
**Pacific Northwest
National Laboratory**

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Model for TCLP Releases From Waste Glasses

D. S. Kim
J. D. Vienna

May 2003

Prepared for the U.S. Department of Energy
under Contract DE-AC06-76RL01830



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Pacific Northwest National Laboratory
Richland, Washington 99352

Summary

A first-order property model for normalized Toxicity Characteristic Leaching Procedure (TCLP) release as a function of glass composition was developed using data collected from various studies. The normalized boron release is used to estimate the release of toxic elements based on the observation that the boron release represents the conservative release for those constituents of interest. The current TCLP model has two targeted application areas: (1) delisting of waste-glass product as radioactive (not mixed) waste and (2) designating the glass wastes generated from waste-glass research activities as hazardous or non-hazardous. This report describes the data collection and model development for TCLP releases and discusses the issues related to the application of the model.

Table S.1 summarizes model coefficients, standard errors, model statistics, and the model validity range in mole fraction of 14 components for the TCLP normalized B release (r_B) model developed in this study.

Table S.1. Model Coefficients and Validity Range for the Normalized B Release (r_B) by TCLP

Component	TCLP r_B Model		Validity Range, Mole Fraction	
	$\ln(r_{B,i}, \text{mg/L})$	Std Error	Minimum	Maximum
Al ₂ O ₃	-11.830	1.637	0.0000	0.1296
B ₂ O ₃	14.155	0.767	0.0165	0.2217
CaO	14.266	0.982	0.0000	0.2269
Fe ₂ O ₃	-9.869	2.027	0.0000	0.0845
K ₂ O	29.025	2.465	0.0000	0.1097
Li ₂ O	10.456	0.937	0.0000	0.2051
MgO	12.980	1.032	0.0000	0.1960
Na ₂ O	18.440	0.874	0.0000	0.2581
SiO ₂	-1.270	0.358	0.3331	0.6458
ZrO ₂	-10.114	2.685	0.0000	0.0908
LN ₂ O ₃	-98.649	7.577	0.0000	0.0231
MnO _x	15.308	6.942	0.0000	0.0795
SrO	8.975	5.238	0.0000	0.1023
Others	9.696	1.116	0.0004	0.1685
Model Statistics		Validity Range for r_B (mg/L)		
Number of Glasses	231	Minimum r_B	Maximum r_B	
R ²	0.870	7.21	3790.57	
R ² (Adjusted)	0.862			
s (RMSE)	0.5825			

Note: Normalized boron release by TCLP is calculated using the formula:

$$\ln[r_B] = \sum_{i=1}^N r_{B,i} x_i \quad (\text{S.1})$$

where x_i is the mole fraction of i -th component in glass, $r_{B,i}$ is the model coefficients for i -th component, and N is the number of components. Then, the TCLP release of each Resource Conservation and Recovery Act (RCRA) element (c_i , mg/L) is calculated by the relation:

$$c_i = r_B f_i \quad (\text{S.2})$$

where f_i is the mass fraction of i -th element in glass.

Abbreviations and Acronyms

AES	atomic emission spectroscopy
ASTM	American Society for Testing and Materials
CFR	U.S. Code of Federal Regulations
DCP	directly coupled plasma
DOE	U.S. Department of Energy
EPA	U.S. Environmental Protection Agency
FR	Federal Regulations
HLW	high-level waste
ICP	inductively coupled plasma
ILAW	immobilized low-activity waste
IHLW	immobilized high-level waste
LANL	Los Alamos National Laboratory
LAW	low-activity waste
LDR	land-disposal restrictions
LLMW	low-level mixed waste
PCT	product consistency test
PNNL	Pacific Northwest National Laboratory
RCRA	Resource Conservation and Recovery Act
RMSE	root mean square error
RPP	River Protection Project
SRS	Savannah River Site
TCLP	Toxicity Characteristic Leaching Procedure
TWRS	Tank Waste Remediation System

UTS	universal treatment standard
VSL	Vitreous State Laboratory
WAC	Washington Administrative Code
WSRC	Westinghouse Savannah River Company
WTP	Waste Treatment Plant

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1.0 Introduction

The United States Department of Energy's (DOE's) Hanford Nuclear Reservation is the current home of approximately 53-million gallons of mixed waste stored in 177 waste tanks. The waste material contains *Resource Conservation and Recovery Act of 1976* (RCRA)-regulated hazardous wastes, including wastes identified in 40 CFR 261.31 through 40 CFR 261.33 and constituents that are subject to the land-disposal restrictions (LDRs) contained in 40 CFR 268 and Washington Administrative Code (WAC) 173-303-140. The RCRA-regulated materials also are subject to management under the analogous provisions of the Washington State Dangerous Waste Regulations found in the WAC, Chapter 173-303. The immobilized high-level waste (IHLW) is intended for disposal at the proposed geologic repository for spent nuclear fuel and high-level radioactive waste (HLW). The federal HLW repository will not be permitted under RCRA or corresponding State regulations and will not accept hazardous wastes for disposal. The immobilized low-activity waste (ILAW) is intended for disposal at a land-disposal unit and is subject to compliance with LDR. Current plans include delisting of IHLW and a LDR treatability variance for both IHLW and ILAW. One of the criteria typically applied to determine whether a material is toxic is to examine the release of certain toxic elements under the conditions of the U.S. Environmental Protection Agency (EPA) Toxicity Characteristic Leaching Procedure (TCLP) (e.g., 62 FR 26041). TCLP determines the release of elements extracted from the solid material to a sodium-buffered leachate at a pH of about 5 over a period of 18 hours at room temperature. The strategy for a successful delisting and LDR treatability variance is based in part on the development of TCLP response models as developed from the evaluation of inactive glasses made from simulated Hanford tank waste.

Currently, glass waste is produced in the glass laboratories at the Pacific Northwest National Laboratory (PNNL) and other facilities for research related to nuclear-waste-vitrification technologies, including glass formulation and various other studies. If no associated TCLP data exist, the glasses produced in these research facilities must be designated based on the components present and are mostly disposed of as hazardous waste. If the glass contains TCLP-listed elements below the applicable limits, it is considered non-regulated. For a small quantity of glasses containing toxic metals, it is typically more economical to dispose of the glass as hazardous waste because of the high cost of the TCLP test. We propose that a TCLP release model be applied to designate the glass wastes while accounting for the appropriate uncertainties in model prediction.

A database of glass properties and associated compositions for simulated HLW and low-activity waste (LAW) glasses has been compiled at PNNL for developing property-composition models (Hrma et al. 2001; Vienna et al. 2002). This effort is aimed at improving the understanding of composition effects on glass properties over the broad composition space of expected waste glasses. With this increased understanding, the ability to predict glass volumes, cleanup cost and schedule, and the impacts of changing property constraints and flowsheet options will be possible. Recently, Vienna et al. (2002) reported the models applicable to Hanford waste glasses for many properties, such as the product consistency test (PCT) (ASTM 1998) response, viscosity, liquidus temperature, and density (using molar volume). However, they did not report a model for TCLP release, mainly because of limited data on TCLP releases contained in the current database. Additional data on TCLP releases were collected for this study. A model to calculate the effects of composition on the normalized release of boron during TCLP was developed, which can be used to estimate the releases of toxic or restricted elements. A wealth of data on the glass responses under a PCT condition exists, which also measures the dissolution of glass

in aqueous solution. Unfortunately, because of the differences in test conditions, such as temperature, duration, and sample surface area to leachate volume ratio, the information gained from the study of PCT cannot be directly applied to TCLP responses. However, the general approach applied to modeling the PCT responses may be applicable to modeling TCLP response.

There have been different approaches at modeling the TCLP releases of elements from simulated waste glasses (Vienna et al. 1998; Pickett and Jantzen 2002; Gan and Pegg 2002). Vienna et al. (1998) selected the TCLP normalized boron release as representative or conservative of normalized releases of toxic or restricted elements and used it to model the TCLP releases for these elements. Pickett and Jantzen (2002) also used normalized boron release as a representative of glass dissolution under TCLP conditions and developed the models for normalized releases of Ni and U using THERMOTM. Gan and Pegg (2002) divided the normalized TCLP elemental releases into three element groups of approximately the same normalized rate:

Group 1: advanced elements (alkalis, alkaline earths, divalent transition metals, B, Ag, U)

Group 2: retarded elements (Si, Tl, Se, Sb, and Pb)

Group 3: slow or irregular elements (Al, Fe, Zr, As, and Cr).

Cadmium was selected as a representative of Group 1 to compare with other elements in this group and also with those elements in other Groups. It was observed that the Group 2 elements are released at about 25% and Group 3 elements at about 10% that of the Group 1 elements. Then the models were fitted to the selected elements, Cd, Ni, and Tl, which were chosen for illustration because of their representative release behavior and significance in HLW glass delisting. In the present report, the TCLP release data were initially evaluated in terms of the relation between each element release to determine the representative element for modeling, which can be used to predict the releases of other elements. Initial models were fit to experimental data and validated before developing the final model as discussed in the remainder of this report.

2.0 Model for TCLP Normalized B Release

2.1 Initial Data Evaluation and Screening

Table 2.1 summarizes the data sets used in this study. The current PNNL database on glass composition and properties (Vienna et al. 2002) contains 165 glasses with TCLP release data from six different studies with the majority of the glasses from one study that had 140 glasses. In addition, 86 more glasses with TCLP data were collected for this modeling effort. The 86 additional glasses are from three studies that were not included in the database (last three studies in Table 2.1), giving a total of 251 glasses for evaluation. Appendix A contains the glass compositions in mass fraction and TCLP release data for all 251 glasses. Although the same TCLP method, SW-846 Method 1311 (EPA 1997), was used for the extractions performed in all these studies, subtle differences in results from different studies can be expected, which can make combining data less ideal for developing property models.^(a)

Table 2.1. Summary of Data Sets Used in this Study

#	Study	Reference	# of Glasses
1	TWRS LAW Formulation 2	Ferrara et al. 1998	3
2	SRS M-Area Mixed Waste	Fu et al. 1997	6
3	TWRS LAW Formulation	Muller and Pegg 1998	4
4	TWRS HLW Glass Formulation	Fu and Pegg 1998	8
5	RPP-WTP LAW Formulation	Muller et al. 2001	4
6	RPP-WTP HLW Formulation	Kot and Pegg 2001	140
7	LANL Glasses	Vienna et al. 1998	37
8	Plutonium Residue Glasses	Bulkley and Vienna 1997	28
9	SRS LLMW Glasses	Cicero-Herman 2002, Not published ^(a)	21
		Total	251

(a) The data were delivered to PNNL in an electronic form from Connie Cicero-Herman, Westinghouse Savannah River Company (WSRC).

The first of these studies, Tank Waste Remediation System (TWRS) LAW Formulation 2 (Ferrara et al. 1998), was a study aimed at demonstrating a typical Hanford LAW product quality. The TCLP extraction and solution analyses were performed by WSRC according to SW-846 Method 1311 and an internal WSRC method for inductively coupled plasma-atomic emission spectroscopy (ICP-AES). The second study, Savannah River Site (SRS) M-area mixed waste (Fu et al. 1997), was aimed at developing an optimized glass formulation for M-area mixed wastes. The TCLP extraction and solution analyses were performed by the Vitreous State Laboratory (VSL) according to SW-846 Method 1311 and an internal VSL method for direct coupled plasma (DCP)-AES. The third study, TWRS LAW formulation (Muller and Pegg 1998), was aimed at developing glass compositions for vitrifying Hanford LAW under the TWRS privatization program. The TCLP extraction and solution analyses were performed by VSL.

(a) The differences in TCLP response between studies come primarily from differences in particle sizing before the extraction, which can cause variation in particle size distribution of the samples. The amount of glass leached is proportional to the surface area of glass exposed to solution.

according to SW-846 Method 1311 and an internal VSL method for DCP-AES. The fourth study, TWRS HLW glass formulation (Fu and Pegg 1998), was aimed at developing glass compositions for vitrifying Hanford HLW under the TWRS privatization program. The TCLP extraction and solution analyses were performed by VSL according to SW-846 Method 1311 and an internal VSL method for DCP-AES. The fifth study, River Protection Project-Waste Treatment Plant (RPP-WTP) LAW Formulation (Muller et al. 2001), was aimed at developing glass compositions for vitrifying Hanford LAW under the WTP. The TCLP extraction and solution analyses were performed by VSL according to SW-846 Method 1311 and an internal VSL method for DCP-AES. The sixth study, RPP-WTP HLW Formulation (Kot and Pegg 2001), was aimed at developing glass compositions for vitrifying Hanford HLW under the WTP. The TCLP extraction and solution analyses were performed by VSL according to SW-846 Method 1311 and an internal VSL method for DCP-AES. The seventh study, Los Alamos National Laboratory (LANL) (Vienna et al. 1998), was aimed at developing glass compositions for vitrifying LANL evaporator bottoms. The TCLP extraction and solution analyses were performed by PNNL according to SW-846 Method 1311 and an internal PNNL method for inductively coupled plasma (ICP)-AES. The eighth study, plutonium residue glasses (Bulkley and Vienna 1997), was aimed at developing glass compositions for vitrifying plutonium-bearing residue materials at Hanford and the Rocky Flats Environmental Technology Site. The TCLP extraction and solution analyses were performed by PNNL according to SW-846 Method 1311 and an internal PNNL method for ICP-AES. The ninth study, SRS low-level mixed waste (LLMW) glasses, was aimed at determining the effect of glass composition on the release of key components of glass during the TCLP and the PCT. The TCLP extraction and solution analyses were performed by WSRC according to SW-846 Method 1311 and an internal WSRC method for ICP-AES.

As discussed below in this Section, evaluating the above data to determine the representative element for TCLP releases suggested that the normalized boron release is most suitable for representing the dissolution of glass and thus for modeling to predict the releases of other elements. The normalized elemental releases, r_i (in mg/L), is defined as below:

$$r_i = \frac{c_i}{f_i} \quad (2.1)$$

where c_i (mg/L) is the TCLP release of i -th element and f_i is the mass fraction of i -th element in glass.

Figure 2.1 is the plot $\ln(r_i)$ versus $\ln(r_B)$ for eight RCRA elements of interest (Ag, As, Ba, Cd, Cr, Ni, Pb, and Se) plus Tl and Zn for the glasses collected from Kot and Pegg (2001). One of the RCRA elements, mercury, is not included because there are no data on the glasses containing HgO as a glass component. Further, of a total of 2001 glasses contained in the current PNNL database, only one glass had a target concentration of 0.01 wt% HgO (Vienna et al. 2002).

