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Calculation of the Proportion of Reactive Waste for Hydrogen Ignition Scenario

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Summary

This study was conducted as outlined in NHC Letter of Instruction 9751330 dated February 24, 1997 and entitled "Analysis by Pacific Northwest National Laboratory to Support a Safety Assessment for Rotary Mode Core Sampling in Flammable Gas Watchlist Tanks." As prescribed in this letter, the results of this study were provided to Los Alamos National Laboratory (LANL) to revise the safety assessment document.

Sampling Hanford tanks with a rotary drill could result in a drill-bit overheating accident which could ignite flammable gases present in the tanks. According to calculations, an overheated drill bit could not get hot enough to ignite the hydrogen directly. However, an overheated drill bit could ignite saltcake waste containing high concentrations of organics, and a local organics burn would achieve sufficient temperature to ignite flammable gas present in the waste. This report estimates one quantity required to evaluate this particular accident scenario; the fraction of reactive waste in the tank waste. Reactive waste is waste that contains sufficient organic carbon and a low enough moisture content to ignite when in contact with an over-heated drill bit.

This report presents a methodology to calculate the proportion of reactive waste for the 100 series tanks, using sampling data from tank characterization studies. The tanks are ranked according to their reactive waste proportions, and confidence limits are assigned to the estimates.

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1 Introduction

One of the safety concerns regarding the Hanford waste storage tanks is the possibility of hydrogen ignition during sampling, due to a local non-propagating reaction. Such a reaction could be caused by rotary sampling drill failure in reactive waste. This drill failure could then cause localized drying of the waste which could in turn lead to a local non-propagating or propagating reaction. In this report, reactive waste is defined as saltcake or sludge waste that contains sufficient total organic carbon (TOC) and that can be dried enough to burn. The objective of this report is to calculate the proportion of reactive waste in the waste solids for each 100-series tank for this hydrogen scenario. These proportions are used to calculate the probability of a gas burn due to local overheating caused by rotary drill sampling.

The proportion of reactive waste in each tank can be calculated from the results of an earlier ANOVA study [4], which produced distributions of moisture content (H_2O) and TOC for every 100-series single-shell tank (SST). This ANOVA work is summarized in Section 2 of this report. Section 3 describes how these ANOVA estimates are used to calculate the proportions of reactive waste. Section 4 adds conservatism to this report by incorporating uncertainties into the calculations of reactive waste proportions. The final results of the reactive waste proportion calculations are also presented in Section 4.

This work is an extension of earlier work [2] which focused on the probability of ignition of reactive wastes by rotary sampling drills in saltcake tanks only, and for three different reactive waste regions. The results of the present study will be used to revise the safety assessment document [5].

2 ANOVA Model

A total of 787 H_2O and 376 TOC measurements were available for the ANOVA fits. The measurements for each location (i.e., the sub-surface or surface results for each riser) were averaged, reducing the number of data points for the ANOVA analysis to 206 and 268 for H_2O and TOC respectively. Table 2 summarizes the ANOVA data, showing the number of TOC and H_2O data points for the top layer (i.e., the upper 0.2 meters of solid waste) and bottom layer (the remaining waste below the top layer) of each tank. The tank group membership for both analytes is also shown. How these tank groups were derived is discussed later in this section. This data was originally compiled on July 24, 1996.

The data were analyzed using a random effects ANOVA model, which produces estimates of TOC and H_2O as well as statements of variability. The formula for the specific model for these analytes is:

$$Y_{ijkl} = \mu + D_i + G_j + DG_{ij} + T_{jk} + DT_{ijk} + E_{ijkl} \qquad (1)$$

where

Y_{ijkl} represents a log_{10}(TOC or H_2O) measurement (expressed in percent) taken under conditions $ijkl$,

μ is the grand mean for TOC or H_2O,

D_i is the tank layer i effect (top or bottom),

G_j is the tank group j effect,

DG_{ij} is an interaction effect of layer i and group j,

T_{jk} is the effect of tank k in group j,

DT_{ijk} is an interaction effect of layer i and tank k in group j,

E_{ijkl} identifies the "replicate" measurements that were made within a layer in a specific tank.

The ANOVA fitting procedure will produce estimates for all the unknown terms in the above equation. Since the terms are considered to be random variables, the fitting procedure also calculates their variances (such as $Var(E_{ijkl}) = \sigma_E^2$, $Var(T_{jk}) = \sigma_T^2$, etc.). These term variance estimates, along with the overall mean estimate for TOC and H_2O, are given in Table 1. The total number of observations for each combination of constituent and tank layer are also given in the table. Note that the variance estimates for σ_{DG}^2 are essentially zero. These variances are used in the ANOVA procedure to calculate uncertainties in the TOC and H_2O estimates.

Table 1: ANOVA Model Parameter Estimates

Parameter Estimates	Log_{10}(TOC)	$Log_{10}(H_2O)$
$\hat{\mu}$	-8.11e-01	1.50e+00
$\hat{\sigma}_D$	1.33e-01	8.12e-02
$\hat{\sigma}_G$	2.94e-01	9.42e-02
$\hat{\sigma}_T$	3.07e-01	8.41e-02
$\hat{\sigma}_{DG}$	1.92e-17	3.25e-14
$\hat{\sigma}_{DT}$	1.65e-01	1.82e-01
$\hat{\sigma}_E$	3.14e-01	1.75e-01
#Obs Top	50	73
#Obs Bottom	218	133

For a tank with data, the "best estimate" for TOC in the top layer of tank k from group j is

$$\hat{\mu}_{top,j,k} = \hat{\mu} + \hat{D}_{top} + \hat{G}_j + \hat{DG}_{top,j} + \hat{T}_{j,k} + \hat{DT}_{top,j,k} \tag{2}$$

while for a tank without data, the "best estimate" for tank k in group j is

$$\hat{\mu}_{top,j,k} = \hat{\mu} + \hat{D}_{top} + \hat{G}_j + \hat{DG}_{top,j}. \tag{3}$$

The latter estimate's uncertainty is inflated by the amount $\sigma_T^2 + \sigma_{DT}^2$. Estimates for the bottom tank layer are calculated in a similar fashion. These constituent estimates for the top and bottom tank layers are provided in Tables 3 and 4 respectively, for all 100-series SSTs. The parameter estimates in these tables are used in Section 3 to specify the log-normal distributions which are in turn used to calculate the proportion of reactive waste in each tank.

2.1 Tank Groups

Tank groups (as identified by index j) were introduced into the ANOVA model to allow prediction of the constituents in unmeasured tanks. Tanks were grouped into three categories for the TOC analysis, based on the chemistry of the principal waste streams contained in the tank (as defined by Agnew). The three categories for the TOC analysis are:

Complexant Tanks: The principal waste stream in the tank contains TOC in complexant form.

Solvent Tanks: The principal waste stream in the tank contains organic solvents.

Non-TOC Tanks: The principal waste stream in the tank contains no organics.

Three categories cannot predict TOC perfectly. For example, a "Non-TOC" tank might still contain TOC because secondary waste streams contain TOC or because of errors in the historical record. Splitting the tanks into more categories would decrease the within-group variation, but would also decrease the data available to estimate TOC for each group. Given this constraint (i.e., data must exist to describe TOC in each group), it was decided to limit the categories to the three described above.

A different tank grouping was used for the H_2O ANOVA model. There are four tank group categories for H_2O. Wastes were assigned to these groups according to their surface dryness and average particle size. Particle size in the waste determines its liquid retention ability. The four groups were defined as follows:

Group I: A small liquid retention capability, large particle size, and dry surface.

