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LIST OF TERMS

95% LL	lower limit of a 95% confidence interval on the mean
95% UL	upper limit of a 95% confidence interval on the mean
ANOVA	analysis of variance
S-104	tank 241-S-104
CI	confidence interval
df	degrees of freedom
.dir	direct
DL	detection limit
GEA	gamma energy analysis
IC	ion chromatography
IC.w.	ion chromatography of a water leached sample
ICP	inductively coupled plasma
ICP.a.	inductively coupled plasma analysis of an acid digested sample
ICP.f.	inductively coupled plasma analysis of a fusion digested sample
ICP.w.	inductively coupled plasma analysis of a water leached sample
KOH/Ni	Potassium Hydroxide/Nickel
Mean/DL	the mean of two sample results (sample and duplicate) divided by the detection limit
mL	milliliters
NA	not available
REML	Restricted Maximum Likelihood Estimation
Spec.w.	spectroscopic method of a water leached sample
TGA	thermal gravimetric analysis
TIC	total inorganic carbon
TOC	total organic carbon
$\bar{y}$	weighted mean of the concentration data
$\hat{\sigma}^2(\bar{y})$	estimated variance of $\bar{y}$
$\mu\text{g/g}$	micrograms per gram
$\mu\text{Ci/g}$	microcuries per gram

STATISTICAL CHARACTERIZATION REPORT
FOR
SINGLE-SHELL TANK 241-S-104

1.0 SUMMARY

This report contains the results of the statistical analysis of data from three core samples obtained from single-shell tank 241-S-104 (S-104).

Section 2.0 contains a description of the core samples and the chemical analyses performed on the core samples.

Section 3.0 contains mean concentration estimates and associated 95% confidence intervals (CIs) on the mean for each of the analytes found in the core samples.

Section 4.0 contains estimates of the spatial variability (variability between cores) and estimates of the analytical variability from the core composite data.

Two types of analytical variability were estimated from the core composite data: (1) sample composite variability (variability between composite samples within the same core) and (2) analytical measurement variability (variability between the primary and duplicate analyses within each core composite sample). Estimates of the analytical measurement variability were used as the reference value to test the significance of the spatial and sample composite variability. Spatial variability was significantly different from zero¹ for 22 out of 63 analytes. The sample composite variance was significantly different from zero for 20 out of the 63 analytes.

¹ Significantly different from zero at the $\alpha = 0.05$ level.

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2.0 INTRODUCTION

Three core samples (cores 42, 43, and 44) were taken from S-104. Cores 42, 43, and 44 were obtained from risers 3, 7, and 2, respectively. The locations of the risers are given in Figure 2-1. The segment recoveries are listed by core number in Table 2-1. Segments 2 and 4 from core 42 had 100% recovery. The recovery from segment 3 of core 42 is unknown since the sample valve was partially open. For cores 43 and 44, 100% segment recovery occurred in segments 2, 3, and 4.

Figure 2-1. Riser Location.

Table 2-1. S-104 Core Recoveries.

Core	Segment number					
	1	2	3	4	5	6
42	75%	100%	*	100%	60%	10%
43	75%	100%	100%	100%	80%	33%
44	50%	100%	100%	100%	33%	50%

* The sampler valve was partially open. Approximately 100 g of tank waste adhered to the outside of the sampler and inside the sleeve. The waste was washed out of the sleeve with Q-water. A total of 223.96 g of solids were recovered from the sampler. There were no drainable liquids (Kocher 1993).

Due to the incomplete core sample recovery, the concentration estimates given in this report are biased. The magnitude of the bias is unknown.

Two core composite samples were made from each core sample from the homogenized solid segment waste. Primary and duplicate results were obtained from each core composite sample.

The chemical analysis of the primary and duplicate samples consisted of the following routine analytical methods and sample preparations (the notation for the method and preparation is also listed):

- inductively coupled plasma (ICP) analysis of an acid digested sample (ICP.a)
- ICP of a potassium hydroxide/nickel (KOH/Ni) fused sample (ICP.f)
- ICP analysis of a water leached sample (ICP.w)
- ion chromatography (IC) of a water leached sample (IC.w)
- radiochemistry
- gamma energy analysis (GEA).

Whenever appropriate, the data given here are identified using the notation in the above list. For example, the notation ICP.a.A1 refers to the A1 concentration from an ICP analysis of an acid digested sample. However, it needs to be noted that, occasionally, other analytical methods are used. The results from such methods are also given in the tables in Sections 3.0 and 4.0 and the table in Appendix A.

The core composite sample data are contained in Table A-1 (Appendix A). In Table A-1, the data from the first composite is above the dashed line and those from the second composite are below the dashed line. Ratios of the mean of each primary and duplicate result divided by the detection limit (DL) for that pair are also included. The ratios are provided to show how large the analyte concentrations are relative to the DL. The data package for S-104 (Kocher 1993) contains a complete report of the sample results along with the laboratory quality control data. The core composite data for each analyte are illustrated in the figures provided in Appendix B.

Analysis of variance (ANOVA) models were fit to the data for all analytes that did not have any "less than" values. All of the data used in the statistical analyses are reported in Table A-1. In addition, this table reports the data for the analytes with "less than" values.

Analytical Evaluation and Reporting personnel, within the Tank Waste Remediation System Information Management Systems, requested that ANOVA models be fit to the data for analytes whose concentrations were greater than ten times the DL. In addition, they identified a list of "special analytes," given in Table 2-2. For this list, they requested that the ANOVA models be fit to the data, provided the concentration values were greater than three times the DL.

Table 2-2. Special Analyte List.

Aluminum	Nitrate
Bismuth	Nitrite
Calcium	Phosphate
Chromium	Carbonate
Iron	Fluoride
Silicon	Chloride
Sodium	Total Organic Carbon
Zirconium	Cyanide

The analytes in Tables 3-1, 4-1, and A-1 are denoted by a "•" or a "★" whenever a concentration is less than three times or ten times the DL. The results for such analytes are to be used with caution.

A close examination of the data plots given in Appendix B revealed several potential anomalies in the core composite data. They are listed below.

- For ICP.f.Ca, ICP.f.Mg, ICP.f.Si, ICP.f.Zn, ICP.w.Ca, ICP.w.Mg, and ICP.w.Si, a single sample result is significantly different than the cluster of remaining sample results within the corresponding core.
- The sample results from core 42, composite 2 were significantly larger than the remaining core composite sample results for ICP.a.Na and ICF.f.Na.
- The sample results from core 44, composite 1 were significantly larger than the remaining core composite sample results for total inorganic carbon (TIC) (TIC.w.CO3).
- For ICP.a.Al, there is a statistical difference between the results reported for the two composites for core 44.

There is no direct evidence that the results noted above are due to analytical measurement error. Consequently, the statistical analysis was performed on the data as reported in Table A-1. The potential anomalies in the data noted above can be clearly seen in the figures in Appendix B.

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3.0 MEAN CONCENTRATION ESTIMATES

One of the tasks outlined in the Tank Waste Characterization Plan, Section 5.1.1.2 (Bell 1993), is to estimate the inventories of the analytes in the waste. The inventories are estimated by computing mean concentration and 95% CIs on the mean concentration for each analyte. The estimate of the inventory and CI on the inventory of an analyte in the tank are equal to the corresponding mean concentration estimates and CI multiplied by the volume of waste in the tank. The estimates of the tank inventory are not given in this document.

Table A-1 contains the core composite data used to compute the mean concentration estimates and the CIs.

3.1 STATISTICAL METHODS

The concentration estimates are given in the form of 95% CIs on the mean concentration. It is assumed that each primary sample and its duplicate are analyzed independently of one another. The two analytical results are used to estimate the analytical measurement variability. Due to the hierarchical structure of the data, the analytical measurement variability alone is not the appropriate variance term to use in computing the CIs. A linear combination of the analytical measurement variance and the spatial variance is the appropriate variance of the mean for the CIs (Snedecor and Cochran 1980). Appendix C contains a description of the statistical model and formulas used to calculate the estimate of the mean, the variance of the mean, and the CI on the mean.

3.2 STATISTICAL RESULTS

Table 3-1 contains the summary statistics, by analyte, for ICP acid digestion, ICP water leach, ICP KOH/Ni fusion dissolution, radiochemistry, IC, and the other analyses. The summary statistics are defined as follows:

$\bar{y}$	mean of the concentration data
$\hat{\sigma}^2(\bar{y})$	estimated variance of $\bar{y}$
df	degrees of freedom
95% LL	lower limit to the 95% CI on the mean
95% UL	upper limit to the 95% CI on the mean.