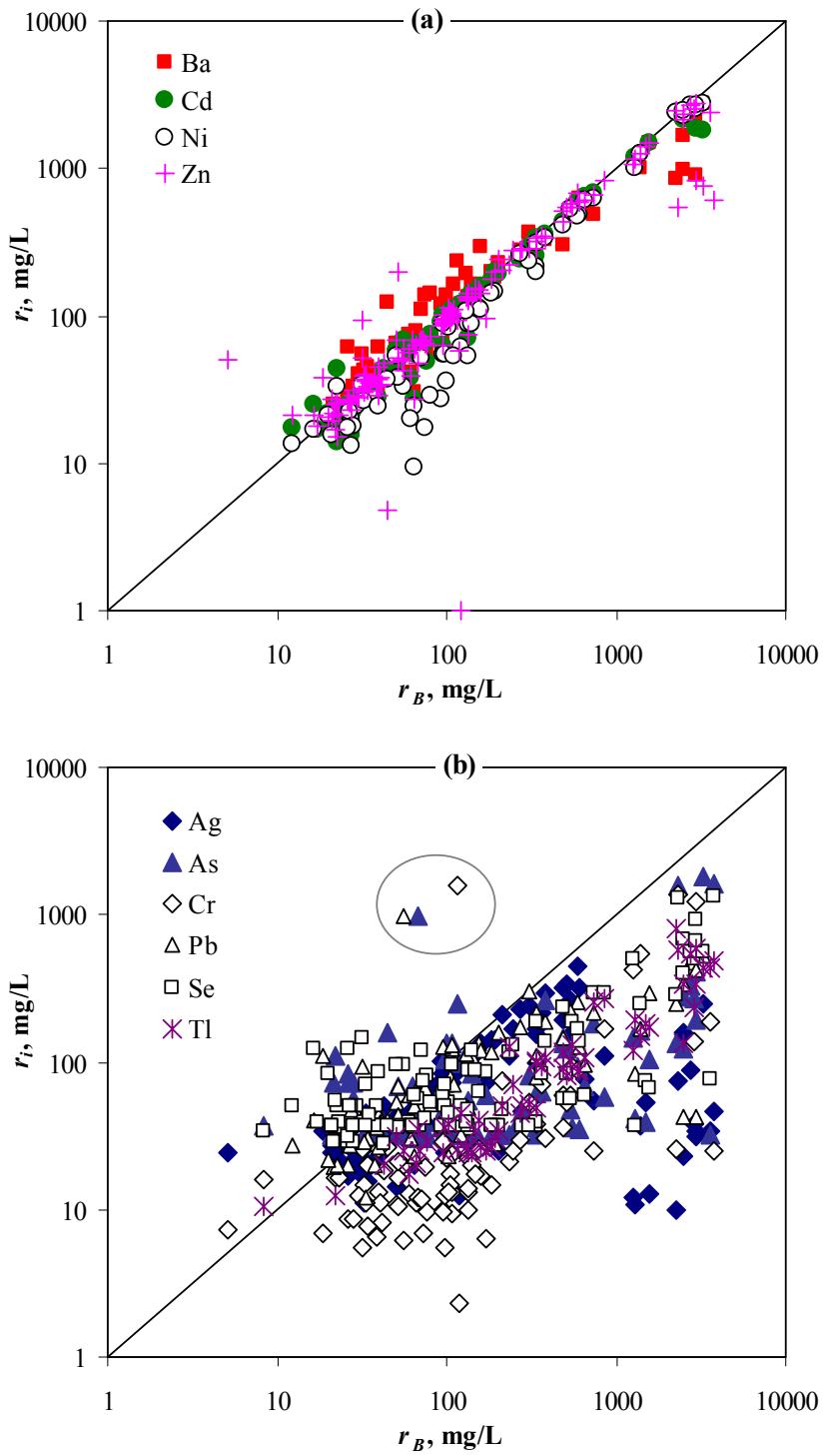


Figure 2.1. $\ln(r_i)$ Versus $\ln(r_B)$ for (a) Ba, Cd, Ni, and Zn and (b) Ag, As, Cr, Pb, Se, and Tl in the Glasses Studied by Kot and Pegg (2001)

Figure 2.1 shows that the normalized releases of all 10 elements are similar to or lower than that of boron except for three glasses that are obvious outliers. The glasses with lower TCLP releases show larger scatter of data, which is presumably caused by the larger uncertainty (sample collection, handling,

and analytical error) involved in the leachate analysis and glass preparation when the elements are present in low concentration and glass dissolution is slow.

The elements in Figure 2.1 were divided into two groups based on their normalized releases compared to normalized boron release: (1) congruent (Ba, Cd, Ni, and Zn) and (2) incongruent (Ag, As, Cr, Pb, Se, and Tl). A similar grouping can also be made to all other elements reported in the study by Kot and Pegg (2001), i.e., some are released at the similar rate as boron and some at a lower rate than boron. The exception was alkali elements—the most mobile elements, K and Li (excluding Na because it is used in TCLP leachate)—that show sometimes higher normalized releases than boron, which indicates that alkali elements can leach out selectively by ion exchange. The evaluation based on Figure 2.1 indicates that normalized boron release can be used to estimate the extent of glass dissolution under TCLP conditions in a similar way as used in the PCT. The lower normalized releases of some elements are due to low solubility of these elements or precipitation in solid forms.

The similar plot for LANL glasses (Vienna et al. 1998) is in Figure 2.2. Figure 2.2 shows the releases of two alkali elements to illustrate the point discussed here. This agrees well with the tendency observed in Figure 2.1 in that Ni is congruent and Cr is incongruent (no comparison is possible for Pb because it has only one data point). Other studies in Table 2.1 did not have both B release and RCRA-element releases together for such an analysis (some studies had B release only, and some had RCRA-element releases without B release).

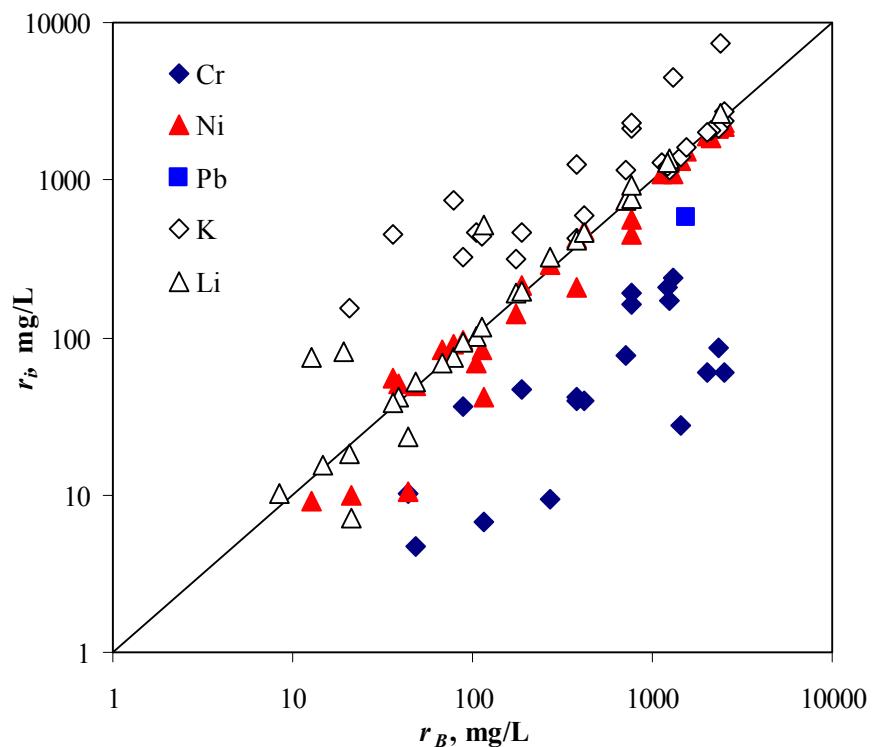


Figure 2.2. $\ln(r_i)$ Versus $\ln(r_B)$ in the Glasses Studied by Vienna et al. (1998)

Of the 251 glasses in Table 2.1, 221 glasses had boron-release data. These 221 glasses were evaluated for concentration distribution, which identified six glasses that had an extreme concentration of SiO₂, B₂O₃, or CaO, which were removed from the data set. During the model fitting, four glasses that constantly had large residuals in ln(r_B) regardless of model components chosen were removed as outliers.^(a) Table 2.2 summarizes the glasses removed from the data set. The remaining 211 glasses were used to develop the model.

Table 2.2. List of Glasses Excluded from TCLP r_B Model Development

Glass	Study	Reason
RFP-4	SRS LLMW Glasses	Extreme SiO ₂ concentration
LANL-1	SRS LLMW Glasses	Extreme SiO ₂ concentration
LANL-13	SRS LLMW Glasses	Extreme SiO ₂ concentration
WETF-7	SRS LLMW Glasses	Extreme B ₂ O ₃ concentration
LANL-8	SRS LLMW Glasses	Extreme B ₂ O ₃ concentration
LANL-3	SRS LLMW Glasses	Extreme CaO concentration
HLW99-04	RPP-WTP HLW Formulation	Model outlier
RFP-8	SRS LLMW Glasses	Model outlier
RFP-9	SRS LLMW Glasses	Model outlier
HLW99-34	RPP-WTP HLW Formulation	Model outlier

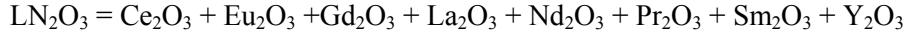
2.2 Composition Conversion

For model calculation, the glass compositions were first converted into mole fractions of oxides (and halogens) by standard methods. Several components were listed in the database with multiple oxidation states. These components were combined into groups of like metal oxides according to:

$$\begin{aligned}
 \text{Ce}_2\text{O}_x &= \text{Ce}_2\text{O}_3 + 0.5 \text{ CeO}_2 & \text{ReO}_x &= \text{ReO}_2 + 2 \text{ Re}_2\text{O}_7 + \text{ReO} \\
 \text{CoO}_x &= \text{CoO} + 2 \text{ Co}_2\text{O}_3 & \text{Rh}_2\text{O}_x &= \text{Rh}_2\text{O}_3 + 0.5 \text{ RhO}_2 \\
 \text{Fe}_2\text{O}_x &= \text{Fe}_2\text{O}_3 + 0.5 \text{ FeO} & \text{Sb}_2\text{O}_x &= \text{Sb}_2\text{O}_3 + \text{Sb}_2\text{O}_5 \\
 \text{MnO}_x &= \text{MnO} + \text{MnO}_2 & \text{SnO}_x &= \text{SnO}_2 + \text{SnO} \\
 \text{MoO}_x &= \text{MoO}_3 + \text{MoO} & \text{Tl}_2\text{O}_x &= \text{Tl}_2\text{O}_3 + \text{Tl}_2\text{O} \\
 \text{PdO}_x &= \text{PdO} + \text{PdO}_2 & \text{UO}_x &= \text{UO}_3 + \text{UO}_2 + 3 \text{ U}_{308} \\
 \text{Pr}_2\text{O}_x &= \text{Pr}_2\text{O}_3 + 3 \text{ Pr}_6\text{O}_{11}
 \end{aligned}$$

When only one oxide form had at least one glass with non-zero concentration, this oxide form was used instead of the combined form, e.g., MnO was used instead of MnO_x if no glass had MnO₂. The resultant compositions were then normalized to 1. In addition, the lanthanide oxides and Y₂O₃ were combined to form a single component—Ln₂O₃:

(a) Although it is preferable to determine whether glasses are “well-predicted” by a more rigorous model using standardized residuals (residual/standard deviation), it is easier to use residuals, and for the purposes of this modeling effort, it was deemed the appropriate level of effort. For detailed discussion of the rigorous methods used to reduce terms in a statistical model see Piepel and Redgate (1997).



because these components were in insufficient concentrations in most glasses and did not, by themselves, have sufficient variation to justify fitting separate coefficients for them. However, combined, they were in sufficient concentration and showed sufficient variation for a combined coefficient. Generally, their effects on glass properties are similar and vary only with ionic radius; however, this variation with radius was not accounted for in this study.

After forming the combined components, the 251 glass compositions were expressed as normalized mole fractions of 44 components. Those components with concentrations greater than 1.5 mole% in at least one glass and with a reasonable distribution were considered as possible model components—leaving 19 components. Only a limited number of components can be included in modeling. In treating the components that are not included in the model components, two different approaches can be applied: (1) use the Others component as a sum of all the components not included in the model or (2) use compositions normalized to sum to one after deleting the components not included in the model. The approach (1) using the Others component was adopted for this study as it was used for models in the recent interim model report for Hanford waste glasses (Vienna et al. 2002).

2.3 Initial Model Development

The natural logarithm of normalized boron release (r_B) was modeled as a linear function of glass composition:

$$\ln[r_B] = \sum_{i=1}^N r_{B,i} x_i \quad (2.2)$$

where $r_{B,i}$ is the model coefficients for i -th glass component, x_i is the mole fraction of i -th component in glass, and N is the number of components. Then, the TCLP release of each RCRA element is calculated by the relation:

$$c_i = r_B f_i \quad (2.3)$$

The calculated c_i is based on the observation that $r_i \leq r_B$ for all RCRA elements as discussed in Section 2.1.

The model coefficients from 211 glasses were initially calculated using 20 components (19 components selected in Section 2.2 plus Others), which were identified as the maximum number of components that have reasonable ranges of mole fractions and distributions of mole-fraction values within the range to consider including them in the model. Then the next models were calculated based on the reduced number of components, removing the component(s) of higher uncertainty or of less importance. Table 2.3 shows which components were included in the 20-, 18-, 17-, 16-, 15-, and 14-component models by providing model coefficient and standard-error values. Summary statistics from the regression analysis for each of these models are also included in Table 2.3.

Table 2.3. Model Coefficients, Standard Error, and Model Statistics for the TCLP Normalized B Release Models

Component	20-Comp.		18-Comp.		16-Comp.		15-Comp.		14-Comp.		13-Comp.	
	Coeff.	Std Error										
Al ₂ O ₃	-13.748	1.989	-12.897	1.980	-12.239	1.882	-12.613	1.815	-12.220	1.784	-15.626	2.457
B ₂ O ₃	14.668	0.805	14.599	0.815	14.551	0.815	14.423	0.797	14.327	0.793	17.105	1.066
CaO	14.541	1.068	14.146	1.061	14.009	1.037	14.165	1.015	14.121	1.015	13.289	1.410
Fe ₂ O ₃	-11.655	2.289	-10.152	2.239	-9.484	2.210	-10.041	2.082	-10.007	2.084	-1.491	2.766
K ₂ O	29.189	2.659	28.766	2.568	28.601	2.567	28.939	2.525	28.861	2.526	22.600	3.456
Li ₂ O	10.157	1.089	10.576	1.081	10.618	1.030	10.576	1.027	10.391	1.015	11.305	1.410
MgO	12.971	1.209	12.326	1.198	12.392	1.198	12.807	1.065	12.949	1.058	14.183	1.467
Na ₂ O	18.743	1.021	18.930	1.030	18.791	1.016	18.659	1.000	18.431	0.981	19.974	1.356
NiO	34.257	29.838	31.691	13.220								
P ₂ O ₅	37.043	33.788	39.090	33.976								
SiO ₂	-1.376	0.394	-1.275	0.396	-1.214	0.395	-1.268	0.388	-1.213	0.386	-2.680	0.516
ZrO ₂	-7.821	3.695	-6.520	3.701	-7.269	3.685	-8.210	3.466	-7.903	3.459	-16.470	4.732
BaO	-116.404	49.319										
CdO	117.390	53.241										
LN ₂ O ₃	-95.087	15.984	-94.319	13.814	-106.239	10.462	-101.081	7.945	-99.609	7.848		
MnO _x	15.481	8.564	22.256	8.159	19.362	7.633	19.747	7.608	19.256	7.602	30.972	10.509
SrO	9.807	6.550	5.009	6.338	5.835	6.033	4.941	5.910	5.774	5.871	2.433	8.161
UO _x	-14.011	23.473	-11.830	23.366	1.654	7.503	0.810	7.412				
ZnO	10.505	13.473	7.103	13.573	0.382	12.668						
Others	7.934	7.427	1.444	6.255	10.983	1.925	9.940	1.346	9.240	1.202	6.274	1.645
Model statistics												
Number of Glasses	211		211		211		211		211		211	
R ²	0.878		0.874		0.872		0.871		0.870		0.748	
R ² (Adjusted)	0.866		0.863		0.862		0.862		0.862		0.733	
s (RMSE)	0.5871		0.5945		0.5960		0.5954		0.5959		0.8291	

The R^2 and root mean square error (RMSE) values do not change significantly with a reduced number of model components until the 14-component model, indicating that those six components deleted may not contribute to improving the model. However, deleting LN_2O_3 from the 14-component model to the 13-component model decreases the R^2 and increases the RMSE significantly. Therefore, the 14-component model (13 components plus Others) was selected for further evaluation. Further reduction would delete or combine SrO and MnO_x because of their high standard error and concentration correlation. However, these two components were deliberately included because these are major components for Hanford HLW glasses, which were not tested extensively because these components became important recently due to the change of the waste-pretreatment process. The plot of calculated $\ln(r_B)$ versus measured $\ln(r_B)$ is in Figure 2.3, which also shows the glasses excluded from the model data as listed in Table 2.2.

