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A Report for Westinghouse Hanford Company

Historical Tank Content Estimate (HTCE) and Sampling Estimate Comparisons

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Prepared for the U.S. Department of Energy
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Pacific Northwest National Laboratory
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Richland, Washington 99352

(a) Westinghouse Hanford Company

Executive Summary

There has been a substantial effort over the years to characterize the waste content in Hanford's waste tanks. This characterization is vital to future efforts to retrieve, pretreat, and dispose of the waste in the proper manner. The present study is being conducted to help escalate this effort.

This study compares estimates from two independent tank characterization approaches. One approach is based on tank sampling while the other is based on historical records.

In order to statistically compare the two independent approaches, quantified variabilities (or uncertainty estimates) around the estimates of the mean concentrations are required. For the sampling-based estimates, the uncertainty estimates are provided in the Tank Characterization Reports (TCR's). However, the historically based estimates are determined from a model, and therefore possess no quantified variabilities. Steps must be taken to provide quantified variabilities for these estimates. These steps involve a parameter influence study (factorial experiment study) and an uncertainty analysis (Monte Carlo study) of the Historical Tank Content Estimate (HTCE). The purpose of the factorial experiment is to identify in the Hanford Defined Wastes (HDW) model which parameters, as they vary, have the largest effect on the HTCE. The results of this study provide the proper input parameters for the Monte Carlo study. The two estimates (HTCE and sampling-based) can then be compared.

The purpose of the Monte Carlo study is to provide estimates of variability around the estimate derived from the historical records.

The statistical comparison of the two estimates revealed the following:

1. In approximately one-fourth (27%) of the comparisons, there were significant differences between the HTCE and sampling estimates at the 95% confidence level. These differences could be due to atypical samples from the tanks. These differences could also be due to deflation of the uncertainties created for the HTCE, because the Monte Carlo simulations did not generate large enough uncertainties.

2. The sampling-based estimates were larger than the HTCE (historical records based) in the majority of cases where significant differences were found. This is evidenced in the following results:

   (a) 26 of the 28 significant differences showed sampling-based estimates to be larger than the HTCE (see Table 1).

   (b) The sampling-based estimates were larger than the HTCE in approximately 59% (61 out of 103) of the comparisons made, whether or not the differences were deemed significant (see Table 1).

   (c) The sampling-based estimates were generally larger than the HTCE for all the tanks in the study (i.e., for every tank, more than 50% of the sampling estimates were larger than the corresponding HTCE), with the exception of tanks T-105 and U-204, whether or not the differences were deemed significant (see Table 2).

   These results may indicate:

   (a) Additional waste stream source terms need to be considered in the HTCE model.

   (b) The waste is more concentrated (contains less water than is represented in the HTCE model).

   (c) The samples extracted are atypical of the waste as a whole in the tank. For example:

      i. The samples were taken through risers located near the inlet and outlet areas of the tank (which is the case for most of the tanks sampled in the Hanford area), and therefore biased the results, causing inflated concentrations in the sampling estimates.

      ii. These particular samples (from which the sampling estimates were derived) were extracted from an area of the tank (not necessarily near the inlet or outlet) that contains irregularly high concentrations of those particular constituents (that show significantly higher mean concentrations than the HTCE).

3. The sampling estimates were larger than the HTCE for chromium and silicon. The chromium differences are particularly pronounced for the tanks containing 2C and 224 waste. This systematic bias could be explained in two ways:

   (a) It could be assumed that the sampling estimates are, indeed, correct and that the HTCE model is lacking chromium and silicon source terms.

   (b) The samples extracted are atypical of the waste as a whole in the tank.

4. The manganese sampling-based estimates are significantly larger than the HTCE values for Tanks B-201 and T-111 which contain 224 waste. For the other 10 tanks, the HTCE values are zero. This means that the HTCE model does not have any manganese source terms for the waste types in these tanks. The practical significance of these statistical differences should be investigated further.

5. Statistically, differences between the sampling estimates and the HTCE cannot be distinguished for water-soluble fluoride, water, total phosphate, and sodium (except for Tank S-104).

6. The HTCE model parameter influence study showed that varying the volume percent solids parameters always had the largest effect on the HTCE values. The parameters considered in this study were volume percent solids, limiting solubility and the waste stream source terms.

Table 1, Table 2, and Table 3 summarize the results of the comparison study.

Table 1: Summary of Comparison Counts

	Number of Comparisons	Sampling > HTCE
Significant Differences	28	26
No Significant Differences	75	35
Total	103	61

Table 2: Summary of Comparison Counts by Tank

Tank	Group	Significant Differences	No Significant Differences	Not Applicable (NA)	Sampling > HTCE
B-110	1	4	5	3	5
B-111	1	4	6	2	7
B-201	1	4	5	3	6
T-111	1	3	7	2	6
BX-107	2	3	7	2	7
C-110	2	2	8	2	5
T-104	2	4	5	3	4
T-105	2	1	7	4	3
T-107	2	0	9	3	5
U-110	2	1	7	4	6
S-104	3	2	4	6	5
U-204	3	0	5	7	2
Total		28	75	41	61

Table 3: Summary of Comparison Counts by Analyte

Analyte	Significant Differences	No Significant Differences	Not Applicable	Sampling > HTCE
Al	2	7	3	5
Bi	2	8	2	5
Cr	6	6	0	10
Cs-137	3	6	3	7
F	0	6	6	3
H2O	0	9	3	2
Mn	2	0	10	2
NO3	5	6	1	8
Na	1	11	0	6
PO4	0	10	2	1
Si	5	6	1	11
TOC	2	0	10	1
Total	28	75	41	61

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List of Terms

ANOVA	Analysis of Variance
HDW/TLM	Hanford Defined Wastes/Tank Layering Model
HTCE	Historical Tank Content Estimates
LANL	Los Alamos National Laboratory
RSD	Relative Standard Deviation
SORWT	Sort on Radioactive Waste Tanks
TCR	Tank Characterization Report
TLM	Tank Layering Model
WHC	Westinghouse Hanford Company
WSTRS	Waste Status and Transaction Record Summary
1C	First cycle decontamination waste
224	Lanthanum fluoride decontamination waste
CW	Cladding waste
REDOX	Reduction/Oxidation
1C44-51/CW	First cycle decontamination waste from BiPO4 process, from 1944 through 1951 - includes cladding waste
1C52-56/CW	First cycle decontanimation waste from BiPO4 process, from 1952 through 1956 - includes cladding waste
2c44-51	Second Cycle decontamination waste from BiPO4 process from 1944 through 1951
CWP/Al56-60	Aluminum cladding Purex wastes from 1956 to 1960
CWP/Al61-72	Aluminum cladding Purex wastes from 1961 to 1972
CWR/Al52-60	Aluminum cladding Redox wastes from 1952 to 1960
CWR/Al61-67	Aluminum cladding Redox wastes from 1961 to 1967
R52-58	Redox waste from 1952 through 1958
CWP/Zr, 66-72	Zircomium cladding waste

1 Introduction

There has been a substantial effort over the years to characterize the waste content in Hanford's population of waste tanks. This characterization is vital to a future effort to retrieve, pretreat, and dispose of the waste in the proper manner. Tank waste characterization has been a difficult effort due to the hazardous and complex nature of the waste.

There have been two independent approaches to characterizing the waste in these tanks. One approach involves sampling the tank waste (i.e., core sampling, auger sampling) while the other utilizes information contained in process history records and tank waste management records. The purpose of this report is to compare these two independent approaches to tank waste characterization, and to determine how well the two independent estimates agree.

This report describes the comparison study between process history-based and sampling-based estimates of tank waste characterization. Since historically based estimates have no quantified variability, steps must be taken to produce variability estimates for them. These steps involve a parameter influence study (factorial experiment analysis) and an uncertainty analysis (Monte Carlo study) on the Historical Tank Content Estimate (HTCE). The purpose of the factorial experiment is to identify, in the Hanford Defined Wastes (HDW) model, which parameters as they vary have the largest effect on the HTCE. This exercise yields the proper input parameters for the Monte Carlo study. The purpose of the Monte Carlo study is to provide estimates of variability around the HTCE. Without this quantified variability, a statistical comparison between the sampling-based estimate (which already has a quantified variability) and the historical records-based estimate cannot be performed.

The main topic of this report is the comparison between the two independent estimates. Independent, in this sense, means that the two estimates of tank analyte concentrations use different sources of information in their calculation. If the two estimates agree, then tank characterization can be made more efficient and less costly in the future, because each tank's contents could be determined from its historical records, rather than by the more time-consuming and costly sampling effort. If the two estimates disagree significantly, useful information can still be obtained. For example, if the process history-based estimates are consistently lower than the sampling-based estimates, this may indicate that there are missing source terms which need to be added to the historical model. Conversely, this could also indicate extremely biased samples for those particular analytes (e.g., the locations (risers) through which the samples were extracted were highly concentrated in those analytes, or the risers were located near the inlet or outlet of the tank, which would have irregularly high concentrations of certain analytes). Furthermore, the information gathered could be useful in the selection of future tanks for sampling. The historically based estimates in this comparison are derived from a combination of two models, the HDW model and the Tank Layering Model (TLM), and are known as Historical Tank Content Estimates (HTCE). The sampling-based estimates are extracted from the Tank Characterization Reports ([3], [4], [6], [7], [8], [9], [11], [14], [15], [16], [18], [19]).

Some caveats should be mentioned with regard to both types of estimates. Since historical process information is incomplete (e.g., some waste transfers were not recorded), physical assumptions had to be made in the models which oversimplify some of the complex chemical relationships in the waste. For sampling-based estimates, several issues cause some samples to be atypical of the waste as a whole in the tank. These drawbacks for both types of estimates introduce random errors and "biases". In general, the magnitude of these biases cannot be evaluated due to insufficient information.

2 Scope

The original scope of this study was to combine the HTCE and sampling characterization estimates (described in the Introduction) into a single estimate using a Bayesian statistical approach. Early work on this task showed many large differences between the HTCE and sampling estimates. Due to this finding, the task scope was changed to a comparison study between the two estimate types. This comparison study focused on estimates from a select group of tanks and target analytes. Results of the comparison study from this set of tanks and analytes will be evaluated to determine whether a full scale comparison study will add value to the tank characterization effort.

HTCE and sampling estimate comparisons are made for the analytes listed in Table 4.

Table 4: Selected Analytes for Comparison Study

Aluminum	Phosphate
Sodium	Cesium-137
Chromium	Nitrate
Bismuth	Fluoride
Manganese	Total Organic Carbon (TOC)
Silicon	Water (Percent)

These analytes were selected for one or more of the following reasons:

1. The constituent is a major component of tank waste at Hanford.
2. The constituent's concentration affects the way the waste must be handled in pretreatment and treatment phases of the waste remediation effort.
3. The constituent's concentration is critical in resolving safety issues associated with the waste tanks.

It should be noted that other analytes exist which fit the above criteria. However, the listed constituents were chosen to keep the task manageable and to construct a foundation on which to build.

Table 5 lists the tanks that were selected for this comparison study. The tanks are classified in three groups by waste type.

Table 5: Selected Tanks for Comparison Study

Group	Waste Types	Tanks	
1	Bismuth Phosphate Process 2C and 224 Wastes	B-110	B-111
		B-201	T-111
2	Bismuth Phosphate Process 1C and CW Wastes	BX-107	C-110
		T-104	T-105
		T-107	U-110
3	REDOX Process Wastes	S-104	U-204

Group 1 includes tanks with simple waste matrices relative to the general population of tanks at Hanford. These tanks contain primarily second cycle decontamination waste (2C waste) and 224 concentration building waste sludges from the bismuth phosphate process.

Like Group 1, Group 2 tanks also contain sludges from the bismuth phosphate process. These tanks contain primarily first cycle decontamination waste (1C waste) and cladding waste (CW).

Tanks in Group 3 contain REDOX process wastes.

3 Brief Discussion of Studies Prior to Comparison Test

To make statistical comparisons between two independent sets of estimates, some measure of uncertainty is required. Estimates of uncertainty are provided in the TCR's for the sampling estimates. However, the HTCE do not have uncertainty estimates. This section briefly describes the steps taken to estimate the HTCE uncertainties so that a statistical comparison can be made between the HTCE and the sampling estimates.

The first step involves identifying all parameters of the HTCE model that could contribute to the uncertainty in the HTCE. Based on discussions with staff at Los Alamos National Laboratory and Westinghouse Hanford Company, a list of parameters were identified.

Next, the identified parameters were used in a factorial experiment (parameter influence study described in Appendix B) to determine the subset of those parameters that significantly affect the concentrations of each target analyte.

Using the significant parameters that were determined in the factorial experiment, a Monte Carlo study was conducted. This study uses simulations to obtain the uncertainty estimates for the HTCE so that the comparisons between the sampling estimates and HTCE can be performed.

Figure 1 displays the elements of the Monte Carlo study. The solid box in the center of the figure represents the HTCE model. It is made up of the following model subcomponents which are described in Reference [2]:

1. Hanford Defined Wastes (HDW)
2. Waste Status and Transaction Record Summary (WSTRS)
3. Tank Layering Model (TLM)

As noted earlier, these model subcomponents are linked together in a series of spreadsheets.

The dashed line box above the HTCE model box represents the inputs to the HTCE model that are potential sources of variability in the estimates of the HTCE model outputs. In this set of HTCE model parameters, the subsets that are significant contributors and can be quantified are identified as 1, 2, 3, ..., n. A probability distribution is placed on each of these model parameters, based on any historical and chemical information that can be gathered. From each of these probability distributions, a large number of realizations are randomly generated and used as inputs into the HTCE model, and the HTCE outputs are recorded. In general, the different sources of variability are considered independently of each other.