Group II: A large liquid retention capability, small particle size, and dry surface.

Group III: A small liquid retention capability, large particle size, and wet surface.

Group IV: A large liquid retention capability, small particle size, and wet surface.

For these group definitions, a large particle size means an average diameter greater than 150 microns. Tanks with wet surfaces are those that showed standing liquid in tank photographs.

Table 2: ANOVA Data Summary

Tank	TOC Data Summary Bottom #Obs	TOC Top #Obs	TOC Group	H_2O Data Summary Bottom #Obs	H_2O Top #Obs	H_2O Group
B103	0	1	complexant	0	2	ii
B106	0	0	complexant	0	0	ii
B108	0	0	complexant	0	0	ii
B109	0	0	complexant	0	0	ii
B112	0	0	complexant	0	2	iv
BX101	0	0	complexant	0	2	ii
BX102	0	0	complexant	0	0	ii
BX103	0	0	complexant	2	2	iv
BX105	1	0	complexant	0	2	iv
BX106	0	0	complexant	0	0	iv
BX110	2	2	complexant	1	2	iv
BX112	2	0	complexant	2	0	ii
SX107	0	0	complexant	0	0	ii
SX108	0	0	complexant	0	0	ii
SX110	0	0	complexant	0	0	ii
SX111	0	0	complexant	0	0	ii
SX112	0	0	complexant	0	0	ii
SX113	0	0	complexant	0	2	ii
SX114	0	0	complexant	0	0	ii
SX115	0	0	complexant	0	0	ii
T101	0	0	complexant	0	0	ii
T102	1	0	complexant	0	0	iv
T103	0	0	complexant	0	0	iv
T105	2	5	complexant	0	1	ii
T106	0	0	complexant	0	2	ii
T107	18	4	complexant	17	4	iv
T108	0	0	complexant	0	2	ii
T109	0	0	complexant	0	0	ii
TX103	0	0	complexant	0	0	ii
TY101	1	0	complexant	0	0	ii
U101	0	0	complexant	0	0	iv
U110	27	6	complexant	27	6	ii
U112	0	0	complexant	0	0	iv
A101	2	0	solvent	2	0	i
A102	2	0	solvent	2	2	iii
A103	2	0	solvent	2	0	iv
A104	0	0	solvent	0	0	ii
A105	0	0	solvent	0	0	ii

Table 2: ANOVA Data Summary

Tank	TOC Data Summary Bottom #Obs	TOC Data Summary Top #Obs	TOC Data Summary Group	H_2O Data Summary Bottom #Obs	H_2O Data Summary Top #Obs	H_2O Data Summary Group
A106	2	0	solvent	2	0	ii
AX101	0	0	solvent	0	0	i
AX102	0	2	solvent	0	2	ii
AX103	0	0	solvent	0	0	ii
AX104	0	0	solvent	0	0	ii
B101	0	0	solvent	0	0	ii
B102	0	0	solvent	0	1	iv
B105	0	0	solvent	0	0	ii
BX104	3	0	solvent	0	0	iv
BX109	0	0	solvent	0	0	ii
BX111	1	0	solvent	1	0	i
BY101	0	0	solvent	0	0	i
BY102	0	0	solvent	0	0	i
BY103	0	0	solvent	0	2	i
BY104	0	0	solvent	0	0	i
BY105	0	0	solvent	0	0	i
BY106	29	0	solvent	27	0	i
BY107	0	0	solvent	0	0	i
BY108	0	0	solvent	0	0	i
BY109	0	0	solvent	0	0	i
BY110	0	0	solvent	0	0	i
BY111	0	0	solvent	0	0	i
BY112	0	0	solvent	0	0	i
C101	0	0	solvent	0	1	ii
C102	0	0	solvent	0	0	ii
C103	4	0	solvent	2	0	iv
C104	1	0	solvent	0	0	ii
C105	2	0	solvent	2	2	ii
C106	2	0	solvent	0	0	iv
C107	0	0	solvent	0	0	ii
C108	0	7	solvent	0	3	ii
C109	9	3	solvent	3	3	iv
C110	6	0	solvent	3	1	iv
C112	16	5	solvent	10	3	ii
S101	0	0	solvent	0	0	iii
S102	0	0	solvent	0	0	i
S103	0	0	solvent	0	0	iii
S104	9	0	solvent	6	3	ii

Table 2: ANOVA Data Summary

Tank	TOC Data Summary Bottom #Obs	TOC Top #Obs	TOC Group	H_2O Data Summary Bottom #Obs	H_2O Top #Obs	H_2O Group
S105	0	0	solvent	0	0	i
S106	0	0	solvent	0	0	iii
S107	0	0	solvent	0	0	iv
S108	0	0	solvent	0	0	i
S109	2	0	solvent	0	0	i
S110	0	0	solvent	0	0	i
S111	3	0	solvent	3	0	iii
S112	0	0	solvent	0	0	i
SX101	0	0	solvent	0	0	iii
SX102	1	1	solvent	0	0	iii
SX103	0	0	solvent	0	0	i
SX104	0	0	solvent	0	0	iii
SX105	0	0	solvent	0	0	iii
SX106	0	0	solvent	0	0	iii
SX109	0	0	solvent	0	0	i
T110	0	0	solvent	0	0	iv
T111	8	0	solvent	2	2	iv
TX101	0	0	solvent	0	0	ii
TX102	0	1	solvent	0	1	ii
TX104	0	0	solvent	0	0	ii
TX105	0	0	solvent	0	0	ii
TX106	0	0	solvent	0	0	ii
TX107	0	0	solvent	0	0	ii
TX108	0	0	solvent	0	0	ii
TX109	0	0	solvent	0	0	i
TX110	0	0	solvent	0	0	ii
TX111	0	0	solvent	0	0	ii
TX112	0	0	solvent	0	0	ii
TX113	0	0	solvent	0	0	ii
TX114	0	0	solvent	0	0	ii
TX115	0	0	solvent	0	0	ii
TX116	0	0	solvent	0	0	i
TX117	0	0	solvent	0	0	ii
TX118	0	1	solvent	0	0	ii
TY102	1	1	solvent	0	1	ii
TY103	2	1	solvent	1	1	ii
TY104	4	4	solvent	2	3	iv
TY105	1	0	solvent	1	0	ii

Table 2: ANOVA Data Summary

Tank	TOC Data Summary Bottom #Obs	Top #Obs	Group	H_2O Data Summary Bottom #Obs	Top #Obs	Group
TY106	4	1	solvent	2	3	ii
U102	0	0	solvent	0	0	iv
U103	1	0	solvent	1	0	iii
U104	0	0	solvent	0	0	ii
U105	1	1	solvent	0	1	iii
U106	0	0	solvent	0	0	iii
U107	0	0	solvent	0	0	iii
U108	0	0	solvent	0	0	iii
U109	0	0	solvent	0	0	iii
U111	0	2	solvent	0	1	i
B104	0	0	non-toc	2	2	ii
B107	0	0	non-toc	0	0	ii
B110	14	0	non-toc	0	0	iv
B111	13	0	non-toc	0	0	iv
BX107	12	0	non-toc	6	0	ii
BX108	0	0	non-toc	0	2	ii
C111	0	1	non-toc	0	2	ii
T104	7	1	non-toc	2	2	iv
T112	0	0	non-toc	0	0	iv

Table 3: Top Layer Parameters for TOC and Moisture Distributions (Log base 10)