The 14-component model was preliminarily applied to calculate the TCLP release of eight RCRA components for the glasses that have resulted from various studies and have been archived for future use whenever necessary. The estimated TCLP releases of toxic components from glasses found in PNNL archives (and in the PNNL database) were compared with the RCRA Toxicity Limits, which will be discussed in Section 3. Of 344 glass compositions calculated, only 3 glasses were predicted to fail TCLP requirements (applying the 95% confidence band using t-distribution). However, 56 glasses could not be accurately predicted by the TCLP model because their compositions were outside of the model validity range. It is believed that most of these glasses would pass the requirements if the model validity range were expanded, considering that their calculated (extrapolated) TCLP releases are far below the toxicity limits. Therefore, it was decided to expand the database by including TCLP data for more glasses.

Twenty glasses with a higher concentration of Al_2O_3 and ZrO_2 were collected from three studies (Crum et al. 1997; Li et al. 1997; Vienna et al. 2001) that did not include TCLP analyses (and so, are not listed in Table 2.1). The TCLP releases of these glasses were obtained for inclusion in the final model.^(a) Al_2O_3 and ZrO_2 were selected because these components had caused the largest number of glasses in the PNNL archive to be outside of the initial model validity range. Appendix A includes the composition and TCLP data for these 20 glasses along with other data used in TCLP model development.

(a) Tests were conducted by Severn Trent laboratories, Inc., 13715 Rider Trail North, Earth City, MO 63045, following the EPA's SW-846 Method 1311 for extraction and Method 6010b for solution analyses by ICP-AES.

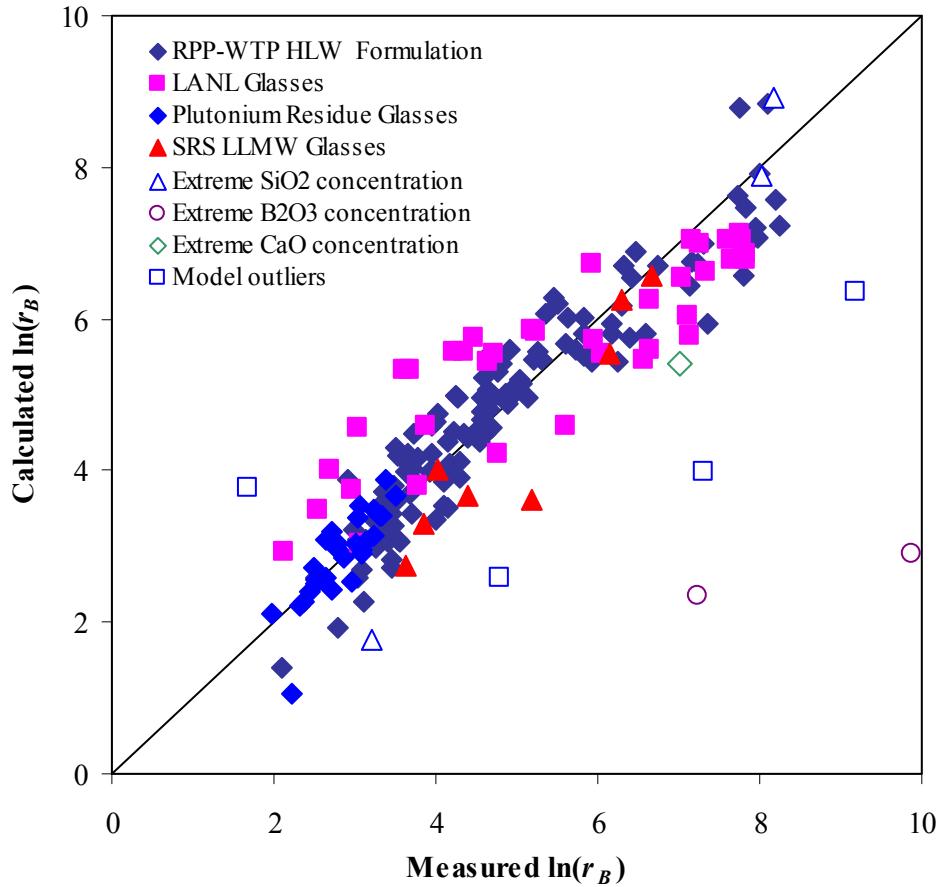


Figure 2.3. Calculated Versus Measured $\ln(r_B)$ Values for Glasses Used in the TCLP Model and Excluded from the Model Based on the 14-Component Model in Table 2.3

2.4 Final Model Development

The 231 glasses discussed in Section 2.3 were used to develop the final model. The composition ranges of these 231 glasses expressed in mole fraction and mass fraction are summarized in Table 2.4 and Table 2.5. The primary determination on whether the glass is within the model validity range is performed based on the mole fraction of 14 model components, including the Others component used in the final model.

The component correlations and scatter-matrix plot of 231 glass compositions used to develop the final model are in Table 2.6 and Figure 2.4. As seen in Table 2.6, there is a strong correlation between MnO_x and SrO , but it was decided to include these two components in the model, considering the importance of these components for glass development for recent estimated Hanford HLW. These two components should be the focus in the future when more glasses are tested to improve the model.

Summary statistics from the regression analysis for the final 14-component model are included in Table 2.7. The plot of calculated $\ln(r_B)$ versus measured $\ln(r_B)$ is in Figure 2.5.

Table 2.4. Mole Fraction Range for Components in 231 Glasses Used to Develop the TCLP r_B Model

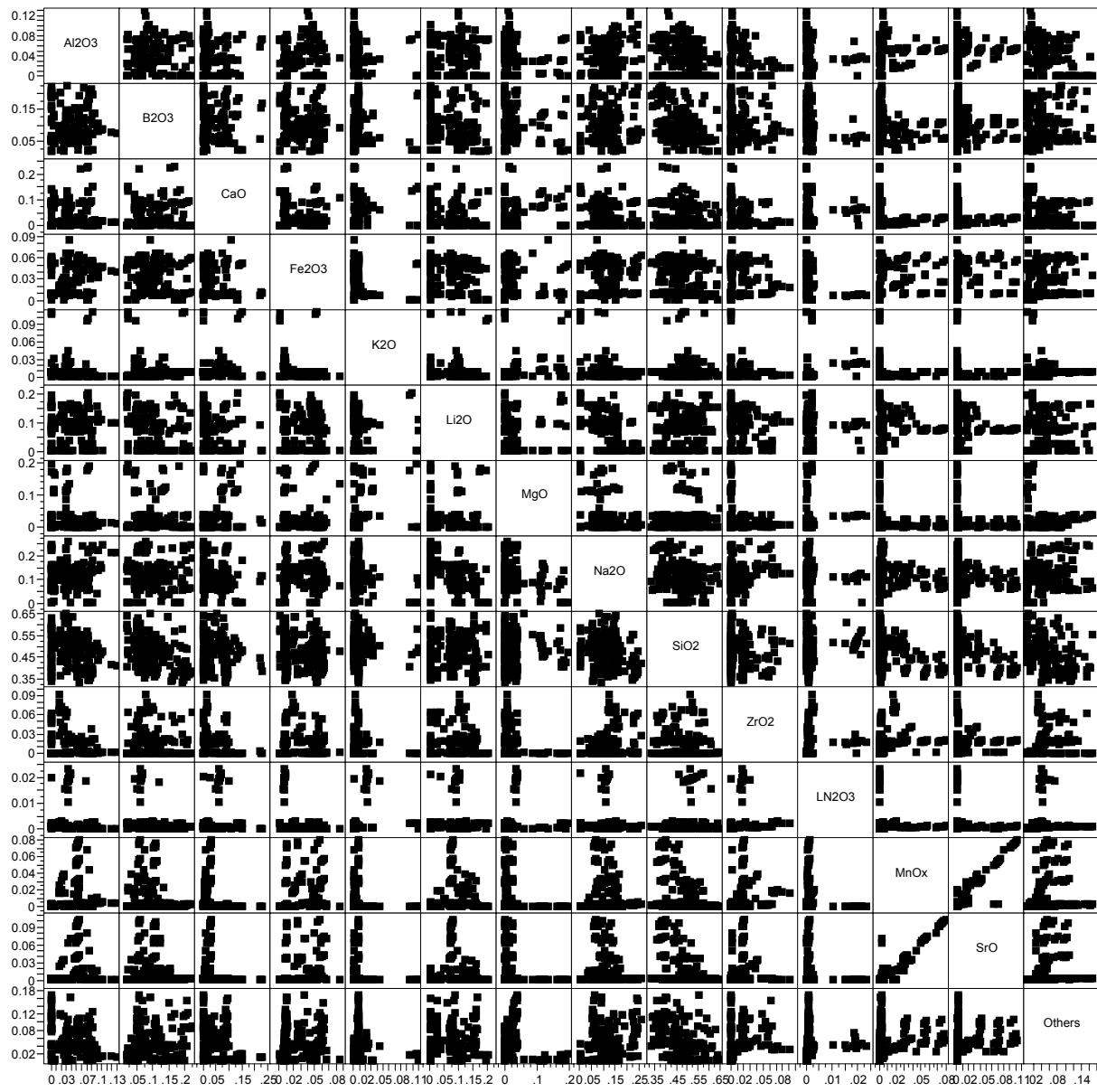
Component	Min	Max	Component	Min	Max	Component	Min	Max
Al ₂ O ₃	0.0000	0.1296	NiO	0.0000	0.0304	PdO	0.0000	0.0003
B ₂ O ₃	0.0165	0.2217	P ₂ O ₅	0.0000	0.0169	Rh ₂ O ₃	0.0000	0.0003
CaO	0.0000	0.2269	Ag ₂ O	0.0000	0.0009	RuO ₂	0.0000	0.0008
Fe ₂ O ₃	0.0000	0.0845	As ₂ O _x	0.0000	0.0008	Sb ₂ O _x	0.0000	0.0010
K ₂ O	0.0000	0.1097	BaO	0.0000	0.0197	SeO ₂	0.0000	0.0017
Li ₂ O	0.0000	0.2051	Bi ₂ O ₃	0.0000	0.0096	SnO _x	0.0000	0.0206
MgO	0.0000	0.1960	CdO	0.0000	0.0177	SO ₃	0.0000	0.0050
Na ₂ O	0.0000	0.2581	Cl	0.0000	0.0108	TeO ₂	0.0000	0.0010
SiO ₂	0.3331	0.6458	CoO	0.0000	0.0064	ThO ₂	0.0000	0.0164
ZrO ₂	0.0000	0.0908	Cr ₂ O ₃	0.0000	0.0086	TiO ₂	0.0000	0.0429
LN ₂ O ₃	0.0000	0.0231	Cs ₂ O	0.0000	0.0027	Tl ₂ O _x	0.0000	0.0009
MnO _x	0.0000	0.0795	CuO	0.0000	0.0020	UO _x	0.0000	0.0237
SrO	0.0000	0.1023	F	0.0000	0.0183	V ₂ O ₅	0.0000	0.0004
Others	0.0004	0.1685	MoO _x	0.0000	0.0034	WO ₃	0.0000	0.0007
			PbO	0.0000	0.0157	ZnO	0.0000	0.0197

Table 2.5. Mass Fraction Range for Components in 231 Glasses Used to Develop the TCLP r_B Model

Component	Min	Max	Component	Min	Max	Component	Min	Max
Al ₂ O ₃	0.0000	0.1929	CeO ₂	0.0000	0.0650	Sb ₂ O ₃	0.0015	0.0023
B ₂ O ₃	0.0200	0.2000	Cl	0.0000	0.0056	Sb ₂ O ₅	0.0000	0.0044
CaO	0.0000	0.2022	CoO	0.0000	0.0063	SeO ₂	0.0000	0.0026
Fe ₂ O ₃	0.0000	0.2030	Cr ₂ O ₃	0.0000	0.0189	SnO	0.0000	0.0400
K ₂ O	0.0000	0.1500	Cs ₂ O	0.0000	0.0111	SnO ₂	0.0000	0.0016
Li ₂ O	0.0000	0.1000	CuO	0.0000	0.0021	SO ₃	0.0000	0.0050
MgO	0.0000	0.1200	F	0.0000	0.0050	SrO	0.0001	0.1399
Na ₂ O	0.0000	0.2123	Gd ₂ O ₃	0.0368	0.0500	TeO ₂	0.0000	0.0021
NiO	0.0000	0.0300	La ₂ O ₃	0.0000	0.0128	ThO ₂	0.0000	0.0591
P ₂ O ₅	0.0000	0.0300	MnO ₂	0.0000	0.0912	TiO ₂	0.0000	0.0500
SiO ₂	0.3000	0.6600	MnO	0.0000	0.0664	Tl ₂ O ₃	0.0000	0.0062
ZrO ₂	0.0000	0.1600	MoO ₃	0.0000	0.0071	UO ₂	0.0000	0.0800
Ag ₂ O	0.0000	0.0026	Nd ₂ O ₃	0.0000	0.0091	UO ₃	0.0044	0.0050
As ₂ O ₃	0.0000	0.0021	PbO	0.0000	0.0500	V ₂ O ₅	0.0000	0.0009
BaO	0.0000	0.0400	PdO	0.0000	0.0004	WO ₃	0.0000	0.0021
Bi ₂ O ₃	0.0000	0.0641	Rh ₂ O ₃	0.0000	0.0008	Y ₂ O ₃	0.0000	0.0001
CdO	0.0000	0.0300	RuO ₂	0.0000	0.0014	ZnO	0.0001	0.0210

Table 2.6. Correlations of 231 Glass Compositions (in Mole Fraction) Used in Model Development

	Al₂O₃	B₂O₃	CaO	Fe₂O₃	K₂O	Li₂O	MgO	Na₂O	SiO₂	ZrO₂	LN₂O₃	MnO_x	SrO	Others
Al ₂ O ₃	1	0.013	-0.128	0.200	-0.121	0.019	-0.224	0.079	-0.259	-0.252	-0.085	0.182	0.214	-0.163
B ₂ O ₃		1	0.017	0.042	-0.090	-0.303	-0.089	0.049	-0.419	-0.123	-0.250	-0.142	-0.092	0.102
CaO			1	-0.283	0.222	-0.191	0.282	-0.153	-0.131	-0.249	0.134	-0.265	-0.229	-0.194
Fe ₂ O ₃				1	-0.202	0.030	-0.217	-0.012	-0.116	-0.060	-0.345	0.124	0.167	-0.008
K ₂ O					1	0.000	0.247	-0.255	0.042	-0.163	0.253	-0.160	-0.137	-0.147
Li ₂ O						1	-0.098	-0.559	0.097	0.046	0.054	0.043	-0.008	-0.054
MgO							1	-0.252	0.060	-0.331	0.028	-0.291	-0.255	-0.298
Na ₂ O								1	-0.214	0.210	-0.065	-0.101	-0.132	0.175
SiO ₂									1	-0.016	0.229	-0.309	-0.326	-0.429
ZrO ₂										1	0.073	0.199	0.044	0.130
LN ₂ O ₃											1	-0.206	-0.199	-0.055
MnO _x												1	0.943	0.129
SrO													1	0.136
Others														1