The dashed box under the HTCE model in Figure 1 represents the distribution of HTCE model results from the Monte Carlo study. The variance of these model results is used as the uncertainty estimate of the HTCE.

Appendix A describes in detail all the studies required prior to the actual statistical comparison.

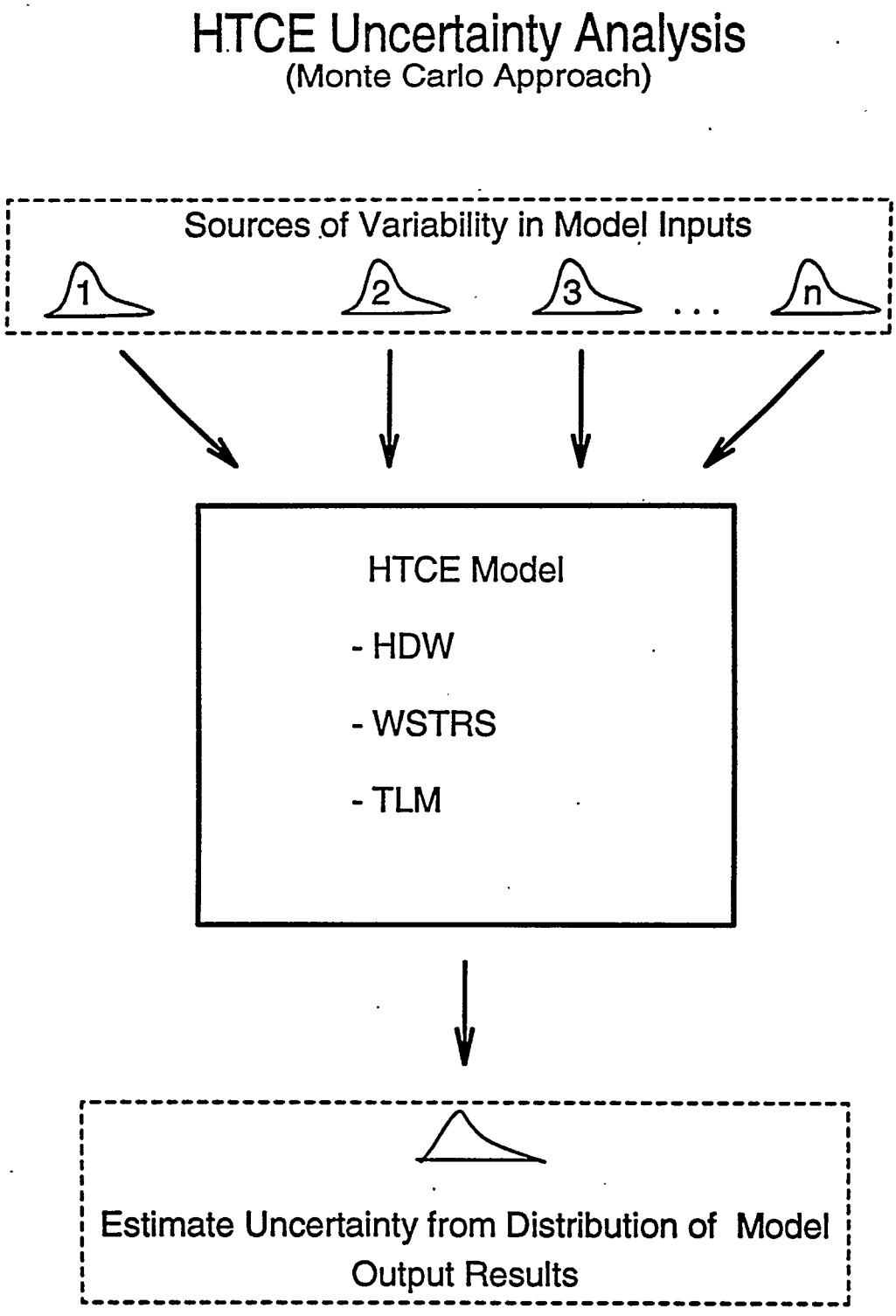


Figure 1: Monte Carlo Study Approach

4 HTCE and Sampling Estimates Comparisons

As described earlier, a Monte Carlo simulation was conducted to establish initial uncertainty estimates for the HTCE model. HTCE model predictions were then compared with estimates based on actual waste measurements. This section discusses the comparison between the HTCE and TCR sampling-based estimates. The sampling-based estimates selected for this comparison, the comparison statistic, and the comparison results are presented. One result of this comparison is that model uncertainties were quantified and overall model behavior and trends were identified. With quantified uncertainties, a model can provide improved inventory estimates and can be used in several stages of the design and construction of the retrieval, treatment and disposal processes at Hanford. The use of this data in appropriate applications may potentially accelerate disposal of the single-shell tank wastes and reduce the overall cost of the characterization effort.

4.1 Sampling Estimate Selection

For several of the target analytes considered in this comparison study, there are multiple analytical methods and/or sample preparation methods. Therefore, there may be several sampling-based estimates from which to choose for comparison with the HTCE. For example, three sampling-based estimates were generally available for aluminum from laboratory analysis of aliquots prepared using KOH/Ni fusion, acid digestion, and water digestion.

The sampling-based estimates used in the comparison with the HTCE were selected based on the following criteria (with few exceptions):

1. The inductively coupled plasma, KOH/Ni fusion method was chosen for the following analytes: aluminum, sodium, chromium, bismuth, manganese, and phosphate (total phosphate converted from phosphorus).

2. The ion chromatography, water digestion method was used for the following anions: nitrate and fluoride.

3. The gamma energy analysis, fusion method was used for the radionuclide, cesium-137.

As an exception to these rules, the aluminum, chromium and manganese estimates for Tank B-110 were taken from ICP analysis on acid-digested samples rather than on fused samples. Estimates from fusion-prepared samples were not available in the TCRs.

4.2 Comparison Statistic

In the past, HTCE and sampling-based estimates were generally compared using the relative percent difference between the two estimates. Only simple comparisons of this type were possible, because no HTCE uncertainty estimates were available. Now that uncertainty estimates are available, a more appropriate comparison can be made, to which a level of confidence can be assigned — given that the HTCE uncertainty was estimated using a reasonable approach.

The statistic used for the comparison between the HTCE and sampling-based estimates is

$$\frac{H - S}{\sqrt{var(H) + var(S)}} \tag{1}$$

where

H is the HTCE

S is the sampling estimate

$var(H)$ is the HTCE uncertainty estimate

$var(S)$ is the sampling uncertainty estimate.

Based on Chebyshev's Inequality ([13]), which does not require any statistical distribution assumptions, values of the comparison statistic that indicate significant differences between the estimates can be identified. If the comparison statistic is greater than 4.5 or less than -4.5, then it is concluded that there is a significant difference between the HTCE and the sampling-based estimates, at the 95% confidence level.

This method of comparison is superior to simply looking at the differences between estimates because it takes into account the quantified variabilities. In some cases, just comparing the estimates would lead to the conclusion that the two estimates were different, when in reality they are statistically indistinguishable when the quantified variabilities are taken into consideration. An example to illustrate this is the phosphate estimates for Tank T-105. The sampling-based estimate from the TCR is 4.68E+03 μg/g (with a relative standard deviation of 27.66%). The HTCE estimate is 7.97E+04 μg/g (with a relative standard deviation of 41.89%). The HTCE estimate is more than an order of magnitude larger than the TCR estimate. If these estimates are considered without any reference to their variability estimates, it might be concluded that they are significantly different. However, when the large variabilities for both of these estimates are taken into consideration (i.e., RSDs greater than 25%), the uncertainty around the estimates is wide enough that these estimates cannot be statistically distinguished from each other.

4.3 Comparison Results and Conclusions

The HTCE uncertainty estimates are presented in this section, along with some general conclusions about the HTCE versus sampling-based estimate comparisons. These are followed by a detailed tabulation and discussion of the results.

Figures 2, 3, 4 and 5 contain four comparison statistic histograms. The first three histogram charts show the comparison statistics for Tank Groups 1, 2, and 3. The fourth includes all comparison statistics across all three tank groups. In each chart, the histograms show the number of tanks within various ranges of the comparison statistic. A negative statistic indicates that the sampling-based estimate is higher than the HTCE, and conversely. A shaded bar indicates that the difference is statistically significant. The histograms also contain the number of comparisons that fall within the range of each bar for each analyte.

The following general conclusions can be drawn from the comparison study:

1. Approximately one-fourth (27%) of the comparisons showed significant differences between the HTCE and sampling-based estimates at the 95% confidence level (28 tanks out of 103).

2. The sampling-based estimates were higher than the HTCE in most cases where significant differences were found (26 out of 28 comparisons, or about 93%). These results may indicate that additional waste stream source terms need to be considered in the HTCE model, or that the waste is more concentrated (contains less water) than the HTCE model assumes.

3. There were 103 available comparisons, because 41 of the 144 possible comparisons either had no available estimate from the sampling, or did not have a quantified variability for the historically-based estimate (i.e., the estimate was equal to zero).

4. For all tanks, at least 50% of the comparisons showed no significant differences between the two estimates.

5. The sampling-based estimates were generally larger than the HTCE for all the tanks in the study (i.e., for every tank, more than 50% of the sampling estimates were larger than the corresponding HTCE), with the exception of tanks T-105 and U-204, whether or not the differences were deemed significant (see Table 8).

The HTCE and sampling-based estimates and their associated uncertainty estimates (reported as relative standard deviations (RSD)) are given in Tables 6 and 7. The relative standard deviation is calculated by dividing the estimated standard deviation by the mean estimate.

