WSRC-STI-2006-00019

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Distribution Coefficient, Solubility,
Stochastic Modeling,
Variability, Heterogeneity,

RETENTION:
Permanent

EARLY GUIDANCE FOR ASSIGNING DISTRIBUTION PARAMETERS TO GEOCHEMICAL INPUT TERMS TO STOCHASTIC TRANSPORT MODELS

Daniel I. Kaplan
Margaret R. Millings

JUNE 30, 2006

Savannah River National Laboratory
Washington Savannah River Company
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Prepared for the U.S. Department of Energy Under Contract Number DE-AC09-96SR18500

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REVIEWS AND APPROVALS

7/20/2006

Daniel I. Kaplan, Co-author, Waste Processing Technology — Date

7/20/2006

Margaret Millings, Co-author, Environmental Science and Biotechnology — Date

8/22/06

James Cook, Peer Reviewer, Waste Processing Technology — Date

8/22/06

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8/23/06

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8/22/06

J. C. Griffin, Level 3 Manager, Waste Processing Technology — Date

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1.0 EXECUTIVE SUMMARY

Stochastic modeling is being used in the Performance Assessment program to provide a probabilistic estimate of the range of risk that buried waste may pose. The objective of this task was to provide early guidance for stochastic modelers for the selection of the range and distribution (e.g., normal, log-normal) of distribution coefficients (K_d) and solubility values (K_{sp}) to be used in modeling subsurface radionuclide transport in E- and Z-Area on the Savannah River Site (SRS). Due to the project's schedule, some modeling had to be started prior to collecting the necessary field and laboratory data needed to fully populate these models. For the interim, the project will rely on literature values and some statistical analyses of literature data as inputs. Based on statistical analyses of some literature sorption tests, the following early guidance was provided:

- Set the range to an order of magnitude for radionuclides with K_d values >1000 mL/g and to a factor of two for K_d values of <1000 mL/g. This decision is based on the literature.
- Set the range to an order of magnitude for radionuclides with K_{sp} values <10^{-6} *M* and to a factor of two for K_d values of >10^{-6} *M*. This decision is based on the literature.
- The distribution of K_d values with a mean >1000 mL/g will be log-normally distributed. Those with a K_d value <1000 mL/g will be assigned a normal distribution. This is based on statistical analysis of non-site-specific data.

Results from on-going site-specific field/laboratory research involving E-Area sediments will supersede this guidance; these results are expected in 2007.

2.0 INTRODUCTION

The objective of this task was to provide early guidance for stochastic modelers who are modeling various aspects of low-level waste disposal in E-Area on the Savannah River Site (SRS). Due to the project's tight schedule, some modeling had to get started prior to collecting the necessary field data needed to fully populate these models. For the interim, we are required to rely on some literature values as inputs. The specific input values that are required are the range and distribution (e.g., normal, log-normal) of distribution coefficients (K_d) and solubility values (K_{sp}), both parameters that quantify the extent that radionuclides partition between the aqueous and solid phases in the subsurface environment.

The approach taken in this task was to use the literature to determine the range of values that others have measured. We were unsuccessful in identifying any citations of published work on the distributions of sorption parameters in sediments. So we elected to use multiple K_d measurement collected from Hanford Site for Sr, Cs, Sr, and U (Kaplan et al. 1998). The statistics and distribution graphs are presented in the Appendix.

3.0 RESULTS

3.1 RANGE OF VALUES

There has not been any work done to date regarding geochemical parameter input variability as it relates to the SRS performance assessment. However, activity to understand variability and uncertainty associated with these parameters is presently underway. Until this site-specific information is available, the general approach adopted by Wieland and Van Loon (2003) will be used. This approach was one based on professional judgment (Wieland and Van Loon 2003). They calculated an uncertainty factor, f_e, which was used to provide upper and lower limits for sorption values:

$$Kd_{\max} = Kd \times f_e \quad (1)$$
$$Kd_{\min} = Kd / f_e \quad (2)$$

The uncertainty range of the sorption values was assumed to be about one order-of-magnitude for the strongly sorbing radionuclides, with Kd • 1000 mL/g. The uncertainty accounts for variability associated with environmental conditions (sediment, groundwater conditions, etc.), contaminant concentrations and speciation, and laboratory technique. They assigned an uncertainty factor, f_e, of 3.3 to Kd values • 1000 mL/g and 1.4 to Kd values <1000 mL/g. The f_e of 3.3 yields a range of about one order of magnitude, whereas the f_e, of 1.4 yields a range of about a factor of 2.

For example, if the Kd value is 1000 mL/g, then using Equation (1), $Kd_{\max}$ = 1000 x 3.3 = 3,300 mL/g, and using Equation (2), $Kd_{\min}$ = 1000/3.3 = 303 mL/g. The range of values would be 3,300 to 303 mL/g, approximately an order of magnitude difference. Similarly, if Kd value is 10 mL/g, then using equation (1), $Kd_{\max}$ = 10 x 1.4 = 14 mL/g, and using

Equation (2), Kd_{min} = 10/1.4 = 7 mL/g. The range of values would be 14 to 7 mL/g, a factor-of-two difference. These estimates of variability will provide early guidance. Both Bradbury and Sarott (1995) and Krupka et al. (2004) recommend that the parameters have a normal distribution. Again, this decision appears to be largely based on professional judgment, rather than on a statistical analysis of data. Additional work clearly needs to be conducted to substantiate the assumptions used to describe the variability of the geochemical parameters.

The method of Wieland and Van Loon will be extended to represent the variability of solubility concentration limits (K_{sp}). K_{sp} values will be varied in a similar manner as *Kd*:

$$K_{sp\text{-},\mathrm{max}} = K_{sp} \times f_e \qquad (3)$$
$$K_{sp\text{-}\mathrm{min}} = K_{sp} / f_e \qquad (4)$$

The uncertainty factors, f_e, will be assigned similar values as those assigned for the *Kd* values in Equation (1) and (2) and the K_{sp} values will be assumed to have a normal distribution. Set the range to an order of magnitude for radionuclides with K_{sp} values $\leq 10^{-6}$ *M* and to a factor of two for K_{sp} values of $>10^{-6}$ *M*.

Kd values and K_{sp} values appropriate for SRS are reported in Kaplan (2006).

3.2 DISTRIBUTION OF VALUES

For the performance assessments, it is important to understand the distributions of *Kd* values within a specific sorption medium. For example, for describing radionuclide transport through the E-Area surface aquifer, we are interested in the variability associated with the *Kd* values within a specific aquifer, not the variability of all the *Kd* values in the literature or not the variability of *Kd* values in various sediments at the SRS.