For some analytes, the lower confidence limit (95% LL) was negative. Since concentrations are greater than or equal to zero, any negative 95% LL values were set equal to zero.

Table 3-1. Concentration Estimate Statistics (Units $\mu\text{g/g}$
Except Radionuclides $\mu\text{Ci/g}$). (sheet 1 of 2)

Analyte	$\bar{y}$	$s^2(\bar{y})$	df	95% LL	95% UL
ICP.a.Al	3.89E+04	5.05E+07	2	8.31E+03	6.94E+04
ICP.a.B*	1.44E+01	1.22E+01	2	0.00	2.94E+01
ICP.a.Ba	2.16E+01	1.01E+00	2	1.72E+01	2.59E+01
ICP.a.Ca*	2.47E+02	6.50E+02	2	1.37E+02	3.56E+02
ICP.a.Ce*	2.21E+01	1.99E+00	2	1.60E+01	2.82E+01
ICP.a.Co*	2.52E+00	2.73E-02	2	1.81E+00	3.23E+00
ICP.a.Cr	2.35E+03	4.01E+03	2	2.08E+03	2.62E+03
ICP.a.Cu	1.94E+01	4.21E+01	2	0.00	4.73E+01
ICP.a.Fe	7.71E+02	5.40E+03	2	4.55E+02	1.09E+03
ICP.a.K	3.00E+02	8.07E+02	2	1.78E+02	4.22E+02
ICP.a.Mg	4.28E+01	2.67E+01	2	2.06E+01	6.50E+01
ICP.a.Mn	9.27E+02	1.86E+04	2	3.40E+02	1.51E+03
ICP.a.Na	1.21E+05	5.22E+06	2	1.11E+05	1.30E+05
ICP.a.Ni	5.60E+01	6.36E+00	2	4.52E+01	6.69E+01
ICP.a.P*	2.12E+01	2.14E+00	2	1.49E+01	2.75E+01
ICP.a.S	3.94E+02	3.87E+02	2	3.10E+02	4.79E+02
ICP.a.Si	1.92E+02	3.47E+02	2	1.12E+02	2.72E+02
ICP.a.Sr	3.26E+02	1.74E+02	2	2.69E+02	3.82E+02
ICP.a.Ti*	6.35E+00	2.84E+00	2	0.00	1.36E+01
ICP.a.Zn*	2.01E+01	1.53E+01	2	3.32E+00	3.69E+01
ICP.a.Zr	3.36E+01	7.62E-01	2	2.99E+01	3.74E+01
ICP.f.AL	1.17E+05	1.69E+06	2	1.11E+05	1.23E+05
ICP.f.Ba	3.31E+01	3.32E+00	2	2.53E+01	4.10E+01
ICP.f.Ca*	4.23E+03	1.14E+07	2	0.00	1.88E+04
ICP.f.Cr	2.35E+03	7.95E+03	2	1.97E+03	2.74E+03
ICP.f.Cu*	5.47E+01	6.08E+01	2	2.12E+01	8.83E+01
ICP.f.Fe	1.72E+03	1.81E+03	2	1.53E+03	1.90E+03
ICP.f.Mg	1.57E+02	5.04E+03	2	0.00	4.62E+02
ICP.f.Mn	1.15E+03	4.73E+04	2	2.15E+02	2.09E+03
ICP.f.Na	1.18E+05	2.77E+06	2	1.11E+05	1.25E+05
ICP.f.Ni	5.01E+03	1.84E+05	2	3.16E+03	6.85E+03
ICP.f.P*	9.31E+01	5.97E+01	2	5.98E+01	1.26E+02
ICP.f.S	4.72E+02	2.00E+02	2	4.11E+02	5.33E+02
ICP.f.Si	1.33E+03	1.52E+04	2	7.97E+02	1.86E+03
ICP.f.Sr	4.24E+02	3.03E+02	2	3.49E+02	1.86E+03

•: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

Table 3-1. Concentration Estimate Statistics (Units $\mu\text{g/g}$
Except Radionuclides $\mu\text{Ci/g}$). (sheet 2 of 2)

Analyte	$\bar{y}$	$\sigma^2(\bar{y})$	df	95% LL	95% UL
ICP.f.Zn*	2.24E+02	2.16E+04	2	0.00	8.56E+02
ICP.f.Zr*	2.12E+01	3.69E+01	2	0.00	4.73E+01
ICP.w.Al	4.68E+03	2.43E+06	2	0.00	1.14E+04
ICP.w.B*	9.08E+00	1.65E+00	2	3.57E+00	1.46E+01
ICP.w.Ca*	1.56E+02	3.35E+03	2	0.00	4.04E+02
ICP.w.Cr	1.90E+03	4.39E+05	2	0.00	4.75E+03
ICP.w.K	2.53E+02	4.62E+03	2	0.00	5.45E+02
ICP.w.Mg*	8.34E+00	1.10E+01	2	0.00	2.26E+01
ICP.w.Na	9.21E+04	7.38E+08	2	0.00	2.09E+05
ICP.w.S	3.40E+02	1.45E+04	2	0.00	8.58E+02
ICP.w.Si*	3.98E+01	2.87E+02	2	0.00	1.13E+02
IC.w.Cl	3.20E+03	8.96E+03	2	2.79E+03	3.61E+03
IC.w.NO2	2.08E+04	2.46E+06	2	1.41E+04	2.76E+04
IC.w.NO3	1.91E+05	3.64E+07	2	1.65E+05	2.17E+05
IC.w.SO4	2.27E+03	3.92E+03	2	2.00E+03	2.54E+03
CN	3.70E+00	4.34E-02	2	2.81E+00	4.60E+00
Percent.H2O	5.16E+01	4.64E+02	2	0.00	1.44E+02
Spec.w.NO2	2.59E+04	1.16E+06	2	2.12E+04	3.05E+04
TIC.w.CO3*	4.14E+03	4.86E+05	2	1.15E+03	7.14E+03
pH	1.29E+01	6.30E-02	2	1.18E+01	1.39E+01
C-14*	9.01E-04	1.42E-08	2	3.88E-04	1.41E-03
GEA.Cs-137	6.23E+01	3.45E+00	2	5.43E+01	7.03E+01
Gross.beta	6.41E+02	7.60E+04	2	0.00	1.83E+03
H-3*	3.38E-03	1.59E-07	2	1.66E-03	5.09E-03
Pu-239/40	2.82E-01	4.67E-03	2	0.00	5.76E-01
Sr-90	3.10E+02	6.23E+01	2	2.76E+02	3.44E+02
Tc-99*	2.42E-02	1.70E-06	2	1.86E-02	2.98E-02
U*	6.69E+03	1.37E+05	2	5.09E+03	8.28E+03

*: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

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4.0 COMPARISON OF THE VARIANCE COMPONENT ESTIMATES

Using the hierarchical structure of the core composite data, estimates of the spatial variability, the sample composite variability, and the analytical measurement variability can be obtained. The spatial variance [$\sigma^2(S)$] is a measure of the variability between cores. The sample composite variance [$\sigma^2(C)$] measures the variability between composite samples within the same core. The analytical measurement variance [$\sigma^2(A)$] includes, among other things, the sample handling variability and the chemical analysis variability. This variance is a measure of the difference between the analytical results from the primary and duplicate samples.

The estimate of the variance of the mean is a linear function of the spatial, sample composite, and analytical measurement variances. To help evaluate the magnitude of these three variance components, estimates of each variance component are given in Table 4-1.

4.1 STATISTICAL METHODS

Estimates of the spatial variance [$\hat{\sigma}^2(S)$], sample composite variance [$\hat{\sigma}^2(C)$], and analytical measurement variance [$\hat{\sigma}^2(A)$] were obtained for each analyte using Restricted Maximum Likelihood Estimation (REML) methods. The REML methods are discussed in Harville (1977).

To test the significance of the variance components, an ANOVA was calculated using the hierarchical statistical model described in Appendix C. The mean square error terms in the ANOVA tables were used to perform F-tests on the spatial variability and F-tests on the composite variability. These tests determine whether or not $\sigma^2(S)$ and $\sigma^2(C)$ are significantly different than zero. The p-values given in Table 4-1 were derived from the results of these tests. The p-value is the attained level of significance of the statistical test.

4.2 STATISTICAL RESULTS

The REML estimates of each component of variability, along with the p-values from the F-tests, are given in Table 4-1. A p-value less than 0.05 indicates that $\sigma^2(S)$ or $\sigma^2(C)$ is significantly different from zero at the 0.05 level of significance.

The p-values from the tests on $\sigma^2(S)$ were less than 0.05 for 22 out of the 63 analytes. For these 22 cases, at least one of the three cores was, statistically, significantly different from the others.