$$RSD = \frac{StandardDeviation}{Mean} \times 100 \qquad (2)$$

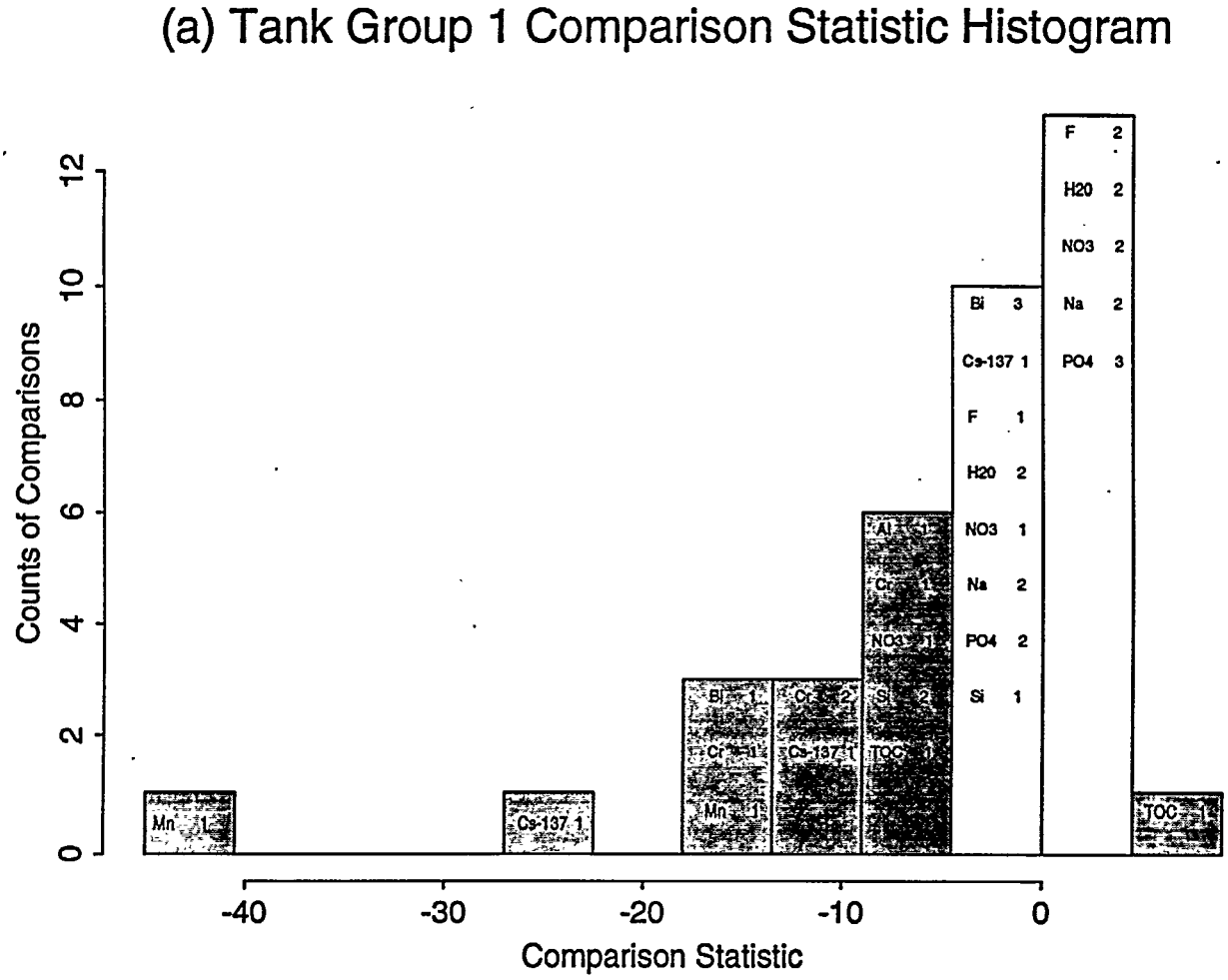


Figure 2: Groups 1 Comparison Statistic Histogram

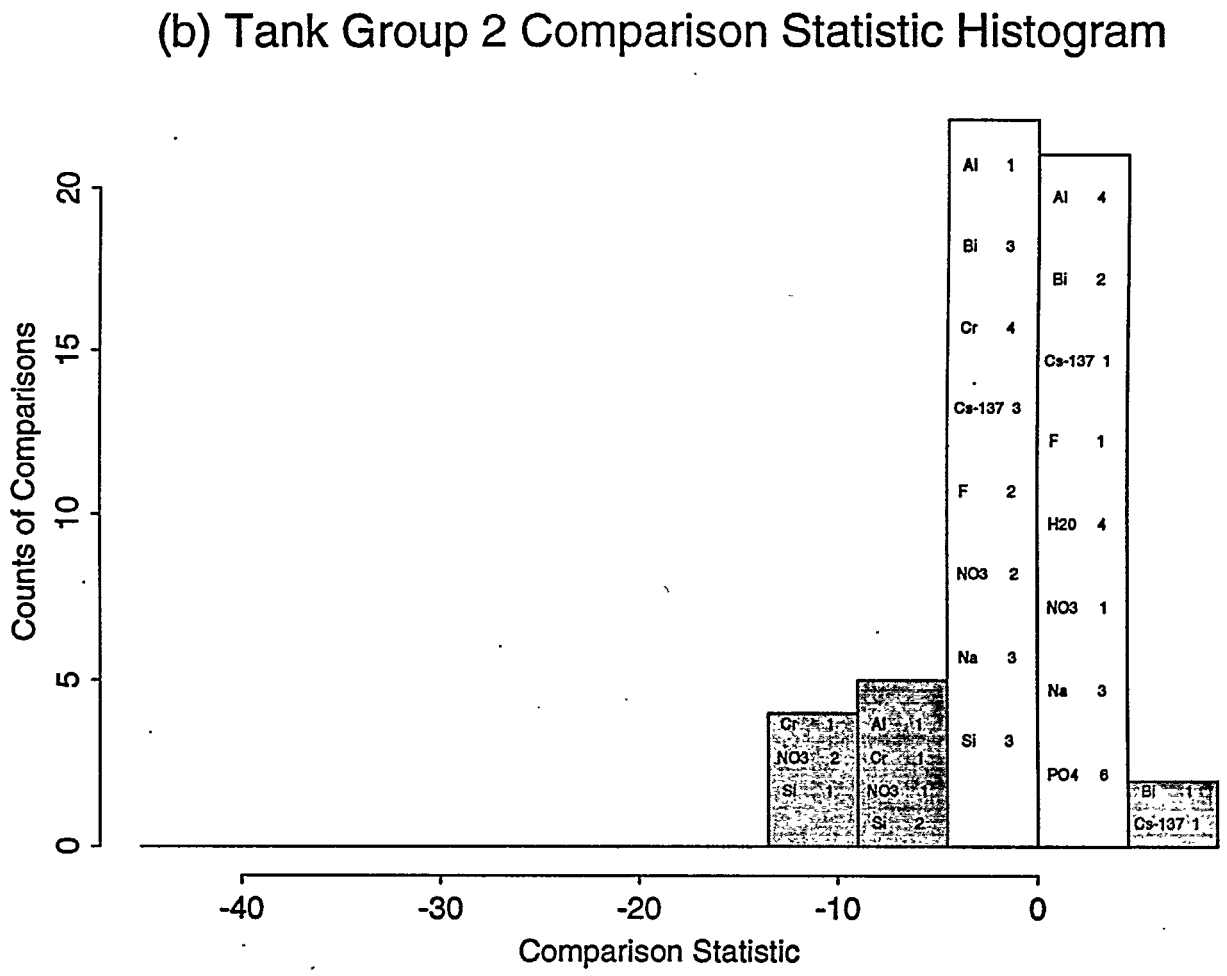


Figure 3: Groups 2 Comparison Statistic Histogram

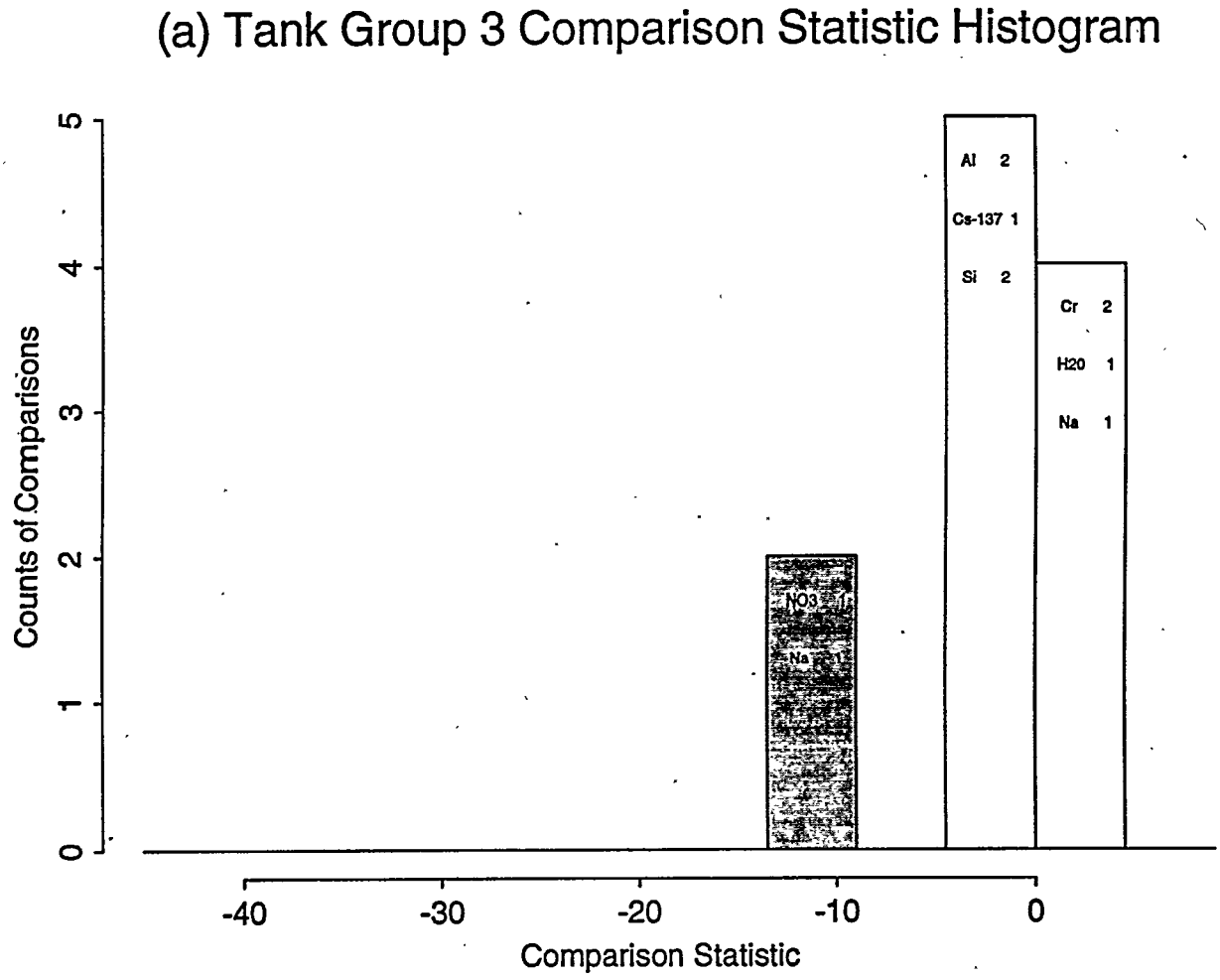


Figure 4: Groups 3 Comparison Statistic Histogram

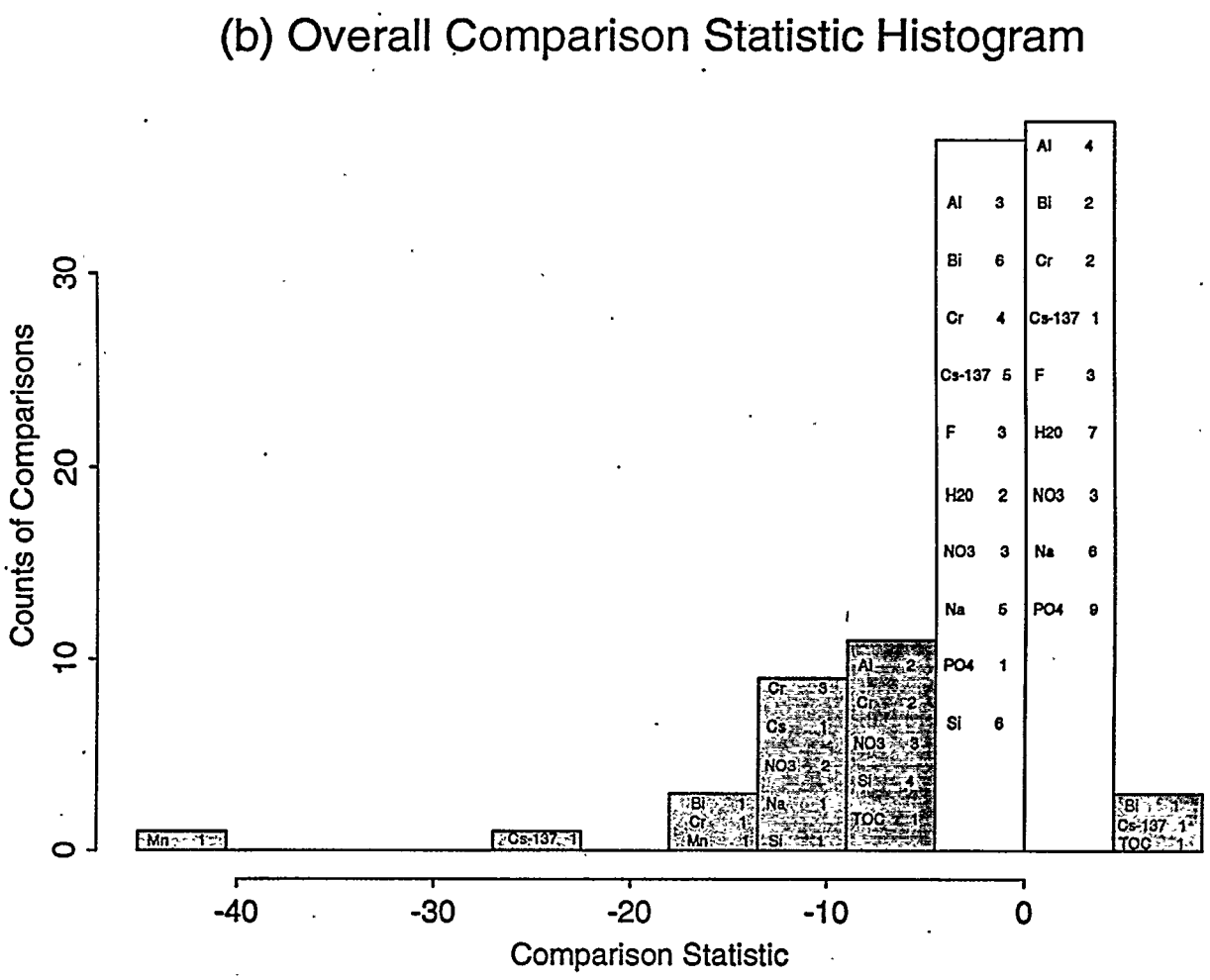


Figure 5: Overall Comparison Statistic Histogram

The RSD thus indicates how large the uncertainty is relative to the estimated mean value. It is important to realize that the RSD's, which are shown in Tables 6 and 7, measure different types of uncertainties for the HTCE than for the sampling estimates. The RSDs for the HTCE measure the variations caused by the inaccuracy in the historical processing and management records. The RSDs for the sampling estimates measure the spatial variations of the contents in a tank as well as the analytical variations. Although the sources of the two RSD's are different, they both indicate the accuracy of their corresponding estimates and therefore are necessary to perform any meaningful comparison between the two entities.

The comparison statistic is also reported in the tables. Table 6 presents the results for each target analyte, and Table 7 presents the results for each tank. In both tables, the statistics that indicate a significant difference between the HTCE and the sampling-based estimates are marked with an asterisk.

It should be noted that some of the analyte concentrations had to be converted to another form in order to make proper comparisons. The following adjustments were made:

1. Phosphorus was changed to total phosphate (PO4) for the sampling-based estimates in order to match what is provided in the historically based estimates. Phosphorus can be converted to total phosphate by multiplying by 3.06.

2. Silicon results are provided in the historical estimates as silica (SiO3), while the sampling-based estimates provide them as silicon (Si). The historical estimates were converted to silicon by multiplying by 0.369.

3. The estimate for fluoride in the sampling-based estimates is for water-soluble fluoride. The HTCE reports total fluoride, but the water-soluble value is retrievable from the HTCE model, and was used in this report.

