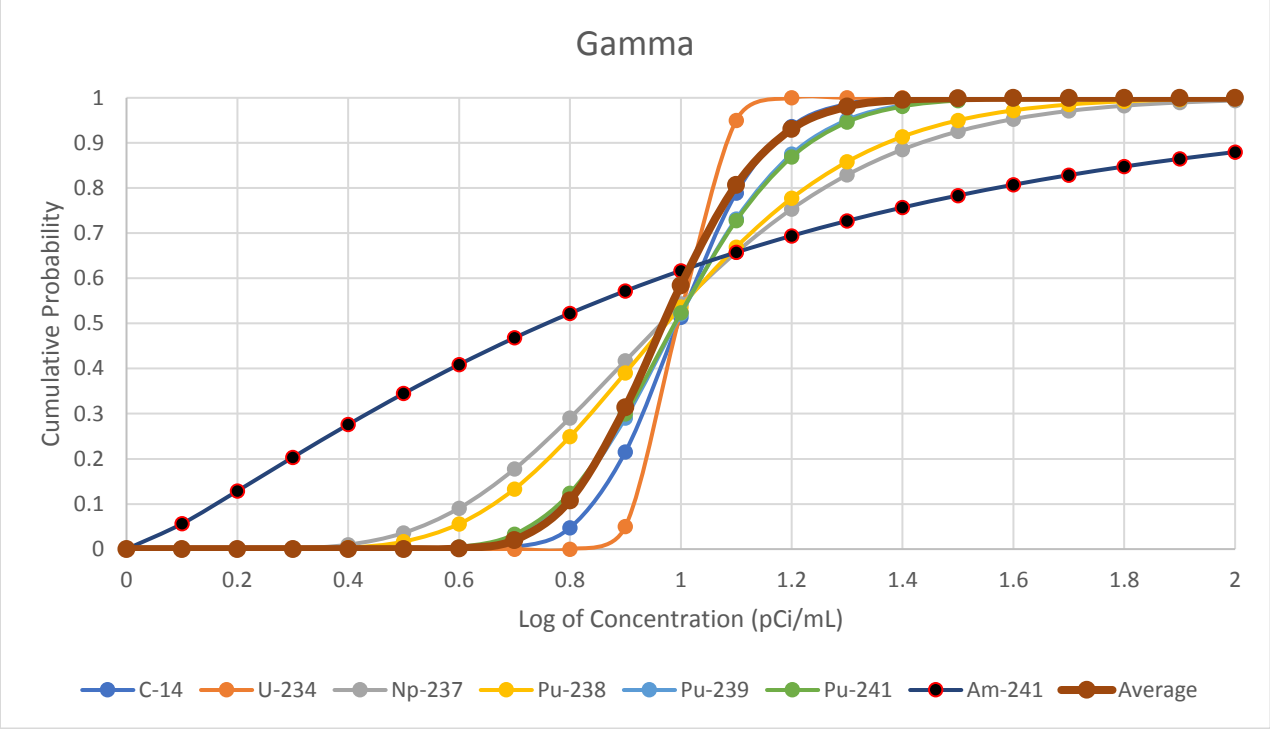