The p-values from the tests on $\sigma^2(C)$ were less than 0.05 for 20 out of the 63 analytes. This implies, that for these 20 analytes, the two composite samples were, statistically, significantly different from each other. Conversely, for 43 out of 63 analytes, differences between composite samples were not, statistically, significantly different from each other.

Table 4-1. Variance Component Estimates. (sheet 1 of 2)

Analyte	$\sigma^2(s)$	Test: $\sigma^2(s)=0$ p-value	$\sigma^2(c)$	Test: $\sigma^2(c)=0$ p-value	$\sigma^2(A)$
ICP.a.Al	6.59E+07	0.311	1.55E+08	0.009	3.30E+07
ICP.a.B*	3.40E+01	0.029	1.96E+00	0.282	6.36E+00
ICP.a.Ba	5.77E-01	0.406	4.69E+00	0.001	4.33E-01
ICP.a.Ca*	1.16E+03	0.231	1.33E+03	0.025	4.78E+02
ICP.a.Ce*	9.03E-17	0.121	9.50E+00	0.029	4.86E+00
ICP.a.Co*	5.40E-02	0.187	3.16E-24	0.482	1.11E-01
ICP.a.Cr	7.18E+03	0.232	7.30E+03	0.069	4.83E+03
ICP.a.Cu	1.26E+02	0.000	7.63E-01	0.018	2.29E-01
ICP.a.Fe	2.48E+03	0.419	2.59E+04	0.002	3.16E+03
ICP.a.K	2.34E+03	0.010	1.27E+02	0.037	5.63E+01
ICP.a.Mg	6.54E+01	0.100	2.41E+01	0.036	1.05E+01
ICP.a.Mn	5.05E+04	0.044	7.54E+03	0.094	6.25E+03
ICP.a.Na	2.60E+06	0.414	2.10E+07	0.043	1.02E+07
ICP.a.Ni	9.20E-25	0.497	3.60E+01	0.002	4.35E+00
ICP.a.P*	2.08E+00	0.357	5.87E+00	0.112	5.64E+00
ICP.a.S	1.09E+03	0.023	4.45E-11	0.503	2.97E+02
ICP.a.Si	7.00E+02	0.189	2.66E+02	0.277	8.28E+02
ICP.a.Sr	9.10E+01	0.412	7.65E+02	0.012	1.93E+02
ICP.a.Ti*	8.23E+00	0.011	5.31E-01	0.010	1.20E-01
ICP.a.Zn*	3.74E+01	0.100	1.08E+01	0.129	1.18E+01
ICP.a.Zr	7.37E-19	0.784	3.87E+00	0.012	1.41E+00
ICP.f.Al	1.30E+06	0.265	1.94E-22	0.676	1.51E+07
ICP.f.Ba	9.02E+00	0.041	1.68E-13	0.489	3.80E+00
ICP.f.Ca*	1.68E+07	0.285	4.97E+06	0.398	5.99E+07
ICP.f.Cr	2.26E+04	0.008	2.68E-20	0.756	5.09E+03
ICP.f.Cu*	5.57E-24	0.668	3.00E+01	0.335	6.70E+02
ICP.f.Fe	1.46E-15	0.518	3.92E+03	0.269	1.39E+04
ICP.f.Mg	7.73E+03	0.275	3.30E+03	0.361	2.29E+04
ICP.f.Mn	1.13E+05	0.113	4.40E+04	0.062	2.71E+04
ICP.f.Na	2.88E+06	0.349	9.33E+06	0.022	3.08E+06
ICP.f.Ni	3.98E-29	0.835	6.71E-23	0.891	2.21E+06
ICP.f.P*	7.12E-11	0.092	5.27E-20	0.964	7.16E+02
ICP.f.S	5.68E-26	0.650	1.60E+02	0.320	2.08E+03
ICP.f.Si	1.31E+04	0.241	1.34E-21	0.701	1.30E+05

•: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

Table 4-1. Variance Component Estimates. (sheet 2 of 2)

Analyte	$\sigma^2(s)$	Test: $\sigma^2(s)=0$ p-value	$\sigma^2(c)$	Test: $\sigma^2(c)=0$ p-value	$\sigma^2(A)$
ICP.f.Sr	3.22E+02	0.345	4.80E+02	0.267	1.38E+03
ICP.f.Zn*	3.52E+04	0.260	7.94E+03	0.401	1.03E+05
ICP.f.Zr*	1.06E+02	0.017	6.85E-01	0.429	1.92E+01
ICP.w.Al	7.25E+06	0.000	9.14E-25	0.901	9.38E+04
ICP.w.B*	4.70E+00	0.017	2.38E-02	0.435	8.90E-01
ICP.w.Ca*	1.08E+03	0.433	1.28E+03	0.427	3.33E+04
ICP.w.Cr	1.31E+06	0.000	1.12E-19	0.872	1.52E+04
ICP.w.K	1.38E+04	0.001	4.96E+01	0.329	2.42E+02
ICP.w.Mg*	2.26E-20	0.569	6.16E-17	0.508	1.33E+02
ICP.w.Na	2.21E+09	0.000	1.31E-27	0.954	2.92E+07
ICP.w.S	4.35E+04	0.000	1.15E-17	0.609	4.53E+02
ICP.w.Si*	6.47E+02	0.115	5.08E-23	0.554	8.52E+02
IC.w.Cl	2.42E+04	0.001	1.62E-42	0.991	1.06E+04
IC.w.NO2	6.92E+06	0.026	2.23E+05	0.356	1.45E+06
IC.w.NO3	4.50E-05	0.487	1.58E+08	0.080	1.21E+08
IC.w.SO4	7.15E+03	0.028	2.29E-24	0.944	1.85E+04
CN	1.85E-20	0.718	2.41E-01	0.002	3.92E-02
Percent.H2O	1.38E+03	0.001	1.78E+01	0.002	1.90E+00
Spec.w.NO2	3.47E-18	0.753	5.28E+06	0.034	3.38E+06
TIC.w.CO3*	5.22E-29	0.700	2.73E+06	0.001	3.63E+05
pH	1.42E-32	0.717	1.72E-21	0.415	7.56E-01
C-14*	5.67E-09	0.425	3.38E-08	0.241	8.08E-08
GEA.f.Cs-137	9.34E+00	0.040	2.01E-18	0.507	3.99E+00
Gross.beta	2.27E+05	0.001	1.98E+03	0.118	2.00E+03
H-3*	3.42E-35	0.813	4.59E-07	0.131	9.89E-07
Pu-239/40	1.34E-02	0.015	9.59E-04	0.043	4.64E-04
Sr-90	5.32E-19	0.929	1.03E+02	0.190	5.41E+02
Tc-99*	2.23E-06	0.310	4.99E-06	0.018	1.49E-06
U*	3.44E+05	0.087	4.45E+04	0.308	1.79E+05

*: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

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5.0 REFERENCES

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- Kocher, K. L., 1993, *Single Shell Tank Waste Characterization, 241-S-104, Cores 42, 43, and 44*, WHC-SD-WM-DP-031, Rev. 0, Westinghouse Hanford Company, Richland, Washington.
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APPENDIX A
CORE COMPOSITE DATA

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Table A-1. Core Composite Data from Two Composite Samples
(Units $\mu\text{g/g}$ Except Radionuclides $\mu\text{Ci/g}$). (sheet 1 of 10)