Table 6: HTCE and Sampling Estimate Comparisons by Analyte

Analyte	Group	Tank	# of Cores	Sampling Est.	Sampling RSD	HTCE Est.	HTCE RSD	Comparison Statistic
				(μg/g)		(μg/g)		
Al	1	B-110	7	1.13e+03	15.62	0.00e+00	NA	NA
Al	1	B-111	2	1.36e+03	16.00	1.03e+02	6.15	-5.77*
Al	1	B-201	2	3.91e+03	71.00	0.00e+00	NA	NA
Al	1	T-111	2	5.70e+02	17.28	0.00e+00	NA	NA
Al	2	BX-107	2	1.43e+04	9.59	2.76e+04	17.38	2.67
Al	2	C-110	3	1.43e+04	1.99	2.76e+04	17.38	2.77
Al	2	T-104	2	1.56e+04	12.12	2.36e+04	14.04	2.10
Al	2	T-105	2	9.51e+04	58.78	4.76e+03	18.07	-1.62
Al	2	T-107	2	1.63e+04	130.14	2.76e+04	17.38	0.52
Al	2	U-110	7	1.50e+05	9.91	1.76e+04	15.50	-8.76*
Al	3	S-104	2	1.17e+05	1.11	8.74e+04	16.86	-2.00
Al	3	U-204	3	2.21e+05	15.69	1.08e+05	13.63	-2.42
				(μg/g)		(μg/g)		
Bi	1	B-110	7	1.85e+04	6.79	1.99e+04	19.73	0.34
Bi	1	B-111	2	2.02e+04	1.00	1.84e+04	19.76	-0.49
Bi	1	B-201	2	9.45e+04	3.00	1.81e+04	27.01	-13.52*
Bi	1	T-111	2	2.36e+04	12.77	2.46e+04	21.87	0.16
Bi	2	BX-107	2	2.23e+04	9.18	1.43e+04	15.35	-2.67
Bi	2	C-110	3	1.37e+04	5.05	1.43e+04	15.35	0.26
Bi	2	T-104	2	1.74e+04	6.32	1.17e+04	13.11	-3.02
Bi	2	T-105	2	1.22e+03	13.36	1.72e+04	17.47	5.31*
Bi	2	T-107	2	1.20e+04	60.90	1.43e+04	15.35	0.30
Bi	2	U-110	7	2.06e+04	24.22	8.20e+03	13.63	-2.42

Table 6: *(continued)*

Analyte	Group	Tank	# of Cores	Sampling Est.	Sampling RSD	HTCE Est.	HTCE RSD	Comparison Statistic
Bi	3	S-104	2	NA	NA	0.00e+00	NA	NA
Bi	3	U-204	3	1.20e+03	68.61	0.00e+00	NA	NA
				(μg/g)		(μg/g)		
Cr	1	B-110	7	8.10e+02	2.54	2.60e+02	27.26	-7.45*
Cr	1	B-111	2	1.15e+03	2.00	2.42e+02	26.74	-13.22*
Cr	1	B-201	2	3.38e+03	8.00	2.78e+02	15.17	-11.33*
Cr	1	T-111	2	1.80e+03	2.19	4.38e+02	19.91	-14.22*
Cr	2	BX-107	2	9.68e+02	6.53	2.55e+02	27.31	-7.58*
Cr	2	C-110	3	4.64e+02	4.57	2.55e+02	27.31	-2.87
Cr	2	T-104	2	8.67e+02	2.20	2.96e+02	18.99	-9.62*
Cr	2	T-105	2	4.32e+02	41.67	2.84e+02	22.48	-0.77
Cr	2	T-107	2	3.60e+02	2.78	2.55e+02	27.31	-1.49
Cr	2	U-110	7	5.35e+02	21.37	3.33e+02	13.81	-1.64
Cr	3	S-104	2	2.35e+03	3.80	2.35e+04	37.21	2.42
Cr	3	U-204	3	1.75e+02	28.81	2.20e+02	18.44	0.70
				(μCi/g)		(μCi/g)		
Cs-137	1	B-110	7	1.49e+01	3.78	4.00e-01	38.67	-24.83*
Cs-137	1	B-111	2	1.58e+02	9.00	2.80e+00	35.50	-10.89*
Cs-137	1	B-201	2	8.00e-01	27.00	0.00e+00	NA	NA
Cs-137	1	T-111	2	1.66e-01	34.94	1.49e-01	20.16	-0.26
Cs-137	2	BX-107	2	1.74e+01	29.02	6.12e+00	26.60	-2.13
Cs-137	2	C-110	3	1.95e+01	12.97	6.12e+00	26.60	-4.45
Cs-137	2	T-104	2	1.99e-01	2.82	2.88e+01	14.43	6.88*
Cs-137	2	T-105	2	4.92e+01	NA	1.43e+01	14.42	NA
Cs-137	2	T-107	2	9.25e+00	59.57	6.12e+00	26.60	-0.54
Cs-137	2	U-110	7	2.82e+01	18.26	5.27e+01	12.78	2.89
Cs-137	3	S-104	2	6.23e+01	2.99	4.70e+01	9.92	-3.05
Cs-137	3	U-204	3	NA	NA	1.83e+00	18.41	NA
				(μg/g)		(μg/g)		
F	1	B-110	7	1.89e+03	6.35	2.39e+03	59.39	0.35
F	1	B-111	2	1.56e+03	2.00	2.39e+03	59.39	0.58
F	1	B-201	2	5.83e+03	2.00	2.96e+03	70.28	-1.38
F	1	T-111	2	2.30e+03	34.95	NA	NA	NA
F	2	BX-107	2	9.19e+03	7.90	2.80e+03	54.48	-3.78
F	2	C-110	3	7.63e+03	13.37	2.80e+03	54.48	-2.63
F	2	T-104	2	8.57e+03	1.91	NA	NA	NA
F	2	T-105	2	NA	NA	NA	NA	NA
F	2	T-107	2	1.14e+03	383.36	2.80e+03	54.48	0.36
F	2	U-110	7	7.05e+03	10.75	NA	NA	NA
F	3	S-104	2	1.45e+02	25.03	0.00e+00	NA	NA
F	3	U-204	3	NA	NA	0.00e+00	NA	NA
				(%)		(%)		
H2O	1	B-110	7	5.81e+01	2.81	6.62e+01	7.82	1.49
H2O	1	B-111	2	6.31e+01	1.17	6.48e+01	7.61	0.34
H2O	1	B-201	2	6.06e+01	1.95	5.62e+01	13.18	-0.59
H2O	1	T-111	2	7.65e+01	6.17	6.86e+01	7.18	-1.16
H2O	2	BX-107	2	5.91e+01	4.75	6.92e+01	6.40	1.93
H2O	2	C-110	3	5.75e+01	3.60	6.92e+01	6.40	2.39

Table 6: *(continued)*

Analyte	Group	Tank	# of Cores	Sampling Est.	Sampling RSD	HTCE Est.	HTCE RSD	Comparison Statistic
H2O	2	T-104	2	7.05e+01	0.28	7.24e+01	4.67	0.56
H2O	2	T-105	2	5.96e+01	48.17	6.90e+01	6.63	0.32
H2O	2	T-107	2	4.98e+01	NA	6.92e+01	6.40	NA
H2O	2	U-110	7	3.15e+01	NA	7.51e+01	3.76	NA
H2O	3	S-104	2	4.29e+01	NA	6.57e+01	3.66	NA
H2O	3	U-204	3	2.60e+01	12.13	6.53e+01	15.18	3.78
				(μg/g)		(μg/g)		
Mn	1	B-110	7	6.67e+01	10.84	0.00e+00	NA	NA
Mn	1	B-111	2	1.11e+02	2.00	0.00e+00	NA	NA
Mn	1	B-201	2	2.29e+04	6.00	1.52e+02	233.46	-16.03*
Mn	1	T-111	2	6.28e+03	2.18	1.33e+01	228.84	-44.62*
Mn	2	BX-107	2	6.46e+01	9.24	0.00e+00	NA	NA
Mn	2	C-110	3	5.63e+01	12.61	0.00e+00	NA	NA
Mn	2	T-104	2	6.18e+01	4.09	0.00e+00	NA	NA
Mn	2	T-105	2	1.04e+04	72.60	0.00e+00	NA	NA
Mn	2	T-107	2	2.13e+02	22.32	0.00e+00	NA	NA
Mn	2	U-110	7	3.46e+03	12.87	0.00e+00	NA	NA
Mn	3	S-104	2	1.15e+03	18.87	0.00e+00	NA	NA
Mn	3	U-204	3	8.20e+01	46.03	0.00e+00	NA	NA
				(μg/g)		(μg/g)		
NO3	1	B-110	7	1.87e+05	8.14	4.49e+04	27.57	-7.24*
NO3	1	B-111	2	8.20e+04	8.00	4.18e+04	27.02	-3.08
NO3	1	B-201	2	4.93e+04	1.00	6.13e+04	14.51	1.35
NO3	1	T-111	2	4.12e+04	6.77	4.63e+04	19.81	0.53
NO3	2	BX-107	2	1.37e+05	6.57	2.00e+04	27.00	-11.15*
NO3	2	C-110	3	1.10e+05	6.85	2.00e+04	27.00	-9.71*
NO3	2	T-104	2	5.80e+04	1.30	2.31e+04	18.92	-7.87*
NO3	2	T-105	2	2.12e+04	26.89	4.08e+04	24.43	1.71
NO3	2	T-107	2	7.45e+04	49.14	2.00e+04	27.00	-1.47
NO3	2	U-110	7	4.51e+04	8.73	2.57e+04	13.90	-3.65
NO3	3	S-104	2	1.91e+05	3.16	7.58e+04	11.37	-10.95*
NO3	3	U-204	3	NA	NA	3.14e+04	19.04	NA
				(μg/g)		(μg/g)		
Na	1	B-110	7	9.77e+04	3.29	9.09e+04	29.41	-0.25
Na	1	B-111	2	9.57e+04	2.00	9.25e+04	26.86	-0.13
Na	1	B-201	2	3.82e+04	2.00	7.72e+04	56.60	0.89
Na	1	T-111	2	3.70e+04	6.62	5.85e+04	49.36	0.74
Na	2	BX-107	2	1.00e+05	1.93	9.00e+04	22.66	-0.49
Na	2	C-110	3	8.26e+04	3.54	9.00e+04	22.66	0.36
Na	2	T-104	2	6.21e+04	2.06	8.19e+04	19.90	1.21
Na	2	T-105	2	4.92e+04	26.22	8.59e+04	27.62	1.36
Na	2	T-107	2	1.17e+05	9.82	9.00e+04	22.66	-1.15
Na	2	U-110	7	1.11e+05	7.12	7.23e+04	17.48	-2.60
Na	3	S-104	2	1.18e+05	1.41	3.94e+04	16.55	-11.68*
Na	3	U-204	3	1.82e+04	19.79	5.26e+04	61.19	1.06
				(μg/g)		(μg/g)		
PO4	1	B-110	7	4.92e+04	13.42	8.20e+04	46.48	0.85
PO4	1	B-111	2	4.87e+04	7.99	7.60e+04	46.88	0.76

Table 6: *(continued)*

Analyte	Group	Tank	# of Cores	Sampling Est.	Sampling RSD	HTCE Est.	HTCE RSD	Comparison Statistic
PO4	1	B-201	2	1.67e+04	13.98	1.07e+04	20.61	-1.87
PO4	1	T-111	2	3.18e+04	8.83	4.18e+04	82.93	0.29
PO4	2	BX-107	2	4.34e+04	3.08	9.82e+04	31.93	1.75
PO4	2	C-110	3	6.21e+04	5.37	9.82e+04	31.93	1.14
PO4	2	T-104	2	7.56e+04	8.66	8.53e+04	29.04	0.38
PO4	2	T-105	2	4.68e+03	27.66	7.97e+04	41.89	2.84
PO4	2	T-107	2	9.82e+04	5.14	9.82e+04	31.93	0.00
PO4	2	U-110	7	4.67e+04	22.12	6.76e+04	28.39	0.96
PO4	3	S-104	2	2.85e+00	NA	0.00e+00	NA	NA
PO4	3	U-204	3	2.15e+03	55.43	0.00e+00	NA	NA
				(μg/g)		(μg/g)		
Si	1	B-110	7	9.35e+03	3.58	2.22e+03	55.01	-5.63*
Si	1	B-111	2	1.04e+04	8.00	2.74e+03	48.95	-4.86*
Si	1	B-201	2	2.02e+04	63.00	0.00e+00	NA	NA
Si	1	T-111	2	5.67e+03	4.10	1.66e+03	70.18	-3.38
Si	2	BX-107	2	6.78e+03	7.09	1.15e+03	50.35	-7.47*
Si	2	C-110	3	7.16e+03	5.91	1.15e+03	50.35	-8.36*
Si	2	T-104	2	6.52e+03	2.79	9.80e+02	47.24	-11.14*
Si	2	T-105	2	6.98e+03	11.23	1.78e+03	52.82	-4.24
Si	2	T-107	2	6.06e+03	39.36	1.15e+03	50.35	-2.00
Si	2	U-110	7	2.22e+04	32.67	7.26e+02	43.01	-2.96
Si	3	S-104	2	1.33e+03	9.25	7.85e+02	57.37	-1.17
Si	3	U-204	3	2.38e+03	65.54	9.51e+02	57.22	-0.87
				(μg/g)		(μg/g)		
TOC	1	B-110	7	3.81e+02	6.08	0.00e+00	NA	NA
TOC	1	B-111	2	8.75e+02	12.00	0.00e+00	NA	NA
TOC	1	B-201	2	5.18e+02	10.00	3.61e-03	15.78	5.41*
TOC	1	T-111	2	3.12e+03	19.84	2.80e-02	16.06	-4.58*
TOC	2	BX-107	2	6.75e+02	NA	0.00e+00	NA	NA
TOC	2	C-110	3	8.02e+02	50.75	0.00e+00	NA	NA
TOC	2	T-104	2	7.06e+02	NA	0.00e+00	NA	NA
TOC	2	T-105	2	4.13e+03	NA	0.00e+00	NA	NA
TOC	2	T-107	2	1.70e+03	30.90	0.00e+00	NA	NA
TOC	2	U-110	7	9.55e+02	515.12	0.00e+00	NA	NA
TOC	3	S-104	2	1.73e+03	NA	0.00e+00	NA	NA
TOC	3	U-204	3	4.69e+02	73.67	0.00e+00	NA	NA

* : HTCE and Sampling estimates significantly different at the 95% confidence level
NA : Not Available or Not Applicable

4.3.1 Comparison Results by Analyte

From an examination of Table 6, the following specific results were noted:

1. The chromium sampling-based estimates are much larger than the HTCE chromium estimates for Group 1, and the differences are statistically significant (see Figure 2). There may be instances where these differences would not be considered practically important. However, this may also mean that a source term for chromium should be included for 2C and 224 Wastes.