	TOC Parameters				H_2O Parameters				
	— μ_2 —		— σ_2 —		— μ_1 —		— σ_1 —		ρ
Tank	Est	StdErr	Est	DOF	Est	StdErr	Est	DOF	Est
A101	-0.18	0.27	0.31	210	1.44	0.21	0.18	144	0.35
A102	-0.16	0.27	0.31	210	1.47	0.11	0.18	144	0.35
A103	-0.15	0.27	0.31	210	1.53	0.20	0.18	144	0.35
A104	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
A105	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
A106	-0.19	0.27	0.31	210	1.49	0.20	0.18	144	0.35
AX101	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
AX102	0.41	0.19	0.31	210	1.48	0.11	0.18	144	0.35
AX103	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
AX104	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
B101	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
B102	-0.42	0.36	0.31	210	1.37	0.13	0.18	144	0.35
B103	-1.01	0.24	0.31	210	1.60	0.11	0.18	144	0.35
B104	-0.94	0.38	0.31	210	1.64	0.11	0.18	144	0.35
B105	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
B106	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
B107	-0.94	0.38	0.31	210	1.48	0.21	0.18	144	0.35
B108	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
B109	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
B110	-1.17	0.24	0.31	210	1.53	0.21	0.18	144	0.35
B111	-0.84	0.24	0.31	210	1.53	0.21	0.18	144	0.35
B112	-0.81	0.37	0.31	210	1.59	0.11	0.18	144	0.35
BX101	-0.81	0.37	0.31	210	1.33	0.11	0.18	144	0.35
BX102	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
BX103	-0.81	0.37	0.31	210	1.71	0.11	0.18	144	0.35
BX104	-0.40	0.26	0.31	210	1.53	0.21	0.18	144	0.35
BX105	-0.71	0.30	0.31	210	1.22	0.11	0.18	144	0.35
BX106	-0.81	0.37	0.31	210	1.53	0.21	0.18	144	0.35
BX107	-0.99	0.25	0.31	210	1.50	0.20	0.18	144	0.35
BX108	-0.94	0.38	0.31	210	1.30	0.11	0.18	144	0.35
BX109	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
BX110	-0.70	0.17	0.31	210	1.39	0.11	0.18	144	0.35
BX111	-0.69	0.29	0.31	210	1.45	0.21	0.18	144	0.35
BX112	-0.53	0.28	0.31	210	1.50	0.20	0.18	144	0.35
BY101	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
BY102	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
BY103	-0.42	0.36	0.31	210	1.33	0.11	0.18	144	0.35

Table 3: Top Layer Parameters for TOC and Moisture Distributions (Log base 10)

	TOC Parameters				H_2O Parameters				
	— μ_2 —		— σ_2 —		— μ_1 —		— σ_1 —		ρ
Tank	Est	StdErr	Est	DOF	Est	StdErr	Est	DOF	Est
BY104	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
BY105	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
BY106	-0.56	0.24	0.31	210	1.40	0.21	0.18	144	0.35
BY107	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
BY108	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
BY109	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
BY110	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
BY111	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
BY112	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
C101	-0.42	0.36	0.31	210	1.42	0.13	0.18	144	0.35
C102	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
C103	-0.22	0.26	0.31	210	1.55	0.20	0.18	144	0.35
C104	-0.32	0.29	0.31	210	1.48	0.21	0.18	144	0.35
C105	-0.43	0.27	0.31	210	1.55	0.11	0.18	144	0.35
C106	-0.49	0.27	0.31	210	1.53	0.21	0.18	144	0.35
C107	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
C108	-0.85	0.11	0.31	210	1.51	0.09	0.18	144	0.35
C109	-0.52	0.15	0.31	210	1.55	0.09	0.18	144	0.35
C110	-0.79	0.25	0.31	210	1.67	0.13	0.18	144	0.35
C111	-1.00	0.24	0.31	210	1.52	0.11	0.18	144	0.35
C112	-0.27	0.12	0.31	210	1.66	0.09	0.18	144	0.35
S101	-0.42	0.36	0.31	210	1.36	0.22	0.18	144	0.35
S102	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
S103	-0.42	0.36	0.31	210	1.36	0.22	0.18	144	0.35
S104	-0.67	0.24	0.31	210	1.57	0.09	0.18	144	0.35
S105	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
S106	-0.42	0.36	0.31	210	1.36	0.22	0.18	144	0.35
S107	-0.42	0.36	0.31	210	1.53	0.21	0.18	144	0.35
S108	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
S109	-0.83	0.27	0.31	210	1.44	0.22	0.18	144	0.35
S110	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
S111	-0.15	0.26	0.31	210	1.32	0.21	0.18	144	0.35
S112	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
SX101	-0.42	0.36	0.31	210	1.36	0.22	0.18	144	0.35
SX102	-0.30	0.22	0.31	210	1.36	0.22	0.18	144	0.35
SX103	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
SX104	-0.42	0.36	0.31	210	1.36	0.22	0.18	144	0.35

Table 3: Top Layer Parameters for TOC and Moisture Distributions (Log base 10)

	TOC Parameters				H_2O Parameters				
	— μ_2 —		— σ_2 —		— μ_1 —		— σ_1 —		ρ
Tank	Est	StdErr	Est	DOF	Est	StdErr	Est	DOF	Est
SX105	-0.42	0.36	0.31	210	1.36	0.22	0.18	144	0.35
SX106	-0.42	0.36	0.31	210	1.36	0.22	0.18	144	0.35
SX107	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
SX108	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
SX109	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
SX110	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
SX111	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
SX112	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
SX113	-0.81	0.37	0.31	210	1.62	0.11	0.18	144	0.35
SX114	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
SX115	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
T101	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
T102	-0.89	0.30	0.31	210	1.53	0.21	0.18	144	0.35
T103	-0.81	0.37	0.31	210	1.53	0.21	0.18	144	0.35
T104	-0.88	0.20	0.31	210	1.61	0.11	0.18	144	0.35
T105	-0.60	0.13	0.31	210	1.61	0.13	0.18	144	0.35
T106	-0.81	0.37	0.31	210	1.30	0.11	0.18	144	0.35
T107	-0.98	0.13	0.31	210	1.30	0.08	0.18	144	0.35
T108	-0.81	0.37	0.31	210	1.00	0.11	0.18	144	0.35
T109	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
T110	-0.42	0.36	0.31	210	1.53	0.21	0.18	144	0.35
T111	-0.36	0.25	0.31	210	1.81	0.11	0.18	144	0.35
T112	-0.94	0.38	0.31	210	1.53	0.21	0.18	144	0.35
TX101	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
TX102	-0.59	0.24	0.31	210	1.58	0.13	0.18	144	0.35
TX103	-0.81	0.37	0.31	210	1.48	0.21	0.18	144	0.35
TX104	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
TX105	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
TX106	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
TX107	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
TX108	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
TX109	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
TX110	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
TX111	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
TX112	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
TX113	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
TX114	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35

Table 3: Top Layer Parameters for TOC and Moisture Distributions (Log base 10)