**Figure 2.4. Scatter Plot Matrix of 231 Glass Compositions
(in Mole Fraction) Used in Model Development**

Table 2.7. Model Coefficients, Standard Error, and Model Statistics for the Final TCLP r_B Model

Component	Final 14-Comp. Model	
	Coeff.	Std Error
Al ₂ O ₃	-11.830	1.637
B ₂ O ₃	14.155	0.767
CaO	14.266	0.982
Fe ₂ O ₃	-9.869	2.027
K ₂ O	29.025	2.465
Li ₂ O	10.456	0.937
MgO	12.980	1.032
Na ₂ O	18.440	0.874
SiO ₂	-1.270	0.358
ZrO ₂	-10.114	2.685
LN ₂ O ₃	-98.649	7.577
MnO _x	15.308	6.942
SrO	8.975	5.238
Others	9.696	1.116
Model Statistics		
Number of Glasses	231	
R ²	0.870	
R ² (Adjusted)	0.862	
s (RMSE)	0.5825	

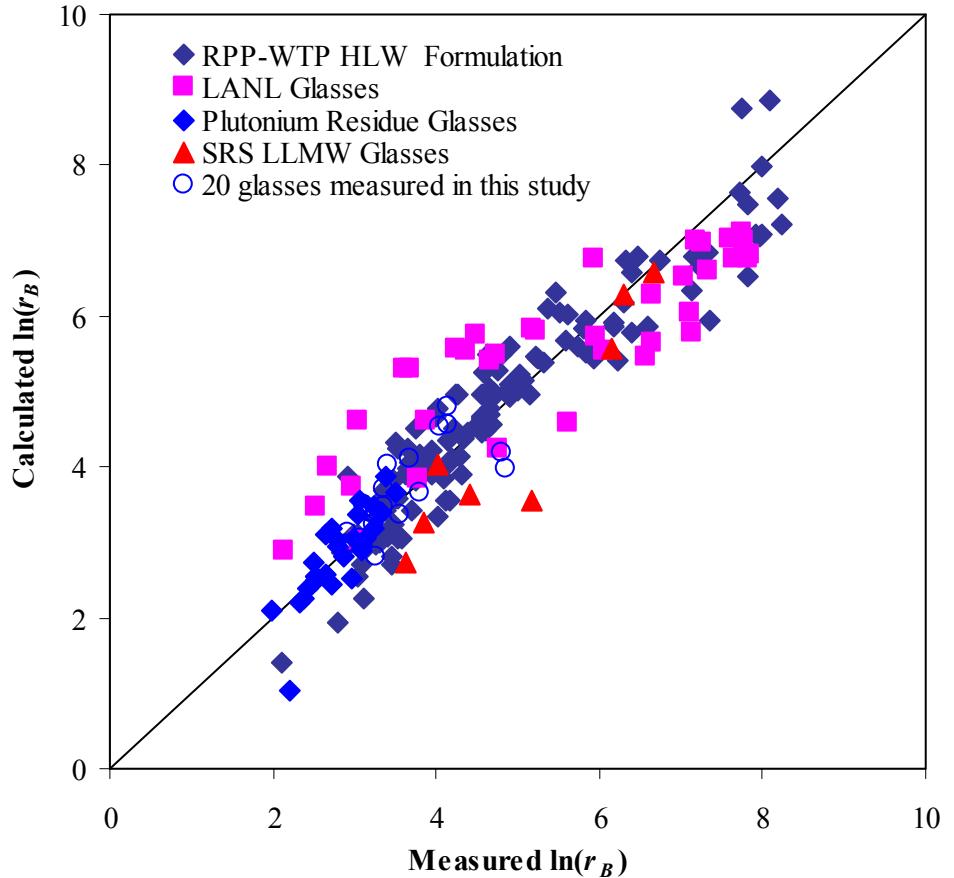


Figure 2.5. Calculated Versus Measured $\ln(r_B)$ Values for Glasses Used in the Final TCLP Model

2.5 Model Validation

To determine how well the model performs for the glasses not used to develop the model, the 231 glasses with r_B data were sorted in the order of r_B and were divided into two subsets by reserving the fifth glass in every five glasses for use to validate the model. This resulted in 46 validation glasses. The other 185 glasses were used for model development (model glasses). The same 14 components used in the final model were used.

Table 2.8 summarizes the model statistics of the reduced-data-set model and the statistics for model validation. The R^2 value in the reduced-data-set model was slightly higher than the full-data-set model because of a slightly narrower composition region. The R^2 (validation) is reasonably good, which was also to be expected, considering that the model coefficients from both models were not much different. Figure 2.6 shows that the model predicts very well the glasses that were not used to develop the model.

Table 2.8. Model Coefficients, Standard Error, and Model statistics for the Final TCLP r_B Model Used for Model Validation

Component	Reduced Data Model	
	Coeff.	Std Error
Al ₂ O ₃	-10.658	1.810
B ₂ O ₃	14.445	0.867
CaO	14.460	1.066
Fe ₂ O ₃	-9.844	2.276
K ₂ O	26.307	3.602
Li ₂ O	10.155	1.038
MgO	14.086	1.314
Na ₂ O	17.244	0.956
SiO ₂	-1.070	0.377
ZrO ₂	-7.330	3.081
LN ₂ O ₃	-100.686	8.758
MnO _x	14.683	7.121
SrO	8.540	5.382
Others	8.953	1.201
Model statistics		
Number of Glasses	185	
R ²	0.878	
R ² (Adjusted)	0.869	
s (RMSE)	0.5664	
Validation Statistics		
Number of Glasses	46	
R ² (Validation)	0.817	

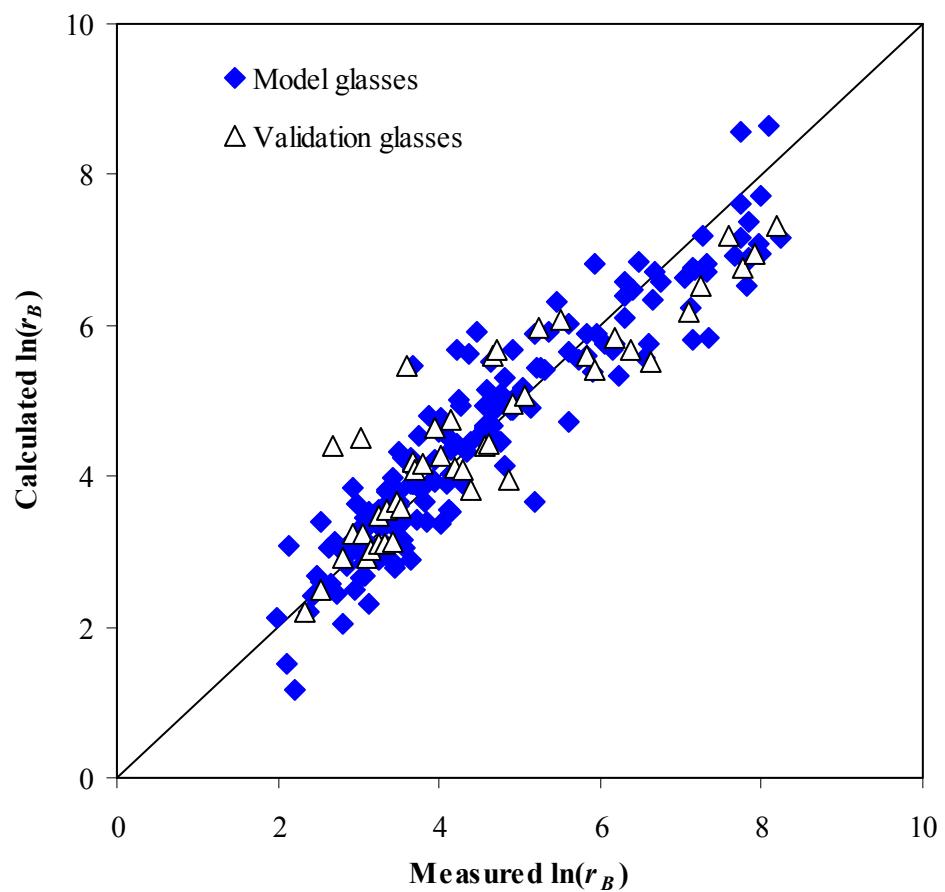


Figure 2.6. Calculated versus Measured $\ln(r_B)$ Values for Glasses Used in the Reduced Data Set Model (Model Glasses) and for Glasses not Used for Model (Validation Glasses)

3.0 Model Applications

The calculated c_i using Equation 2.3 is based on the observation that generally $r_i \leq r_B$ for all RCRA elements, which provides a reasonable estimation for congruent elements (Ba, Cd, Ni, and Zn) and a conservative estimation for “incongruent” elements (Ag, As, Cr, Pb, and Se). It will be necessary to develop the separate models for these incongruent elements if they become a limiting factor that causes the glasses to fail the TCLP requirements because the current model predicts higher than measured releases for these components, in most cases. The development of separate models would require a larger number of data than currently available. As a first step, it was attempted to develop the model for TCLP Cd release (third in number of data after B and Ba, but Ba is less important because its regulatory limit is high), but this effort was not successful, primarily because of limited data on Cd release and possibly because of the dominant effect of CdO concentration in glass. The component coefficients changed erratically with the change of model components, even though the model had higher R^2 values than the r_B model.

Table 3.1 summarizes the regulatory limits used by EPA for designating wastes (55 FR 22520) and the LDR universal treatment standard (UTS) (61 FR 2338; 62 FR 26041). UTS limits are lower than the toxicity limits for all elements except for As and Se.

Table 3.1. RCRA Toxicity Limits by TCLP and Corresponding Glass Oxide Concentration (see text)

Element	Ag	As	Ba	Cd	Cr	Hg	Ni	Pb	Se
RCRA Toxicity Limit (mg/L)	5	5	100	1	5	0.2	--	5	1
RCRA UTS Limit (mg/L)	0.14	5	21	0.11	0.6	0.025	11	0.75	5.7

Figure 3.1 shows the plots of calculated versus measured releases of eight RCRA elements for 231 glasses used in the model development. Also included in Figure 3.1 are the lines representing the values of RCRA toxicity and UTS limits. In terms of pass/fail classification, the data points in the top-left rectangle separated by each line of regulatory limit represent the false classification of non-hazardous glasses as hazardous (“false positive”), and the bottom right represents the false classification of hazardous glasses as non-hazardous (“false negative”). Figure 3.1 shows that there are two glasses in the bottom-right rectangle of “false negative” classification based on RCRA toxicity limits (blue solid lines, one each for c_{Cd} and c_{Cr}), which are predicted to be non-hazardous but are hazardous based on TCLP measurements.

Figure 3.2 illustrates the classification errors using c_{Cd} and its RCRA toxicity limit as an example. To decrease the probability of “false negative” classification, it is necessary to apply the prediction uncertainty, u .^(a) The method for uncertainty calculation will depend on the nature of application and

(a) Typically, u is calculated using either the t-statistic according to $u = \sqrt{s^2 T \mathbf{x}' (\mathbf{X}' \mathbf{X})^{-1} \mathbf{x}}$ or the f-statistic according to $u = \sqrt{ps^2 F \mathbf{x}' (\mathbf{X}' \mathbf{X})^{-1} \mathbf{x}}$, where s is the root mean square error, T is the t-statistic at the appropriate confidence (e.g., 95% one sided) and degrees of freedom, \mathbf{x} is the composition vector, \mathbf{X} is the

governing regulations. Figure 3.2 shows that one glass is in the “false negative” region and four glasses are in the “false positive” if the classification is based on as-predicted values. However, by applying the upper bound [$\ln(c_{Cd})+u$] of the confidence band [$\ln(c_{Cd})\pm u$] as a limit (here, u was assumed as a constant value arbitrarily chosen for the purpose of this illustration), the one glass in the “false negative” region is eliminated, but the four glasses in the “false positive” region increase to 12.

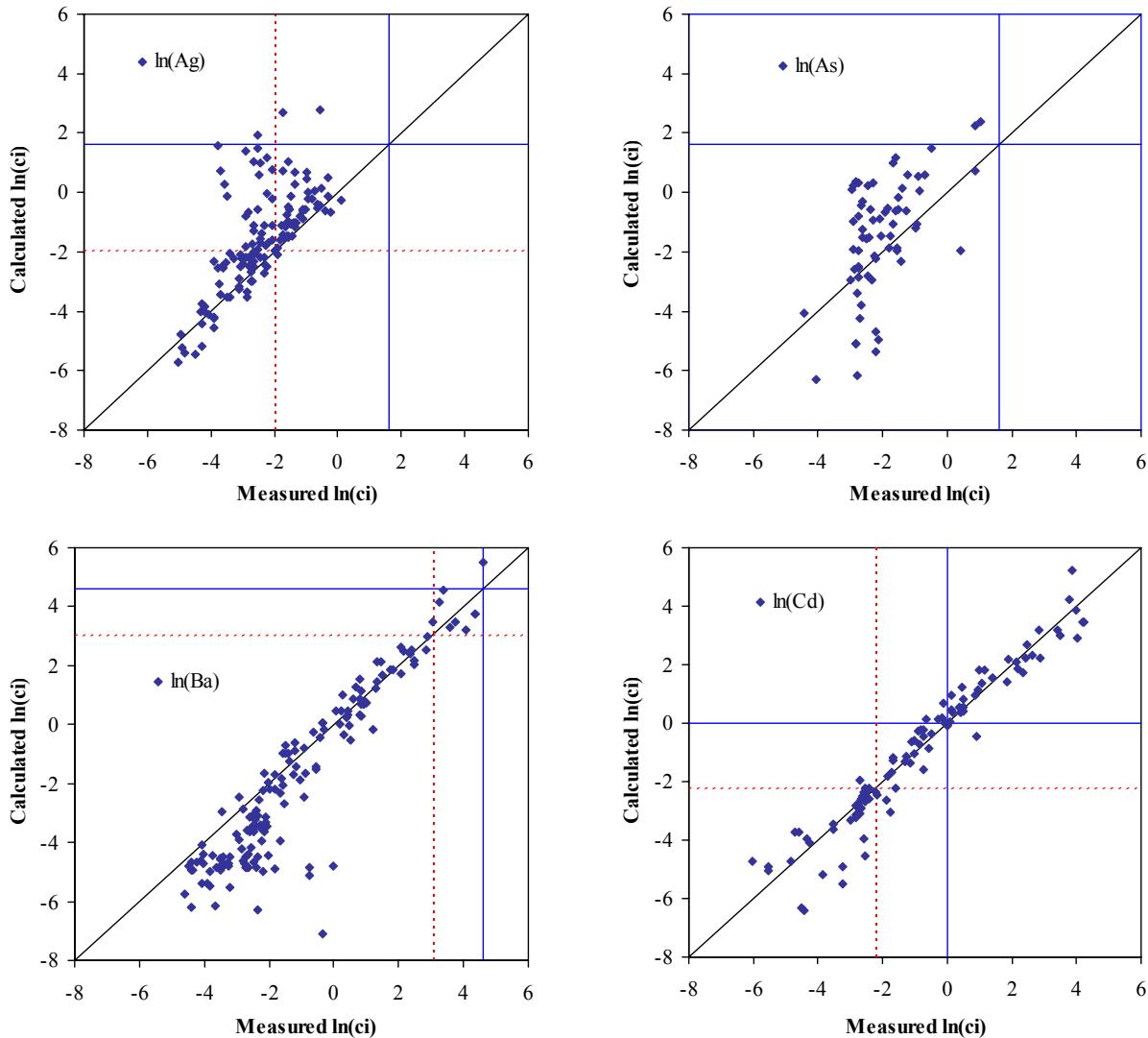


Figure 3.1. Plots of Calculated vs. Measured TCLP Releases of Eight RCRA Elements (no data exist on Hg) for 231 Glasses Used in the Model Development. (Solid lines represent the RCRA toxicity limits and dotted lines the RCRA UTS limits.)

matrix of compositions used in model fitting, p is the number of model coefficients, and F is the f-statistic at the appropriate confidence and degrees of freedom. The appropriate method depends upon the application.