There is no site specific data available for calculating the distribution of *Kd* values or solubility constants. Furthermore, there are no reports of the distribution of these parameters in the literature. Consequently, we calculated these based on a data set from the Hanford site (Kaplan et al. 1998). Table A1 in the Appendix provides the laboratory measured *Kd* values for the Hanford boring 299-E17-21. These *Kd* values represent the mean of three replicates for each sample. The reported *Kd* values were collected primarily from two formations. It was statistically determined that the *Kd* values between the two formations were not statistically different for Cs and U. However, the *Kd* values between the two formations were found to be significantly different for Sr. These differences were attributed to differences in pH and cation exchange between the two formations (Kaplan et al. 1998). Statistical analyses were conducted on data sets combining the *Kd* values from both formations (n = 20) for all of the chemical parameters as well as for each formation (n = 10; Appendix) for Sr.

Table 1 in the Appendix shows summary statistics for the *Kd* values from the Hanford boring. The table includes the (arithmetic) sample mean, a minimum and maximum value of the sample population, the variance of the sample population, and the variance of the sample mean. The variance of the sample population is defined by:

$$s_{X_i}^2 = \frac{1}{n-1}\sum\left(X_i - \overline{X}\right)^2 \qquad (5)$$

where $s_{X_i}^2$ is the variance of the sample population (s_{X_i} is the standard deviation of the sample population), n is the number of samples, X_i represents each observation and $\overline{X}$ reflects the mean of a randomly sampled population. It reflects the amount of spread in the sample data.

The variance of the sample mean is defined by:

$$s_{\overline{X}}^2 = \frac{s_{X_i}^2}{n} \text{ or } s_{\overline{X}} = \frac{s_{X_i}}{\sqrt{n}} \qquad (6)$$

where $s_{\overline{X}}$ is the estimated standard deviation of the (arithmetic) sample mean, s_{X_i} is the estimated standard deviation of the population, and n is the number of samples (Walpole and Myers 1978). $s_{\overline{X}}$ is the standard error of the mean.

Table 1 also includes skewness and kurtosis. Understanding these two parameters is key for determining if a data set is normally distributed. Skewness is a measure of the symmetry of a distribution about a mean. A skewness value that is far from zero indicates an asymmetric distribution (positive value corresponds to a long right tail and a negative value corresponds to a long left tail). The coefficients of skewness are provided on Table 1. One method of evaluating the skewness value is by comparing it to the standard error of skewness. Values equal to two standard errors of skewness or more can be considered to be significantly skewed. Only Cs has a skewness value (2.1) that is greater than two standard errors of skewness (1.1). The skewness value is less for the transformed Cs dataset (LnCs). The skewness of Cs is discussed further below in the graphical evaluation of the parameter distributions.

A kurtosis value far greater than zero indicates that the distribution has longer tails than a normal distribution whereas a value far less than zero reflects a distribution that is flatter than a normal distribution. The coefficients of kurtosis are provided on Table 1. Values equal to two standard errors of kurtosis or more can be considered to be significant. The kurtosis values for Cs and U are greater than two standard errors of kurtosis and indicate that their distributions have longer tails than what would be expected with a normal distribution. Again, the kurtosis value improves for Cs when the dataset is transformed (LnCs).

For this evaluation, summary statistics were performed in Excel and confirmed by using SYSTAT 10.2. Numerical calculations such as skewness and kurtosis can be used as guides for evaluating distributions. However, it should be noted that the values can widely vary for small datasets even for populations that are normally distributed.

Table 1. Summary statistics of Kd measurements in Hanford sediments.

Statistic	K_d (mL/g)[1]			
	Cs	LnCs	Sr	U
mean	2055.1	7.60	14.74	0.62
min	1373.9	7.23	12.18	0.30
max	4068.2	8.31	16.92	0.94
median	2034.3	7.62	14.25	0.60
count	20.0	20	20	20
std deviation of sample mean (standard error)	133.4	0.06	0.36	0.03
std deviation of sample population	596.5	0.25	1.60	0.12
skewness	2.1	1.03	0.09	0.10
standard error skewness[2]	0.55	0.55	0.55	0.55
kurtosis	6.4	2.35	-1.22	3.57
standard error kurtosis[2]	1.10	1.10	1.10	1.10
distribution	lognormal	normal	normal	normal

[1]Average pH of samples = 8.75, with min of 8.5 and maximum of 8.96
[2]Standard error of skewness approximated by sqrt(6/n) and standard error of kurtosis approximated by sqrt(24/n), where n equals the count

Graphical methods are also helpful in evaluating whether a distribution is normal. Figures 1 through 6 provide graphs for Cs, the natural log of Cs (LnCs), Sr, and U, were generated using SYSTAT 10.2. For each parameter, the top graph shows a normal probability plot in which the measured values are plotted against the expected values (assuming a normal distribution). On these graphs, the straight line reflects a normal distribution. The left side of the each plot shows the number of standard deviations with "0" corresponding to the mean value of the graphed population. The size of the data points show the influence that each point has on a linear fit (or the amount that the correlation would change if that particular point was deleted). A small box plot along the top of each graph also shows the distribution of the data. 50% of the data lie within the box with the box ends representing the 25th and 75th percentiles. The vertical line inside the box reflects the median of the data. Whiskers on the outside of the box show the 10th and 90th percentile. Data outside of the 10th and 90th percentile are plotted as lone points. In addition to the probability plots, a dot histogram with a smoothing line is also provided to show each parameter's distribution.

For Cs, all the data except one, are represented by a small Pearson r Influence dot in the upper Probability Plot in Figure 1. The one data point representing a *Kd* value of 4068 mL/g, is larger than the rest because it influences the representation of the distribution more than the other data points (*i.e*., it pulls the data more from a normal to a log-normal distribution).

Given the high skewness value, 2.1 and kurtosis value, 6.4 (Table 1) of this data set, the data was replotted in a log-normal distribution (Figure 2). Note that the skewness and kurtosis in Table 1 decrease and that deviation of the data from the line in the probability plot is smaller in Figure 2. Also the influence of the single large *Kd* value, ln(CsKd) = 8.31, was greatly diminished.

Strontium *Kd* value distributions are presented in Figure 3. The data are scattered and the data are normally distributed. As noted above, Kaplan et al. (1998) determined that Sr *Kd* values were significantly different between the two formations. Therefore, separate statistics were conducted on the *Kd* values from each of the two individual formations (Table 3 in Appendix). The statistics became weaker due to the smaller population size (n=10 for layer 2 and n=9 for layer 1), but the result was the same, that Sr was normally distributed (Appendix).

Uranium was normally distributed and the dot histogram shows a near classical distribution of data with a few data points at the extremes and most points in the middle (Figure 4; Table 1).

The two data sets that had low *Kd* values, Sr and U, had normal distributions, whereas the only data set with a high *Kd* value, Cs, was log-normally distributed. The cause for this is not known.

