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Preliminary Enhanced LAW Glass Formulation Algorithm

January 2023

NA Lumetta
DS Kim
JD Vienna

U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

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Richland, Washington 99354

Summary

This report summarizes the Preliminary Enhanced Low-Activity Waste Glass Formulation Algorithm (GFA), its background information, and the calculations it performs.

The Preliminary Enhanced Low-Activity Waste GFA is a tool developed in MATLAB to formulate glass for a given waste composition while attempting to maximize waste loading. It is intended for use at the Waste Treatment and Immobilization Plant, where nuclear waste will be vitrified into glass. The formulated glass is required to satisfy several processing and product quality constraints. In addition, calculations must account for associated uncertainties in constraint prediction and measurement. The GFA adheres to Pacific Northwest National Laboratory nuclear quality assurance procedures and has been validated and verified.

In this second revision to the report, two constraints: the lithium and zirconia target constraints were amended to Table 3.1 and programmed into the algorithm. Additionally, three sections were added. Section 3.2.1 includes the Enhanced LAW Correlation Rules, an addition to the glass optimality criteria. Section 4.0 discusses a stepped process approach taken to ensure the algorithm can adequately react to differences between its recommended output and the actual measurements and transfers made during plant operation, and calculation of specific radionuclide concentrations. Section 5.2 describes changes to the user interaction with the algorithm program including the addition of a graphical user interface and compilation of the software.

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Acronyms and Abbreviations

CRV	concentrate receipt vessel
DF	decontamination factor
DFLAW	Direct Feed Low-Activity Waste
DOE	U.S. Department of Energy
EMF	Effluent Management Facility
GFA	glass formulation algorithm
GFC	glass-forming chemical
GUI	graphical user interface
ID	identification
ILAW	immobilized low-activity waste
K-3	Monofrax K-3 refractory material
LAW	low-activity waste
MFPV	melter feed preparation vessel
MFV	melter feed vessel
NQAP	Nuclear Quality Assurance Program
PCT	product consistency test
PERT	Program Evaluation and Review Technique
PNNL	Pacific Northwest National Laboratory
RSD	relative standard deviation
SUCI	simultaneous upper confidence interval
TOC	total organic carbon
TSCR	Tank Side Cesium Removal
VHT	vapor hydration test
WTP	Waste Treatment and Immobilization Plant

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1.0 Background

The U.S. Department of Energy (DOE) is responsible for managing the legacy tank waste stored at the Hanford Site. To facilitate treatment, the low-activity waste (LAW) fraction will be separated from the waste managed as high-level waste, with each waste fraction having specific constraints surrounding its processing. To initiate treatment in a timely manner, the LAW fraction will be treated in advance of completion of the Waste Treatment and Immobilization Plant (WTP) through the Direct Feed Low-Activity Waste (DFLAW) process that will use the WTP LAW Facility, the Effluent Management Facility (EMF), the WTP Analytical Laboratory, and supporting facilities. The current DFLAW flowsheet is graphically summarized in Figure 1.1. Double-shell tank waste will be filtered, and Cs will be removed by ion exchange in the Tank Side Cesium Removal (TSCR) Facility and returned to the interim LAW storage tank (ILST, nominally 241-AP-106). Decontaminated waste will be blended with melter off-gas condensate concentrate in the concentrate receipt vessel (CRV). The CRV will be sampled, and the LAW samples will be analyzed for chemical and radiochemical composition at the WTP Analytical Laboratory. Based on the analysis results, a compliant and processable glass will be formulated using the Glass Formulation Algorithm (GFA). The formulation prescribed amount of LAW and glass-forming chemicals (GFCs) will be transferred to the melter feed preparation vessel (MFPV). The melter feed batch will be mixed, sampled, and then transferred to the melter feed vessel (MFV), where it will be continuously fed to the melter. Melter feed will be converted to a molten glass and off-gas in the melter. Off-gases will be treated with a fraction of the off-gas content being collected for recycle and the remainder being captured on filters or discharged. Off-gas condensate will be transferred to the EMF and evaporated with the concentrate stream being recycled to the CRV and the dilute stream being condensed and discharged to the Liquid Effluent Retention Facility/Effluent Treatment Facility. The glass melt will be poured into containers and cooled into a solid glass waste form called immobilized low-activity waste (ILAW). ILAW will be disposed onsite in the Integrated Disposal Facility. This flowsheet model can be seen in Figure 1.1.