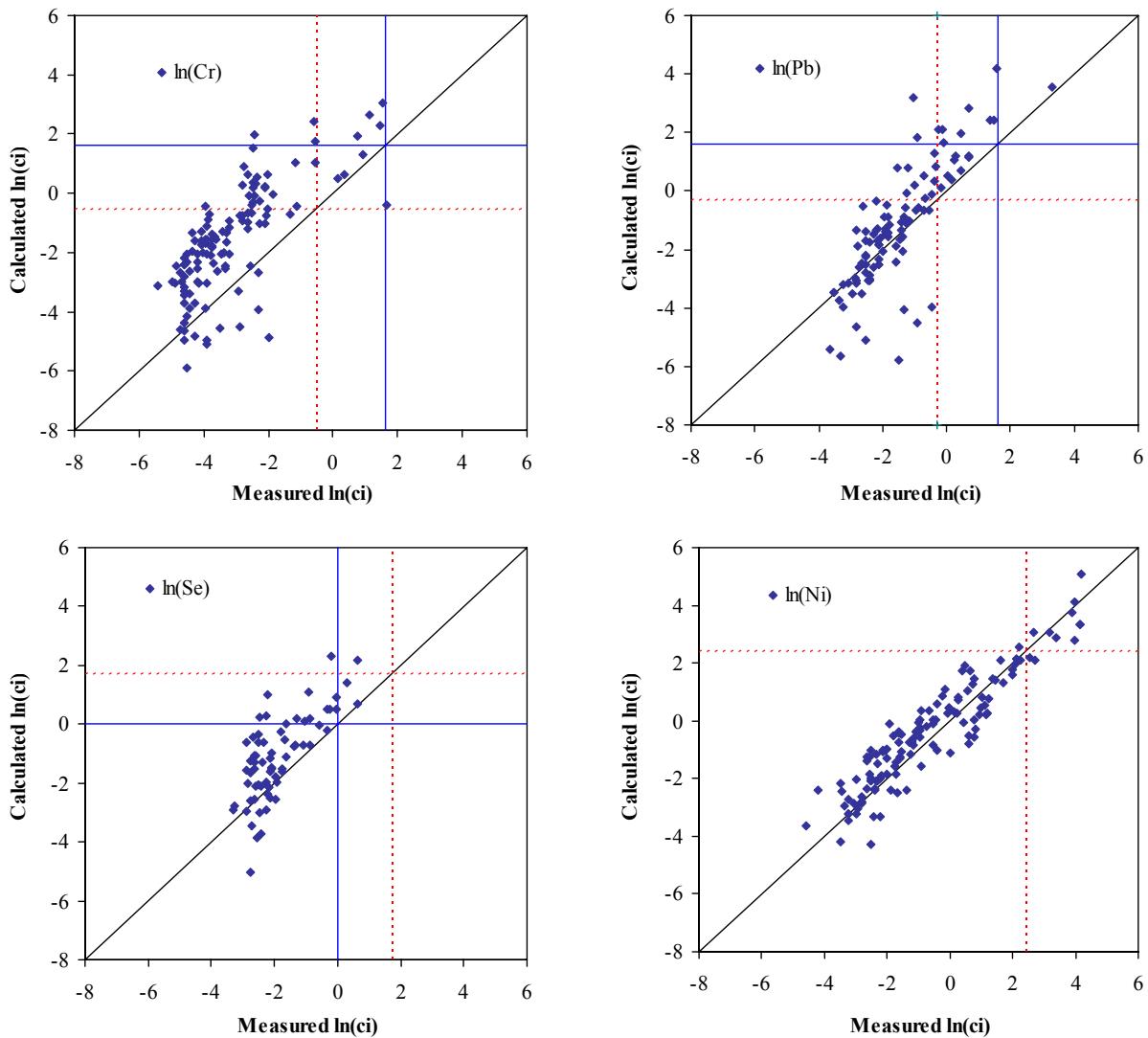


Figure 3.1 (cont'd)

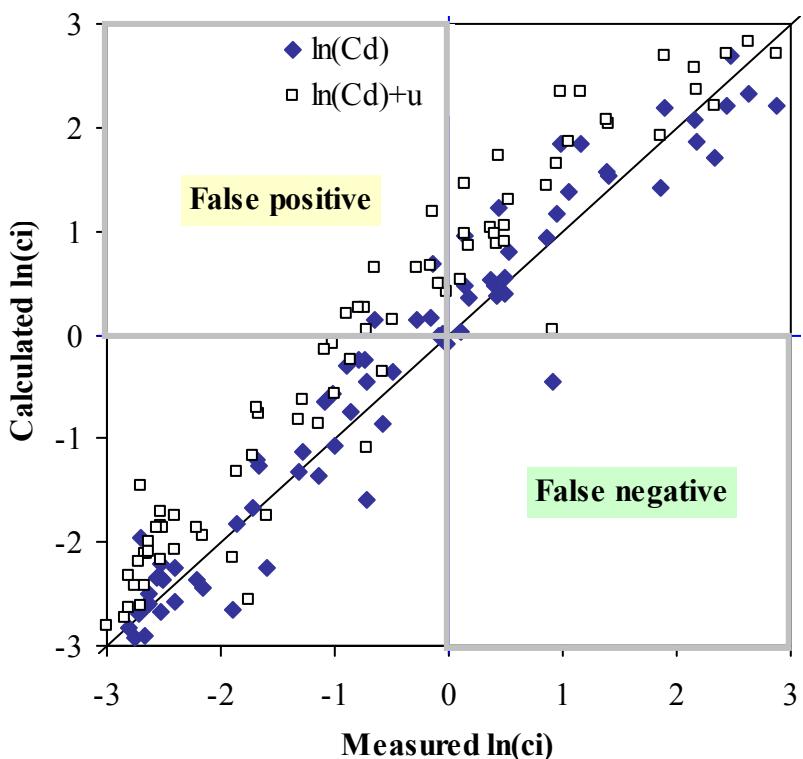


Figure 3.2. Plot of Calculated vs. Measured TCLP Releases of Cd

The normalized release, r_i , represents the amount of glass dissolved in the TCLP condition if it is assumed that the glass dissolves congruently, i.e., all the elements in glass release at the same rate. If the glass sample were entirely dissolved in TCLP and the dissolution were congruent, then $r_i = 50,000$ for all elements. Similar to PCT, boron is believed to be the most appropriate element to represent the glass network dissolution, neither participating in the precipitation of mineral phases nor preferentially releasing elements like alkalis by ion exchange (see Hrma et al. 1994 for example).

Of 241 glasses with boron-release data (initial 221 plus the additional 20 glasses), the r_B was below 3800 mg/L for all glasses but one (RFP-8), which is an obvious outlier.^(a) The maximum release of 3800-mg/L corresponds to the glass dissolution of 7.6% under TCLP conditions. Assuming conservatively that 10% is the maximum glass dissolution for typical waste glasses, we can calculate the corresponding release of these elements based on glass composition if congruent dissolution is assumed. Table 3.2 shows the concentration of oxides in glass that correspond to the TCLP limits of each element when it is assumed that the glass dissolves congruently at the maximum rate of 10% for typical glasses. This information can be used as a good preliminary screening of glasses that will pass the TCLP requirements based only on the oxide concentration of RCRA elements without having to apply the TCLP model. For example, if the oxide concentrations of all RCRA elements are lower than the values in Table 3.2 for each requirement (toxicity and UTS), the glass will pass that TCLP requirement. However, if a

(a) This glass had 9694 mg/L. Reviewing the composition of this glass compared with other glasses did not suggest any reason that this particular glass should dissolve more than twice the maximum dissolution in the other 240 glasses. This composition needs to be tested again to confirm this assumption.

glass has a concentration of just one component higher than the values listed in Table 3.2, then the TCLP model must be applied.

**Table 3.2. RCRA Toxicity Limits by TCLP and Corresponding Glass Oxide Concentration
(see text)**

Element	Ag	As	Ba	Cd	Cr	Hg	Ni	Pb	Se
RCRA Toxicity Limit (mg/L)	5	5	100	1	5	0.2	--	5	1
RCRA UTS Limit (mg/L)	0.14	5	21	0.11	0.6	0.025	11	0.75	5.7
Oxide*	Ag ₂ O	As ₂ O ₃	BaO	CdO	Cr ₂ O ₃	HgO	NiO	PbO	SeO ₂
For RCRA Toxicity Limit (wt%)	0.1074	0.1320	2.2330	0.0228	0.1462	0.0043	--	0.1077	0.0281
For RCRA UTS Limit (wt%)	0.0030	0.1320	0.4689	0.0025	0.0175	0.0005	0.2800	0.0162	0.1602

4.0 References

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Appendix A

Glass Composition and TCLP Release Data Collected for This Study

Appendix A: Glass Composition and TCLP Release Data Collected for This Study

Appendix A. Glass Composition and TCLP Release Data

TWRS LAW Formulation 2 (Ferrara et al. 1998)

Glass ID	MoO	MoO ₃	Nd ₂ O ₃	PbO	PdO	ReO ₂	Rh ₂ O ₃	RuO ₂	Sb ₂ O ₃	Sb ₂ O ₅	SeO ₂	SnO	SnO ₂
Envelope A													
Envelope B													
Envelope C													

SRS M-Area Mixed Waste (Fu et al 1997)

SRM-20													
SRM-21													
SRM-22													
SRM-12													
SRM-26													
SRM-18													

TWRS LAW Formulation (Muller and Pegg 1998)

LAWA23				0									0
LAWA24				0.001									0
LAWB29				0									0
LAWPC10				0.0002									0

TWRS HLW Glass Formulation (Fu and Pegg 1998)

HLWD1-08	0.003		0.0081	0.0048	0	0		0		0	0	0	
HLWD1-09	0.003		0.0081	0.0048	0	0		0		0	0	0	
HLWD1-10	0.0029		0.0076	0.0045	0	0		0		0	0	0	
HLWD3-03	0		0	0	0	0		0		0	0	0	
HLWD3-04	0.0059		0	0.0093	0	0		0		0.0088	0.0057	0	
HLWD3-06	0		0	0	0	0		0		0	0	0	
HLWD3-08	0		0	0.0019	0.0005	0.0003		0.0013		0.0009	0.0009	0	
EnvDSR1	0		0	0.0018	0	0		0		0	0	0	

RPP-WTP LAW Formulation (Muller et al. 2001)

LAWA44				0.00001		0.001							
LAWA102S						0.001							
LAWB45						0.001							
LAWC21S						0.001							

RPP-WTP HLW Formulation (Kot and Pegg 2001)

HLW98-01				0.0022					0.0019	0.0019			
HLW98-02				0.0023					0.002	0.002			
HLW98-03				0.0047	0.0024				0.0005	0.0005			

Appendix A. Glass Composition and TCLP Release Data

Glass ID	MoO	MoO ₃	Nd ₂ O ₃	PbO	PdO	ReO ₂	Rh ₂ O ₃	RuO ₂	Sb ₂ O ₃	Sb ₂ O ₅	SeO ₂	SnO	SnO ₂
HLW99-81				0	0.0004		0.0008	0.0014		0.0021	0.0021		
HLW99-82				0.0063	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-83				0	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-84				0.0037	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-85				0.0031	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-86				0	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-87				0.0021	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-88				0.0063	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-89				0	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-90R				0	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-91				0	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-92				0.0063	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-93R2				0	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-94				0	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-95				0	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-96				0.0031	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-97				0.0042	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-98R				0.0063	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-99				0	0.0004		0.0008	0.0013		0.002	0.002		
HLW99-100				0	0.0004		0.0008	0.0013		0.002	0.002		

LANL Glasses (Vienna et al. 1998)

LANL-A		0	0.000161										
LANL-B		0	0.000161										
LANL-C		0	0.000161										
LANL-D		0	0.000161										
LANL-E		0	0.000161										
LANL-F		0	0.000161										
LANL-G		0	0.000161										
LANL-H		0	0.000161										
LANL-I		0	0.000161										
LANL-J		0	0.000161										
LANL-K		0	0.000241										
LANL-L		0	0.000161										
LANL-M		0	0.050008										
LANL-N		0	0.000161										
LANL-O		0	0.000161										
LANL-P		0	0.000161										
LANL-Q		0	0.000161										

Appendix A. Glass Composition and TCLP Release Data

Glass ID	SO3	SrO	TeO2	ThO2	TiO2	Tl2O3	U3O8	UO2	UO3	V2O5	WO3	Y2O3	ZnO	Sum
HLW99-81	0.0026	0.0986	0.0021	0	0	0.0021		0			0.0021		0.021	0.9998
HLW99-82	0.0025	0.0545	0.002	0	0.0063	0.002		0			0.002		0.02	1.0002
HLW99-83	0.0025	0.1001	0.002	0	0	0.002		0			0.002		0.02	1.0000
HLW99-84	0.0025	0.1007	0.002	0	0.0037	0.002		0			0.002		0.02	1.0002
HLW99-85	0.0025	0.0545	0.002	0	0.0031	0.002		0			0.002		0.02	1.0001
HLW99-86	0.0025	0.0545	0.002	0	0	0.002		0			0.002		0.02	1.0000
HLW99-87	0.0025	0.1332	0.002	0	0.0021	0.002		0			0.002		0.02	1.0001
HLW99-88	0.0025	0.0545	0.002	0	0.0063	0.002		0			0.002		0.02	1.0002
HLW99-89	0.0025	0.0545	0.002	0	0	0.002		0			0.002		0.02	1.0000
HLW99-90R	0.0025	0.095	0.002	0	0	0.002		0			0.002		0.02	1.0000
HLW99-91	0.0025	0.1332	0.002	0	0	0.002		0			0.002		0.02	1.0000
HLW99-92	0.0025	0.1283	0.002	0	0.0063	0.002		0			0.002		0.02	1.0002
HLW99-93R2	0.0025	0.1332	0.002	0	0	0.002		0			0.002		0.02	1.0000
HLW99-94	0.0025	0.0545	0.002	0	0	0.002		0			0.002		0.02	1.0000
HLW99-95	0.0025	0.0545	0.002	0	0	0.002		0			0.002		0.02	1.0000
HLW99-96	0.0025	0.095	0.002	0	0.0031	0.002		0			0.002		0.02	1.0001
HLW99-97	0.0025	0.0545	0.002	0	0.0042	0.002		0			0.002		0.02	1.0002
HLW99-98R	0.0025	0.0981	0.002	0	0.0063	0.002		0			0.002		0.02	1.0002
HLW99-99	0.0025	0.1332	0.002	0	0	0.002		0			0.002		0.02	1.0000
HLW99-100	0.0025	0.0938	0.002	0	0	0.002		0			0.002		0.02	1.0000

LANL Glasses (Vienna et al. 1998)

LANL-A														1.0000
LANL-B														1.0000
LANL-C														1.0000
LANL-D														1.0000
LANL-E														1.0000
LANL-F														1.0000
LANL-G														1.0000
LANL-H														1.0000
LANL-I														1.0000
LANL-J														1.0000
LANL-K														1.0000
LANL-L														1.0000
LANL-M														1.0000
LANL-N														1.0000
LANL-O														1.0000
LANL-P														1.0000
LANL-Q														1.0000