Figure 1. Probability Plot (top) and Dot Histogram (bottom) for Cs Kd Values

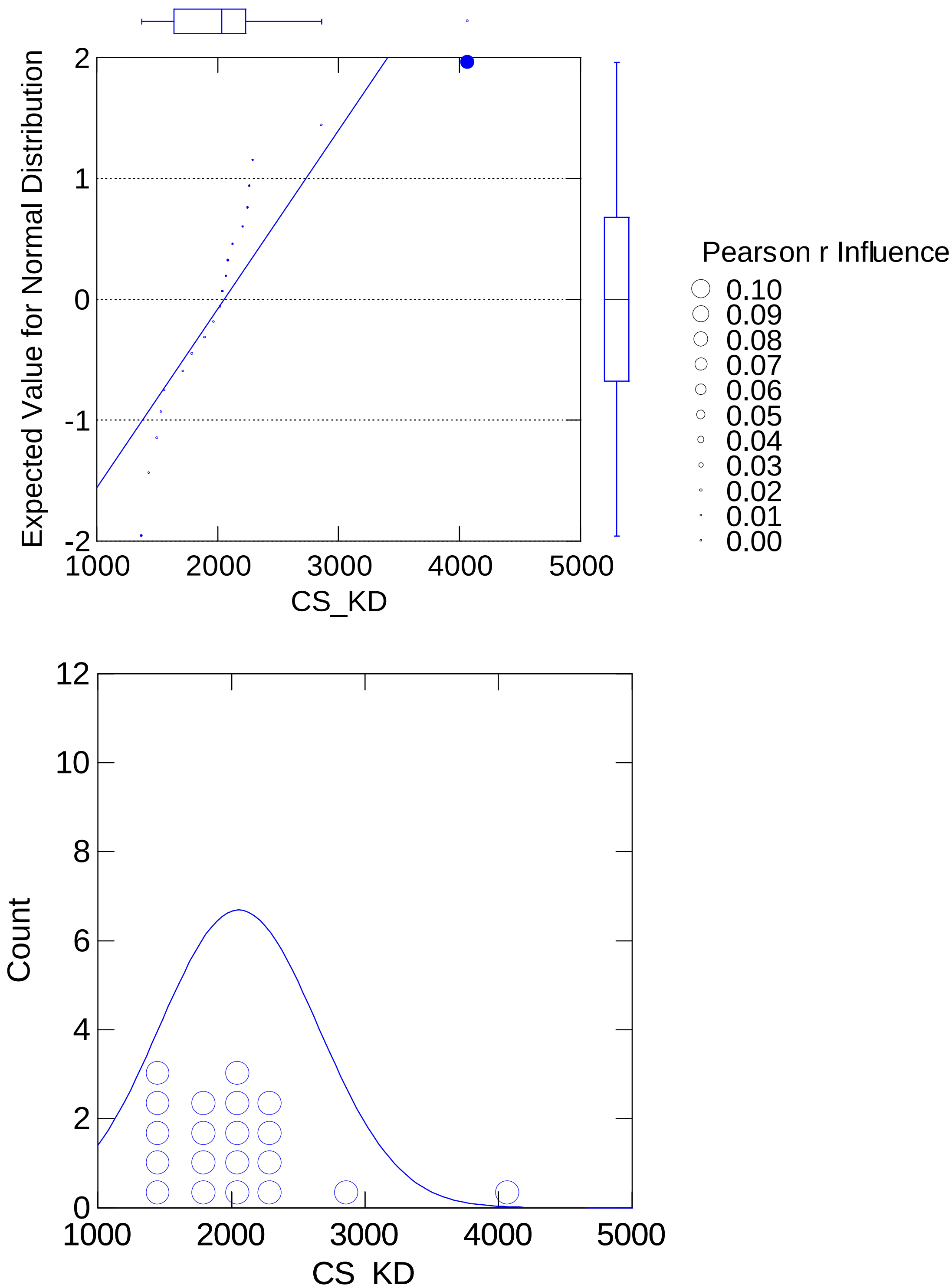


Figure 2. Probability Plot (top) and Dot Histogram (bottom) for LnCs-Kd

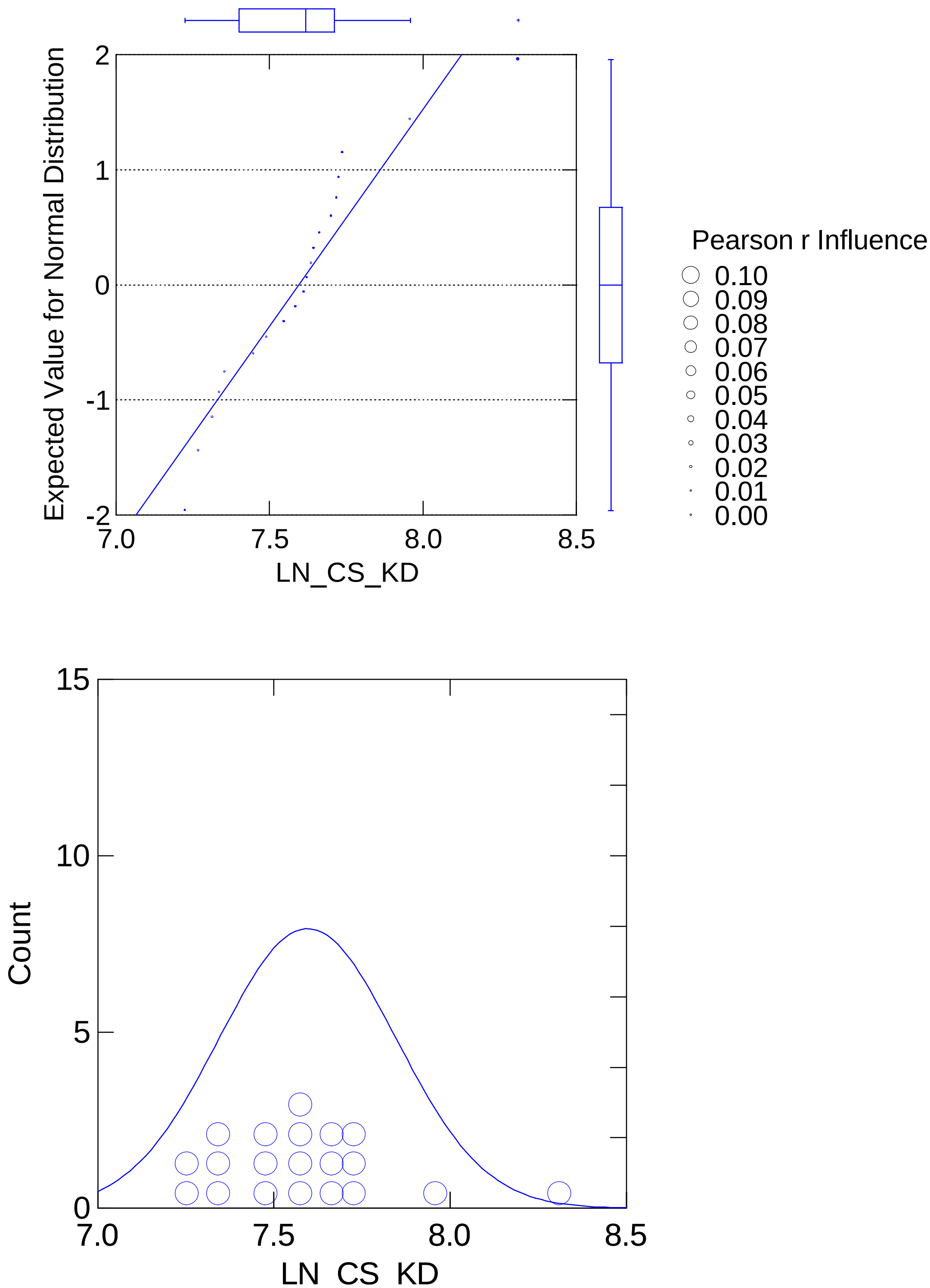