	TOC Parameters				H_2O Parameters				
	— μ_2 —		— σ_2 —		— μ_1 —		— σ_1 —		ρ
Tank	Est	StdErr	Est	DOF	Est	StdErr	Est	DOF	Est
TX115	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
TX116	-0.42	0.36	0.31	210	1.44	0.22	0.18	144	0.35
TX117	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
TX118	-0.18	0.24	0.31	210	1.48	0.21	0.18	144	0.35
TY101	-0.89	0.30	0.31	210	1.48	0.21	0.18	144	0.35
TY102	-0.72	0.22	0.31	210	1.64	0.13	0.18	144	0.35
TY103	-0.77	0.21	0.31	210	1.62	0.13	0.18	144	0.35
TY104	-0.60	0.13	0.31	210	1.68	0.09	0.18	144	0.35
TY105	-0.64	0.29	0.31	210	1.48	0.20	0.18	144	0.35
TY106	-0.74	0.20	0.31	210	1.52	0.09	0.18	144	0.35
U101	-0.81	0.37	0.31	210	1.53	0.21	0.18	144	0.35
U102	-0.42	0.36	0.31	210	1.53	0.21	0.18	144	0.35
U103	-0.24	0.29	0.31	210	1.31	0.21	0.18	144	0.35
U104	-0.42	0.36	0.31	210	1.48	0.21	0.18	144	0.35
U105	0.21	0.22	0.31	210	1.34	0.14	0.18	144	0.35
U106	-0.42	0.36	0.31	210	1.36	0.22	0.18	144	0.35
U107	-0.42	0.36	0.31	210	1.36	0.22	0.18	144	0.35
U108	-0.42	0.36	0.31	210	1.36	0.22	0.18	144	0.35
U109	-0.42	0.36	0.31	210	1.36	0.22	0.18	144	0.35
U110	-1.12	0.11	0.31	210	0.82	0.07	0.18	144	0.35
U111	-0.32	0.19	0.31	210	1.52	0.14	0.18	144	0.35
U112	-0.81	0.37	0.31	210	1.53	0.21	0.18	144	0.35

Table 4: Bottom Layer Parameters for TOC and Moisture Distributions (Log base 10)

	TOC Parameters				H_2O Parameters				
	— μ_2 —		— σ_2 —		— μ_1 —		— σ_1 —		ρ
Tank	Est	StdErr	Est	DOF	Est	StdErr	Est	DOF	Est
A101	-0.28	0.19	0.31	210	1.57	0.11	0.18	144	0.35
A102	-0.26	0.19	0.31	210	1.52	0.11	0.18	144	0.35
A103	-0.25	0.19	0.31	210	1.61	0.11	0.18	144	0.35
A104	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
A105	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
A106	-0.30	0.19	0.31	210	1.63	0.11	0.18	144	0.35
AX101	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
AX102	0.05	0.27	0.31	210	1.58	0.20	0.18	144	0.35
AX103	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
AX104	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
B101	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
B102	-0.60	0.36	0.31	210	1.61	0.21	0.18	144	0.35
B103	-1.13	0.30	0.31	210	1.60	0.20	0.18	144	0.35
B104	-1.12	0.38	0.31	210	1.65	0.11	0.18	144	0.35
B105	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
B106	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
B107	-1.12	0.38	0.31	210	1.58	0.21	0.18	144	0.35
B108	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
B109	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
B110	-1.41	0.08	0.31	210	1.64	0.21	0.18	144	0.35
B111	-0.98	0.09	0.31	210	1.64	0.21	0.18	144	0.35
B112	-0.98	0.37	0.31	210	1.64	0.20	0.18	144	0.35
BX101	-0.98	0.37	0.31	210	1.56	0.20	0.18	144	0.35
BX102	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
BX103	-0.98	0.37	0.31	210	1.55	0.11	0.18	144	0.35
BX104	-0.57	0.16	0.31	210	1.64	0.21	0.18	144	0.35
BX105	-0.85	0.24	0.31	210	1.58	0.20	0.18	144	0.35
BX106	-0.98	0.37	0.31	210	1.64	0.21	0.18	144	0.35
BX107	-1.17	0.09	0.31	210	1.70	0.07	0.18	144	0.35
BX108	-1.12	0.38	0.31	210	1.55	0.20	0.18	144	0.35
BX109	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
BX110	-1.18	0.17	0.31	210	1.67	0.13	0.18	144	0.35
BX111	-0.94	0.24	0.31	210	1.64	0.14	0.18	144	0.35
BX112	-0.63	0.19	0.31	210	1.71	0.11	0.18	144	0.35
BY101	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
BY102	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
BY103	-0.60	0.36	0.31	210	1.52	0.21	0.18	144	0.35

Table 4: Bottom Layer Parameters for TOC and Moisture Distributions (Log base 10)

	TOC Parameters				H_2O Parameters				
	— μ_2 —		— σ_2 —		— μ_1 —		— σ_1 —		ρ
Tank	Est	StdErr	Est	DOF	Est	StdErr	Est	DOF	Est
BY104	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
BY105	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
BY106	-0.77	0.06	0.31	210	1.36	0.03	0.18	144	0.35
BY107	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
BY108	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
BY109	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
BY110	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
BY111	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
BY112	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
C101	-0.60	0.36	0.31	210	1.57	0.20	0.18	144	0.35
C102	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
C103	-0.34	0.14	0.31	210	1.71	0.11	0.18	144	0.35
C104	-0.46	0.24	0.31	210	1.58	0.21	0.18	144	0.35
C105	-0.60	0.19	0.31	210	1.42	0.11	0.18	144	0.35
C106	-0.68	0.19	0.31	210	1.64	0.21	0.18	144	0.35
C107	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
C108	-0.93	0.24	0.31	210	1.59	0.20	0.18	144	0.35
C109	-0.57	0.10	0.31	210	1.54	0.09	0.18	144	0.35
C110	-1.06	0.12	0.31	210	1.74	0.09	0.18	144	0.35
C111	-1.16	0.30	0.31	210	1.59	0.20	0.18	144	0.35
C112	-0.56	0.07	0.31	210	1.68	0.05	0.18	144	0.35
S101	-0.60	0.36	0.31	210	1.46	0.22	0.18	144	0.35
S102	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
S103	-0.60	0.36	0.31	210	1.46	0.22	0.18	144	0.35
S104	-0.91	0.10	0.31	210	1.63	0.07	0.18	144	0.35
S105	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
S106	-0.60	0.36	0.31	210	1.46	0.22	0.18	144	0.35
S107	-0.60	0.36	0.31	210	1.64	0.21	0.18	144	0.35
S108	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
S109	-1.12	0.19	0.31	210	1.54	0.22	0.18	144	0.35
S110	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
S111	-0.24	0.16	0.31	210	1.24	0.09	0.18	144	0.35
S112	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
SX101	-0.60	0.36	0.31	210	1.46	0.22	0.18	144	0.35
SX102	-0.56	0.21	0.31	210	1.46	0.22	0.18	144	0.35
SX103	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
SX104	-0.60	0.36	0.31	210	1.46	0.22	0.18	144	0.35

Table 4: Bottom Layer Parameters for TOC and Moisture Distributions (Log base 10)