Appendix A. Glass Composition and TCLP Release Data

Glass ID	TCLP B (mg/L)	TCLP Ag (mg/L)	TCLP As (mg/L)	TCLP Ba (mg/L)	TCLP Cd (mg/L)	TCLP Cr (mg/L)	TCLP Ni (mg/L)	TCLP Pb (mg/L)	TCLP Se (mg/L)	TCLP Zn (mg/L)
HLW99-81	2.171	0.254	0.049	1.169	0.101	0.019	0.039	0.124	0.072	2.155
HLW99-82	5.748	0.334	0.049	4.458	2.875	0.02	2.089	0.69	0.0532	2.823
HLW99-83	1.971	0.111	0.105	1.019	0.016	<0.0055	<0.0079	0.044	0.0532	1.097
HLW99-84	4.03	0.231	0.172	2.512	1.2	<0.0055	0.937	0.388	0.055	2.171
HLW99-85	1.374	0.081	0.238	1.373	0.337	0.036	0.27	0.115	0.0532	0.0779
HLW99-86	1.232	0.07	0.049	0.816	0.011	0.035	0.039	<0.0243	0.121	0.73
HLW99-87	9.597	0.559	0.122	2.737	1.64	0.073	1.171	0.583	0.0532	4.627
HLW99-88	2.92	0.233	0.055	2.659	1.508	<0.0055	0.399	0.416	0.0532	1.376
HLW99-89	1.027	0.105	0.049	0.807	0.017	0.015	<0.0079	<0.0243	0.0532	0.649
HLW99-90R	3.254	0.201	0.049	0.767	<0.0027	0.02	0.015	0.085	0.0532	1.714
HLW99-91	2.96	0.18	<0.049	0.819	0.011	<0.0055	<0.0079	0.066	<0.0532	1.627
HLW99-92	8.366	0.527	0.063	6.268	4.021	0.04	3.913	1.016	<0.0532	4.434
HLW99-93R2	15.072	0.739	0.224	1.415	<0.0027	0.081	0.019	0.233	0.081	8.326
HLW99-94	4.177	0.253	0.083	1.206	0.072	0.019	0.061	0.055	<0.0532	2.307
HLW99-95	3.212	0.195	0.083	0.974	<0.0027	0.018	<0.0079	<0.0243	0.064	1.812
HLW99-96	2.499	0.164	<0.0490	1.605	0.616	<0.0055	0.212	0.147	0.075	1.151
HLW99-97	3.446	0.225	<0.0490	2.453	1.151	<0.0055	0.523	0.275	<0.0532	1.781
HLW99-98R	16.871	0.605	0.072	10.716	8.643	0.081	7.903	1.292	0.081	9.125
HLW99-99	4.592	0.267	<0.0490	1.262	0.018	0.024	0.009	0.077	0.125	2.486
HLW99-100	15.874	0.795	0.186	1.627	0.02	0.072	0.022	0.227	0.12	8.829

LANL Glasses (Vienna et al. 1998)

LANL-A	13.1253			0.03444	0.0387	0.12057	1.02933			
LANL-B	1.45275			0.01434			0.12591			
LANL-C	3.29358			0.01746			0.19824			
LANL-D	115.7718			0.08067		0.09246	3.09501			
LANL-E	108.32994			0.07389		0.13149	2.97954			
LANL-F	4.89279			0.01152			0.09693			
LANL-G	117.61176			0.10524			3.26493			
LANL-H	5.23701			0.01797			0.11772			
LANL-I	98.60685			0.09222			2.60763			
LANL-J	93.5427			0.08604		0.09345	2.64261			
LANL-K	66.37953			0.06129		0.06411	2.81679			
LANL-L	53.05995			0.0501			1.51941			
LANL-M	71.20971			0.07347			2.15244	26.95101		
LANL-N	19.5414			0.0687	0.02127	0.26736	1.79145			
LANL-O	17.78376			0.03249		0.06102	0.59286			
LANL-P	19.70343			0.03777		0.06111	0.65973			
LANL-Q	1.06527			0.01227			0.11706			

Appendix A. Glass Composition and TCLP Release Data

LANL Glasses (Vienna et al. 1998)

Glass ID	Al ₂ O ₃	B ₂ O ₃	CaO	Fe ₂ O ₃	K ₂ O	Li ₂ O	MgO	Na ₂ O	NiO	P ₂ O ₅	SiO ₂	ZrO ₂	Ag ₂ O	As ₂ O ₃
LANL-R	0.006818	0.050007	0.066975	0.019067	0.016633	0.050007	0.120017	0.100836	0.00178		0.563478			
LANL-S	0.010228	0.050011	0.100469	0.028602	0.024951	0.050011	0.11462	0.064717	0.002671		0.547148			
LANL-T	0.050024	0.050007	0.066975	0.019067	0.050007	0.050007	0.120017	0.0828	0.00178		0.504934			
LANL-U	0.006821	0.116772	0.066977	0.019072	0.016632	0.058656	0.076418	0.056506	0.00178		0.575988			
LANL-U	0.006821	0.116772	0.066977	0.019072	0.016632	0.058656	0.076418	0.056506	0.00178		0.575988			
LANL-V	0	0.200002	0	0.120001	0.150002	0.0309	0	0.069101	0.00024		0.429004			
LANL-X	0.12	0.2	0.12	0	0	0.0823	0	0	0.00971		0.4377			
LANL-Y	0	0.2	0.12	0.12	0	0.052	0	0	0.00971		0.468			
LANL-Z	0.12	0.0218	0.12	0	0.15	0.1	0	0	0.00971		0.4482			
LANL-AA	0.12	0.02	0	0.12	0	0.0876	0.12	0.0924	0.00971		0.4			
LANL-AB	0.12	0.0536	0	0	0.15	0.1	0.12	0	0.00971		0.4164			
LANL-AC	0	0.02	0	0.120001	0	0.099701	0	0.150302	0.00024		0.609006			
LANL-AD	0.0416	0.02	0	0	0	0.0784	0	0.16	0.00971		0.66			
LANL-AE	0.120001	0.02	0.120001	0.120001	0.150002	0.0476	0	0	0.00024		0.421404			
LANL-AF	0.120001	0.200002	0	0.120001	0	0.0406	0.118401	0	0.00024		0.400004			
LANL-AG	0.120001	0.200002	0	0	0	0.099901	0	0	0.00024		0.579106			
LANL-AH	0	0.2	0	0	0.15	0	0	0.0968	0.00971		0.5132			
LANL-AI	0	0.02	0.12	0.12	0.15	0	0.12	0.0017	0.00971		0.4283			
LANL-AJ	0.12	0.02	0.12	0.12	0	0.0106	0	0.16	0.00971		0.4094			
LANL-AK	0	0.02	0	0.12	0	0.0889	0.12	0	0.00971		0.6111			

Plutonium Residue Glasses (Bulkley and Vienna 1997)

SRC-BL	0.05	0.06	0.049	0.016	0.03	0.04	0.02	0.1	0.005	0.003	0.45	0.03		
SRC-Al-1	0	0.063158	0.051579	0.016842	0.031579	0.042105	0.021053	0.105263	0.005263	0.003158	0.473684	0.031579		
SRC-Al-2	0.1	0.056842	0.046421	0.015158	0.028421	0.037895	0.018947	0.094737	0.004737	0.002842	0.426316	0.028421		
SRC-B-2	0.051064	0.04	0.050043	0.01634	0.030638	0.040851	0.020426	0.102128	0.005106	0.003064	0.459574	0.030638		
SRC-B-3	0.046809	0.12	0.045872	0.014979	0.028085	0.037447	0.018723	0.093617	0.004681	0.002809	0.421277	0.028085		
SRC-Ca-1	0.052576	0.063091	0	0.016824	0.031546	0.042061	0.02103	0.105152	0.005258	0.003155	0.473186	0.031546		
SRC-Ca-2	0.051525	0.06183	0.02	0.016488	0.030915	0.04122	0.02061	0.103049	0.005152	0.003091	0.463722	0.030915		
SRC-Ca-3	0.04837	0.058044	0.08	0.015478	0.029022	0.038696	0.019348	0.09674	0.004837	0.002902	0.435331	0.029022		
SRC-Ce-1	0.052356	0.062827	0.051309	0.016754	0.031414	0.041885	0.020942	0.104712	0.005236	0.003141	0.471204	0.031414		
SRC-Ce-2	0.051047	0.061257	0.050026	0.016335	0.030628	0.040838	0.020419	0.102094	0.005105	0.003063	0.459424	0.030628		
SRC-Ce-3	0.048953	0.058743	0.047974	0.015665	0.029372	0.039162	0.019581	0.097906	0.004895	0.002937	0.440576	0.029372		
SRC-K-1	0.051546	0.061856	0.050515	0.016495	0	0.041237	0.020619	0.103093	0.005155	0.003093	0.463918	0.030928		
SRC-K-2	0.048454	0.058144	0.047485	0.015505	0.06	0.038763	0.019381	0.096907	0.004845	0.002907	0.436082	0.029072		
SRC-Li-1	0.052083	0.0625	0.051042	0.016667	0.03125	0	0.020833	0.104167	0.005208	0.003125	0.46875	0.03125		
SRC-Li-2	0.051302	0.061563	0.050276	0.016417	0.030781	0.015	0.020521	0.102604	0.00513	0.003078	0.461719	0.030781		
SRC-Li-3	0.04974	0.059688	0.048745	0.015917	0.029844	0.045	0.019896	0.099479	0.004974	0.002984	0.447656	0.029844		
SRC-Na-1	0.055556	0.066667	0.054444	0.017778	0.033333	0.044444	0.022222	0	0.005556	0.003333	0.5	0.033333		

Appendix A. Glass Composition and TCLP Release Data

LANL Glasses (Vienna et al. 1998)

Glass ID	BaO	Bi2O3	CdO	CeO2	Cl	CoO	Cr2O3	Cs2O	CuO	F	Gd2O3	La2O3	MnO2	MnO
LANL-R	4E-05		2E-05	0.0019			0.00226							
LANL-S	6E-05		3E-05	0.00285			0.003391							
LANL-T	4E-05		2E-05	0.0019			0.00226							
LANL-U	4E-05		2E-05	0.0019			0.00226							
LANL-U	4E-05		2E-05	0.0019			0.00226							
LANL-V	0		0	4E-05			0.00047							
LANL-X	0.00011		0	0.00167			0.01891							
LANL-Y	0.00011		0	0.00167			0.01891							
LANL-Z	0.00011		0	0.00167			0.01891							
LANL-AA	0.00011		0	0.00167			0.01891							
LANL-AB	0.00011		0	0.00167			0.01891							
LANL-AC	0		0	4E-05			0.00047							
LANL-AD	0.00011		0	0.00167			0.01891							
LANL-AE	0		0	4E-05			0.00047							
LANL-AF	0		0	4E-05			0.00047							
LANL-AG	0		0	4E-05			0.00047							
LANL-AH	0.00011		0	0.00167			0.01891							
LANL-AI	0.00011		0	0.00167			0.01891							
LANL-AJ	0.00011		0	0.00167			0.01891							
LANL-AK	0.00011		0	0.00167			0.01891							

Plutonium Residue Glasses (Bulkley and Vienna 1997)

SRC-BL	0.0022			0.045	0.005		0.004	0.01	0.0004	0.001	0.045			
SRC-Al-1	0.002316			0.047368	0.005263		0.004211	0.010526	0.000421	0.001053	0.047368			
SRC-Al-2	0.002084			0.042632	0.004737		0.003789	0.009474	0.000379	0.000947	0.042632			
SRC-B-2	0.002247			0.045957	0.005106		0.004085	0.010213	0.000409	0.001021	0.045957			
SRC-B-3	0.00206			0.042128	0.004681		0.003745	0.009362	0.000374	0.000936	0.042128			
SRC-Ca-1	0.002313			0.047319	0.005258		0.004206	0.010515	0.000421	0.001052	0.047319			
SRC-Ca-2	0.002267			0.046372	0.005152		0.004122	0.010305	0.000412	0.00103	0.046372			
SRC-Ca-3	0.002128			0.043533	0.004837		0.00387	0.009674	0.000387	0.000967	0.043533			
SRC-Ce-1	0.002304			0	0.005236		0.004188	0.010471	0.000419	0.001047	0.04712			
SRC-Ce-2	0.002246			0.025	0.005105		0.004084	0.010209	0.000408	0.001021	0.045942			
SRC-Ce-3	0.002154			0.065	0.004895		0.003916	0.009791	0.000392	0.000979	0.044058			
SRC-K-1	0.002268			0.046392	0.005155		0.004124	0.010309	0.000412	0.001031	0.046392			
SRC-K-2	0.002132			0.043608	0.004845		0.003876	0.009691	0.000388	0.000969	0.043608			
SRC-Li-1	0.002292			0.046875	0.005208		0.004167	0.010417	0.000417	0.001042	0.046875			
SRC-Li-2	0.002257			0.046172	0.00513		0.004104	0.01026	0.00041	0.001026	0.046172			
SRC-Li-3	0.002189			0.044766	0.004974		0.003979	0.009948	0.000398	0.000995	0.044766			
SRC-Na-1	0.002444			0.05	0.005556		0.004444	0.011111	0.000444	0.001111	0.05			

Appendix A. Glass Composition and TCLP Release Data

LANL Glasses (Vienna et al. 1998)

Glass ID	MoO	MoO ₃	Nd ₂ O ₃	PbO	PdO	ReO ₂	Rh ₂ O ₃	RuO ₂	Sb ₂ O ₃	Sb ₂ O ₅	SeO ₂	SnO	SnO ₂
LANL-R			0	0.000161									
LANL-S			0	0.000241									
LANL-T			0	0.000161									
LANL-U			0	0.00016									
LANL-U			0	0.00016									
LANL-V			0.00023	1E-05									
LANL-X			0.0091	0.0005									
LANL-Y			0.0091	0.0005									
LANL-Z			0.0091	0.0005									
LANL-AA			0.0091	0.0005									
LANL-AB			0.0091	0.0005									
LANL-AC			0.00023	1E-05									
LANL-AD			0.0091	0.0005									
LANL-AE			0.00023	1E-05									
LANL-AF			0.00023	1E-05									
LANL-AG			0.00023	1E-05									
LANL-AH			0.0091	0.0005									
LANL-AI			0.0091	0.0005									
LANL-AJ			0.0091	0.0005									
LANL-AK			0.0091	0.0005									

Plutonium Residue Glasses (Bulkley and Vienna 1997)

SRC-BL		0.0064	0.008	0.01								0	
SRC-Al-1		0.006737	0.008421	0.010526								0	
SRC-Al-2		0.006063	0.007579	0.009474								0	
SRC-B-2		0.006536	0.00817	0.010213								0	
SRC-B-3		0.005991	0.007489	0.009362								0	
SRC-Ca-1		0.00673	0.008412	0.010515								0	
SRC-Ca-2		0.006595	0.008244	0.010305								0	
SRC-Ca-3		0.006191	0.007739	0.009674								0	
SRC-Ce-1		0.006702	0.008377	0.010471								0	
SRC-Ce-2		0.006534	0.008168	0.010209								0	
SRC-Ce-3		0.006266	0.007832	0.009791								0	
SRC-K-1		0.006598	0.008247	0.010309								0	
SRC-K-2		0.006202	0.007753	0.009691								0	
SRC-Li-1		0.006667	0.008333	0.010417								0	
SRC-Li-2		0.006567	0.008208	0.01026								0	
SRC-Li-3		0.006367	0.007958	0.009948								0	
SRC-Na-1		0.007111	0.008889	0.011111								0	

Appendix A. Glass Composition and TCLP Release Data

LANL Glasses (Vienna et al. 1998)