Figure 3. Probability Plot (top) and Dot Histogram (bottom) for Sr Kd Values

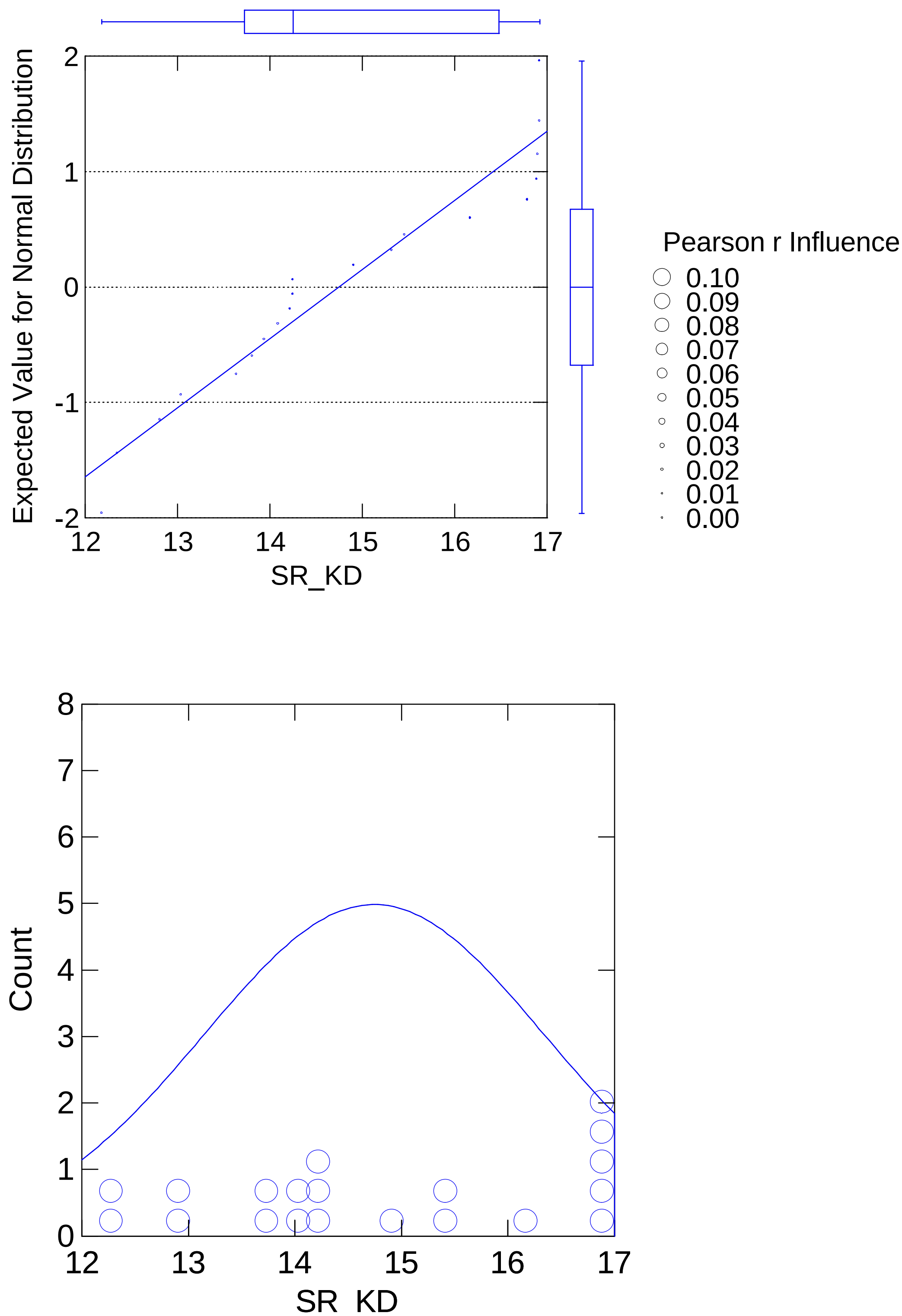
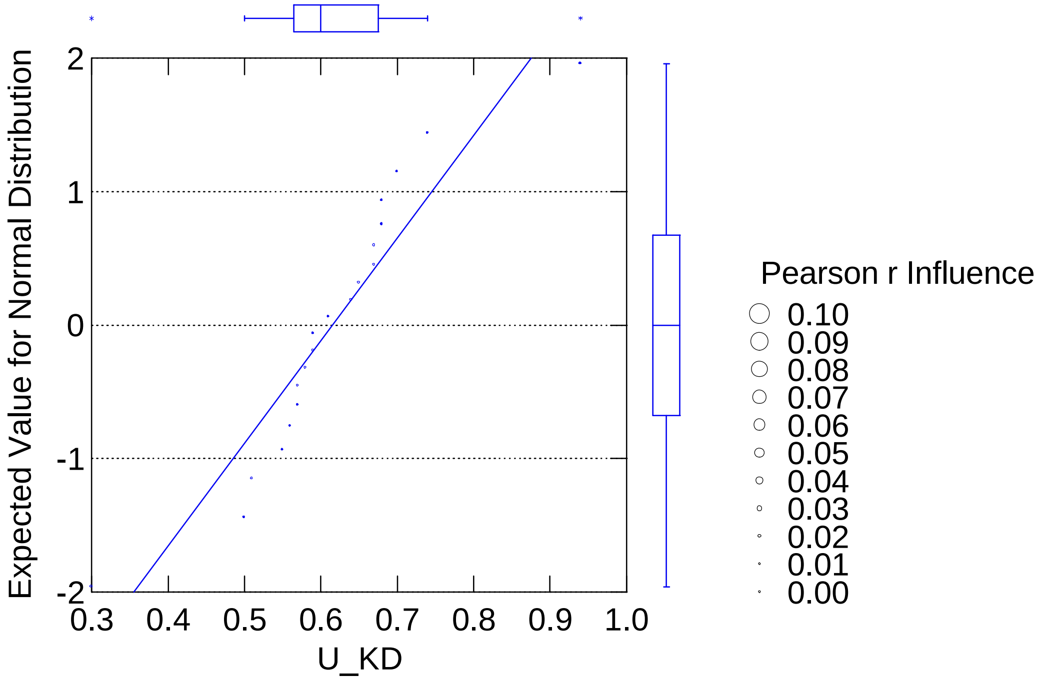
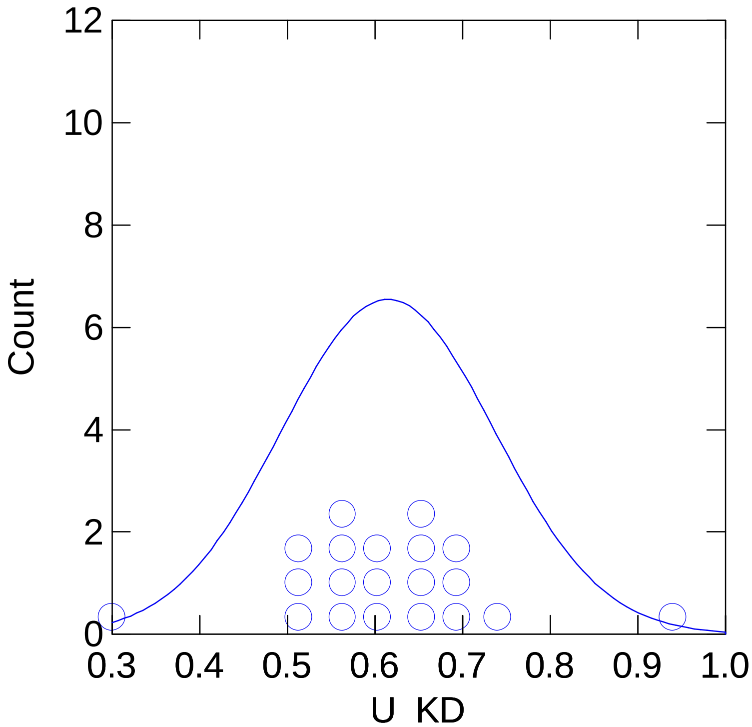