Analyte	Core 42	Mean/DL	Core 43	Mean/DL	Core 44	Mean/DL
ICP.a.Ag	<9.58E-01 <9.67E-01	NA	<9.65E-01 <9.53E-01	NA	<9.84E-01 <9.62E-01	NA
	<9.90E-01 <9.57E-01	NA	<9.80E-01 <9.86E-01	NA	<9.68E-01 <9.52E-01	NA
ICP.a.Al	4.23E+04 3.00E+04	1.03E+04	2.14E+04 2.22E+04	6.41E+03	6.31E+04 6.15E+04	1.83E+04
	4.29E+04 5.82E+04	1.44E+04	2.94E+04 2.68E+04	8.26E+03	3.49E+04 3.38E+04	1.01E+04
ICP.a.B*	1.05E+01 1.35E+01	1.20E+01	9.13E+00 9.48E+00	4.90E+00	2.16E+01 1.75E+01	1.03E+01
	8.82E+00 1.05E+01	9.66E+00	1.55E+01 9.95E+00	6.70E+00	2.12E+01 2.53E+01	1.22E+01
ICP.a.Ba	2.08E+01 2.00E+01	6.80E+01	2.05E+01 1.92E+01	6.62E+01	2.59E+01 2.58E+01	8.62E+01
	2.21E+01 2.29E+01	7.50E+01	2.04E+01 1.94E+01	6.63E+01	2.14E+01 2.03E+01	6.95E+01
ICP.a.Be	<2.87E-01 <2.90E-01	NA	<2.90E-01 <2.86E-01	NA	<2.95E-01 <2.88E-01	NA
	<2.97E-01 <2.87E-01	NA	<2.94E-01 <2.96E-01	NA	<2.90E-01 <2.85E-01	NA
ICP.a.Bi	<5.56E+00 <5.61E+00	NA	<8.20E+00 <8.10E+00	NA	<8.37E+00 <8.17E+00	NA
	5.74E+00 5.55E+00	9.73E-01	<8.33E+00 <8.38E+00	NA	<8.23E+00 <8.09E+00	NA
ICP.a.Ca*	1.96E+02 1.78E+02	6.88E+00	3.27E+02 3.30E+02	1.37E+02	2.77E+02 2.65E+02	1.13E+02
	2.13E+02 2.02E+02	7.63E+00	2.69E+02 2.03E+02	9.83E+01	2.64E+02 2.36E+02	1.04E+02
ICP.a.Cd	<6.70E-01 <6.77E-01	NA	<6.76E-01 <6.67E-01	NA	7.54E-01 9.17E-01	1.19E+00
	7.35E-01 <6.70E-01	NA	<6.86E-01 <6.90E-01	NA	6.87E-01 9.37E-01	1.16E+00
ICP.a.Ce*	2.04E+01 1.84E+01	1.98E+00	2.93E+01 2.58E+01	3.20E+00	2.03E+01 2.53E+01	2.65E+00
	2.51E+01 2.30E+01	2.45E+00	2.18E+01 1.99E+01	2.42E+00	1.65E+01 1.95E+01	2.09E+00
ICP.a.Co*	2.62E+00 2.49E+00	2.56E+00	3.03E+00 2.30E+00	2.22E+00	1.80E+00 2.10E+00	1.63E+00
	3.15E+00 2.53E+00	2.84E+00	2.81E+00 2.57E+00	2.24E+00	2.17E+00 2.70E+00	2.03E+00
ICP.a.Cr	2.55E+03 2.49E+03	2.10E+03	2.29E+03 2.19E+03	1.60E+03	2.17E+03 2.20E+03	1.56E+03
	2.50E+03 2.37E+03	2.03E+03	2.28E+03 2.39E+03	1.67E+03	2.45E+03 2.33E+03	1.71E+03

•: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

NA: Not available.

Table A-1. Core Composite Data from Two Composite Samples
(Units $\mu\text{g/g}$ Except Radionuclides $\mu\text{Ci/g}$). (sheet 2 of 10)

Analyte	Core 42	Mean/DL	Core 43	Mean/DL	Core 44	Mean/DL
ICP.a.Cu	3.15E+01	7.85E+01	1.35E+01	2.16E+01	1.35E+01	2.28E+01
	3.13E+01		1.24E+01		1.39E+01	
	3.39E+01	8.35E+01	1.25E+01	2.06E+01	1.30E+01	2.13E+01
	3.29E+01		1.22E+01		1.25E+01	
ICP.a.Fe	7.55E+02	4.57E+02	6.17E+02	3.14E+02	1.03E+03	5.28E+02
	6.17E+02		6.39E+02		1.08E+03	
	8.50E+02	6.03E+02	6.56E+02	3.19E+02	7.40E+02	3.57E+02
	9.58E+02		6.20E+02		6.86E+02	
ICP.a.K	3.57E+02	2.78E+01	2.79E+02	2.02E+01	2.53E+02	1.94E+01
	3.61E+02		2.57E+02		2.64E+02	
	3.55E+02	2.74E+01	2.67E+02	2.03E+01	2.89E+02	2.17E+01
	3.53E+02		2.74E+02		2.88E+02	
ICP.a.La	<1.53E+00	NA	<2.03E+00	NA	<2.07E+00	NA
	<1.55E+00		<2.00E+00		<2.02E+00	
	<1.58E+00	NA	<2.06E+00	NA	<2.03E+00	NA
	<1.53E+00		<2.07E+00		<2.00E+00	
ICP.a.Mg	3.37E+01	4.83E+01	3.84E+01	6.13E+01	5.87E+01	9.75E+01
	3.39E+01		3.51E+01		5.83E+01	
	3.63E+01	5.41E+01	4.52E+01	7.08E+01	5.16E+01	7.88E+01
	3.94E+01		3.98E+01		4.29E+01	
ICP.a.Mn	6.81E+02	2.64E+03	8.35E+02	2.58E+03	1.34E+03	4.42E+03
	9.05E+02		7.10E+02		1.31E+03	
	8.13E+02	2.62E+03	8.38E+02	2.70E+03	1.10E+03	3.58E+03
	7.60E+02		7.83E+02		1.05E+03	
ICP.a.Na	1.32E+05	4.68E+04	1.18E+05	1.34E+04	1.14E+05	1.36E+04
	1.30E+05		1.16E+05		1.22E+05	
	1.17E+05	4.25E+04	1.15E+05	1.35E+04	1.20E+05	1.40E+04
	1.21E+05		1.20E+05		1.23E+05	
ICP.a.Ni	5.20E+01	3.65E+01	5.20E+01	2.78E+01	6.56E+01	3.73E+01
	5.03E+01		4.79E+01		6.87E+01	
	5.73E+01	4.14E+01	5.53E+01	3.09E+01	5.67E+01	3.02E+01
	5.85E+01		5.58E+01		5.21E+01	
ICP.a.P*	2.52E+01	2.54E+00	1.82E+01	2.54E+00	2.16E+01	2.65E+00
	2.50E+01		2.24E+01		2.08E+01	
	1.92E+01	2.02E+00	1.31E+01	2.03E+00	2.28E+01	3.03E+00
	2.08E+01		1.93E+01		2.57E+01	
ICP.a.Pb	3.73E+01	5.70E+00	3.66E+01	5.22E+00	<8.37E+00	NA
	4.36E+01		5.21E+01		<8.17E+00	
	4.26E+01	4.15E+00	1.19E+01	1.62E+00	2.14E+01	2.32E+00
	1.63E+01		1.56E+01		1.81E+01	
ICP.a.S	4.18E+02	9.59E+01	4.35E+02	6.87E+01	3.50E+02	5.81E+01
	4.45E+02		3.89E+02		3.47E+02	
	4.15E+02	9.10E+01	4.14E+02	6.68E+01	3.67E+02	6.05E+01
	4.04E+02		3.88E+02		3.59E+02	

*: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

NA: Not available.

Table A-1. Core Composite Data from Two Composite Samples
(Units $\mu\text{g/g}$ Except Radionuclides $\mu\text{Ci/g}$). (sheet 3 of 10)

Analyte	Core 42	Mean/DL	Core 43	Mean/DL	Core 44	Mean/DL
ICP.a.Sb	<3.51E+01 <3.54E+01	NA	<3.44E+01 3.40E+01	NA	3.58E+01 3.81E+01	1.04E+00
	<3.62E+01 <3.50E+01	NA	<3.49E+01 <3.51E+01	NA	<3.45E+01 4.05E+01	NA
ICP.a.Si	1.60E+02 1.75E+02	3.90E+01	1.67E+02 1.89E+02	7.74E+01	3.01E+02 2.09E+02	1.11E+02
	1.65E+02 1.45E+02	3.60E+01	2.02E+02 1.96E+02	8.65E+01	2.05E+02 1.87E+02	8.52E+01
ICP.a.Sn	<2.20E+00 <2.22E+00	NA	<1.54E+00 <1.53E+00	NA	<1.57E+00 <1.54E+00	NA
	<2.28E+00 <2.20E+00	NA	<1.57E+00 1.84E+00	NA	1.77E+00 <1.52E+00	NA
ICP.a.Sr	3.38E+02 2.96E+02	7.93E+02	3.27E+02 3.28E+02	5.46E+02	3.21E+02 3.29E+02	5.42E+02
	3.68E+02 3.58E+02	9.08E+02	3.45E+02 3.50E+02	5.79E+02	2.83E+02 2.64E+02	4.56E+02
ICP.a.Ti*	4.84E+00 5.16E+00	1.25E+01	4.04E+00 3.56E+00	7.60E+00	9.02E+00 8.63E+00	1.77E+01
	6.42E+00 5.79E+00	1.53E+01	4.09E+00 3.93E+00	8.02E+00	1.07E+01 9.97E+00	2.07E+01
ICP.a.Zn*	2.62E+01 3.26E+01	1.18E+01	2.65E+01 2.36E+01	1.00E+01	1.35E+01 1.17E+01	5.04E+00
	2.15E+01 1.86E+01	8.02E+00	2.60E+01 1.70E+01	8.60E+00	1.20E+01 1.22E+01	4.84E+00
ICP.a.Zr	3.23E+01 3.09E+01	3.95E+01	3.48E+01 3.36E+01	3.11E+01	3.45E+01 3.55E+01	3.18E+01
	3.70E+01 3.45E+01	4.47E+01	3.43E+01 3.55E+01	3.17E+01	3.15E+01 2.93E+01	2.76E+01
ICP.f.Ag	<5.00E+00 <5.00E+00	NA	<4.47E+00 <4.45E+00	NA	<4.93E+00 <5.00E+00	NA
	<4.93E+00 <4.96E+00	NA	<4.41E+00 <4.39E+00	NA	<4.95E+00 <4.96E+00	NA
ICP.f.Al	1.16E+05 1.11E+05	6.49E+03	1.19E+05 1.22E+05	4.73E+03	1.15E+05 1.23E+05	7.00E+03
	1.19E+05 1.13E+05	6.63E+03	1.22E+05 1.14E+05	4.63E+03	1.17E+05 1.13E+05	6.76E+03
ICP.f.B	<5.00E+00 <5.00E+00	NA	4.05E+01 2.99E+01	7.04E+00	<9.37E+00 1.06E+01	NA
	<4.93E+00 <4.96E+00	NA	1.65E+02 2.00E+01	1.85E+01	1.02E+01 1.41E+01	1.28E+00
ICP.f.Ba	2.93E+01 2.69E+01	1.87E+01	3.34E+01 3.43E+01	1.69E+01	3.36E+01 3.88E+01	2.41E+01
	3.15E+01 3.06E+01	2.07E+01	3.51E+01 3.41E+01	1.73E+01	3.67E+01 3.33E+01	2.33E+01