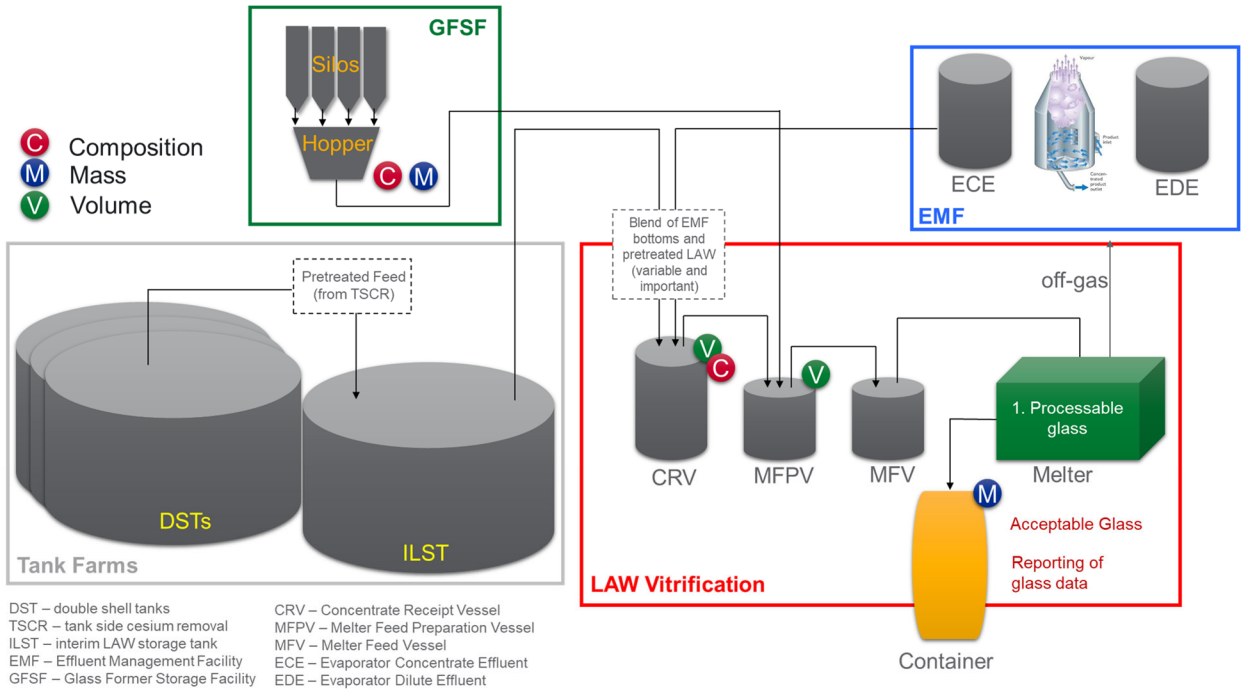

Figure 1.1. Simplified DFLAW Flowsheet

The ability to increase the ratio of waste to GFCs in glass, also referred to as waste loading, is favorable. It decreases the required number of containers that need to be handled and may increase the rate at which LAW is processed.

The purpose of the Preliminary Enhanced LAW GFA is to computationally formulate LAW glass compositions given a waste composition and specific constraints, while applying all property and measurement uncertainties. It does this by determining the addition of GFCs and their relative ratio to the waste.

All the calculations performed in the algorithm are based on those found in the *Preliminary ILAW Formulation Algorithm Description, 24590-LAW-RPT-RT-04-0003, Rev. 1* (Kim and Vienna 2012). Additionally, this document uses the processing and product quality models described in Vienna et al. (2022).

1.1 Quality Assurance

This work was performed in accordance with the Pacific Northwest National Laboratory (PNNL) Nuclear Quality Assurance Program (NQAP). The NQAP complies with DOE Order 414.1D, *Quality Assurance*, and 10 CFR 830, Subpart A, *Quality Assurance Requirements*. The NQAP uses American Society of Mechanical Engineers Standard NQA-1-2012, *Quality Assurance Requirements for Nuclear Facility Application*, as its consensus standard, and NQA-1-2012, Subpart 4.2.1, as the basis for its graded approach to quality.