	TOC Parameters				H_2O Parameters				
	— μ_2 —		— σ_2 —		— μ_1 —		— σ_1 —		ρ
Tank	Est	StdErr	Est	DOF	Est	StdErr	Est	DOF	Est
SX105	-0.60	0.36	0.31	210	1.46	0.22	0.18	144	0.35
SX106	-0.60	0.36	0.31	210	1.46	0.22	0.18	144	0.35
SX107	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
SX108	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
SX109	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
SX110	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
SX111	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
SX112	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
SX113	-0.98	0.37	0.31	210	1.61	0.20	0.18	144	0.35
SX114	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
SX115	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
T101	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
T102	-1.09	0.24	0.31	210	1.64	0.21	0.18	144	0.35
T103	-0.98	0.37	0.31	210	1.64	0.21	0.18	144	0.35
T104	-1.25	0.11	0.31	210	1.77	0.11	0.18	144	0.35
T105	-0.70	0.17	0.31	210	1.61	0.20	0.18	144	0.35
T106	-0.98	0.37	0.31	210	1.55	0.20	0.18	144	0.35
T107	-1.15	0.07	0.31	210	1.69	0.04	0.18	144	0.35
T108	-0.98	0.37	0.31	210	1.50	0.20	0.18	144	0.35
T109	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
T110	-0.60	0.36	0.31	210	1.64	0.21	0.18	144	0.35
T111	-0.51	0.11	0.31	210	1.82	0.11	0.18	144	0.35
T112	-1.12	0.38	0.31	210	1.64	0.21	0.18	144	0.35
TX101	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
TX102	-0.72	0.29	0.31	210	1.60	0.20	0.18	144	0.35
TX103	-0.98	0.37	0.31	210	1.58	0.21	0.18	144	0.35
TX104	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
TX105	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
TX106	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
TX107	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
TX108	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
TX109	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
TX110	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
TX111	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
TX112	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
TX113	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
TX114	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35

Table 4: Bottom Layer Parameters for TOC and Moisture Distributions (Log base 10)

	TOC Parameters				H_2O Parameters				
	— μ_2 —		— σ_2 —		— μ_1 —		— σ_1 —		ρ
Tank	Est	StdErr	Est	DOF	Est	StdErr	Est	DOF	Est
TX115	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
TX116	-0.60	0.36	0.31	210	1.54	0.22	0.18	144	0.35
TX117	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
TX118	-0.40	0.29	0.31	210	1.58	0.21	0.18	144	0.35
TY101	-1.09	0.24	0.31	210	1.58	0.21	0.18	144	0.35
TY102	-1.04	0.21	0.31	210	1.61	0.20	0.18	144	0.35
TY103	-0.92	0.18	0.31	210	1.66	0.13	0.18	144	0.35
TY104	-0.74	0.13	0.31	210	1.71	0.11	0.18	144	0.35
TY105	-0.87	0.24	0.31	210	1.59	0.13	0.18	144	0.35
TY106	-0.81	0.14	0.31	210	1.59	0.11	0.18	144	0.35
U101	-0.98	0.37	0.31	210	1.64	0.21	0.18	144	0.35
U102	-0.60	0.36	0.31	210	1.64	0.21	0.18	144	0.35
U103	-0.36	0.24	0.31	210	1.17	0.14	0.18	144	0.35
U104	-0.60	0.36	0.31	210	1.58	0.21	0.18	144	0.35
U105	0.07	0.21	0.31	210	1.46	0.21	0.18	144	0.35
U106	-0.60	0.36	0.31	210	1.46	0.22	0.18	144	0.35
U107	-0.60	0.36	0.31	210	1.46	0.22	0.18	144	0.35
U108	-0.60	0.36	0.31	210	1.46	0.22	0.18	144	0.35
U109	-0.60	0.36	0.31	210	1.46	0.22	0.18	144	0.35
U110	-1.03	0.06	0.31	210	1.59	0.03	0.18	144	0.35
U111	-0.51	0.27	0.31	210	1.55	0.21	0.18	144	0.35
U112	-0.98	0.37	0.31	210	1.64	0.21	0.18	144	0.35

3 Reactive Waste Calculations

These calculations employ two definitions of reactive waste, so that the sensitivity of the desired value (proportion of reactive waste) can be determined. Each definition equates reactive waste with a certain region in (H_2O, TOC) space. The two regions are defined as follows:

Region 1: $H_2O\% < 91\%$ and $TOC\% > 1.34 - 0.0134 \cdot H_2O\%$

Region 2: $H_2O\% < 85\%$ and $TOC\% > 0.83 - 0.0083 \cdot H_2O\%$

where H_2O and TOC are wet basis results. Region 1 is a Low Heat of Reaction Region (i.e., heat of reaction is -6.0 $kcal/gTOC$). Region 2 is a High Heat of Reaction Region (i.e., heat of reaction is -9.7 $kcal/gTOC$).

As discussed in the last section, the ANOVA study partitioned each 100-series single-shell tank into two layers (i.e., top and bottom). The top layer comprised the top 0.2 meters of solid waste. The remaining waste below this layer was assigned to the bottom layer. The waste was partitioned in this fashion because of the differing properties of waste that exist between the surface and sub-surface layers for many Hanford waste tanks. ANOVA model parameter estimates were obtained for both waste layers. The remaining reactive waste calculations described in this section were made on each waste layer separately.

The proportion of reactive waste in any tank and layer combination is calculated by integrating the joint distribution of H_2O and TOC in the tank over the reactive region:

$$\text{Proportion Reactive Waste} = \int_{R_i} f(log(x), log(y))dxdy \qquad (4)$$

where x and y are the concentrations of H_2O and TOC respectively, and R_i represents one of the reactive waste regions defined above.

Reactive waste proportions for the top (p_T) and bottom (p_B) layers can be calculated by integrating the distributions over one of the reactive regions. The overall proportion of reactive waste in a tank was estimated as

$$\text{Proportion of Reactive Waste} = \frac{p_T \cdot v_T + p_B \cdot v_B}{v_T + v_B} \qquad (5)$$

where v_T and v_B are the solid waste volumes of the top and bottom layers, respectively. This estimate of the proportion of reactive waste is specific to the solid waste (i.e., the sludge and saltcake) in the tanks. The supernate volumes in the tanks were not considered.

The ANOVA residual plots show that both moisture content (H_2O) and TOC are log-normally distributed (approximately). Thus, the form of the distribution function $f(log(x), log(y))$ is

$$f(log(x), log(y)) = C_0 exp\left(-\frac{1}{2}\begin{bmatrix} log(x) - \mu_1 \\ log(y) - \mu_2 \end{bmatrix}^T \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}^{-1} \begin{bmatrix} log(x) - \mu_1 \\ log(y) - \mu_2 \end{bmatrix}\right) \qquad (6)$$

where subscripts 1 and 2 refer to moisture content and TOC respectively, μ is the estimated mean of the log values for the tank, σ^2 is their estimated variability, ρ is the correlation factor between moisture content and TOC, and the constant C_0 in the formula is defined as:

$$C_0 = \frac{1}{2\pi\sqrt{1-\rho^2}\sigma_1\sigma_2} \tag{7}$$

It should also be noted that the logarithms in the above equation are to the base 10.

The proportion of reactive waste in a tank can be calculated from Equations 4 and 6, given suitable estimates of the distribution parameters μ_1, μ_2, σ_1, σ_2, and ρ. These parameter estimates were obtained from References [4] and [3] for each combination of tank (100-series SST) and waste layer, and are listed in Tables 3 and 4, along with the standard error (StdErr) and degrees of freedom (DOF) for each estimate. Table 3 contains the parameter estimates information for the top layer and Table 4 contains the parameter estimates information for the bottom layer. The estimates in these tables are in units of log_{10} of weight percent. The standard error columns in the tables represent the uncertainties associated with the estimates, and the "DOF" columns represent the amount of data used to estimate the sigma parameters. The DOF is a measure of the uncertainties in the sigma's. The other parameter needed to solve Equations 4 and 6 is the correlation factor ρ. This parameter was assumed equal to 0.35, based on [4].

4 Uncertainty Analysis

No estimate is ever completely accurate. An advantage of ANOVA is that uncertainties (in the form of standard errors) are given for the estimates. Since some estimates contain substantial uncertainty, it is important to account for this in the reactive waste estimates. Simply plugging the ANOVA estimates into formulas 4 and 6 may produce a non-conservative result. To assess the uncertainty, a Monte Carlo simulation [1] was performed.