•: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

NA: Not available.

Table A-1. Core Composite Data from Two Composite Samples
(Units $\mu\text{g/g}$ Except Radionuclides $\mu\text{Ci/g}$). (sheet 4 of 10)

Analyte	Core 42	Mean/DL	Core 43	Mean/DL	Core 44	Mean/DL
ICP.f.Be	<1.50E+00 <1.50E+00	NA	<1.49E+00 <1.48E+00	NA	<1.48E+00 <1.50E+00	NA
	<1.48E+00 <1.49E+00	NA	<1.47E+00 <1.46E+00	NA	<1.49E+00 <1.49E+00	NA
ICP.f.Bi	<2.90E+01 <2.90E+01	NA	<4.57E+01 <4.55E+01	NA	<4.19E+01 <4.25E+01	NA
	<2.86E+01 <2.88E+01	NA	<4.51E+01 <4.49E+01	NA	<4.21E+01 <4.22E+01	NA
ICP.f.Ca*	9.72E+02 4.23E+02	5.13E+00	8.33E+02 6.96E+02	3.06E+02	4.05E+03 3.45E+03	3.13E+02
	5.55E+02 5.30E+02	3.99E+00	1.91E+03 8.88E+02	5.60E+02	3.16E+04 4.82E+03	1.52E+03
ICP.f.Cd	<3.50E+00 <3.50E+00	NA	3.93E+00 3.57E+00	1.07E+00	<3.45E+00 <3.50E+00	NA
	<3.45E+00 <3.47E+00	NA	<3.43E+00 3.58E+00	NA	<3.47E+00 <3.47E+00	NA
ICP.f.Ce	<4.90E+01 <4.90E+01	NA	<6.36E+01 <6.32E+01	NA	<4.24E+01 <4.30E+01	NA
	<4.83E+01 <4.86E+01	NA	<6.27E+01 <6.25E+01	NA	<4.26E+01 <4.27E+01	NA
ICP.f.Co	<5.00E+00 <5.00E+00	NA	<9.44E+00 <9.39E+00	NA	<5.92E+00 <6.00E+00	NA
	<4.93E+00 <4.96E+00	NA	<9.31E+00 <9.28E+00	NA	<5.94E+00 7.34E+00	NA
ICP.f.Cr	2.53E+03 2.47E+03	4.17E+02	2.30E+03 2.40E+03	3.13E+02	2.10E+03 2.27E+03	3.12E+02
	2.62E+03 2.46E+03	4.23E+02	2.30E+03 2.30E+03	3.07E+02	2.20E+03 2.29E+03	3.21E+02
ICP.f.Cu*	5.67E+01 6.19E+01	2.97E+01	8.54E+01 3.77E+01	2.05E+01	6.31E+01 8.04E+01	2.39E+01
	3.70E+01 1.10E+02	3.68E+01	3.28E+01 3.03E+01	1.05E+01	3.57E+01 2.57E+01	1.02E+01
ICP.f.Fe	1.56E+03 1.45E+03	2.01E+02	1.74E+03 1.81E+03	2.22E+02	1.66E+03 1.85E+03	1.76E+02
	1.90E+03 1.63E+03	2.35E+02	1.76E+03 1.69E+03	2.16E+02	1.67E+03 1.86E+03	1.77E+02
ICP.f.La	<8.00E+00 <8.00E+00	NA	<9.94E+00 <9.88E+00	NA	<1.04E+01 <1.05E+01	NA
	<7.89E+00 <7.94E+00	NA	<9.80E+00 <9.77E+00	NA	<1.04E+01 <1.04E+01	NA
ICP.f.Mg	8.05E+01 6.94E+01	2.14E+01	9.25E+01 9.14E+01	6.13E+01	1.50E+02 1.49E+02	4.98E+01
	7.93E+01 7.61E+01	2.22E+01	1.09E+02 8.99E+01	6.63E+01	7.09E+02 1.85E+02	1.49E+02

•: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

NA: Not available.

Table A-1. Core Composite Data from Two Composite Samples
(Units $\mu\text{g/g}$ Except Radionuclides $\mu\text{Ci/g}$). (sheet 5 of 10)

Analyte	Core 42	Mean/DL	Core 43	Mean/DL	Core 44	Mean/DL
ICP.f.Mn	8.15E+02 1.09E+03	6.35E+02	1.07E+03 9.90E+02	6.87E+02	1.52E+03 1.96E+03	1.16E+03
	1.22E+03 1.13E+03	7.83E+02	6.53E+02 5.83E+02	4.12E+02	1.29E+03 1.48E+03	9.23E+02
ICP.f.Na	1.24E+05 1.25E+05	8.89E+03	1.19E+05 1.20E+05	5.98E+03	1.14E+05 1.13E+05	2.61E+03
	1.16E+05 1.19E+05	8.39E+03	1.16E+05 1.19E+05	5.88E+03	1.15E+05 1.19E+05	2.69E+03
ICP.f.Ni	4.26E+03 5.35E+03	6.86E+02	5.91E+03 5.19E+03	7.40E+02	5.75E+03 2.88E+03	4.79E+02
	5.16E+03 4.58E+03	6.96E+02	5.42E+03 4.31E+03	6.49E+02	2.80E+03 8.46E+03	6.26E+02
ICP.f.P*	1.47E+02 7.36E+01	2.23E+00	1.02E+02 5.65E+01	2.26E+00	6.14E+01 1.09E+02	2.13E+00
	1.19E+02 8.72E+01	2.08E+00	7.41E+01 1.15E+02	2.70E+00	7.45E+01 9.76E+01	2.15E+00
ICP.f.Pb	<3.55E+01 <3.55E+01	NA	<3.88E+01 <3.85E+01	NA	<4.19E+01 <4.25E+01	NA
	<3.50E+01 <3.52E+01	NA	<3.82E+01 <3.81E+01	NA	<4.21E+01 <4.22E+01	NA
ICP.f.S	4.64E+02 4.67E+02	2.07E+01	4.63E+02 4.82E+02	2.42E+01	4.39E+02 4.59E+02	1.50E+01
	4.73E+02 4.62E+02	2.08E+01	4.49E+02 4.30E+02	2.25E+01	6.15E+02 4.61E+02	1.79E+01
ICP.f.Sb	<1.83E+02 <1.83E+02	NA	<7.55E+01 <7.51E+01	NA	<1.76E+02 <1.78E+02	NA
	<1.80E+02 <1.82E+02	NA	<7.45E+01 <7.42E+01	NA	<1.76E+02 <1.77E+02	NA
ICP.f.Si	1.03E+03 1.04E+03	4.81E+01	1.23E+03 1.13E+03	6.94E+01	1.44E+03 1.40E+03	1.23E+02
	1.18E+03 1.09E+03	5.28E+01	2.31E+03 9.47E+02	9.58E+01	1.57E+03 1.55E+03	1.36E+02
ICP.f.Sn	<1.15E+01 <1.15E+01	NA	<8.95E+00 <8.89E+00	NA	<7.89E+00 <8.00E+00	NA
	<1.13E+01 <1.14E+01	NA	<8.82E+00 <8.79E+00	NA	<7.92E+00 <7.94E+00	NA
ICP.f.Sr	4.16E+02 4.01E+02	2.04E+02	4.15E+02 4.40E+02	2.85E+02	3.71E+02 4.88E+02	1.43E+02
	4.34E+02 3.99E+02	2.08E+02	5.03E+02 4.74E+02	3.26E+02	3.72E+02 3.73E+02	1.24E+02
ICP.f.Ti	3.50E+00 <2.00E+00	NA	1.15E+01 8.68E+00	2.88E+00	1.01E+01 7.18E+00	3.46E+00
	4.45E+00 3.46E+00	1.98E+00	6.98E+00 6.60E+00	1.94E+00	1.17E+01 1.39E+01	5.12E+00

•: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

NA: Not available.