Figure 4. Probability Plot (top) and Dot Histogram (bottom) for U-Kd Values





4.0 CONCLUSIONS

Based on statistical analyses of some literature sorption tests, the following early guidance has been provided:

- Set the range to an order of magnitude for radionuclides with K_d values >1000 mL/g and to a factor of two for K_d values of <1000 mL/g. This decision is based on the literature.
- Set the range to an order of magnitude for radionuclides with K_{sp} values $<10^{-6}$ *M* and to a factor of two for K_d values of $>10^{-6}$ *M*. This decision is based on the literature.
- The distribution of K_d values with a mean >1000 mL/g will be log-normally distributed. Those with a K_d value <1000 mL/g will be assigned a normal distribution. This is based on our field measurements.

The range and distribution of solubility and Kd values based on the above guidance and the mean values provided in Kaplan (2006) are provided in Appendix B.

This guidance for stochastic modeling will provide a probabilistic estimate of the range of risk that buried waste may pose. Results from on-going site-specific field/laboratory research involving E-Area sediments will supersede this guidance; these results are expected in 2007.

5.0 REFERENCES

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APPENDIX A: STATISTICS OF Kd DISTRIBUTIONS

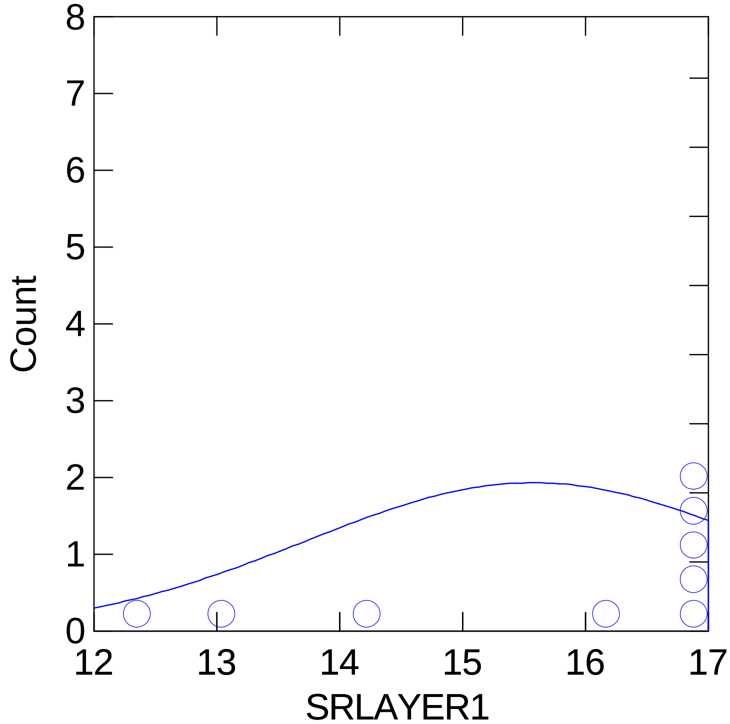
Table 2. Kd (mL/g) Values from Borehole 299-E17-21 at Hanford.

Sample ID	Depth (m)		pH	CEC (meq/100g)	Cs		Sr		U	
					value (mL/g)	+/-	value (mL/g)	+/-	value (mL/g)	+/-
07A	14	14.6	8.54	5.07	2044.8	275	14.09	0.83	0.94	0.12
10A	17.6	18.2	8.8	4.73	2090	305	14.25	0.49	0.67	0.08
12A	21.2	21.6	8.77	4.6	2023.8	305	13.81	0.78	0.64	0.1
14A	24.5	25.2	8.73	4.62	1969.8	39.5	13.94	0.5	0.67	0.05
15A	27.6	28.3	8.75	4.11	1502.1	80.1	13.64	0.85	0.74	0.05
16A	30.6	31.4	8.77	2.32	1535.9	270	12.81	0.33	0.57	0.04
17A	33.5	34.2	8.52	4.98	2267.2	388	15.46	0.33	0.68	0.15
19A	36.9	37.6	8.5	4.72	2861.7	396	14.25	0.45	0.51	0.08
20A	39.5	40.3	8.52	4.67	2251.8	292	15.32	0.37	0.65	0.08
21A	43.1	43.9	8.56	4.56	2072.5	409	14.91	0.63	0.57	0.09
22A	46.3	47.1	8.94	7.33	1373.9	332	12.18	0.29	0.59	0.08
23A	48.9	49.7	8.82	8.41	2295.2	280	13.04	0.95	0.58	0.05
24A	55.1	55.7	8.81	9.03	2213.3	455	16.92	0.92	0.55	0.05
25A	57.8	58.5	8.89	6.63	1716.9	484	12.35	0.85	0.56	0.07
27A	59.2	61.4	8.88	8.36	1563	259	16.17	1.42	0.59	0.08
29A	64.3	64.4	8.84	7.77	2128.7	423	14.22	0.34	0.5	0.13
31A	65.4	67.8	8.56	10.98	4068.2	259	16.9	0.11	0.3	0.12
32A	69.8	70.5	8.93	8.39	1792	315	16.89	1.72	0.7	0.11
34A	72	72.6	8.92	6.21	1897	178	16.92	1.53	0.61	0.16
35A	73	73.6	8.89	6.65	1435	133	16.79	2.68	0.68	0.13