2. The sampling-based estimates and HTCE values for percent water are not statistically different from each other, based on the criteria used in these comparisons. This could indicate agreement between the two independent estimates.

3. The manganese sampling-based estimates are significantly larger than the HTCE values for both available comparisons (Tanks B-201 and T-111, which contain mostly 224 waste). For the other 10 tanks, the HTCE values are zero. This means that the HTCE model does not have a source term for manganese for any of the waste types contained in these tanks, with the exception of 224 Waste. The practical significance of these statistical differences should be investigated further.

4. The sodium sampling-based estimates and HTCE values for tank Groups 1 and 2 are not statistically different, nor is one consistently higher than the other (see Figure 2 and 3). However, note that the HTCE uncertainties are relatively large.

5. The phosphate sampling-based estimates and HTCE values cannot be statistically distinguished from each other at the 95% confidence level. Note again that the HTCE uncertainties are somewhat large. Also, the HTCE phosphate values are generally larger than the sampling-based estimates.

6. The sampling-based estimates are larger than the HTCE values for silicon in every instance (see Figure 5). This difference is significant in five of the cases listed. This consistent pattern may indicate that there are missing silicon source terms for the waste types considered here.

Since most of the comparisons indicate that the sampling-based estimates were generally larger than the historically-based estimates, it is recommended that improvements be considered to the HDW model, i.e., that appropriate source terms be investigated to improve the agreement between the two estimates. However, this recommendation assumes that the sampling estimates are correct. It is possible that the samples extracted are atypical of the waste as a whole in the tank.

4.3.2 Comparison Results by Tank

Table 6 contains the same comparison statistics as Table 7, but ordered by tank rather than by analyte.

Table 7: HTCE and Sampling Estimate Comparisons by Tank

Analyte	Group	Tank	# of Cores	Sampling Est.	Sampling RSD	HTCE Est.	HTCE RSD	Comparison Statistic
Al	1	B-110	7	1.13e+03	15.62	0.00e+00	NA	NA
Bi	1	B-110	7	1.85e+04	6.79	1.99e+04	19.73	0.34
Cr	1	B-110	7	8.10e+02	2.54	2.60e+02	27.26	-7.45*
Cs-137	1	B-110	7	1.49e+01	3.78	4.00e-01	38.67	-24.83*
F	1	B-110	7	1.89e+03	6.35	2.39e+03	59.39	0.35
H2O	1	B-110	7	5.81e+01	2.81	6.62e+01	7.82	1.49
Mn	1	B-110	7	6.67e+01	10.84	0.00e+00	NA	NA
NO3	1	B-110	7	1.87e+05	8.14	4.49e+04	27.57	-7.24*
Na	1	B-110	7	9.77e+04	3.29	9.09e+04	29.41	-0.25
PO4	1	B-110	7	4.92e+04	13.42	8.20e+04	46.48	0.85
Si	1	B-110	7	9.35e+03	3.58	2.22e+03	55.01	-5.63*
TOC	1	B-110	7	3.81e+02	6.08	0.00e+00	NA	NA
Al	1	B-111	2	1.36e+03	16.00	1.03e+02	6.15	-5.77*
Bi	1	B-111	2	2.02e+04	1.00	1.84e+04	19.76	-0.49
Cr	1	B-111	2	1.15e+03	2.00	2.42e+02	26.74	-13.22*
Cs-137	1	B-111	2	1.58e+02	9.00	2.80e+00	35.50	-10.89*
F	1	B-111	2	1.56e+03	2.00	2.39e+03	59.39	0.58
H2O	1	B-111	2	6.31e+01	1.17	6.48e+01	7.61	0.34
Mn	1	B-111	2	1.11e+02	2.00	0.00e+00	NA	NA

Table 7: *(continued)*

Analyte	Group	Tank	# of Cores	Sampling Est.	Sampling RSD	HTCE Est.	HTCE RSD	Comparison Statistic
NO3	1	B-111	2	8.20e+04	8.00	4.18e+04	27.02	-3.08
Na	1	B-111	2	9.57e+04	2.00	9.25e+04	26.86	-0.13
PO4	1	B-111	2	4.87e+04	7.99	7.60e+04	46.88	0.76
Si	1	B-111	2	1.04e+04	8.00	2.74e+03	48.95	-4.86*
TOC	1	B-111	2	8.75e+02	12.00	0.00e+00	NA	NA
Al	1	B-201	2	3.91e+03	71.00	0.00e+00	NA	NA
Bi	1	B-201	2	9.45e+04	3.00	1.81e+04	27.01	-13.52*
Cr	1	B-201	2	3.38e+03	8.00	2.78e+02	15.17	-11.33*
Cs-137	1	B-201	2	8.00e-01	27.00	0.00e+00	NA	NA
F	1	B-201	2	5.83e+03	2.00	2.96e+03	70.28	-1.38
H2O	1	B-201	2	6.06e+01	1.95	5.62e+01	13.18	-0.59
Mn	1	B-201	2	2.29e+04	6.00	1.52e+02	233.46	-16.03*
NO3	1	B-201	2	4.93e+04	1.00	6.13e+04	14.51	1.35
Na	1	B-201	2	3.82e+04	2.00	7.72e+04	56.60	0.89
PO4	1	B-201	2	1.67e+04	13.98	1.07e+04	20.61	-1.87
Si	1	B-201	2	2.02e+04	63.00	0.00e+00	NA	NA
TOC	1	B-201	2	5.18e+02	10.00	3.61e+03	15.78	5.41*
Al	1	T-111	2	5.70e+02	17.28	0.00e+00	NA	NA
Bi	1	T-111	2	2.36e+04	12.77	2.46e+04	21.87	0.16
Cr	1	T-111	2	1.80e+03	2.19	4.38e+02	19.91	-14.22*
Cs-137	1	T-111	2	1.66e-01	34.94	1.49e-01	20.16	-0.26
F	1	T-111	2	2.30e+03	34.95	NA	NA	NA
H2O	1	T-111	2	7.65e+01	6.17	6.86e+01	7.18	-1.16
Mn	1	T-111	2	6.28e+03	2.18	1.33e+01	228.84	-44.62*
NO3	1	T-111	2	4.12e+04	6.77	4.63e+04	19.81	0.53
Na	1	T-111	2	3.70e+04	6.62	5.85e+04	49.36	0.74
PO4	1	T-111	2	3.18e+04	8.83	4.18e+04	82.93	0.29
Si	1	T-111	2	5.67e+03	4.10	1.66e+03	70.18	-3.38
TOC	1	T-111	2	3.12e+03	19.84	2.80e+02	16.06	-4.58*
Al	2	BX-107	2	1.43e+04	9.59	2.76e+04	17.38	2.67
Bi	2	BX-107	2	2.23e+04	9.18	1.43e+04	15.35	-2.67
Cr	2	BX-107	2	9.68e+02	6.53	2.55e+02	27.31	-7.58*
Cs-137	2	BX-107	2	1.74e+01	29.02	6.12e+00	26.60	-2.13
F	2	BX-107	2	9.19e+03	7.90	2.80e+03	54.48	-3.78
H2O	2	BX-107	2	5.91e+01	4.75	6.92e+01	6.40	1.93
Mn	2	BX-107	2	6.46e+01	9.24	0.00e+00	NA	NA
NO3	2	BX-107	2	1.37e+05	6.57	2.00e+04	27.00	-11.15*
Na	2	BX-107	2	1.00e+05	1.93	9.00e+04	22.66	-0.49
PO4	2	BX-107	2	4.34e+04	3.08	9.82e+04	31.93	1.75
Si	2	BX-107	2	6.78e+03	7.09	1.15e+03	50.35	-7.47*
TOC	2	BX-107	2	6.75e+02	NA	0.00e+00	NA	NA
Al	2	C-110	3	1.43e+04	1.99	2.76e+04	17.38	2.77
Bi	2	C-110	3	1.37e+04	5.05	1.43e+04	15.35	0.26
Cr	2	C-110	3	4.64e+02	4.57	2.55e+02	27.31	-2.87
Cs-137	2	C-110	3	1.95e+01	12.97	6.12e+00	26.60	-4.45
F	2	C-110	3	7.63e+03	13.37	2.80e+03	54.48	-2.63
H2O	2	C-110	3	5.75e+01	3.60	6.92e+01	6.40	2.39
Mn	2	C-110	3	5.63e+01	12.61	0.00e+00	NA	NA

Table 7: *(continued)*

Analyte	Group	Tank	# of Cores	Sampling Est.	Sampling RSD	HTCE Est.	HTCE RSD	Comparison Statistic
NO3	2	C-110	3	1.10e+05	6.85	2.00e+04	27.00	-9.71*
Na	2	C-110	3	8.26e+04	3.54	9.00e+04	22.66	0.36
PO4	2	C-110	3	6.21e+04	5.37	9.82e+04	31.93	1.14
Si	2	C-110	3	7.16e+03	5.91	1.15e+03	50.35	-8.36*
TOC	2	C-110	3	8.02e+02	50.75	0.00e+00	NA	NA
Al	2	T-104	2	1.56e+04	12.12	2.36e+04	14.04	2.10
Bi	2	T-104	2	1.74e+04	6.32	1.17e+04	13.11	-3.02
Cr	2	T-104	2	8.67e+02	2.20	2.96e+02	18.99	-9.62*
Cs-137	2	T-104	2	1.99e-01	2.82	2.88e+01	14.43	6.88*
F	2	T-104	2	8.57e+03	1.91	NA	NA	NA
H2O	2	T-104	2	7.05e+01	0.28	7.24e+01	4.67	0.56
Mn	2	T-104	2	6.18e+01	4.09	0.00e+00	NA	NA
NO3	2	T-104	2	5.80e+04	1.30	2.31e+04	18.92	-7.87*
Na	2	T-104	2	6.21e+04	2.06	8.19e+04	19.90	1.21
PO4	2	T-104	2	7.56e+04	8.66	8.53e+04	29.04	0.38
Si	2	T-104	2	6.52e+03	2.79	9.80e+02	47.24	-11.14*
TOC	2	T-104	2	7.06e+02	NA	0.00e+00	NA	NA
Al	2	T-105	2	9.51e+04	58.78	4.76e+03	18.07	-1.62
Bi	2	T-105	2	1.22e+03	13.36	1.72e+04	17.47	5.31*
Cr	2	T-105	2	4.32e+02	41.67	2.84e+02	22.48	-0.77
Cs-137	2	T-105	2	4.92e+01	NA	1.43e+01	14.42	NA
F	2	T-105	2	NA	NA	NA	NA	NA
H2O	2	T-105	2	5.96e+01	48.17	6.90e+01	6.63	0.32
Mn	2	T-105	2	1.04e+04	72.60	0.00e+00	NA	NA
NO3	2	T-105	2	2.12e+04	26.89	4.08e+04	24.43	1.71
Na	2	T-105	2	4.92e+04	26.22	8.59e+04	27.62	1.36
PO4	2	T-105	2	4.68e+03	27.66	9.97e+04	33.49	2.84
Si	2	T-105	2	6.98e+03	11.23	1.78e+03	52.82	-4.24
TOC	2	T-105	2	4.13e+03	NA	0.00e+00	NA	NA
Al	2	T-107	2	1.63e+04	130.14	2.76e+04	17.38	0.52
Bi	2	T-107	2	1.20e+04	60.90	1.43e+04	15.35	0.30
Cr	2	T-107	2	3.60e+02	2.78	2.55e+02	27.31	-1.49
Cs-137	2	T-107	2	9.25e+00	59.57	6.12e+00	26.60	-0.54
F	2	T-107	2	1.14e+03	383.36	2.80e+03	54.48	0.36
H2O	2	T-107	2	4.98e+01	NA	6.92e+01	6.40	NA
Mn	2	T-107	2	2.13e+02	22.32	0.00e+00	NA	NA
NO3	2	T-107	2	7.45e+04	49.14	2.00e+04	27.00	-1.47
Na	2	T-107	2	1.17e+05	9.82	9.00e+04	22.66	-1.15
PO4	2	T-107	2	9.82e+04	5.14	9.82e+04	31.93	0.00
Si	2	T-107	2	6.06e+03	39.36	1.15e+03	50.35	-2.00
TOC	2	T-107	2	1.70e+03	30.90	0.00e+00	NA	NA
Al	2	U-110	7	1.50e+05	9.91	1.76e+04	15.50	-8.76*
Bi	2	U-110	7	2.06e+04	24.22	8.20e+03	13.63	-2.42
Cr	2	U-110	7	5.35e+02	21.37	3.33e+02	13.81	-1.64
Cs-137	2	U-110	7	2.82e+01	18.26	5.27e+01	12.78	2.89
F	2	U-110	7	7.05e+03	10.75	NA	NA	NA
H2O	2	U-110	7	3.15e+01	NA	7.51e+01	3.76	NA
Mn	2	U-110	7	3.46e+03	12.87	0.00e+00	NA	NA