Table A-1. Core Composite Data from Two Composite Samples
(Units $\mu\text{g/g}$ Except Radionuclides $\mu\text{Ci/g}$). (sheet 6 of 10)

Analyte	Core 42	Mean/DL	Core 43	Mean/DL	Core 44	Mean/DL
ICP.f.Zn*	7.79E+01 6.93E+01	5.89E+00	9.69E+01 4.52E+01	2.84E+01	2.34E+02 2.06E+02	1.76E+01
	5.54E+01 9.54E+01	6.03E+00	1.17E+02 5.99E+01	3.54E+01	1.37E+03 2.63E+02	6.53E+01
ICP.f.Zr*	1.31E+01 8.63E+00	2.72E+00	2.60E+01 2.83E+01	4.53E+00	2.29E+01 2.03E+01	3.93E+00
	4.85E+00 1.25E+01	2.17E+00	2.97E+01 3.79E+01	5.63E+00	2.09E+01 2.94E+01	4.57E+00
ICP.w.Ag	1.43E+00 2.03E+00	1.73E+00	1.42E+00 <1.00E+00	NA	<1.02E+00 <1.02E+00	NA
	<1.02E+00 <1.02E+00	NA	<1.01E+00 <1.01E+00	NA	<1.02E+00 <1.02E+00	NA
ICP.w.Al	6.67E+03 6.31E+03	1.85E+03	6.08E+03 6.07E+03	1.79E+03	1.19E+03 1.89E+03	4.53E+02
	6.54E+03 5.93E+03	1.78E+03	5.98E+03 6.30E+03	1.81E+03	1.93E+03 1.26E+03	4.69E+02
ICP.w.B*	1.09E+01 1.08E+01	1.09E+01	1.00E+01 1.10E+01	5.53E+00	5.62E+00 7.92E+00	3.56E+00
	9.20E+00 9.33E+00	9.27E+00	1.09E+01 1.07E+01	5.68E+00	7.35E+00 5.27E+00	3.32E+00
ICP.w.Ba	<3.05E-01 1.61E+00	NA	3.14E-01 <3.00E-01	NA	<3.05E-01 <3.06E-01	NA
	<3.05E-01 <3.06E-01	NA	<3.04E-01 3.19E-01	NA	3.29E-01 <3.06E-01	NA
ICP.w.Be	<3.05E-01 <3.03E-01	NA	<3.00E-01 <3.00E-01	NA	<3.05E-01 <3.06E-01	NA
	<3.05E-01 <3.06E-01	NA	<3.04E-01 <3.03E-01	NA	<3.05E-01 <3.06E-01	NA
ICP.w.Bi	<5.89E+00 <5.86E+00	NA	<8.50E+00 <8.50E+00	NA	<8.65E+00 <8.67E+00	NA
	<5.89E+00 <5.92E+00	NA	<8.60E+00 <8.58E+00	NA	<8.65E+00 <8.66E+00	NA
ICP.w.Ca*	1.21E+02 7.47E+02	1.60E+01	1.02E+02 1.28E+02	4.79E+01	1.15E+02 9.23E+01	4.32E+01
	6.72E+01 1.48E+02	3.96E+00	1.08E+02 9.09E+01	4.14E+01	7.89E+01 6.78E+01	3.06E+01
ICP.w.Cd	<7.11E-01 9.00E-01	NA	<7.00E-01 <7.00E-01	NA	<7.13E-01 <7.14E-01	NA
	<7.11E-01 <7.14E-01	NA	<7.08E-01 <7.07E-01	NA	<7.13E-01 <7.13E-01	NA
ICP.w.Ce	<9.96E+00 <9.90E+00	NA	<8.60E+00 <8.60E+00	NA	<8.75E+00 <8.77E+00	NA
	<9.96E+00 <1.00E+01	NA	<8.70E+00 <8.69E+00	NA	<8.75E+00 <8.76E+00	NA

•: Analytes with a portion of the data below three times the DL.
 *: Analytes with a portion of the data below ten times the DL.
 NA: Not available.

Table A-1. Core Composite Data from Two Composite Samples
(Units $\mu\text{g/g}$ Except Radionuclides $\mu\text{Ci/g}$). (sheet 7 of 10)

Analyte	Core 42	Mean/DL	Core 43	Mean/DL	Core 44	Mean/DL
ICP.W.Co	<1.02E+00 <1.01E+00	NA	<1.20E+00 <1.20E+00	NA	1.36E+00 <1.22E+00	NA
	<1.02E+00 <1.02E+00	NA	<1.21E+00 <1.21E+00	NA	<1.22E+00 <1.22E+00	NA
ICP.W.Cr	2.70E+03 2.55E+03	2.19E+03	2.44E+03 2.53E+03	1.78E+03	4.39E+02 7.24E+02	4.15E+02
	2.68E+03 2.42E+03	2.13E+03	2.54E+03 2.61E+03	1.84E+03	6.85E+02 4.38E+02	4.01E+02
ICP.W.Cu	8.32E-01 8.88E+00	1.21E+01	6.91E-01 <6.00E-01	NA	<6.11E-01 <6.12E-01	NA
	1.35E+00 1.32E+00	3.34E+00	6.21E-01 <6.06E-01	NA	9.45E-01 <6.11E-01	NA
ICP.W.Fe	4.18E+00 1.06E+02	3.67E+01	3.76E+00 <2.00E+00	NA	<2.04E+00 <2.04E+00	NA
	3.26E+00 1.35E+01	5.59E+00	4.59E+00 3.24E+00	1.96E+00	<2.04E+00 <2.04E+00	NA
ICP.W.K	3.36E+02 3.51E+02	2.66E+01	3.26E+02 3.11E+02	2.39E+01	1.08E+02 1.19E+02	8.53E+00
	3.21E+02 3.13E+02	2.46E+01	2.87E+02 3.17E+02	2.27E+01	1.39E+02 1.02E+02	9.06E+00
ICP.W.La	<1.63E+00 <1.62E+00	NA	<2.10E+00 <2.10E+00	NA	<2.14E+00 <2.14E+00	NA
	<1.63E+00 <1.63E+00	NA	<2.12E+00 <2.12E+00	NA	<2.14E+00 <2.14E+00	NA
ICP.W.Mg*	2.44E+00 4.45E+01	3.35E+01	6.39E+00 7.99E+00	1.20E+01	4.93E+00 5.09E+00	8.35E+00
	1.89E+00 5.76E+00	5.46E+00	6.15E+00 6.10E+00	1.02E+01	5.11E+00 3.74E+00	7.38E+00
ICP.W.Mn	<3.05E-01 2.58E+00	NA	<3.00E-01 <3.00E-01	NA	<3.05E-01 <3.06E-01	NA
	<3.05E-01 5.10E-01	NA	<3.04E-01 <3.03E-01	NA	<3.05E-01 <3.06E-01	NA
ICP.W.Na	1.16E+05 1.20E+05	4.21E+04	1.18E+05 1.20E+05	1.37E+04	2.80E+04 4.55E+04	4.22E+03
	1.18E+05 1.24E+05	4.32E+04	1.21E+05 1.17E+05	1.37E+04	4.43E+04 3.33E+04	4.46E+03
ICP.W.Ni	<1.42E+00 1.78E+00	NA	<1.80E+00 <1.80E+00	NA	<1.83E+00 <1.84E+00	NA
	<1.42E+00 1.61E+00	NA	<1.82E+00 <1.82E+00	NA	<1.83E+00 <1.83E+00	NA
ICP.W.P	<1.01E+01 1.60E+01	NA	8.44E+00 <8.00E+00	NA	<8.14E+00 <8.16E+00	NA
	<1.01E+01 <1.01E+01	NA	9.67E+00 <8.08E+00	NA	<8.14E+00 <8.15E+00	NA

*: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

NA: Not available.