The Monte Carlo method uses standard Bayesian posterior distributions to describe parameter uncertainty. The means, μ, of the logged data were assumed to be normally distributed about their estimated means, and the sigma terms, σ, were assumed to have an inverse chi-square distribution defined by their estimates. These distribution parameters were simulated 1000 times, based on their calculated variabilities, and the proportion of reactive waste was calculated for each simulation. For each tank, the results were formed into an empirical distribution, as illustrated in Figure 1 for Tank A-101.

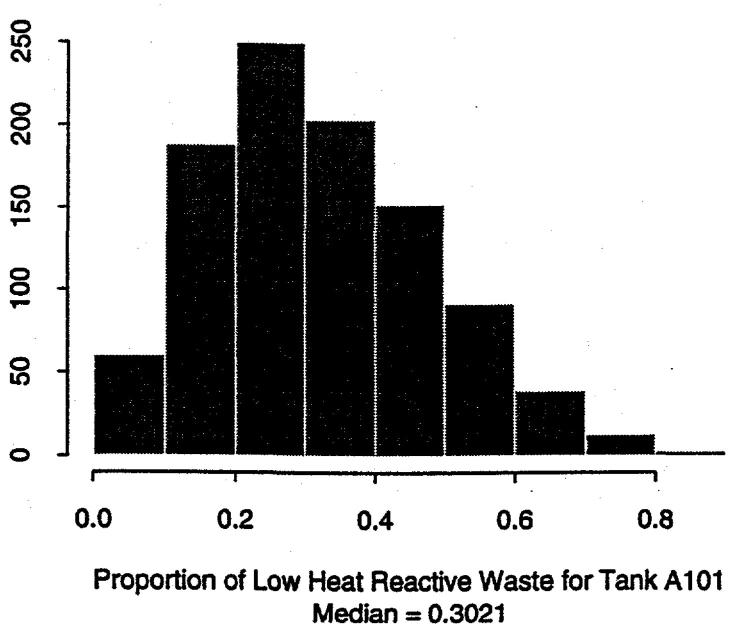

Figure 1: Distribution of Calculated Reactive Waste Proportion, Tank A-101

This distribution describes the uncertainty associated with the reactive waste calculation for this particular tank. From the figure, the percentage of reactive waste is most probably about 30%. On the other hand, there is a small chance that the percentage might be as high as 80% or more. The uncertainty presented in this plot is typical of the reactive waste estimates.

Table 5 contains the final reactive waste proportion estimates for each 100-series SST. This table lists the following quantities:

- A solids volume estimate, in cubic meters, for each tank;
- The average TOC and H_2O concentrations in the original units of weight percent ("NA" indicates that no data was available for the particular tank);
- The median and upper 95% percentile of reactive waste proportions for the low heat region; and
- The median and upper 95% percentile of reactive waste proportions for the high heat region.

The tanks in Table 5 are listed in ascending order of the median reactive waste proportion for the high heat region. We can see that for both regions, Tank B-110 has the lowest estimated reactive waste proportions, at less than 1% for the high heat region; while Tank AX-102 has the highest, at 86% for the high heat region.

Table 5: Reactive Waste Proportions

Tank	Solid Volume (M^3)	Average TOC (wt%)	Average H_2O (wt%)	Reactive Waste Proportions ——Low Heat—— Median	Low Heat Upper-95%	——High Heat—— Median	High Heat Upper-95%
B110	927	0.04	NA	0.002	0.007	0.004	0.013
T104	1673	0.09	55.16	0.008	0.021	0.015	0.037
S109	2150	0.05	NA	0.007	0.049	0.018	0.089
T107	655	0.09	48.60	0.010	0.022	0.021	0.042
BX107	1302	0.07	52.23	0.011	0.025	0.022	0.046
BX108	98	NA	28.88	0.007	0.148	0.025	0.314
BX110	772	0.21	35.59	0.011	0.043	0.026	0.081
C111	216	0.09	34.06	0.011	0.066	0.026	0.134
B107	621	NA	NA	0.012	0.143	0.028	0.255
U110	704	0.13	33.50	0.012	0.022	0.028	0.048
B104	1400	NA	47.86	0.015	0.182	0.029	0.327
TY101	447	0.07	NA	0.014	0.079	0.030	0.143
B103	223	0.07	44.85	0.014	0.076	0.030	0.146
T106	72	NA	17.23	0.008	0.247	0.036	0.475
T112	254	NA	NA	0.019	0.154	0.042	0.252
T108	167	NA	14.13	0.014	0.172	0.045	0.303
B111	893	0.11	NA	0.022	0.060	0.045	0.100
T102	72	0.07	NA	0.020	0.214	0.050	0.351
SX114	685	NA	NA	0.024	0.210	0.051	0.354
C110	674	0.08	58.09	0.028	0.064	0.051	0.109
C108	250	0.15	35.18	0.023	0.109	0.055	0.198
TX103	594	NA	NA	0.025	0.219	0.056	0.357
SX111	473	NA	NA	0.026	0.205	0.057	0.355
BY106	2430	0.42	24.88	0.017	0.034	0.058	0.096
SX112	348	NA	NA	0.026	0.192	0.059	0.318
B109	481	NA	NA	0.027	0.202	0.059	0.334
SX115	45	NA	NA	0.023	0.350	0.060	0.547
BX102	363	NA	NA	0.028	0.204	0.060	0.338
B108	356	NA	NA	0.028	0.231	0.061	0.358
BX101	159	NA	18.71	0.024	0.199	0.062	0.314
T101	382	NA	NA	0.029	0.232	0.063	0.382
SX107	394	NA	NA	0.028	0.191	0.064	0.313
B106	439	NA	NA	0.029	0.199	0.065	0.321
T109	220	NA	NA	0.031	0.216	0.069	0.329
T103	87	NA	NA	0.033	0.339	0.069	0.500
BX111	613	0.06	51.90	0.034	0.141	0.070	0.243
SX108	329	NA	NA	0.032	0.197	0.071	0.311
TY102	242	0.13	58.00	0.038	0.125	0.075	0.201