Note: values for each sample represent mean +/- standard deviation based on 3 replicates; only one replicate was used for pH and cation exchange (CEC)

Figure 5: Dot Histograms for Sr Kd Values for Layer 1 (top) and Layer 2 (bottom) (n=10)

Layer 1



Layer 2

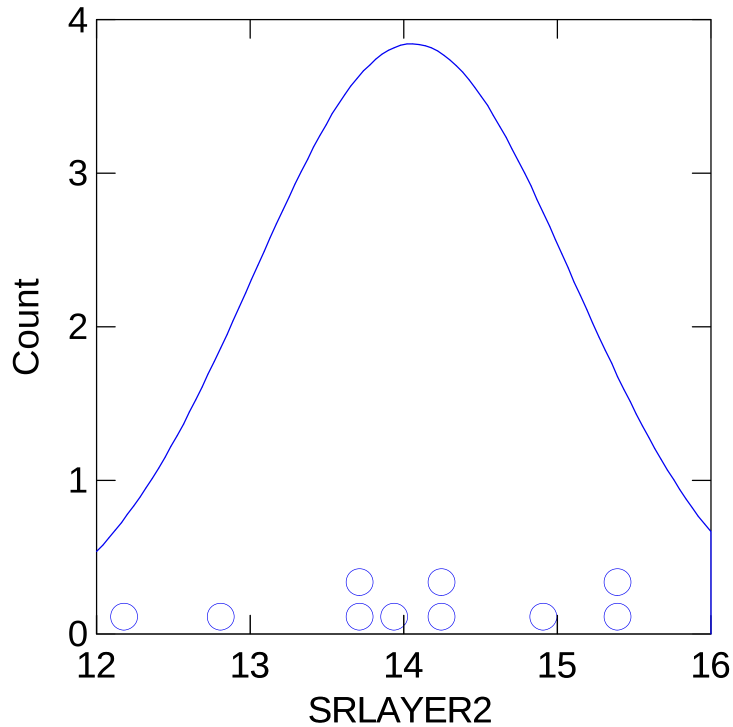
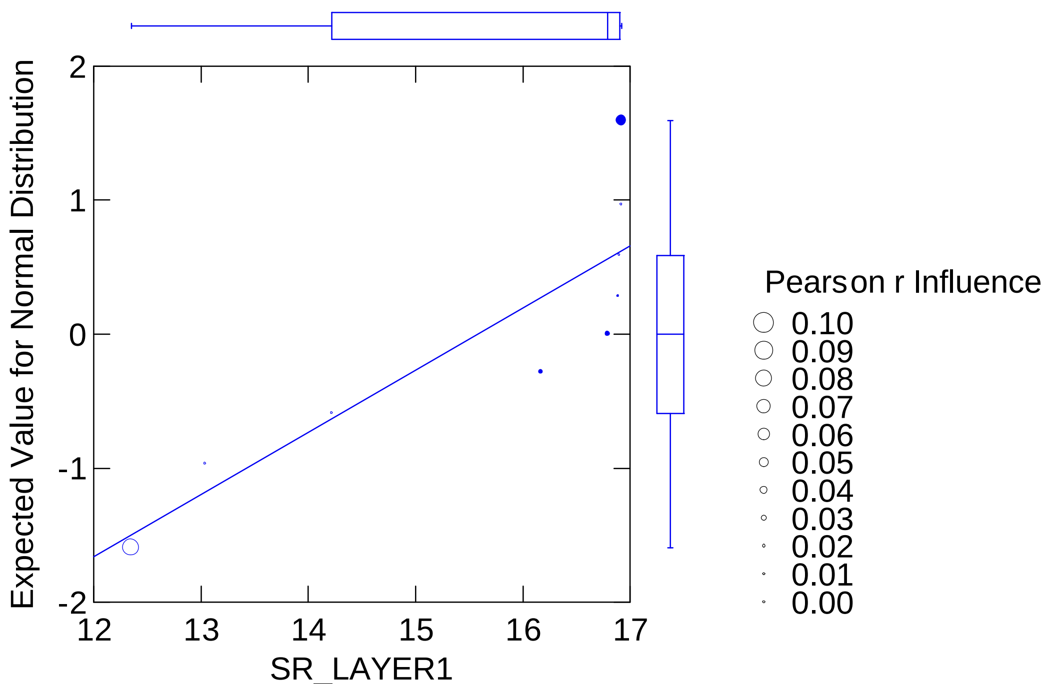


Figure 6: Probability Plots for Sr Kd Values for Layer 1 (top) and Layer 2 (bottom) (n=10)