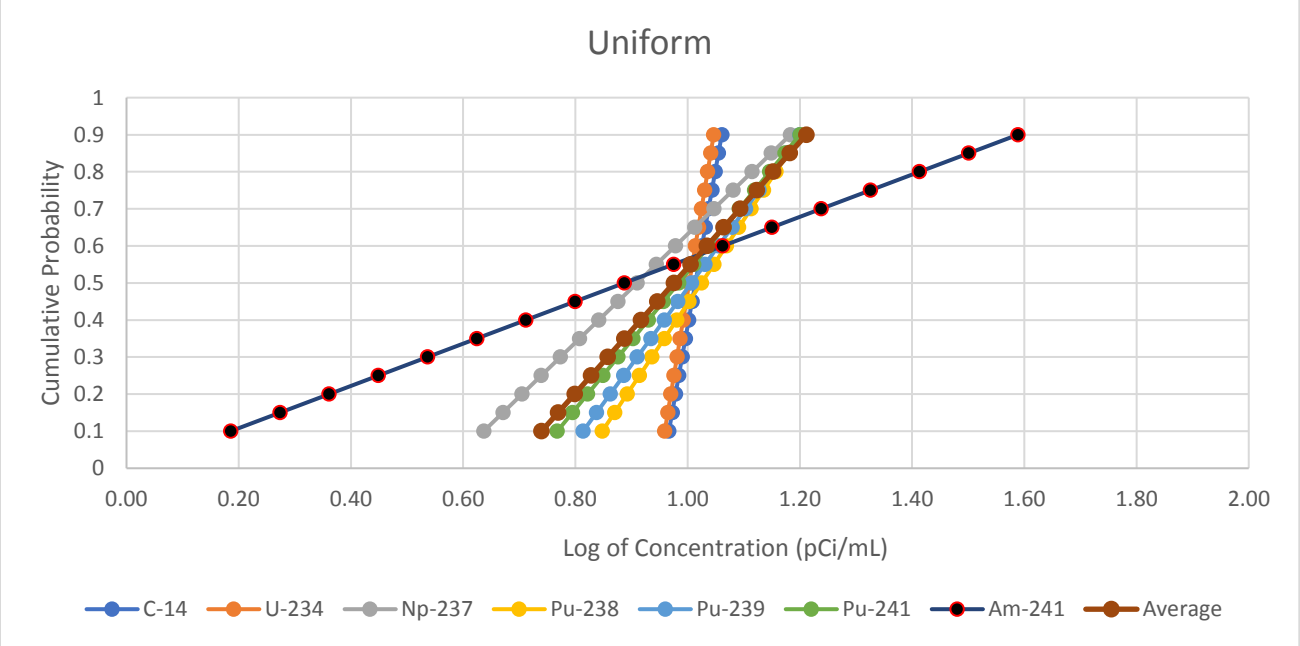