Table A-1. Core Composite Data from Two Composite Samples
(Units $\mu\text{g/g}$ Except Radionuclides $\mu\text{Ci/g}$). (sheet 8 of 10)

Analyte	Core 42	Mean/DL	Core 43	Mean/DL	Core 44	Mean/DL
ICP.w.Pb	<7.21E+00 <7.17E+00	NA	<8.50E+00 <8.50E+00	NA	<8.65E+00 <8.67E+00	NA
	<7.21E+00 <7.24E+00	NA	<8.60E+00 <8.58E+00	NA	<8.65E+00 <8.66E+00	NA
ICP.w.S	4.78E+02 4.70E+02	1.05E+02	4.45E+02 4.55E+02	7.50E+01	7.49E+01 1.23E+02	1.65E+01
	4.67E+02 4.31E+02	9.98E+01	4.59E+02 4.80E+02	7.83E+01	1.21E+02 7.71E+01	1.65E+01
ICP.w.Sb	<3.72E+01 <3.70E+01	NA	<3.56E+01 <3.56E+01	NA	<3.62E+01 <3.63E+01	NA
	<3.72E+01 <3.73E+01	NA	<3.60E+01 <3.60E+01	NA	<3.62E+01 <3.63E+01	NA
ICP.w.Si*	4.46E+01 1.46E+02	2.22E+01	4.66E+01 2.16E+01	1.48E+01	1.52E+01 1.81E+01	7.24E+00
	5.58E+01 4.34E+01	1.15E+01	2.77E+01 2.96E+01	1.25E+01	1.67E+01 1.27E+01	6.39E+00
ICP.w.Sn	2.51E+00 <2.32E+00	NA	3.98E+00 2.27E+00	1.95E+00	<1.63E+00 <1.63E+00	NA
	<2.34E+00 <2.35E+00	NA	2.52E+00 3.17E+00	1.78E+00	<1.63E+00 <1.63E+00	NA
ICP.w.Sr	<4.06E-01 1.08E+00	NA	7.77E-01 9.27E-01	1.42E+00	6.88E-01 <6.12E-01	NA
	<4.06E-01 <4.08E-01	NA	6.95E-01 8.33E-01	1.27E+00	8.24E-01 <6.11E-01	NA
ICP.w.Ti	<4.06E-01 3.48E+00	NA	7.84E-01 <5.00E-01	NA	<5.09E-01 <5.10E-01	NA
	<4.06E-01 <4.08E-01	NA	<5.06E-01 <5.05E-01	NA	<5.09E-01 <5.09E-01	NA
ICP.w.Zn	1.95E+01 4.46E+01	1.28E+01	1.39E+01 1.39E+01	5.56E+00	<2.54E+00 <2.55E+00	NA
	1.94E+01 1.82E+01	7.52E+00	1.19E+01 1.19E+01	4.76E+00	7.12E+00 <2.55E+00	NA
ICP.w.Zr	<8.13E-01 <8.08E-01	NA	<1.10E+00 <1.10E+00	NA	<1.12E+00 <1.12E+00	NA
	<8.13E-01 <8.16E-01	NA	<1.11E+00 <1.11E+00	NA	1.20E+00 <1.12E+00	NA
IC.w.Cl	3.22E+03 3.08E+03	3.15E+02	3.14E+03 3.00E+03	3.07E+02	3.34E+03 3.42E+03	3.38E+02
	3.13E+03 3.10E+03	3.12E+02	2.95E+03 3.22E+03	3.09E+02	3.26E+03 3.52E+03	3.39E+02
IC.w.F	<1.10E+02 <1.09E+02	NA	<1.08E+02 <1.08E+02	NA	<2.16E+02 <2.19E+02	NA
	<1.10E+02 <1.10E+02	NA	<1.09E+02 <1.09E+02	NA	<2.19E+02 <2.18E+02	NA

*: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

NA: Not available.

Table A-1. Core Composite Data from Two Composite Samples
(Units $\mu\text{g/g}$ Except Radionuclides $\mu\text{Ci/g}$). (sheet 9 of 10)

Analyte	Core 42	Mean/DL	Core 43	Mean/DL	Core 44	Mean/DL
IC.W.NO2	2.21E+04	2.14E+02	1.92E+04	1.79E+02	2.28E+04	2.28E+02
	2.06E+04		1.66E+04		2.27E+04	
	1.98E+04	1.99E+02	1.77E+04	1.85E+02	2.33E+04	2.45E+02
	1.99E+04		1.93E+04		2.57E+04	
IC.W.NO3	1.70E+05	1.84E+03	1.95E+05	1.92E+03	2.09E+05	2.08E+03
	1.97E+05		1.89E+05		2.07E+05	
	1.97E+05	2.04E+03	1.57E+05	1.67E+03	1.86E+05	1.91E+03
	2.11E+05		1.77E+05		1.95E+05	
IC.W.PO4	<1.10E+03	NA	<1.08E+03	NA	<2.16E+03	NA
	<1.09E+03		<1.08E+03		<2.19E+03	
	<1.10E+03	NA	<1.09E+03	NA	<2.19E+03	NA
	<1.10E+03		<1.09E+03		<2.18E+03	
IC.W.SO4	2.52E+03	2.39E+01	2.41E+03	2.21E+01	2.20E+03	2.19E+01
	2.25E+03		2.01E+03		2.17E+03	
	2.52E+03	2.40E+01	2.37E+03	2.31E+01	2.17E+03	2.17E+01
	2.27E+03		2.24E+03		2.16E+03	
CN	3.96E+00	4.04E+01	4.15E+00	4.00E+01	4.30E+00	4.12E+01
	4.12E+00		3.84E+00		3.94E+00	
	2.98E+00	2.85E+01	4.08E+00	3.91E+01	3.21E+00	3.31E+01
	2.72E+00		3.74E+00		3.40E+00	
Percent.H2O	2.39E+01	NA	2.94E+01	NA	9.52E+01	NA
	2.55E+01		2.86E+01		9.49E+01	
	3.60E+01	NA	2.97E+01	NA	9.38E+01	NA
	3.39E+01		3.35E+01		9.47E+01	
Spec.w.NO2	2.84E+04	5.31E+02	2.98E+04	5.53E+02	2.65E+04	5.22E+02
	2.58E+04		2.66E+04		2.67E+04	
	2.61E+04	4.99E+02	2.04E+04	4.08E+02	2.48E+04	5.31E+02
	2.48E+04		2.12E+04		2.94E+04	
TIC.W.CO3•	2.49E+03	5.51E+00	3.33E+03	6.51E+00	3.54E+03	2.97E+00
	3.02E+03		3.18E+03		2.39E+03	
	4.98E+03	9.13E+00	3.28E+03	7.93E+00	7.55E+03	7.35E+00
	4.15E+03		4.65E+03		7.14E+03	
Total organic carbon (TOC)	2.19E+03	4.15E+00	2.35E+03	4.01E+00	<1.10E+03	NA
	2.38E+03		2.06E+03		<1.10E+03	
	1.30E+03	2.36E+00	1.19E+03	2.07E+00	<1.10E+03	NA
	1.30E+03		1.09E+03		<1.10E+03	
pH	1.02E+01	NA	1.29E+01	NA	1.31E+01	NA
	1.33E+01		1.26E+01		1.32E+01	
	1.33E+01	NA	1.31E+01	NA	1.31E+01	NA
	1.34E+01		1.31E+01		1.31E+01	
C-14•	1.00E-03	1.19E+01	5.08E-04	1.25E+01	1.02E-03	2.44E+01
	6.94E-05		6.15E-04		1.18E-03	
	9.07E-04	2.25E+00	1.08E-03	2.26E+01	1.14E-03	2.62E+01
	1.12E-03		9.58E-04		1.22E-03	

•: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

NA: Not available.