Table 7: *(continued)*

Analyte	Group	Tank	# of Cores	Sampling Est.	Sampling RSD	HTCE Est.	HTCE RSD	Comparison Statistic
NO3	2	U-110	7	4.51e+04	8.73	2.57e+04	13.90	-3.65
Na	2	U-110	7	1.11e+05	7.12	7.23e+04	17.48	-2.60
PO4	2	U-110	7	4.67e+04	22.12	6.76e+04	28.39	0.96
Si	2	U-110	7	2.22e+04	32.67	7.26e+02	43.01	-2.96
TOC	2	U-110	7	9.55e+02	515.12	0.00e+00	NA	NA
Al	3	S-104	2	1.17e+05	1.11	8.74e+04	16.86	-2.00
Bi	3	S-104	2	NA	NA	0.00e+00	NA	NA
Cr	3	S-104	2	2.35e+03	3.80	2.35e+04	37.21	2.42
Cs-137	3	S-104	2	6.23e+01	2.99	4.70e+01	9.92	-3.05
F	3	S-104	2	1.45e+02	25.03	0.00e+00	NA	NA
H2O	3	S-104	2	4.29e+01	NA	6.57e+01	3.66	NA
Mn	3	S-104	2	1.15e+03	18.87	0.00e+00	NA	NA
NO3	3	S-104	2	1.91e+05	3.16	7.58e+04	11.37	-10.95*
Na	3	S-104	2	1.18e+05	1.41	3.94e+04	16.55	-11.68*
PO4	3	S-104	2	2.85e+00	NA	0.00e+00	NA	NA
Si	3	S-104	2	1.33e+03	9.25	7.85e+02	57.37	-1.17
TOC	3	S-104	2	1.73e+03	NA	0.00e+00	NA	NA
Al	3	U-204	3	2.21e+05	15.69	1.08e+05	36.41	-2.16
Bi	3	U-204	3	1.20e+03	68.61	0.00e+00	NA	NA
Cr	3	U-204	3	1.75e+02	28.81	2.20e+02	18.44	0.70
Cs-137	3	U-204	3	NA	NA	1.83e+00	18.41	NA
F	3	U-204	3	NA	NA	0.00e+00	NA	NA
H2O	3	U-204	3	2.60e+01	12.13	6.53e+01	15.18	3.78
Mn	3	U-204	3	8.20e+01	46.03	0.00e+00	NA	NA
NO3	3	U-204	3	NA	NA	3.14e+04	19.04	NA
Na	3	U-204	3	1.82e+04	19.79	5.26e+04	61.19	1.06
PO4	3	U-204	3	2.15e+03	55.43	0.00e+00	NA	NA
Si	3	U-204	3	2.38e+03	65.54	9.51e+02	57.22	-0.87
TOC	3	U-204	3	4.69e+02	73.67	0.00e+00	NA	NA

* : HTCE and Sampling estimates significantly different at the 95% confidence level
NA: Not Available or Not Applicable

Tables 8 and 9 summarize the results in Table 6 concisely. From Table 8, the following can be stated:

1. No tank had more than 4 significant differences among the available comparisons
2. 103 comparisons were available of the 144 possible comparisons
3. 75 of the 103 comparisons (73%) showed no distinguishable differences could be found between the two estimates; conversely, 28 of 103 (27%) showed significant differences between the two estimates.
4. All tanks showed no significant differences between the two estimates for at least 50% of the comparisons made. However, this does not necessarily indicate statistical agreement between the two methods for any particular analyte.

Table 8: Summary of Comparison Counts by Tank

Tank	Significant Differences	No Significant Differences	Not Applicable (NA)	Sampling > HTCE
B-110	4	5	3	5
B-111	4	6	2	7
B-201	4	5	3	6
T-111	3	7	2	6
BX-107	3	7	2	7
C-110	2	8	2	5
T-104	4	5	3	4
T-105	1	7	4	3
T-107	0	9	3	5
U-110	1	7	4	6
S-104	2	4	6	5
U-204	0	5	7	2
Total	28	75	41	61

Table 9: Summary of Comparison Counts by Analyte

Analyte	Significant Differences	No Significant Differences	Not Applicable	Sampling > HTCE
Al	2	7	3	5
Bi	2	8	2	5
Cr	6	6	0	10
Cs-137	3	6	3	7
F	0	6	6	3
H2O	0	9	3	2
Mn	2	0	10	2
NO3	5	6	1	8
Na	1	11	0	6
PO4	0	10	2	1
Si	5	6	1	11
TOC	2	0	10	1
Total	28	75	41	61

5 Summary and Conclusions

This study was conducted to help escalate the existing effort to characterize the contents of Hanford's waste tanks. Two independent approaches, one consisting of the actual tank sampling and the other based on the historical records, were compared and the following conclusions drawn.

1. In approximately one-fourth (27%) of the comparisons, there were significant differences between the HTCE and sampling estimates at the 95% confidence level. These differences could be due to atypical samples from the tanks. These differences could also be due to deflation of the uncertainties created for the HTCE, because the Monte Carlo simulations did not generate large enough uncertainties.

2. The sampling-based estimates were larger than the HTCE (historical records based) in the majority of cases where significant differences were found. This is evidenced in the following results:

   (a) 26 of the 28 significant differences showed sampling-based estimates to be larger than the HTCE (see Table 10).

   (b) The sampling-based estimates were larger than the HTCE in approximately 59% (61 out of 103) of the comparisons made, whether or not the differences were deemed significant (see Table 10).

   (c) The sampling-based estimates were generally larger than the HTCE for all the tanks in the study (i.e., for every tank, more than 50% of the sampling estimates were larger than the corresponding HTCE), with the exception of tanks T-105 and U-204 whether or not the differences were deemed significant (see Table 8).

   These results may indicate:

   (a) Additional waste stream source terms need to be considered in the HTCE model.

   (b) The waste is more concentrated (contains less water than is represented in the HTCE model).

   (c) The samples extracted are atypical of the waste as a whole in the tank. For example:

      i. The samples were taken through risers located near the inlet and outlet areas of the tank (which is the case for most of the tanks sampled in the Hanford area), and therefore biased the results, causing inflated concentrations in the sampling estimates.

      ii. These particular samples (from which the sampling estimates were derived) were extracted from an area of the tank (not necessarily near the inlet or outlet) that contains irregularly high concentrations of those particular constituents (that show significantly higher mean concentrations than the HTCE).

3. The sampling estimates were larger than the HTCE for chromium and silicon. This systematic bias could be explained in two ways:

   (a) It could be assumed that the sampling estimates are, indeed, correct and that the HTCE model is lacking chromium and silicon source terms.

   (b) The samples extracted are atypical of the waste as a whole in the tank.

4. Statistically, differences between the sampling estimates and the HTCE cannot be distinguished for water-soluble fluoride, water, total phosphate, and sodium (except for Tank S-104).

5. The HTCE model parameter influence study showed that varying the volume percent solids parameters always had the largest effect on the HTCE values. The parameters considered in this study were volume percent solids, limiting solubility and the waste stream source terms.

Table 10: Summary of Comparison Counts

	Number of Comparisons	Sampling > HTCE
Significant Differences	28	26
No Significant Differences	75	35
Total	103	61

Table 10, Table 8 (found in Section 4), and Table 9 (also found in Section 4) summarize the results of the comparison study.

In the cases where the sampling estimates were significantly higher than the historically based estimates, the HDW model could be missing source terms for certain analytes and therefore consistently underestimating the tank concentrations. This finding leads to the recommendation that improvements be made to the model to correct for this systematic bias. If these corrections to the model are successful, the overall effort of tank characterization will be facilitated. The sampling effort could be reduced in the future because the HDW model could reasonably predict a tank's contents simply from its historical information. It is recommended that this model improvement effort be pursued. On the other hand, the sampling estimates may be higher because the samples were extracted from areas of the tank that were highly concentrated in those analytes.

The results of this study complement the results of another study of tank grouping completed by Pacific Northwest Laboratory for Westinghouse Hanford Company[1]. This other study uses a statistical cluster analysis to group tanks naturally by their similarities in measured properties. Underlying this approach is the belief that tanks which are grouped together by the analysis will have similar concentrations for each analyte. The results of that grouping study, coupled with the results of this comparison of HTCE and sampling estimates, are contributing toward the overall effort of characterizing Hanford's population of waste tanks.

[1]Letter report written to Susan Eberlein of WHC entitled "Hanford Single Shell Tank Grouping Study" dated August 24, 1995.

References

[1] Agnew SF, Watkins JG, 1994. "Estimation of Limiting Solubilities for Ionic Species in Hanford Waste Tank Supernates," LAUR-94-3590, Los Alamos National Laboratories, Los Alamos, NM.

[2] Agnew SF, 1994. "Hanford Defined Wastes: Chemical and Radionuclide Compositions," LAUR-94-2657, Los Alamos National Laboratories, Los Alamos, NM.

[3] Amato LC, DeLorenzo DS, DiCenso AT, Rutherford JH, Stephens RH, Heasler PG, Brown TM, Simpson BC, 1994. "Tank Characterization Report for Single-Shell Tank 241-B-110," WHC-SD-WM-ER-368, Rev. 0. Westinghouse Hanford Company, Richland, WA.

[4] Amato LC, Nuttall GL, Johnson KW, Lambie RW, DiCenso AT, 1994. "Tank Characterization Report for Single-Shell Tank 241-C-110," WHC-SD-WM-ER-367, Rev 0, Westinghouse Hanford Company, Richland, WA.

[5] Brevick CH, Gaddis LA, Pickett WW, 1994. "Historical Tank Content Estimate for Northeast Quadrant of the Hanford 200 East Areas," WHC-SD-WM-ER-349, Westinghouse Hanford Company, Richland WA.

[6] Cromar RD, Wilmarth SR, Jensen L, 1994, "Statistical Characterization Report for Single- Shell Tank 241-T-104," WHC-SD-WM-TI-658, Rev 0, Westinghouse Hanford Company, Richland, WA.

[7] DiCenso AT, Amato LC, Franklin JD, Nuttall GL, Johnson KW, 1994. "Tank Characterization Report for Single-Shell Tank 241-S-104," WHC-SD-WM-ER-370, Rev 0, Westinghouse Hanford Company, Richland, WA.

[8] DiCenso AT, Amato LC, Franklin JD, Nuttall GL, Johnson KW, 1994. "Tank Characterization Report for Single-Shell Tank 241-T-105," WHC-SD-WM-ER-369, Rev 0, Westinghouse Hanford Company, Richland, WA.

[9] Heasler PG, Remund KM, Tingey JM, Baird DB, Ryan FM, 1994. "Tank Characterization Report for Single-Shell Tank B-201," PNL-10100/UC-2070, Pacific Northwest Laboratory, Richland, WA.

[10] Hill JG, Anderson GS, Simpson BC, 1995. "The Sort on Radioactive Waste Type Model: A Method to Sort Single-Shell Tanks into Characteristic Groups," PNL-9814, Rev 2, Pacific Northwest Laboratory, Richland WA.

[11] Jensen L, Remund KM, 1993. "Statistical Characterization Report For Single-Shell Tank 241-U-110," WHC-SD-WM-TI-560, Rev. 0, Westinghouse Hanford Company, Richland, WA.

[12] Jungfleisch FM and Simpson BC, 1993. "A Preliminary Estimation of the Waste Inventories in Hanford Tanks Through 1980," SD-WM-TI-057, Rev. 0-A, Westinghouse Hanford Company, Richland WA.

[13] Mendenhall W, Scheaffer RL, Wackerly DD, 1990. "Mathematical Statistics with Applications," PWS-Kent Publishing Company, Boston MA.

[14] Raphael, GF, 1995. "Tank Characterization Report for Single-Shell Tank 241-BX-107," WHC-EP-0739, Westinghouse Hanford Company, Richland, WA.

[15] Raphael, GF, Tran TT, 1994. "Tank Characterization Report for Single-Shell Tank 241-U-204," WHC-SD-WM-ER-486, Rev. 0, Westinghouse Hanford Company, Richland, WA.

[16] Remund, KM, Tingey JM, Heasler PG, Toth JJ, Ryan FM, Hartley SA, Simpson DB, Simpson BC, 1994. "Tank Characterization Report for Single-Shell Tank B-111," PNL-10099/UC-2070, Pacific Northwest Laboratory, Richland, WA.

[17] Shaver, RL, 1993. "PNL 325 Laboratories Single Shell Tank Waste Characterization, Tank B-201 Core 26 and 27," WHC-SD-WM-DP-037, Westinghouse Hanford Company, Richland WA.

[18] Simpson, BC, 1994. "Tank 241-T-111 Characterization Report," WHC-EP-0806, Westinghouse Hanford Company, Richland, WA.

[19] Valenzuela BD, Jensen L, 1994. "Tank Characterization Report for Single-Shell Tank 241-T-107," WHC-SD-ER-382, Rev. 0, Westinghouse Hanford Company, Richland, WA.

APPENDIX A

HTCE UNCERTAINTY ANALYSIS

A HTCE Uncertainty Analysis

To make statistical comparisons between two independent sets of estimates, some measure of the uncertainty in the estimates is required. This uncertainty reflects different sources of variability in the process of obtaining the estimates. Some of these sources include spatial variability (differences in sample properties due to the spatial position from which that sample was taken), and random and systematic error in the laboratory results for samples and duplicates. Estimates of uncertainty are provided in the TCRs for the sampling estimates. However, the HTCE do not have uncertainty estimates. This section describes the steps taken to estimate the HTCE uncertainties so that a statistical comparison can be made between the HTCE and sampling estimates. These steps involve factorial experiments and Monte Carlo studies, which are both described later in this section.

A.1 Potential Influential Model Parameters

The first step is to identify all parameters of the HTCE model that could contribute to the uncertainty in the HTCE. The following list of HTCE variance contributing parameters were identified, based on discussions with the staff at Los Alamos National Laboratory (LANL) and Westinghouse Hanford Company (WHC):

1. Percent solids in each waste stream, by volume
2. Limiting solubilities for the target analytes
3. Waste stream source terms
4. Unknown tank transfers.