Layer 1



Layer 2

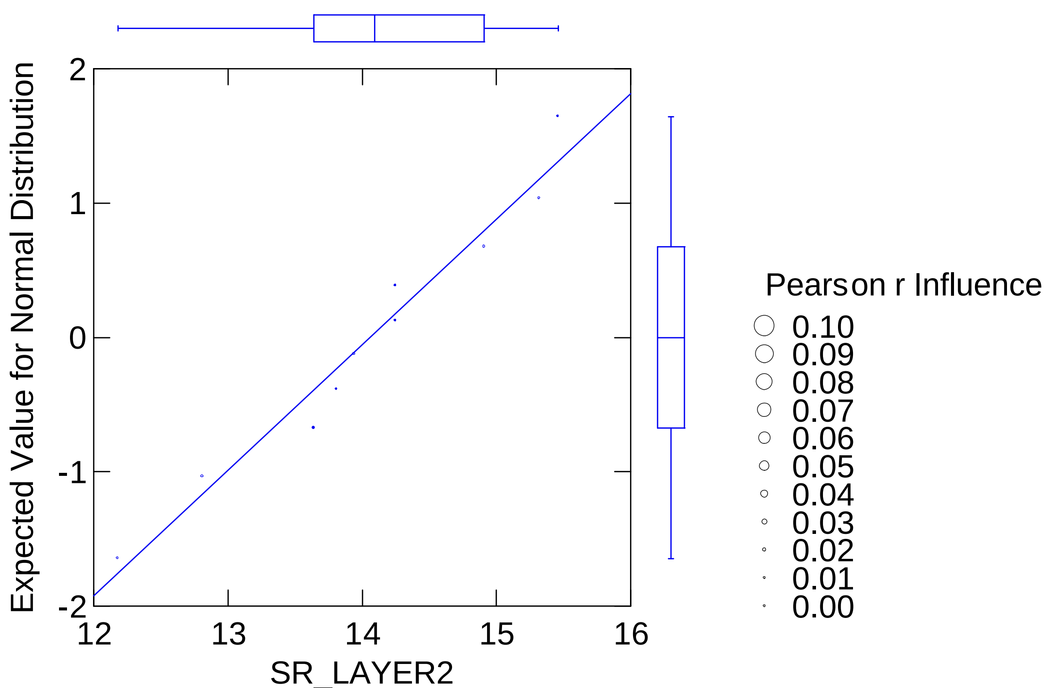


Table 3: Summary statistics of Kd measurements for Sr for Layers 1 & 2

Statistic	K_d (mL/g)[1]	
	Layer 1 Sr	Layer 2 Sr
mean	15.58	14.06
min	12.35	12.18
max	16.92	15.46
median	16.79	14.10
count	9	10
std deviation of sample mean (standard error)	0.62	0.33
std deviation of sample population	1.86	1.04
skewness	-1.03	-0.40
standard error skewness[2]	0.82	0.77
kurtosis	-0.78	-0.23
standard error kurtosis[2]	1.63	1.55

[1]Average pH of samples = 8.75, with min of 8.5 and maximum of 8.96

[2]Standard error of skewness approximated by sqrt(6/n) and standard error of kurtosis approximated by sqrt(24/n), where n equals the count

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APPENDIX B: RANGE AND DISTRIBUTION OF Kd AND SOLUBILITY VALUES USED IN E- AND Z-AREA PERFORMANCE ASSESSMENT CALCULATIONS

Table 4. Distribution Coefficicients (Kd values, mL/g) ranges and distributions in Sandy and Clayey Sediments.

	Sandy Sediment					Clayey Sediment				
Radionuclide	Best Kd	Distribution	fe	Lower Limit	Upper Limit	Best Kd	Distribution	fe	Lower Limit	Upper Limit
^{3}H, Kr, Rn, Ar	0	Normal	1.4	0	0	0	Normal	1.4	0	0
Cl, Nb	0	Normal	1.4	0	0	0	Normal	1.4	0	0
Ac, Am, Bk, Cf, Cm, Eu, Gd, Sm	1100	Log-Normal	3.3	333	3630	8500	Log-Normal	3.3	2576	28050
Inorganic C	0	Normal	1.4	0	0	0	Normal	1.4	0	0
Cs, Rb, Fr	50	Normal	1.4	36	70	250	Normal	1.4	179	350
Co	7	Normal	1.4	5	10	30	Normal	1.4	21	42
I, At	0	Normal	1.4	0	0	0.6	Normal	1.4	0	1
Ni	7	Normal	1.4	5	10	30	Normal	1.4	21	42
Np, Pa	0.6	Normal	1.4	0	1	35	Normal	1.4	25	49
Pu(V/VI)	16	Normal	1.4	11	22	5000	Log-Normal	3.3	1515	16500
Pu(III/IV)	300	Normal	1.4	214	420	6000	Log-Normal	3.3	1818	19800
Pu(combo)	270	Normal	1.4	193	378	5900	Log-Normal	3.3	1788	19470
Th,Zr	900	Normal	1.4	643	1260	2000	Log-Normal	3.3	606	6600
Pb, Po, Sn	2000	Log-Normal	3.3	606	6600	5000	Log-Normal	3.3	1515	16500
Sr, Ra, Ba	5	Normal	1.4	4	7	17	Normal	1.4	12	24
Se, Te	1000	Log-Normal	3.3	303	3300	1000	Log-Normal	3.3	303	3300
Tc, Re	0.1	Normal	1.4	0	0	0.2	Normal	1.4	0	0
U	200	Normal	1.4	143	280	300	Normal	1.4	214	420

Best Kds taken from Table 10 in Kaplan (2006).
"fe" = uncertainty factor, defined in equations 1 and 2.

Table 5. Apparent solubility concentration limits (mol/L) for Oxidizing Cementitious Solids

	Young Cement, 1st Stage					Moderately-aged Cement, 2nd Stage					Aged Cement, 3rd Stage				
Radionuclide	Best	Distribution	fe	Low Kd	Upper Kd	Best	Distribution	fe	Low Kd	Upper Kd	Best	Distribution	fe	Low Kd	Upper Kd
^{3}H, Cl, Tc, Re, Kr, Rn, Ar, Nb, Se, Te, I, At, Cs, Fr, Rb	NA			NA	NA	NA			NA	NA	NA			NA	NA
C	1.00E-06	Log-Normal	3.3	3.0E-07	3.3E-06	1.00E-04	Normal	1.4	7.1E-05	1.4E-04	1.00E-04	Normal	1.4	7.1E-05	1.4E-04
Ac, Am, Bk, Cf, Cm, Eu, Gd, Sm	1.00E-11	Log-Normal	3.3	3.0E-12	3.3E-11	1.00E-08	Log-Normal	3.3	3.0E-09	3.3E-08	1.00E-07	Log-Normal	3.3	3.0E-08	3.3E-07
Co, Ni	1.00E-07	Log-Normal	3.3	3.0E-08	3.3E-07	1.00E-07	Log-Normal	3.3	3.0E-08	3.3E-07	1.00E-06	Log-Normal	3.3	3.0E-07	3.3E-06
Np, Pa	1.00E-08	Log-Normal	3.3	3.0E-09	3.3E-08	1.00E-08	Log-Normal	3.3	3.0E-09	3.3E-08	1.00E-07	Log-Normal	3.3	3.0E-08	3.3E-07
Ra	1.00E-06	Log-Normal	3.3	3.0E-07	3.3E-06	1.00E-06	Log-Normal	3.3	3.0E-07	3.3E-06	1.00E-06	Log-Normal	3.3	3.0E-07	3.3E-06
Sr, Ba	1.00E-05	Normal	1.4	7.1E-06	1.4E-05	1.00E-05	Normal	1.4	7.1E-06	1.4E-05	NA			NA	NA
Pb, Po, Pu(V/VI), Pu(III/IV), Pu(combo), Th, Zr, Sn	1.00E-08	Log-Normal	3.3	3.0E-09	3.3E-08	1.00E-08	Log-Normal	3.3	3.0E-09	3.3E-08	1.00E-07	Log-Normal	3.3	3.0E-08	3.3E-07
U(VI)	1.00E-07	Log-Normal	3.3	3.0E-08	3.3E-07	1.00E-07	Log-Normal	3.3	3.0E-08	3.3E-07	1.00E-06	Log-Normal	3.3	3.0E-07	3.3E-06

Best Kds taken from Table 11 in Kaplan (2006).