Table A-1. Core Composite Data from Two Composite Samples
(Units $\mu\text{g/g}$ Except Radionuclides $\mu\text{Ci/g}$). (sheet 10 of 10)

Analyte	Core 42	Mean/DL	Core 43	Mean/DL	Core 44	Mean/DL
GEA.Cs-137	6.75E+01	9.45E+02	6.02E+01	1.58E+03	6.31E+01	4.44E+03
	6.20E+01		6.03E+01		6.40E+01	
	6.61E+01	9.39E+02	5.83E+01	1.50E+03	6.39E+01	4.47E+03
	6.26E+01		5.57E+01		6.40E+01	
Gross.alpha	7.01E-01	NA	8.07E-01	3.97E+00	4.32E-01	4.61E+00
	<3.52E-01		7.79E-01		4.89E-01	
	5.78E-01	NA	9.98E-01	4.79E+00	3.90E-01	3.15E+00
	<7.20E-01		9.16E-01		2.39E-01	
Gross.beta	8.03E+01	6.07E+02	9.30E+02	4.85E+02	8.65E+02	2.68E+03
	8.97E+01		9.14E+02		1.01E+03	
	9.48E+01	7.03E+02	9.85E+02	5.19E+02	7.95E+02	2.34E+03
	1.02E+02		9.86E+02		8.46E+02	
H-3*	1.90E-03	6.09E+00	3.16E-03	9.84E+00	3.19E-03	4.83E+00
	2.00E-03		3.14E-03		3.28E-03	
	3.34E-03	1.43E+01	2.77E-03	9.22E+00	3.21E-03	6.54E+00
	5.83E-03		3.13E-03		5.56E-03	
Hg	<1.23E-01	NA	<1.25E-01	NA	<1.25E-01	NA
	<1.26E-01		<1.25E-01		<1.25E-01	
	<1.26E-01	NA	<1.25E-01	NA	<1.25E-01	NA
	<1.21E-01		<1.25E-01		<1.25E-01	
NH4	<4.50E+03	NA	<4.50E+03	NA	<9.00E+03	NA
	<4.50E+03		<4.50E+03		<9.00E+03	
	<4.50E+03	NA	<4.50E+03	NA	<9.00E+03	NA
	<4.50E+03		<4.50E+03		<9.00E+03	
Pu-239/40	1.37E-01	2.13E+01	2.96E-01	2.35E+01	3.65E-01	2.96E+01
	1.36E-01		3.14E-01		4.04E-01	
	1.57E-01	2.43E+01	3.85E-01	2.87E+01	3.66E-01	2.60E+01
	1.54E-01		3.61E-01		3.10E-01	
Sr-90	2.95E+02	8.73E+01	3.05E+02	2.75E+02	2.99E+02	2.98E+02
	2.81E+02		3.00E+02		3.56E+02	
	3.39E+02	9.83E+01	3.10E+02	2.98E+02	2.72E+02	2.61E+02
	3.10E+02		3.45E+02		3.03E+02	
Tc-99*	2.71E-02	5.88E+00	2.29E-02	2.45E+01	2.81E-02	3.32E+01
	2.35E-02		2.12E-02		2.83E-02	
	2.61E-02	6.03E+00	2.13E-02	2.34E+01	2.18E-02	2.99E+01
	2.58E-02		2.09E-02		2.31E-02	
U*	7.10E+03	4.86E+00	7.06E+03	6.17E+00	6.14E+03	1.29E+01
	6.51E+03		6.52E+03		6.21E+03	
	6.90E+03	5.05E+00	7.53E+03	6.84E+00	5.15E+03	1.19E+01
	7.27E+03		7.51E+03		6.32E+03	

•: Analytes with a portion of the data below three times the DL.

*: Analytes with a portion of the data below ten times the DL.

NA: Not available.

APPENDIX B
CORE COMPOSITE DATA PLOTS

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B-3

ICP.a.Al

ICP.a.B

ICP.a.Ba

ICP.a.Ca

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

ICP.a.Ce

ICP.a.Co

ICP.a.Cr

ICP.a.Cu

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

ICP.a.Na

ICP.a.Ni

ICP.a.P

ICP.a.S

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

ICP.a.Si

ICP.a.Sr

ICP.a.Ti

ICP.a.Zn

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

Composite 1 = O , Composite 2 = X
Units ug/g, except radionuclides uCi/g

ICP.f.Mn

ICP.f.Na

ICP.f.Ni

ICP.f.P

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

ICP.f.Zr

ICP.w.B

ICP.w.Al

ICP.w.Ca

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

ICP.W.Cr

ICP.W.K

ICP.W.Mg

ICP.W.Na

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

ICP.W.S

ICP.W.SI

IC.W.Cl

IC.W.NO2

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

IC.W.NO3

IC.W.SO4

B-15

CN

Percent.H2O

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

Spec.W.NO2

TIC.W.CO3

pH

C-14

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

GEA.I.Cs-137

Gross, beta

B-17

H-3

Pu-239/40

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

U

Composite 1 = O, Composite 2 = X
Units ug/g, except radionuclides uCi/g

APPENDIX C
MEAN CONCENTRATION CALCULATION METHODS

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This appendix includes a description of the statistical model that describes the structure of the data from core samples taken from tank 241-S-104. Equations are also presented for estimates of the mean concentration, the variance for the mean concentration, and the confidence interval (CI) on the mean concentration.

The statistical model that describes the structure of the core composite data is

$$y_{ijk} = \mu + S_i + C_{ij} + A_{ijk}, \quad i=1, \dots, a, \quad j=1, \dots, b_i, \quad k=1, \dots, n_{ij}, \quad (1)$$

where

y_{ijk} = laboratory results from the k^{th} duplicate of the j^{th} composite of the i^{th} core from the tank

μ = the grand mean

S_i = the effect of the i^{th} core (spatial effect)

C_{ij} = the effect of the j^{th} composite sample from the i^{th} core

A_{ijk} = the analytical error associated with the k^{th} duplicate in the j^{th} composite from the i^{th} core

a = the number of cores

b_i = the number of composite samples in the i^{th} core

n_{ij} = the number of analytical results from the j^{th} composite sample in the i^{th} core.

For cores 42, 43 and 44, there are two core composite samples (i.e., $b_i = 2$).

The variables S_i and C_{ij} are treated as random effects. It is assumed that S_i , C_{ij} , and A_{ijk} are each distributed normally with mean zero and variances $\sigma^2(S)$, $\sigma^2(C)$, and $\sigma^2(A)$, respectively. Estimates of $\sigma^2(S)$, $\sigma^2(C)$, and $\sigma^2(A)$ were obtained using Restricted Maximum Likelihood Estimation (REML). This method applied to variance component estimation is described in Harville (1977).

The mean concentration of each analyte of interest in the tank was calculated using the following equation:

$$\bar{y} = \frac{1}{a} \sum_{i=1}^a \bar{y}_{i++} = \frac{1}{a} \sum_{i=1}^a \frac{\sum_{j=1}^{b_i} \sum_{k=1}^{n_{ij}} y_{ijk}}{n_{i+}} = \frac{1}{a} \sum_{i=1}^a \frac{\sum_{j=1}^{b_i} \sum_{k=1}^{n_{ij}} (\mu + S_i + C_{ij} + A_{ijk})}{n_{i+}}, \quad (2)$$

where

$$\bar{y}_{i++} = \frac{\sum_{j=1}^{b_i} \sum_{k=1}^{n_{ij}} y_{ijk}}{n_{i+}} \quad \text{and} \quad n_{i+} = \sum_{j=1}^{b_i} n_{ij}. \quad (3)$$

This mean gives the results from each core the same weight regardless of the unbalance that may exist for a particular analyte.

The variance of $\bar{y}$ is

$$V(\bar{y}) = C_1 \sigma^2(S) + C_2 \sigma^2(C) + C_3 \sigma^2(A) \quad (4)$$

where

$$C_1 = \frac{1}{a}, \quad C_2 = \frac{1}{a^2} \sum_{i=1}^a \left(\frac{1}{n_{i+}} \right)^2 \left[\sum_{j=1}^{b_i} n_{ij}^2 \right], \quad C_3 = \frac{1}{a^2} \sum_{i=1}^a \left(\frac{1}{n_{i+}} \right). \quad (5)$$

Using $\hat{\sigma}^2(S)$, $\hat{\sigma}^2(C)$, and $\hat{\sigma}^2(A)$ (REML variance component estimates), an estimated variance of $\bar{y}$ is

$$\hat{\sigma}^2(\bar{y}) = C_1\hat{\sigma}^2(S) + C_2\hat{\sigma}^2(C) + C_3\hat{\sigma}^2(A). \quad (6)$$

The approximate degrees of freedom used for $\hat{\sigma}^2(\bar{y})$ is the number of cores with data minus one.

The lower and upper 95% CI limits (95% LL and 95% UL, respectively) on the mean concentration are

$$95\% \text{ LL} = \bar{y} - t_{0.975} \sqrt{\hat{\sigma}^2(\bar{y})} \quad \text{and} \quad 95\% \text{ UL} = \bar{y} + t_{0.975} \sqrt{\hat{\sigma}^2(\bar{y})} \quad (7)$$

where $t_{0.975}$ is the 0.975 percentile from a Student's t-distribution with the approximate degrees of freedom associated with $\hat{\sigma}^2(\bar{y})$.