Glass ID	SO ₃	SrO	TeO ₂	ThO ₂	TiO ₂	Tl ₂ O ₃	U ₃ O ₈	UO ₂	UO ₃	V ₂ O ₅	WO ₃	Y ₂ O ₃	ZnO	Sum
LANL-R														1.0000
LANL-S														1.0000
LANL-T														1.0000
LANL-U														1.0000
LANL-U														1.0000
LANL-V														1.0000
LANL-X														1.0000
LANL-Y														1.0000
LANL-Z														1.0000
LANL-AA														1.0000
LANL-AB														1.0000
LANL-AC														1.0000
LANL-AD														1.0000
LANL-AE														1.0000
LANL-AF														1.0000
LANL-AG														1.0000
LANL-AH														1.0000
LANL-AI														1.0000
LANL-AJ														1.0000
LANL-AK														1.0000

Plutonium Residue Glasses (Bulkley and Vienna 1997)

SRC-BL					0.01									1.0000
SRC-AI-1						0.010526								1.0000
SRC-AI-2							0.009474							1.0000
SRC-B-2							0.010213							1.0000
SRC-B-3							0.009362							1.0000
SRC-Ca-1							0.010515							1.0000
SRC-Ca-2							0.010305							1.0000
SRC-Ca-3							0.009674							1.0000
SRC-Ce-1							0.010471							1.0000
SRC-Ce-2							0.010209							1.0000
SRC-Ce-3							0.009791							1.0000
SRC-K-1							0.010309							1.0000
SRC-K-2							0.009691							1.0000
SRC-Li-1							0.010417							1.0000
SRC-Li-2							0.01026							1.0000
SRC-Li-3							0.009948							1.0000
SRC-Na-1							0.011111							1.0000

Appendix A. Glass Composition and TCLP Release Data

LANL Glasses (Vienna et al. 1998)

Glass ID	TCLP B (mg/L)	TCLP Ag (mg/L)	TCLP As (mg/L)	TCLP Ba (mg/L)	TCLP Cd (mg/L)	TCLP Cr (mg/L)	TCLP Ni (mg/L)	TCLP Pb (mg/L)	TCLP Se (mg/L)	TCLP Zn (mg/L)
LANL-R	2.88666			0.02373		0.07278	0.29586			
LANL-S	1.36494			0.01716		0.08469	0.19932			
LANL-T	18.88569			0.05925	0.03909	0.3249	1.80783			
LANL-U	1.42386			0.0123			0.07074			
LANL-U	1.31898			0.01293			0.0771			
LANL-V	147.56388			0.01806			0.40101			
LANL-X	2.97198			0.01608		0.06102	0.37692			
LANL-Y	16.96671			0.06138		0.12033	2.24241			
LANL-Z	5.15775			0.06867		2.49396	3.4875			
LANL-AA	0.72159			0.02202		0.08667	0.31491			
LANL-AB	12.76827			0.03162		2.12643	4.27473			
LANL-AC	0.12081			0.01788						
LANL-AD	0.07827			0.01002			0.06963			
LANL-AE	0.12831			0.01293						
LANL-AF	0.90909			0.0147						
LANL-AG	0.52509			0.01161						
LANL-AH	80.91507			0.1371		3.10026	8.25039			
LANL-AI	2.34852			0.05286		0.54342	1.57932			
LANL-AJ	0.27108			0.01695		0.13329	0.07932			
LANL-AK	0.13272			0.01209			0.07623			

Plutonium Residue Glasses (Bulkley and Vienna 1997)

SRC-BL	0.41									
SRC-Al-1	0.5									
SRC-Al-2	0.27									
SRC-B-2	0.15									
SRC-B-3	1.24									
SRC-Ca-1	0.21									
SRC-Ca-2	0.24									
SRC-Ca-3	0.51									
SRC-Ce-1	0.58									
SRC-Ce-2	0.4									
SRC-Ce-3	0.35									
SRC-K-1	0.22									
SRC-K-2	0.39									
SRC-Li-1	0.2									
SRC-Li-2	0.24									
SRC-Li-3	0.43									
SRC-Na-1	0.19									

Appendix A. Glass Composition and TCLP Release Data

Plutonium Residue Glasses (Bulkley and Vienna 1997)

Glass ID	Al ₂ O ₃	B ₂ O ₃	CaO	Fe ₂ O ₃	K ₂ O	Li ₂ O	MgO	Na ₂ O	NiO	P ₂ O ₅	SiO ₂	ZrO ₂	Ag ₂ O	As ₂ O ₃
SRC-Na-2	0.051111	0.061333	0.050089	0.016356	0.030667	0.040889	0.020444	0.08	0.005111	0.003067	0.46	0.030667		
SRC-Pb-1	0.050505	0.060606	0.049495	0.016162	0.030303	0.040404	0.020202	0.10101	0.005051	0.00303	0.454545	0.030303		
SRC-Pb-2	0.04798	0.057576	0.04702	0.015354	0.028788	0.038384	0.019192	0.09596	0.004798	0.002879	0.431818	0.028788		
SRC-Si-1	0.054545	0.065455	0.053455	0.017455	0.032727	0.043636	0.021818	0.109091	0.005455	0.003273	0.4	0.032727		
SRC-Si-2	0.040909	0.049091	0.040091	0.013091	0.024545	0.032727	0.016364	0.081818	0.004091	0.002455	0.55	0.024545		
SRC-Sn-1	0.049	0.0588	0.04802	0.01568	0.0294	0.0392	0.0196	0.098	0.0049	0.00294	0.441	0.0294		
SRC-Sn-2	0.048	0.0576	0.04704	0.01536	0.0288	0.0384	0.0192	0.096	0.0048	0.00288	0.432	0.0288		
SRC-Ti-1	0.050505	0.060606	0.049495	0.016162	0.030303	0.040404	0.020202	0.10101	0.005051	0.00303	0.454545	0.030303		
SRC-Ti-2	0.04798	0.057576	0.04702	0.015354	0.028788	0.038384	0.019192	0.09596	0.004798	0.002879	0.431818	0.028788		
SRC-Zr-1	0.051546	0.061856	0.050515	0.016495	0.030928	0.041237	0.020619	0.103093	0.005155	0.003093	0.463918	0		
SRC-Zr-2	0.048969	0.058763	0.04799	0.01567	0.029381	0.039175	0.019588	0.097938	0.004897	0.002938	0.440722	0.05		

SRS LLMW Glasses (Cicero-Herman 2002)

WETF-1	0.108797	0.163839	0.192348	0.025534	0.001855	8.61E-05	0.00849	0.10638	0.001393	0.01025	0.375105	2.7E-05		
WETF-2	0.11131	0.177138	0.192754	0.024419	0.001735	2.15E-05	0.008192	0.108006	0.001215	0.009609	0.350032	2.7E-05		
WETF-3	0.095476	0.06437	0.202184	0.018343	0.000617	0.044191	0.015074	0.093867	0.001088	0.012583	0.444055	0.006497		
WETF-7	0.162585	0.000397	0.199143	0.014135	0.030511	3.59E-05	0.008037	0.034437	0.000681	0.007062	0.501088	2.36E-05		
RFP-2	0.045021	0.153663	0.025055	0.054624	0.002646	2.15E-05	0.013631	0.108181	0.000753	0.000595	0.581262	0.001021		
RFP-4	0.04153	0.070359	0.024519	0.047528	0.003336	2.15E-05	0.015378	0.077532	0.000634	0.00058	0.706853	0.00075		
RFP-5	0.06587	0.157302	0.022578	0.052375	0.002553	2.15E-05	0.017633	0.100165	0.000662	0.000458	0.592964	0.000646		
RFP-6	0.05448	0.094499	0.091209	0.203027	0.001109	2.15E-05	0.08082	0.06474	0.001175	0.000458	0.429343	0.000958		
RFP-7	0.044492	0.095412	0.042965	0.104745	0.002378	2.15E-05	0.035051	0.078341	0.000927	0.000458	0.596194	0.001063		
RFP-8	0.026297	0.077263	0.133605	0.173151	0.002439	2.7E-05	0.058946	0.158311	0.001433	0.000574	0.363457	0.001645		
RFP-9	0.041756	0.09612	0.072632	0.168524	0.001577	2.15E-05	0.056161	0.082466	0.001175	0.000564	0.444946	0.000125		
RFP-10	0.041942	0.112435	0.061318	0.15579	0.001666	2.15E-05	0.051009	0.079321	0.000974	0.000534	0.494906	0.000125		
LANL-1	0.150751	0.252434	0.212226	0.044406	9.44E-05	2.15E-05	0.021984	0.104888	0.001629	0.000641	0.218644	8.08E-05		
LANL-3	0.073275	0.071916	0.284098	0.047252	0.000675	3.59E-05	0.028871	0.03725	0.000755	0.0009	0.452334	8.59E-05		
LANL-4	0.410996	0.000129	0.252038	0.081236	0.000345	3.23E-05	0.039476	0.005271	0.000165	0.000458	0.234318	0.001		
LANL-5	0.236194	0.000429	0.227258	0.069178	0.000366	8.61E-05	0.03263	0.008731	0.00109	0.001235	0.40877	0.000126		
LANL-6	0.147469	0.000569	0.220514	0.137056	0.000387	0.000237	0.05798	0.035942	0.000954	0.000839	0.371076	0.000147		
LANL-7	0.173154	0.000161	0.278982	0.050402	0.004676	2.87E-05	0.027865	0.000449	0.000721	0.000808	0.446358	7.58E-05		
LANL-8	0.087427	0.000215	0.165926	0.032383	0.029432	6.46E-05	0.016495	0.021307	0.000901	0.000717	0.647545	7.58E-05		
LANL-9	0.134438	0.000537	0.25125	0.039641	0.000169	2.15E-05	0.025565	0.000256	0.000734	0.000656	0.540544	7.58E-05		
LANL-13	0.100307	0.259207	0.233209	0.037515	0.000149	4.31E-05	0.02263	0.11467	0.001179	0.000641	0.216469	7.58E-05		

TRU Study (Crum et al. 1997)

TRU-AZ-1	0.03	0.08027	0.009613	0.042886	0.002659	0.04515	0.00259	0.11221	0.00067	0.00858	0.46058	0.113	0.000197	
TRU-NL-1	0.02351	0.08342	0.00999	0.044564	0.002763	0.01	0.002692	0.13	0.000696	0.00891	0.4786	0.10948	0.000205	
TRU-ZN-1	0.02211	0.07845	0.009395	0.041913	0.002599	0.04413	0.002532	0.13	0.000655	0.00838	0.45013	0.12	0.000193	

Appendix A. Glass Composition and TCLP Release Data

Plutonium Residue Glasses (Bulkley and Vienna 1997)

Glass ID	BaO	Bi2O3	CdO	CeO2	Cl	CoO	Cr2O3	Cs2O	CuO	F	Gd2O3	La2O3	MnO2	MnO
SRC-Na-2	0.002249			0.046	0.005111		0.004089	0.010222	0.000409	0.001022	0.046			
SRC-Pb-1	0.002222			0.045455	0.005051		0.00404	0.010101	0.000404	0.00101	0.045455			
SRC-Pb-2	0.002111			0.043182	0.004798		0.003838	0.009596	0.000384	0.00096	0.043182			
SRC-Si-1	0.0024			0.049091	0.005455		0.004364	0.010909	0.000436	0.001091	0.049091			
SRC-Si-2	0.0018			0.036818	0.004091		0.003273	0.008182	0.000327	0.000818	0.036818			
SRC-Sn-1	0.002156			0.0441	0.0049		0.00392	0.0098	0.000392	0.00098	0.0441			
SRC-Sn-2	0.002112			0.0432	0.0048		0.00384	0.0096	0.000384	0.00096	0.0432			
SRC-Ti-1	0.002222			0.045455	0.005051		0.00404	0.010101	0.000404	0.00101	0.045455			
SRC-Ti-2	0.002111			0.043182	0.004798		0.003838	0.009596	0.000384	0.00096	0.043182			
SRC-Zr-1	0.002268			0.046392	0.005155		0.004124	0.010309	0.000412	0.001031	0.046392			
SRC-Zr-2	0.002155			0.044072	0.004897		0.003918	0.009794	0.000392	0.000979	0.044072			

SRS LLMW Glasses (Cicero-Herman 2002)

WETF-1	0.000466		8.75E-06	0.000246			0.002236		0.000789					4.75E-05
WETF-2	0.000373		8.75E-06	0.000233			0.001973		0.000688					0
WETF-3	0.000361		1.14E-05	0.000246			0.001959		0.000701					0
WETF-7	0.000676		8.75E-06	0.000909			0.000207		0.000655					0.000622
RFP-2	2.61E-05		5.33E-05				0.000805		1.41E-05					0.000153
RFP-4	4.09E-05		3.05E-05				0.00058		1.41E-05					0.000153
RFP-5	0		3.05E-05				0.000608		1.41E-05					0.0001
RFP-6	0		0.000388				0.000978		1.41E-05					0.000227
RFP-7	0		0.000137				0.000729		1.41E-05					0.0002
RFP-8	0		0.000339				0.001189		1.76E-05					0.000159
RFP-9	0		0.000346				0.001136		1.41E-05					0.000158
RFP-10	0		0.000366				0.000935		1.41E-05					0.000195
LANL-1	0.00047		0.00033	0.001425			0.000982		1.25E-05					0.00057
LANL-3	0.000602		0.000242	0.001159			0.000683		1.25E-05					3.17E-05
LANL-4	0.000419		9.63E-05	0.000246			0.001434		4.19E-05					0.000111
LANL-5	0.000365		0.000236	0.002244			0.001027		2.09E-05					0.000264
LANL-6	0.000489		0.000324	0.000348			0.001151		3.34E-05					0.000269
LANL-7	0.000637		0.000268	0.000246			0.00084		1.25E-05					1.58E-05
LANL-8	0.000466		0.000231	0.000246			0.001087		8.35E-05					0.000744
LANL-9	0.000474		0.000321	0.000246			0.000734		1.25E-05					2.64E-05
LANL-13	0.000951		0.000622	0.000246			0.000906		1.25E-05					3.17E-05

TRU Study (Crum et al. 1997)

TRU-AZ-1	0.000433	0.05334		0			0.003546		0.000158	0.004137			0.010638		0.01704
TRU-NL-1	0.00045	0.05543		0			0.003685		0.000164	0.004299			0.011054		0.017707
TRU-ZN-1	0.000424	0.05213		0			0.003465		0.000154	0.004043			0.010396		0.016654

Appendix A. Glass Composition and TCLP Release Data

Plutonium Residue Glasses (Bulkley and Vienna 1997)

Glass ID	MoO	MoO ₃	Nd ₂ O ₃	PbO	PdO	ReO ₂	Rh ₂ O ₃	RuO ₂	Sb ₂ O ₃	Sb ₂ O ₅	SeO ₂	SnO	SnO ₂
SRC-Na-2		0.006542	0.008178	0.010222								0	
SRC-Pb-1		0.006465	0.008081	0								0	
SRC-Pb-2		0.006141	0.007677	0.05								0	
SRC-Si-1		0.006982	0.008727	0.010909								0	
SRC-Si-2		0.005236	0.006545	0.008182								0	
SRC-Sn-1		0.006272	0.00784	0.0098								0.02	
SRC-Sn-2		0.006144	0.00768	0.0096								0.04	
SRC-Ti-1		0.006465	0.008081	0.010101								0	
SRC-Ti-2		0.006141	0.007677	0.009596								0	
SRC-Zr-1		0.006598	0.008247	0.010309								0	
SRC-Zr-2		0.006268	0.007835	0.009794								0	

SRS LLMW Glasses (Cicero-Herman 2002)