"fe" = uncertainty factor, defined in equations 3 and 4.

Table 6. Apparent solubility concentration limits (mol/L) for Reducing Cementitious Solids.

	Young Cement, 1st Stage					Moderately-aged Cement, 2nd Stage					Aged Cement, 3rd Stage				
Radionuclide	Best	Distribution	fe	Low Kd	Upper Kd	Best Kd	Distribution	fe	Low Kd	Upper Kd	Best Kd	Distribution	fe	Low Kd	Upper Kd
^{3}H, Cl, Kr, Rn, Sr, Ra, Zr, Th, Nb, Sn, I, Cs, Ac, Am, Cf, Cm, Eu, Po, Se, C, Co, Ni, Pb, Bk, Sm, Fr, Gd, At, Ar, Te, Ba	See Oxidizing Cementitious Solids (See Table 5)														
Tc (IV), Re(IV)	1.00E-10	Log-Normal	3.3	3.0E-11	3.3E-10	1.00E-10	Log-Normal	3.3	3.0E-11	3.3E-10	1.00E-10	Log-Normal	3.3	3.0E-11	3.3E-10
Np(IV), Pa(IV)	1.00E-06	Log-Normal	3.3	3.0E-07	3.3E-06	1.00E-06	Log-Normal	3.3	3.0E-07	3.3E-06	1.00E-05	Normal	1.4	7.1E-06	1.4E-05
Pu(III/IV)	1.00E-10	Log-Normal	3.3	3.0E-11	3.3E-10	1.00E-10	Log-Normal	3.3	3.0E-11	3.3E-10	1.00E-09	Log-Normal	3.3	3.0E-10	3.3E-09
Pu(combo)	1.00E-10	Log-Normal	3.3	3.0E-11	3.3E-10	1.00E-10	Log-Normal	3.3	3.0E-11	3.3E-10	1.00E-09	Log-Normal	3.3	3.0E-10	3.3E-09
U	1.00E-06	Log-Normal	3.3	3.0E-07	3.3E-06	1.00E-07	Log-Normal	3.3	3.0E-08	3.3E-07	1.00E-07	Log-Normal	3.3	3.0E-08	3.3E-07

Best Kds taken from Table 12 in Kaplan (2006).

"fe" = uncertainty factor, defined in equations 3 and 4.

Table 7. Distribution coefficients (Kd, mL/g) for Oxidizing Cementitious Solids.

	Young Cement, 1st Stage					Moderately-aged Cement, 2nd Stage					Aged Cement, 3rd Stage				
Radionuclide	Best Kd	Distribution	fe	Low Kd	Upper Kd	Best Kd	Distribution	fe	Low Kd	Upper Kd	Best Kd	Distribution	fe	Low Kd	Upper Kd
Tc(VII), Re, Kr, Rn, Ar,	0	Normal	1.4	0	0	0	Normal	1.4	0	0	0	Normal	1.4	0	0
3-H	0	Normal	1.4	0	0	0	Normal	1.4	0	0	0	Normal	1.4	0	0
Cl	0.8	Normal	1.4	0.6	1.1	2	Normal	1.4	1	3	0	Normal	1.4	0	0
I, At	8	Normal	1.4	6	11	20	Normal	1.4	14	28	0	Normal	1.4	0	0
Inorganic C	20	Normal	1.4	14	28	10	Normal	1.4	7	14	0	Normal	1.4	0	0
Ac, Am, Bk, Cf, Cm, Eu, Gd, Sm	5000	Log-Normal	3.3	1515	16500	5000	Log-Normal	3.3	1515	16500	500	Normal	1.4	357	700
Co, Ni,	1000	Log-Normal	3.3	303	3300	1000	Log-Normal	3.3	303	3300	500	Normal	1.4	357	700
Ra, Ba	100	Normal	1.4	71	140	100	Normal	1.4	71	140	70	Normal	1.4	50	98
Sr	1	Normal	1.4	1	1	1	Normal	1.4	1	1	0.8	Normal	1.4	1	1
Sn	4000	Log-Normal	3.3	1212	13200	4000	Log-Normal	3.3	1212	13200	2000	Log-Normal	3.3	606	6600
Cs, Fr	2	Normal	1.4	1	3	4	Normal	1.4	3	6	2	Normal	1.4	1	3
Nb	1000	Normal	1.4	714	1400	1000	Log-Normal	3.3	303	3300	500	Normal	1.4	357	700
Np, Pa	2000	Log-Normal	3.3	606	6600	2000	Log-Normal	3.3	606	6600	200	Normal	1.4	143	280
Se, Te	300	Normal	1.4	214	420	300	Normal	1.4	214	420	150	Normal	1.4	107	210
Pb, Po,	500	Normal	1.4	357	700	500	Normal	1.4	357	700	250	Normal	1.4	179	350
Pb, Po, Pu(V/VI), Pu(III/IV), Pu(combo), Th, Zr	5000	Log-Normal	3.3	1515	16500	5000	Log-Normal	3.3	1515	16500	500	Normal	1.4	357	700
U	1000	Log-Normal	3.3	303	3300	1000	Log-Normal	3.3	303	3300	70	Normal	1.4	50	98

Best Kds taken from Table 13 in Kaplan (2006).
"fe" = uncertainty factor, defined in equations 1 and 2.

Table 8. Distribution coefficients (Kd, mL/g) for Reducing Cementitious Solids.

	Young Cement, 1st Stage					Moderately-aged Cement, 2nd Stage					Aged Cement, 3rd Stage				
Radionuclide	Best Kd	Distribution	fe	Low Kd	Upper Kd	Best Kd	Distribution	fe	Low Kd	Upper Kd	Best Kd	Distribution	fe	Low Kd	Upper Kd
All rads except the following	Same values as reported in Table7.														
Tc, Re	5000	Log-Normal	3.3	1515	16500	5000	Log-Normal	3.3	1515	16500	5000	Log-Normal	3.3	1515	16500
U	5000	Log-Normal	3.3	1515	16500	5000	Log-Normal	3.3	1515	16500	5000	Log-Normal	3.3	1515	16500

Best Kds taken from Table 14 in Kaplan (2006).
"fe" = uncertainty factor, defined in equations 1 and 2.

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