Table 5: Reactive Waste Proportions

Tank	Solid Volume (M^3)	Average TOC (wt%)	Average H_2O (wt%)	Reactive Waste Proportions: Low Heat Median	Low Heat Upper-95%	High Heat Median	High Heat Upper-95%
SX110	235	NA	NA	0.035	0.197	0.075	0.317
TY103	613	0.11	51.93	0.038	0.108	0.075	0.188
S104	1109	0.13	42.84	0.037	0.078	0.077	0.151
BX105	174	0.18	12.56	0.030	0.156	0.078	0.288
U101	83	NA	NA	0.033	0.391	0.079	0.590
BX106	117	NA	NA	0.037	0.283	0.083	0.442
TY105	874	0.08	39.40	0.040	0.167	0.085	0.292
U112	170	NA	NA	0.041	0.232	0.087	0.350
BX103	235	NA	46.68	0.049	0.219	0.092	0.343
B112	114	NA	41.25	0.051	0.275	0.104	0.418
TY106	64	0.160	36.270	0.042	0.178	0.106	0.347
SX113	98	NA	46.60	0.051	0.356	0.107	0.511
TX102	821	0.19	44.51	0.061	0.315	0.122	0.468
T105	371	0.31	51.97	0.074	0.194	0.147	0.319
C106	746	0.27	NA	0.086	0.242	0.160	0.386
SX105	2585	NA	NA	0.071	0.493	0.162	0.678
U108	1681	NA	NA	0.076	0.561	0.165	0.724
S105	1726	NA	NA	0.081	0.498	0.165	0.675
SX101	1722	NA	NA	0.076	0.519	0.168	0.686
S106	1798	NA	NA	0.076	0.578	0.169	0.729
SX103	2464	NA	NA	0.083	0.502	0.171	0.671
S102	2078	NA	NA	0.084	0.503	0.172	0.688
BY110	1506	NA	NA	0.088	0.538	0.173	0.721
BY103	1514	NA	19.69	0.084	0.537	0.173	0.710
S108	2286	NA	NA	0.088	0.503	0.174	0.697
S101	1571	NA	NA	0.080	0.511	0.176	0.694
U109	1681	NA	NA	0.082	0.525	0.178	0.712
U106	799	NA	NA	0.088	0.526	0.178	0.702
SX106	1805	NA	NA	0.077	0.481	0.178	0.692
TX116	2388	NA	NA	0.092	0.527	0.178	0.704
SX104	2324	NA	NA	0.078	0.543	0.179	0.718
TX106	1715	NA	NA	0.095	0.539	0.180	0.722
C105	511	0.35	30.53	0.084	0.243	0.181	0.429
AX101	2831	NA	NA	0.091	0.545	0.182	0.732
SX109	924	NA	NA	0.089	0.508	0.183	0.694
BY107	1007	NA	NA	0.089	0.490	0.183	0.664
TX117	2369	NA	NA	0.097	0.550	0.183	0.700
BY104	1537	NA	NA	0.090	0.560	0.183	0.731

Table 5: Reactive Waste Proportions

Tank	Solid Volume (M^3)	Average TOC (wt%)	Average H_2O (wt%)	Reactive Waste Proportions ——Low Heat—— Median	Upper-95%	——High Heat—— Median	Upper-95%
TX114	2025	NA	NA	0.094	0.502	0.184	0.663
S110	1476	NA	NA	0.088	0.553	0.184	0.709
BY112	1101	NA	NA	0.091	0.531	0.185	0.697
BY111	1737	NA	NA	0.092	0.528	0.185	0.700
BY105	1904	NA	NA	0.092	0.522	0.186	0.701
TX109	1453	NA	NA	0.094	0.522	0.187	0.704
TX113	2297	NA	NA	0.093	0.559	0.188	0.721
BY101	1465	NA	NA	0.092	0.561	0.188	0.714
S103	874	NA	NA	0.085	0.515	0.189	0.702
S112	1980	NA	NA	0.091	0.496	0.190	0.684
U107	1419	NA	NA	0.087	0.546	0.191	0.738
BY109	1601	NA	NA	0.095	0.509	0.191	0.682
TX105	2305	NA	NA	0.101	0.532	0.192	0.712
TX112	2456	NA	NA	0.094	0.543	0.192	0.716
B105	1158	NA	NA	0.102	0.548	0.194	0.689
TX111	1400	NA	NA	0.101	0.520	0.194	0.695
C102	1196	NA	NA	0.104	0.541	0.195	0.706
C107	897	NA	NA	0.104	0.544	0.197	0.720
BY102	1048	NA	NA	0.099	0.499	0.197	0.655
TY104	163	0.24	52.57	0.111	0.195	0.197	0.310
TX115	2422	NA	NA	0.103	0.505	0.198	0.688
TX110	1749	NA	NA	0.106	0.586	0.200	0.743
SX102	2055	0.51	NA	0.091	0.336	0.201	0.514
U102	1347	NA	NA	0.112	0.533	0.201	0.701
BY108	863	NA	NA	0.103	0.501	0.207	0.663
T110	1423	NA	NA	0.113	0.564	0.208	0.717
BX109	731	NA	NA	0.112	0.530	0.210	0.701
S107	1370	NA	NA	0.115	0.502	0.213	0.674
TX108	507	NA	NA	0.125	0.517	0.221	0.658
U104	462	NA	NA	0.132	0.481	0.222	0.637
BX112	621	0.51	57.47	0.131	0.308	0.226	0.455
AX103	424	NA	NA	0.130	0.498	0.228	0.642
C109	235	0.28	36.79	0.109	0.195	0.228	0.349
B101	428	NA	NA	0.139	0.526	0.238	0.692
TX101	318	NA	NA	0.138	0.490	0.240	0.653
C101	333	NA	23.97	0.136	0.486	0.243	0.631
BX104	363	0.30	NA	0.145	0.303	0.251	0.457
B102	106	NA	17.34	0.128	0.553	0.253	0.712

Table 5: Reactive Waste Proportions

Tank	Solid Volume (M^3)	Average TOC (wt%)	Average H_2O (wt%)	Reactive Waste Proportions: Low Heat Median	Low Heat Upper-95%	High Heat Median	High Heat Upper-95%
TX104	242	NA	NA	0.145	0.459	0.254	0.618
U111	1245	0.53	39.12	0.148	0.491	0.274	0.679
A104	106	NA	NA	0.150	0.604	0.275	0.744
U103	1722	0.69	8.70	0.117	0.485	0.280	0.727
T111	1688	0.33	77.86	0.199	0.315	0.285	0.436
TX107	132	NA	NA	0.162	0.524	0.288	0.648
AX104	26	NA	NA	0.145	0.717	0.292	0.852
A105	72	NA	NA	0.161	0.707	0.309	0.849
C104	1117	0.44	NA	0.175	0.492	0.313	0.666
C112	394	0.36	50.00	0.199	0.273	0.328	0.425
TX118	1313	1.06	NA	0.214	0.626	0.367	0.779
S111	2218	1.33	15.40	0.219	0.476	0.437	0.717
C103	235	0.59	57.69	0.334	0.526	0.482	0.668
A106	473	0.67	44.05	0.321	0.574	0.489	0.741
A101	3607	0.71	38.28	0.302	0.614	0.501	0.786
A103	1385	0.79	40.20	0.363	0.645	0.551	0.797
A102	140	0.76	33.64	0.355	0.628	0.558	0.793
U105	1442	2.75	20.80	0.620	0.896	0.788	0.961
AX102	136	5.65	30.50	0.759	0.912	0.861	0.963

5 Conclusions

Figures 2 and 3 compare the proportions of reactive waste calculated under the two definitions. Figure 2 plots the tank medians for each method, while Figure 3 plots the upper 95% bound of the resulting distributions. Each point represents a tank, while the line in the figures is the locus of agreement (i.e., where the parameters are equal). Both figures show that the medians and upper 95% bounds of reactive waste proportion are consistently higher for the high heat reactive region, as expected. Note the curvature in the cloud of points in each plot. This is particularly apparent in Figure 3 for the Upper 95% limit. The pattern shows that the points converge to the locus of agreement line when reactive waste proportions of 0 or 1 are approached. This is simply due to the physical constraint that the reactive waste proportion cannot be less than zero or greater than 100%.

The reactive waste proportions calculated in this study (Table 5) are much higher than those reported in [2], due to the much more conservative regions defined for the present study.