This is not an all-inclusive list. Other parameters could contribute to the variability of the HTCE. The last item in the list, unknown tank transfers, is a significant candidate as a likely contributor to the random error and biases of the HTCE. Note that the HTCE model treats the volume percent solids and waste stream source term parameters as being specific to the waste types, whereas the limiting solubilities are considered the same for all waste types. A subject for future study would be defining limiting solubilities for specific waste types.

The list of parameters given above was later restricted to the limiting solubility, volume percent solids, and waste stream source term parameters. There were two reasons for this decision. First, LANL and WHC staff felt that these three parameters contribute most to the uncertainty of the HTCE. Second, sufficient information was available for these parameters to determine their probability distributions. The lack of available information on the fourth parameter, unknown tank transfers, precluded their consideration in this study.

A.2 Parameter Influence Study

The parameters selected for study include volume percent solids for each waste type, the largest waste stream source terms for each waste type, and the limiting solubilities for constituents of interest (assumes that the limiting solubility distributions are the same across all waste types). Varying all of these parameters in a Monte Carlo Study is difficult and probably unnecessary. A parameter influence study was first conducted to determine the subset of these parameters that significantly affects the concentrations of each target analyte.

Appendix B gives a simple example of a factorial experiment similar to the one used in this parameter influence study. This appendix also provides some details on the experimental setup and the analysis of results.

The following general conclusions were drawn from this factorial experiment:

1. The volume percent solids parameters nearly always had the largest effect on the HTCE for the target analytes.

2. The limiting solubility for the constituent of interest and the limiting solubilities for fluoride and phosphate were large contributors to the variability of the HTCE. In order of contribution, these limiting solubility parameters were usually second only to the volume percent solids parameters.

3. The waste stream source terms usually made only marginal contributions to the variability in the HTCE.

A.3 Monte Carlo Study Approach

The HTCE are obtained from a model that is built into a series of EXCEL[2] spreadsheets. These estimates do not have closed forms and must be obtained iteratively. Due to the complexity of these estimates, a straightforward explicit form for the uncertainty of the HTCE does not exist.

A common method of estimating the uncertainty in similar situations is a Monte Carlo simulation. Figure 6 illustrates how a Monte Carlo approach can be used to obtain the HTCE uncertainty estimates.

The solid box in the center of the figure represents the HTCE model. It is made up of the following model subcomponents which are described in Reference [2]:

1. Hanford Defined Wastes (HDW)

2. Waste Status and Transaction Record Summary (WSTRS)

3. Tank Layering Model (TLM)

As noted earlier, these model subcomponents are linked together in a series of spreadsheets.

The dashed line box above the HTCE model box represents the inputs to the HTCE model that are potential sources of variability in the estimates of the HTCE model outputs. In this set of HTCE model parameters, the subsets that are significant contributors and can be quantified are identified as 1, 2, 3, ..., n. A probability distribution is placed on each of these model parameters, based on any historical and chemical information that can be gathered. From each of these probability distributions, a large number of realizations are randomly generated and used as inputs into the HTCE model, and the HTCE outputs are recorded. In general, the different sources of variability are considered independently of each other.

The dashed box under the HTCE model in Figure 1 represents the distribution of HTCE model results from the Monte Carlo study. The variance of these model results is used as the uncertainty estimate of the HTCE.

A.4 Parameter Distributions

Probability distributions were defined for each of the HTCE model parameters, based upon historical sampling information and engineering judgment. These distributions are used in the Monte Carlo study (HTCE uncertainty analysis) to obtain randomly selected realizations of each of these model parameters.

Obtaining reasonable distributions for the HTCE model parameters is critical if realistic HTCE uncertainty estimates are to be obtained. If the information used to place distributions on the HTCE model parameters is inaccurate or incomplete, then the HTCE uncertainty estimates are also inaccurate or incomplete.

A.4.1 Limiting Solubility Distributions

Limiting solubility distributions for the parameters noted earlier were estimated using supernatant data provided in Reference [1]. The limiting solubilities were calculated in this referenced paper by calculating the mean after the lower 75% of the supernatant data had been removed for each analyte of interest. Following a similar pattern, the limiting solubility distributions were calculated for each target analyte in the present study by first placing a beta distribution ([13]) on all of the supernatant data; and then truncating the distribution so that the selected random values exceeded the 75th percentile from the distribution.

[2]EXCEL is a product of the Microsoft Corporation

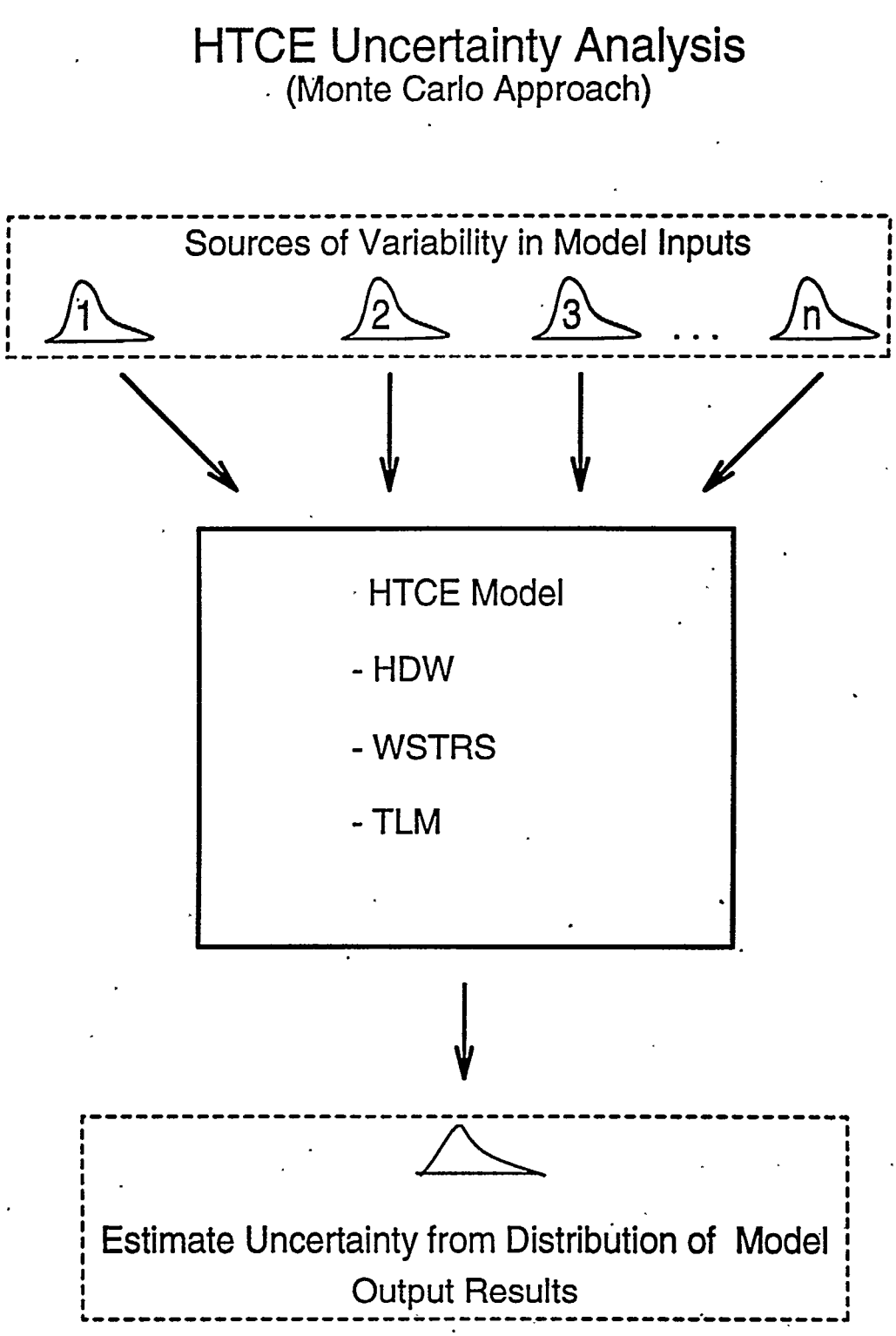


Figure 6: Monte Carlo Study Approach

Figure 7 illustrates this process for the limiting solubility distributions for phosphate and fluoride. The histograms represent the raw supernatant data. The solid curved lines that roughly mimic the histograms are the beta distributions that are placed on the data. The vertical dashed line is the 75th percentile from the beta distributions. Realizations were generated only from the upper tail of these distributions (i.e., the upper 25% of the probability distribution).

A.4.2 Volume Percent Solids Distributions

There is no sampling information available to aid in fitting probability distributions to the volume percent solids parameters s_v for each waste type. Based upon discussions with WHC staff, the following definitions were established for the volume percent solids parameter distributions of each waste type:

1. A minimum - s_v is certainly no lower than this value
2. A typical value - the value of s_v used in the HTCE model
3. 95th percentile - s_v is very unlikely to be higher than this value
4. A maximum - s_v is certainly no higher than this value.

The values of these characteristics for each waste type were supplied by WHC, based on process knowledge and engineering judgment, and are given in Table 11.

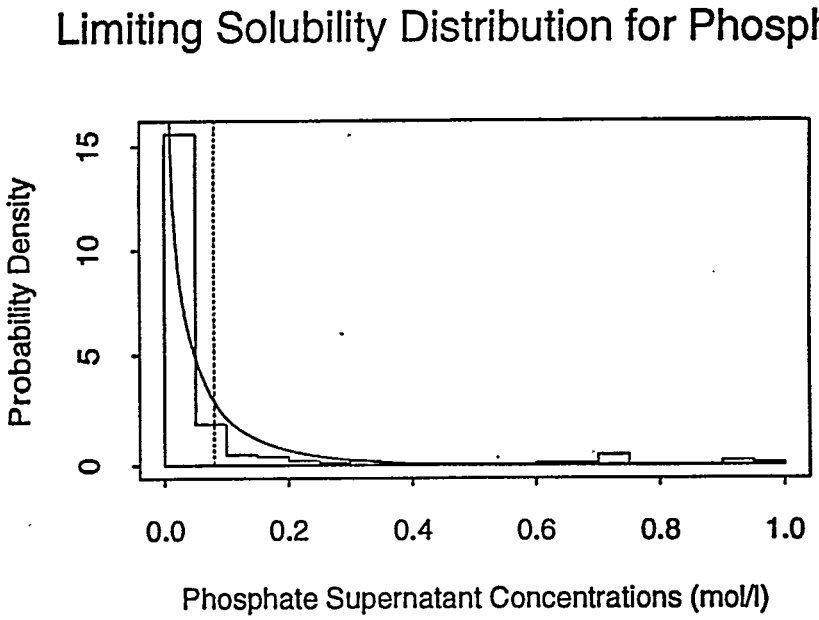
A beta probability distribution ([13]) was selected to simulate the behavior of volume percent solids parameters. The beta distribution is a reasonable choice because it can easily accommodate different data distribution shapes. As the parameters of the data distribution change, the beta distribution becomes symmetric, skewed left, or skewed right. The beta distribution thus appropriately represents the characteristics of volume percent solids parameters for different waste types. Furthermore, the range of a beta distribution is from zero to one, and is easily transformed to other ranges. A beta distribution for the volume percent solids parameter was determined according to the characteristics given in Table 11. The distribution was chosen such that it always fell within the range of the minimum and maximum values, provided the largest probability density at the typical value, and possessed the given 95th percentile. Figure 8 illustrates the volume percent solids beta distributions for 2C and 224 Wastes (Group 1).