Table 12: Summary of Recommended Uniform Distributions

Radionuclide	Slope	Intercept
C-14	0.118	0.955
U-234	0.109	0.948
Np-237	0.683	0.568
Pu-238	0.442	0.804
Pu-239	0.483	0.765
Pu-241	0.541	0.714
Am-241	1.754	0.010
Average	0.590	0.681

Figure 3: Uniform Distribution Plot



Recommendations and Goodness-of-Fit Statistics

Because there was limited data available for testing and analysis, the recommended approach was to take the average of the mean and standard deviations listed in Table 10, which combines the seven distributions into a universal 'average' normal distribution, 'average' uniform distribution, and an 'average' gamma distribution. Combining all seven distributions into one simultaneously gives the best estimate to the behavior of available data without being overly conservative with the multiplier value. A plot of the Normal, Gamma, and Uniform distributions is shown in Figure 4, overlaid with the average data point values for a comparison of best fit.

Figure 4: Average Normal, Uniform, and Gamma Plot

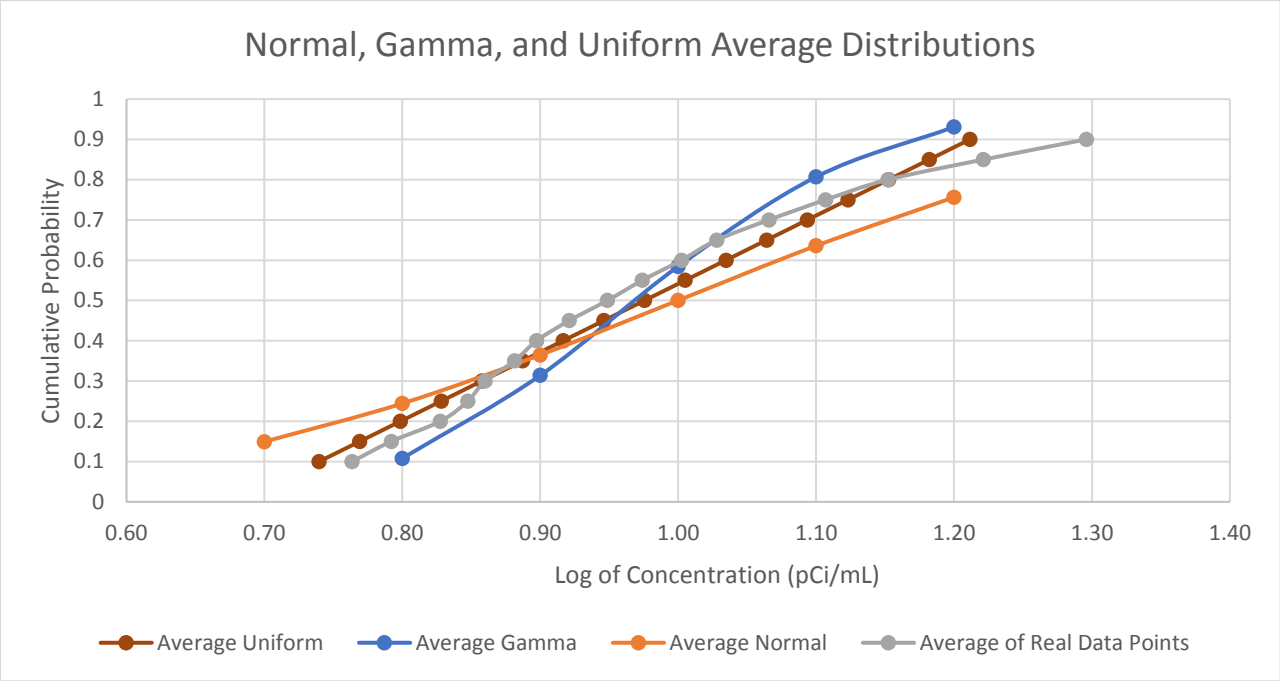


Table 13 displays the goodness-of-fit statistics to select the best distribution to fit the data. Table 13 data indicates that the uniform distribution fits best because it has the smallest Root Mean Square Error (RMSE) and has a very high R-square value. The RMSE is a measure of how much error is in the data, so a value closer to 0 indicates better fit. The R-squared coefficient measures how two data sets correlate together, with a value of 1 indicating a perfect positive correlation, 0 indicating no correlation, and -1 indicating a perfect negative correlation.

Table 13: Goodness-of-Fit Statistics

Distribution	RMSE	R-squared Coefficient
Normal	0.072	0.964
Gamma	0.048	0.976
Uniform	0.032	0.954

Recommendation for Modeling

Given the logarithmic behavior of the data, it is recommended that probabilistic modeling apply the following equation:

$$r^P \quad \text{(Eq. 1-1)}$$

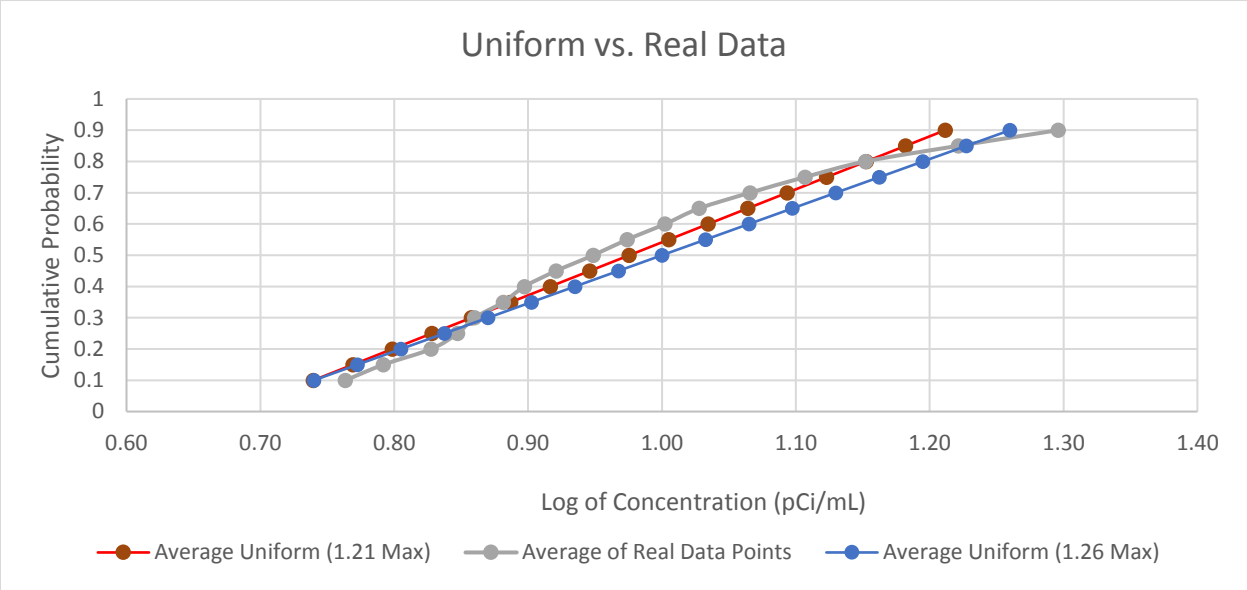
where r is a recommended inventory value in Ci and *P* is a probabilistically sampled model element with a uniform distribution with a minimum value of 0.74 and a maximum value of 1.26. These minimum and

maximum values were calculated by the relative minimum and maximum of the uniform distribution data set. In Table 14, the average uniform distribution values are displayed along with the average number of the data set itself. The minimum value in the data set, 0.74 has a delta of 0.26 from 1. The maximum value has a 0.21 delta from 1. To be conservative, the 0.26 delta will be added to 1 to get a maximum value of 1.26 for the uniform distribution, rather than the suggested value of 1.21. Thus, for probabilistic modeling, the maximum value should be 1.26 and the minimum value should be 0.74. Figure 5 shows that the recommended distribution (with the higher maximum of 1.26) provides a slightly more conservative comparison to the measured concentrations when compared to the average uniform distribution (with the lower maximum value of 1.21).

Table 14: Derivation of Minimum and Maximum Values

Probability	Uniform Average Value
0.9	1.21
0.85	1.18
0.8	1.15
0.75	1.12
0.7	1.09
0.65	1.06
0.6	1.03
0.55	1.01
0.5	0.98
0.45	0.95
0.4	0.92
0.35	0.89
0.3	0.86
0.25	0.83
0.2	0.80
0.15	0.77
0.1	0.74
Average of the Data Set:	0.98

Figure 5: Uniform Comparisons to Real Data



For demonstration purposes, let r be equal to 800 Ci of a hypothetical radionuclide "X" for modeling input. Then using Equation 1-1, the model (simulated for 10,000 realizations) computes the following "X" inventory estimates at various percentiles:

Table 11: Eq. 1-1 Output Example

1st Percentile	25th Percentile	50th Percentile	75th Percentile	99th Percentile
146 Ci	336 Ci	800 Ci	1908 Ci	4934 Ci

The data ranges from 336 to 1908 Ci of the 25th-75th percentile is a reasonable range of values, given the assumed 800 Ci, while the extreme values provide a greater range for exploring the effects of uncertainty. Therefore, applying Equation 1-1 where P is a probabilistically sampled model element with a uniform distribution with a minimum value of 0.74 and a maximum value of 1.26 is a valid approach for modeling SDF inventory for radionuclides wherein there is significant uncertainty.

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