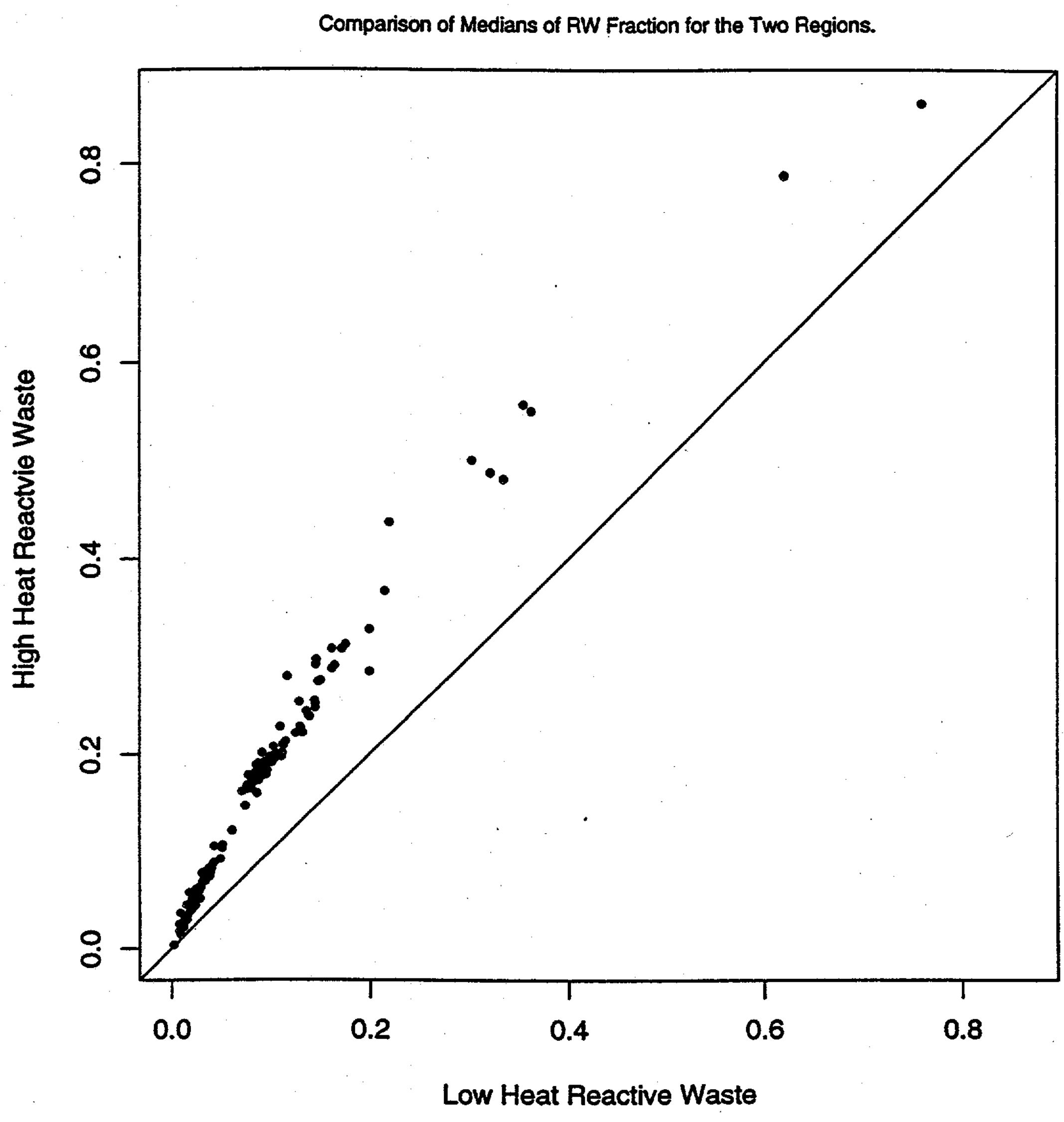

Figure 2: Median Proportion of Reactive Waste for Two Regions.

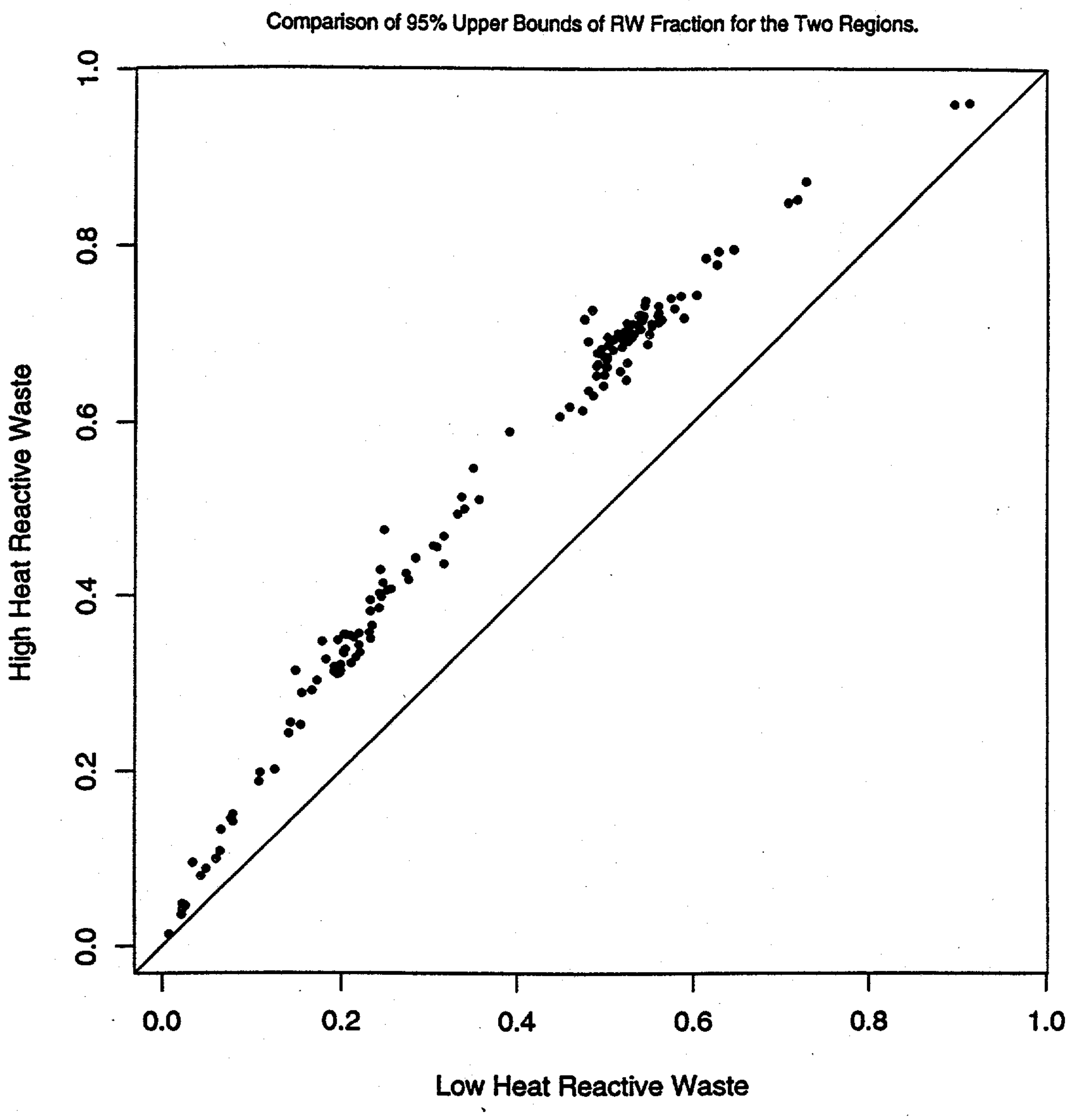

Figure 3: Upper 95% Limit Proportion of Reactive Waste for Two Regions.

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