Table 11: Characteristics of Volume Percent Solid Parameters

Waste Type	Min	Typical	95th	Max
2C	2.8	6.8	8.8	13.5
224	2.8	3.9	NA	13.5
1C/CW/44-51	6.8	13.7	19.0	25.0
1C/CW/52-56	12.0	25.0	27.0	31.0
R/52-58	3.5	8.9	12.5	15.0
CWR/Al/52-60	4.0	8.1	15.0	17.0
CWP/Zr/66-72	1.5	4.0	8.0	12.0

A.4.3 Waste Stream Source Term Distributions

There is little information available to help estimate the distributions for the waste stream source terms. For this reason, a very simple approach was used to obtain these distributions from the Hanford Defined Wastes (HDW) estimates given in Reference [2]. For each waste stream source term, a normal distribution was fit which had a mean equal to the HDW estimate and first and ninety-ninth percentiles equal to +/- 20% of the HDW estimate, respectively. The range of +/- 20% was considered reasonable because it is assumed that



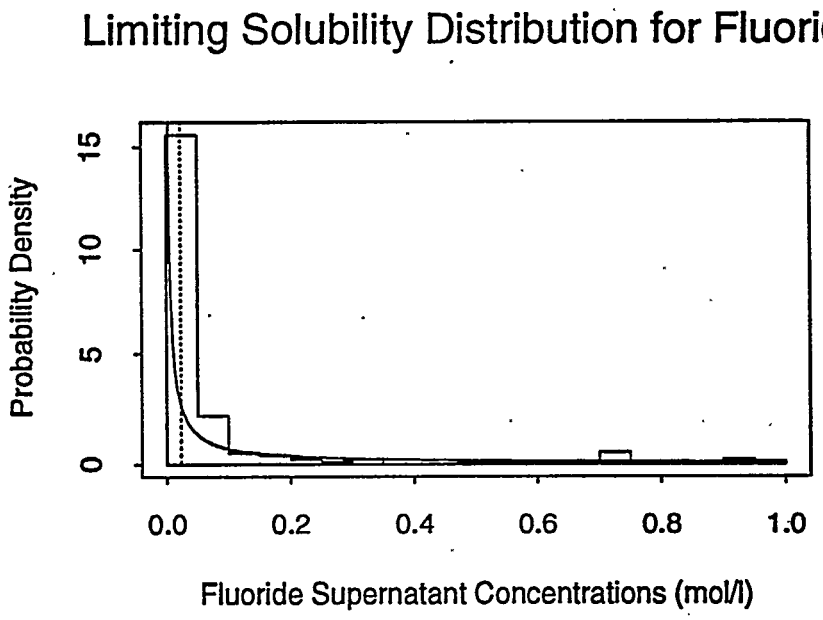
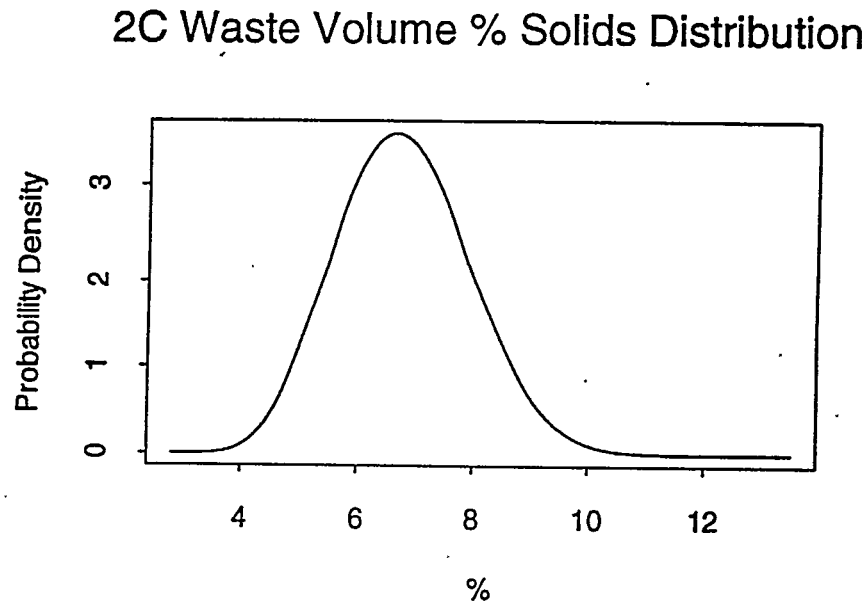


Figure 7: Limiting Solubility Distributions for Phosphate and Fluoride



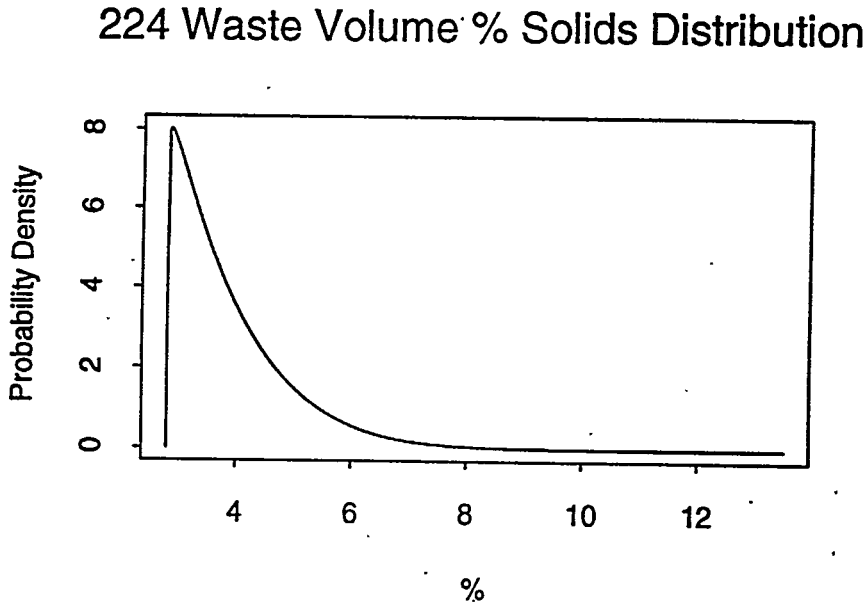


Figure 8: Volume % Solids Distributions for 2C and 224 Wastes

nearly all of the waste stream concentrations fall within those limits. Table 12 displays the source terms, their respective HDW values, and the first and ninety-ninth percentile values by waste type.

Table 12: Source Terms and Values by Waste Type

Waste Type	Source Terms	Hanford Defined Wastes Value mol/L	-20% mol/L	+20% mol/L
2C	HNO3	1.1500	0.9200	1.3800
	NaOH*	0.0400	0.0320	0.0480
	Na3PO4	0.2000	0.1600	0.2400
	NaF	0.2200	0.1760	0.2640
224	HNO3	1.0600	0.8480	1.2720
	NaOH*	0.0400	0.0320	0.0480
	NaF	0.3100	0.2480	0.3720
1C44-51/1C52-56	NaOH	0.0400	0.0320	0.0480
	HNO3	0.5000	0.4000	0.6000
	NaPO4	0.3100	0.2480	0.3720
	NaAlO2	0.2330	0.1864	0.2796
R'52-58	HNO3	2.3000	1.8400	2.7600
	NaAlO2	0.6500	0.5200	0.7800
	NaOH	1.9280	1.5424	2.3136
CWR/Al, 52-60	HNO3	0.8000	0.6400	0.9600
	NaAlO2	2.0000	1.6000	2.4000
	NaOH	0.5180	0.4144	0.6216
	NaNO2	1.4000	1.1200	1.6800
CWP/Zr, 66-72	NaOH*	0.0400	0.0320	0.0480
	NaF	0.7700	0.6160	0.9240
	KNO3	0.2200	0.1760	0.2640

*Note that, because of the solution chemistry of the waste material, the sodium hydroxide (NaOH) source term depends upon the ferric nitrate (Fe(NO3)3) source term. In the Monte Carlo study, the ferric nitrate parameter was therefore adjusted to obtain the desired NaOH values. The values shown in the last three columns are for ferric nitrate, not NaOH. This exception applies to 2C, 224, and CWP waste types; but not to 1C, R, or CWR waste types.

A.5 Monte Carlo Study Setup and Results

Given the probability distributions and variability estimates for the input parameters, the Monte Carlo study can be implemented. For a given target analyte, the following parameters were randomly varied in the Monte Carlo study:

1. Volume percent solids for each waste type
2. Important limiting solubilities (usually phosphate or fluoride)
3. Limiting solubility for the target analyte (if applicable)
4. Major waste stream source term parameters for each waste type.

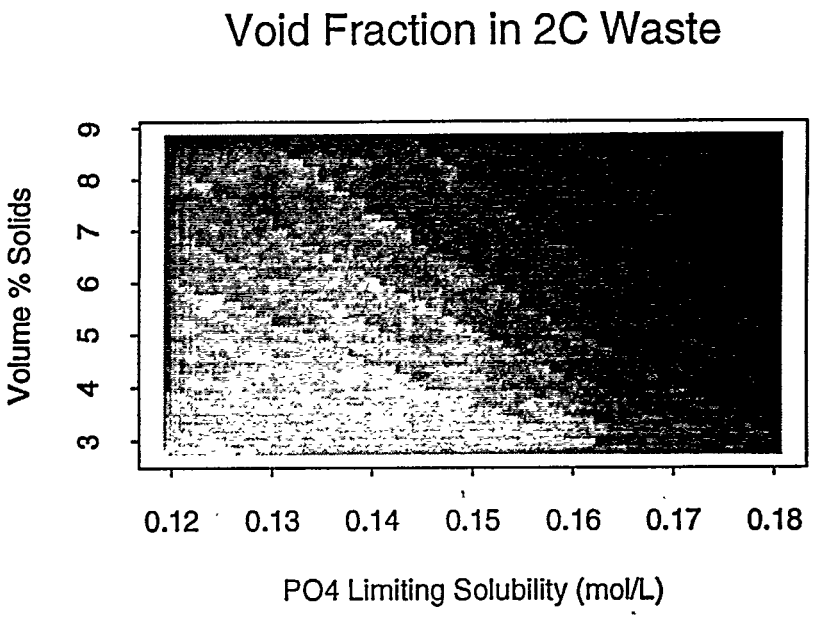
The random values were generated from each of these distributions independently of one another, with few exceptions. As an example, one exception was made for 2C waste. The factorial experiment showed that for 2C waste, when low volume percent solids values and low phosphate limiting solubility values were

paired together in the same run, void fractions below 0.4 occurred. Void fractions are measures of the total space between the grains that make up various sludges and slurries. The degree of packing within these sludges and slurries will have bearing on the concentration for any particular analyte. Since the materials being investigated are analogous to sludges and slurries, the lower boundary for is 0.4 (i.e., the void fraction lower boundary for sludges and slurries is 0.4). Discussions with LANL and WHC technical staff confirmed this. The relationships between volume percent solids, phosphate limiting solubility and void fraction can be seen in Figure 9. The upper part of the figure is an image plot of 2C Waste void fractions, as volume percent solids and limiting solubility for phosphate are varied together. Low void fractions are in the lightly shaded region at the bottom left-hand corner of the plot and high void fractions are in the dark region at the upper right-hand corner. The lower part of the figure is a contour plot of the 2C waste void fraction as the same two parameters are varied. A regression line was fit to the 0.4 void fraction contour. This regression equation was then used to discard random pairs of these two parameters that fell in the region below the 0.4 void fraction contour line.

Similar dependencies were found between volume percent solids, limiting solubility and waste stream source term parameters for both of the 1C/CW waste types. These dependencies were resolved in similar fashion, by excluding certain of the randomly generated values.

For each target analyte, 250 sets of random parameter values were generated. Each set of parameter values was run through the HTCE model in turn. The HTCE model was allowed to iterate until relative convergence was achieved, as indicated by the near-equality of successive solutions (convergence was usually achieved at 3 iterations, but 5 iterations were performed to ensure convergence).

The results were recorded and the variance of these results was used as the HTCE uncertainty estimate. These HTCE uncertainties are reported and discussed in Section 4.



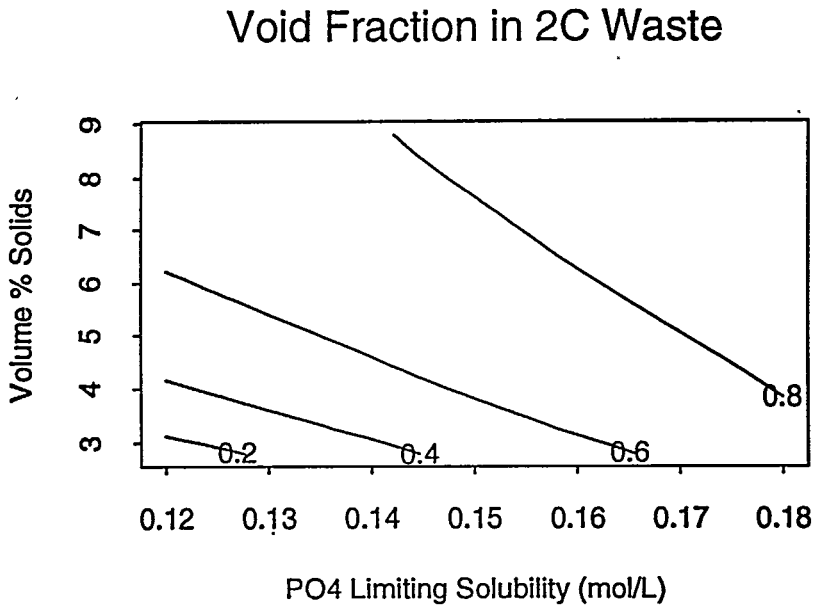


Figure 9: 2C Waste Void Fraction Plots

APPENDIX B

FACTORIAL EXPERIMENT EXAMPLE AND DETAILS

B Factorial Experiment Example and Details

Table 13 contains an example of a simple factorial experiment similar to the one described in Appendix A. In this example, the objective is to determine which of the three parameters shown in the table (i.e., limiting solubility for phosphate and volume percent solids for 2C and 224 Wastes) or which combination of these three parameters significantly affect the HTCE estimates of target analyte concentrations. High and low levels are assigned to each of the three parameters. All possible levels of these three parameters are included in the experiment. For this example, there are 2^3 or 8 possible combinations. These combinations would each in turn be input into the HTCE model. After each model run, the HTCE output values are recorded.

Table 13: Factorial Experiment Example

Run	L.S. PO4	Vol. % Sol. 2C	Vol. % Sol. 224
1	Low	Low	Low
2	Low	Low	High
3	Low	High	Low
4	Low	High	High
5	High	Low	Low
6	High	Low	High
7	High	High	Low
8	High	High	High

The model results from this factorial experiment would be analyzed using analysis of variance (ANOVA) to identify the significant parameters, which are then included in the uncertainty analysis for the HTCE.

This simple example has exactly the same setup as the factorial experiments that were run in the parameter influence studies described in this report — with one exception. Instead of three parameters of interest, there are nine in our study. To get all possible combinations of high and low levels for all nine parameters, 2^9 or 512 runs are required, rather than only 8 as in the example.

The high and low levels for the limiting solubility parameters included in the factorial experiment were the upper and lower 95% confidence limits from the upper 25% of the supernatant data for the given analyte, taken from Reference [1]. The high and low levels for the volume percent solids parameters were the two extremes that were used in the distribution fits for these parameters.

All 512 combinations of high and low parameter settings were run through the HTCE model and the results were recorded. ANOVA was used to determine which parameters and combinations of parameters significantly contributed to the HTCE variability for each target analyte. These were the parameters that were varied in the HTCE uncertainty analysis.

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