WETF-1				0.000452									
WETF-2				0.000215									
WETF-3				0.000215									
WETF-7				0.000215									
RFP-2				0.000215									
RFP-4				0.000215									
RFP-5				0.000215									
RFP-6				0.000215									
RFP-7				0.000215									
RFP-8				0.00027									
RFP-9				0.0053									
RFP-10				0.000205									
LANL-1				0.00056									
LANL-3				0.000596									
LANL-4				0.000242									
LANL-5				0.000689									
LANL-6				0.000725									
LANL-7				0.0007									
LANL-8				0.000406									
LANL-9				0.0006									
LANL-13				0.000697									

TRU Study (Crum et al. 1997)

TRU-AZ-1				0.001133									
TRU-NL-1				0.001177									
TRU-ZN-1				0.001107									

Appendix A. Glass Composition and TCLP Release Data

Plutonium Residue Glasses (Bulkley and Vienna 1997)

Glass ID	SO ₃	SrO	TeO ₂	ThO ₂	TiO ₂	Tl ₂ O ₃	U ₃ O ₈	UO ₂	UO ₃	V ₂ O ₅	WO ₃	Y ₂ O ₃	ZnO	Sum
SRC-Na-2					0.010222									1.0000
SRC-Pb-1					0.010101									1.0000
SRC-Pb-2					0.009596									1.0000
SRC-Si-1					0.010909									1.0000
SRC-Si-2					0.008182									1.0000
SRC-Sn-1					0.0098									1.0000
SRC-Sn-2					0.0096									1.0000
SRC-Ti-1					0									1.0000
SRC-Ti-2					0.05									1.0000
SRC-Zr-1					0.010309									1.0000
SRC-Zr-2					0.009794									1.0000

SRS LLMW Glasses (Cicero-Herman 2002)

WETF-1					0.000984								0.00112	1.0005
WETF-2					0.000784								0.001207	0.9899
WETF-3					5E-05								0.001245	1.0031
WETF-7					0.00035								0.000112	0.9619
RFP-2					0.001268								0.000481	0.9895
RFP-4					0.001562								0.000477	0.9921
RFP-5					0.001195								0.000581	1.0160
RFP-6					0.000734								0.000448	1.0248
RFP-7					0.001151								0.000531	1.0050
RFP-8					0.000369								0.00051	1.0000
RFP-9					0.000812								0.000514	0.9743
RFP-10					0.000878								0.000423	1.0031
LANL-1					1.67E-05								3.73E-05	1.0122
LANL-3					0.000467								1.24E-05	1.0013
LANL-4					0.000384								0.000205	1.0286
LANL-5					0.000595								1.24E-05	0.9915
LANL-6					0.000161								7.47E-05	0.9767
LANL-7					3.89E-05								0.000162	0.9866
LANL-8					0.000484								3.32E-05	1.0063
LANL-9					2.78E-05								1.24E-05	0.9963
LANL-13					3.34E-05								1.24E-05	0.9896

TRU Study (Crum et al. 1997)

TRU-AZ-1		0.000591											0.000512	0.9999
TRU-NL-1		0.000614											0.000532	0.9999
TRU-ZN-1		0.000578											0.000501	0.9999

Appendix A. Glass Composition and TCLP Release Data

Plutonium Residue Glasses (Bulkley and Vienna 1997)

Glass ID	TCLP B (mg/L)	TCLP Ag (mg/L)	TCLP As (mg/L)	TCLP Ba (mg/L)	TCLP Cd (mg/L)	TCLP Cr (mg/L)	TCLP Ni (mg/L)	TCLP Pb (mg/L)	TCLP Se (mg/L)	TCLP Zn (mg/L)
SRC-Na-2	0.27									
SRC-Pb-1	0.31									
SRC-Pb-2	0.36									
SRC-Si-1	0.55									
SRC-Si-2	0.11									
SRC-Sn-1	0.3									
SRC-Sn-2	0.25									
SRC-Ti-1	0.41									
SRC-Ti-2	0.27									
SRC-Zr-1	0.49									
SRC-Zr-2	0.32									

SRS LLMW Glasses (Cicero-Herman 2002)

WETF-1	27.59275			0.56925			0.16275			
WETF-2	43.27325			0.5655			0.1935			
WETF-3	9.31825			0.4075			0.0995			
WETF-7	2.328			0.84			0.171			
RFP-2	8.449			0.717	0.012	0.101				
RFP-4	0.503			0.729		0.091	0.103	0.353		
RFP-5	2.273			0.504		0.056	0.08			
RFP-6	1.624			0.931	0.013	0.054		0.408		
RFP-7	1.128			0.648	0.011	0.137		0.22		
RFP-8	222.91			0.386	2.196	3.078	0.407	0.431		
RFP-9	44.87			0.525	0.448	0.729	0.153	0.221		
RFP-10	2.849			0.608						
LANL-1	229.14			0.564	0.159		0.166			
LANL-3	22.432			0.764	0.347		0.307			
LANL-4				0.462	0.016					
LANL-5				0.384						
LANL-6				0.32	0.013					
LANL-7				0.506	0.028					
LANL-8	0.083			0.625				0.214		
LANL-9				0.398						
LANL-13	269.18			0.745	0.08		0.051			

TRU Study (Crum et al. 1997)

TRU-AZ-1	0.65		0.064	0.066						
TRU-NL-1	0.48	0.011		0.062	0.0029					
TRU-ZN-1	0.7		0.079	0.078		0.011		0.046		

Appendix A. Glass Composition and TCLP Release Data

TRU Study (Crum et al. 1997)

Glass ID	Al ₂ O ₃	B ₂ O ₃	CaO	Fe ₂ O ₃	K ₂ O	Li ₂ O	MgO	Na ₂ O	NiO	P ₂ O ₅	SiO ₂	ZrO ₂	Ag ₂ O	As ₂ O ₃
TRU-ABZ-1	0.04	0.1	0.009159	0.040858	0.002534	0.04302	0.002468	0.1069	0.000638	0.00817	0.43881	0.12	0.000188	
TRU-NBZ-1	0.02271	0.06	0.009654	0.043065	0.002671	0.04534	0.002601	0.13	0.000673	0.00861	0.4625	0.12	0.000198	
TRU-B-2	0.0245	0.02	0.01041	0.04646	0.002881	0.04891	0.00281	0.12155	0.000726	0.00929	0.49891	0.11413	0.000213	
TRU-Li-2	0.02371	0.08413	0.01008	0.04495	0.002787	0.015	0.00272	0.1176	0.000702	0.00899	0.48272	0.11043	0.000206	
TRU-Si-1	0.02545	0.09032	0.01082	0.04825	0.002992	0.0508	0.00292	0.12625	0.000754	0.00965	0.41	0.11854	0.000222	
TRU-Si-3	0.02718	0.09644	0.01154	0.05152	0.003195	0.05425	0.00311	0.1348	0.000805	0.0103	0.37	0.12658	0.000237	
TRU-Zr-2	0.02263	0.08031	0.00962	0.0429	0.002661	0.04517	0.00259	0.11226	0.00067	0.00858	0.46078	0.12	0.000197	
TRU-Zr-3	0.02212	0.07848	0.00939	0.04193	0.0026	0.04415	0.00253	0.10971	0.000655	0.00839	0.45031	0.14	0.000193	
TRU-Zr-4	0.0216	0.07666	0.00917	0.04095	0.00254	0.04312	0.00247	0.10715	0.00064	0.00819	0.43984	0.16	0.000188	

SP3, SPx4, Misc. (Vienna et al. 2001)

c106b-2	0.144	0.1094	0.0018	0.0781	0	0.0599	0.0005	0.1311	0	0.0094	0.4501	0.0005	0.001496	0.00034
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Nepheline Precipitation Study (Li et al. 1997)

NP-Al-3	0.1768	0.0764	0.0107	0.0949	0.001	0.043	0.0065	0.1936	0.000662	0.009458	0.3664	0.0028	0.001324	0.000189
NP-Al-4	0.1929	0.0749	0.0105	0.093	0.0009	0.0421	0.0064	0.1898	0.000655	0.009356	0.3592	0.0027	0.00131	0.000187
NP-Na-1	0.1496	0.087	0.0122	0.1081	0.0011	0.0489	0.0074	0.133	0.000762	0.010881	0.4174	0.0032	0.001523	0.000218
NP-Na-2	0.147	0.0855	0.012	0.1062	0.0011	0.0481	0.0073	0.1481	0.000747	0.010678	0.4101	0.0031	0.001495	0.000214
NP-Li-1	0.1441	0.0838	0.0117	0.1041	0.001	0	0.0071	0.2123	0.000736	0.010508	0.4019	0.003	0.001471	0.00021
NP-Ca-1	0.1392	0.0809	0	0.1005	0.001	0.0455	0.0069	0.2051	0.000707	0.010102	0.3882	0.0029	0.001414	0.000202
NP-Fe-2	0.1408	0.0819	0.0115	0.0795	0.001	0.046	0.007	0.2075	0.000691	0.009864	0.3927	0.003	0.001381	0.000197

Appendix A. Glass Composition and TCLP Release Data

TRU Study (Crum et al. 1997)

Glass ID	BaO	Bi ₂ O ₃	CdO	CeO ₂	Cl	CoO	Cr ₂ O ₃	Cs ₂ O	CuO	F	Gd ₂ O ₃	La ₂ O ₃	MnO ₂	MnO
TRU-ABZ-1	0.000413	0.05082		0			0.003378		0.00015	0.003941		0.010135		0.016234
TRU-NBZ-1	0.000435	0.05356		0			0.003561		0.000158	0.004154		0.010682		0.017111
TRU-B-2	0.000469	0.05778		0			0.003841		0.000171	0.004481		0.011523		0.018458
TRU-Li-2	0.000454	0.0559		0			0.003716		0.000165	0.004336		0.011149		0.017859
TRU-Si-1	0.000488	0.06001		1E-07			0.00399		0.000177	0.004654		0.011969		0.019172
TRU-Si-3	0.000521	0.06408		0			0.00426		0.000189	0.00497		0.01278		0.020472
TRU-Zr-2	0.000434	0.05336		1E-07			0.003547		0.000158	0.004139		0.010642		0.017048
TRU-Zr-3	0.000424	0.05215		0			0.003467		0.000154	0.004045		0.010401		0.01666
TRU-Zr-4	0.000414	0.05094		0			0.003386		0.00015	0.003951		0.010159		0.016273

SP3, SPx4, Misc. (Vienna et al. 2001)

c106b-2	0.000258	0	0	0	0		0.001692	0	0.000246	0		0		0.003853
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Nepheline Precipitation Study (Li et al. 1997)

NP-Al-3	0.003216		0.000189				0.001892		0.000284					0.003972
NP-Al-4	0.003181		0.000187				0.001871		0.000281					0.003929
NP-Na-1	0.0037		0.000218				0.002176		0.000326					0.00457
NP-Na-2	0.003631		0.000214				0.002136		0.00032					0.004485
NP-Li-1	0.003573		0.00021				0.002102		0.000315					0.004414
NP-Ca-1	0.003435		0.000202				0.00202		0.000303					0.004243
NP-Fe-2	0.003354		0.000197				0.001973		0.000296					0.004143

Appendix A. Glass Composition and TCLP Release Data

TRU Study (Crum et al. 1997)

Glass ID	MoO	MoO ₃	Nd ₂ O ₃	PbO	PdO	ReO ₂	Rh ₂ O ₃	RuO ₂	Sb ₂ O ₃	Sb ₂ O ₅	SeO ₂	SnO	SnO ₂
TRU-ABZ-1				0.001079									
TRU-NBZ-1				0.001137									
TRU-B-2				0.001227									
TRU-Li-2				0.001187									
TRU-Si-1				0.001274									
TRU-Si-3				0.001361									
TRU-Zr-2				0.001133									
TRU-Zr-3				0.001107									
TRU-Zr-4				0.001082									

SP3, SPx4, Misc. (Vienna et al. 2001)

c106b-2	0	0	0	0	0	0	0	0.002302	0.001198		
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Nepheline Precipitation Study (Li et al. 1997)

NP-Al-3				0.002648				0.001513		0.000757		
NP-Al-4				0.00262				0.001497		0.000748		
NP-Na-1				0.003047				0.001741		0.000871		
NP-Na-2				0.00299				0.001708		0.000854		
NP-Li-1				0.002942				0.001681		0.000841		
NP-Ca-1				0.002828				0.001616		0.000808		
NP-Fe-2				0.002762				0.001578		0.000789		

Appendix A. Glass Composition and TCLP Release Data

TRU Study (Crum et al. 1997)

Glass ID	SO ₃	SrO	TeO ₂	ThO ₂	TiO ₂	Tl ₂ O ₃	U ₃ O ₈	UO ₂	UO ₃	V ₂ O ₅	WO ₃	Y ₂ O ₃	ZnO	Sum
TRU-ABZ-1		0.000563											0.000488	0.9999
TRU-NBZ-1		0.000593											0.000514	0.9999
TRU-B-2		0.00064											0.000555	0.9999
TRU-Li-2		0.000619											0.000537	0.9999
TRU-Si-1		0.000665											0.000576	0.9999
TRU-Si-3		0.00071											0.000615	0.9999
TRU-Zr-2		0.000591											0.000512	0.9999
TRU-Zr-3		0.000578											0.000501	0.9999
TRU-Zr-4		0.000564											0.000489	0.9999

SP3, SPx4, Misc. (Vienna et al. 2001)

c106b-2	0	8.59E-05	0		0.000365		0				0	0	8.04E-05	0.9967
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Nepheline Precipitation Study (Li et al. 1997)

NP-Al-3		9.46E-05			0.001608								9.46E-05	1.0000
NP-Al-4		9.36E-05			0.001591								9.36E-05	1.0000
NP-Na-1		0.000109			0.00185								0.000109	1.0000
NP-Na-2		0.000107			0.001815								0.000107	1.0000
NP-Li-1		0.000105			0.001786								0.000105	1.0000
NP-Ca-1		0.000101			0.001717								0.000101	1.0000
NP-Fe-2		9.86E-05			0.001677								9.86E-05	1.0000

Appendix A. Glass Composition and TCLP Release Data

TRU Study (Crum et al. 1997)

Glass ID	TCLP B (mg/L)	TCLP Ag (mg/L)	TCLP As (mg/L)	TCLP Ba (mg/L)	TCLP Cd (mg/L)	TCLP Cr (mg/L)	TCLP Ni (mg/L)	TCLP Pb (mg/L)	TCLP Se (mg/L)	TCLP Zn (mg/L)
TRU-ABZ-1	0.8	0.0073		0.095	0.0027	0.009		0.053		
TRU-NBZ-1	0.53		0.065	0.073	0.003	0.015				
TRU-B-2	0.16	0.0066		0.11		0.0044				
TRU-Li-2	0.47			0.065		0.0091				
TRU-Si-1	1.1		0.075	0.084		0.023				
TRU-Si-3	1.7		0.071	0.12		0.013				
TRU-Zr-2	0.61		0.11	0.13		0.012				
TRU-Zr-3	0.62	0.008	0.044	0.085	0.0029	0.0099				
TRU-Zr-4	0.51			0.072		0.0074				

SP3, SPx4, Misc. (Vienna et al. 2001)

c106b-2	0.77	0.024		0.069						
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Nepheline Precipitation Study (Li et al. 1997)

NP-Al-3	2.9	0.061	0.11	0.41		0.079		0.12		
NP-Al-4	3	0.1		0.35	0.0024	0.099		0.25		
NP-Na-1	0.94	0.045	0.11	0.19				0.12		
NP-Na-2	1.2	0.044	0.058	0.21	0.004					
NP-Li-1	0.79	0.027		0.16				0.061		
NP-Ca-1	1.6	0.069	0.067	0.25		0.015		0.079	0.037	
NP-Fe-2	1.6	0.054		0.24		0.024		0.17		

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