The NQAP works in conjunction with PNNL's laboratory-level Quality Management Program, which is based on the requirements as defined in DOE Order 414.1D, *Quality Assurance*, and 10 CFR 830, *Nuclear Safety Management*, Subpart A, *Quality Assurance Requirements*.

The work of this report was performed with a technology readiness level of 8 due to the high-assurance classification of the software under PNNL's NQAP.

2.0 Process Description

The Preliminary Enhanced LAW GFA follows all the assumptions used in Kim and Vienna (2012) regarding the LAW Facility process and the WTP Analytical Laboratory's analytical methods and uncertainties. Waste compositions are assumed to be analyzed for all components in the CRV, using three samples. This means that only two composition inputs are used for glass formulation: CRV waste composition and GFC compositions. The GFC compositions and composition uncertainties are specified by the vendor. GFC additions are the same as those specified in Kim and Vienna (2012), with the addition of chromium, vanadium, and tin oxides and the removal of sodium carbonate, borax, and hematite. The GFC additions to the waste are used to obtain the necessary composition of the final glass waste form to satisfy the associated regulatory and property constraints. This process flow can be seen in Figure 2.1. Per the process described by Kim and Vienna (2012), analytes are converted into their corresponding oxides, and radionuclide masses are added element by element to determine concentration.

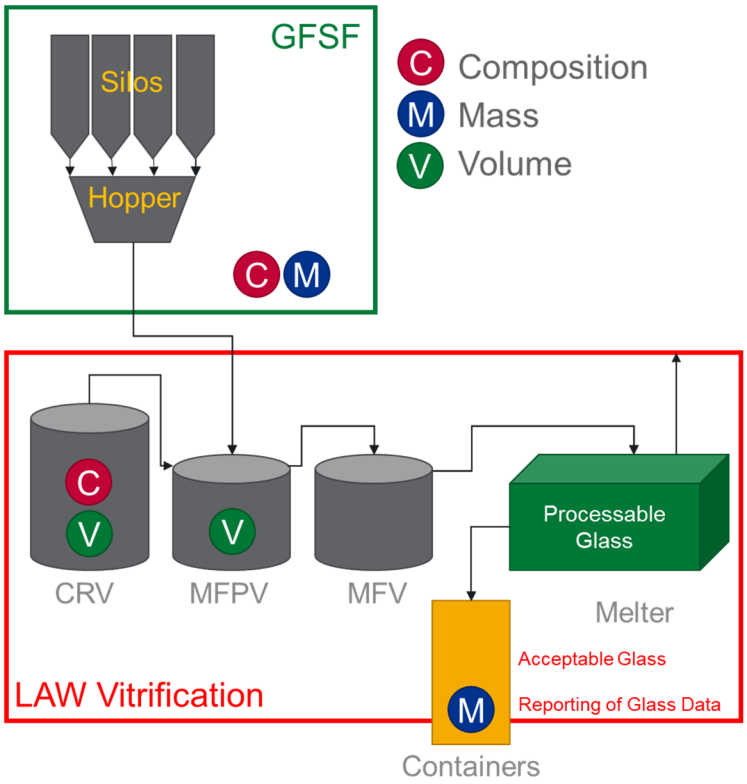

Figure 2.1. Visual Depiction of Glass Formulation Method Used by the Preliminary Enhanced LAW Glass Formulation Algorithm Associated with Plant Operations

The off-gas system captures varying amounts of specific melter feed components that partition to off-gas during melter operations, as indicated by the retention factors (v_i) in Appendix A. During plant operations, the EMF concentrates are recycled to the CRV (Figure 1.1). The EMF is not specifically accounted for in the GFA as analyses of CRV content are used in glass formulation. The specific retention factors used in the algorithm are assumptions and may change in the future.

3.0 Calculations

This section summarizes the calculations used in the Preliminary Enhanced LAW GFA. For a detailed description of all the equations used to model optimization and uncertainty, see Kim and Vienna (2012). The calculation validation methodology is described in Section 6.0.

3.1 LAW Glass Formulation Constraints and Property Models

3.1.1 Property and Composition Constraints

Glass formulation is subject to property and composition constraints to meet criteria for processing and storage. Overall waste loading is limited by alkali and sulfur content, and other property constraints use a mix of linear and quadratic terms to limit specific components. A summary of these constraints, taken from Vienna et al. (2022), can be found in Table 3.1. The model coefficients used to predict each of these properties can be found in Appendix C.

Table 3.1. LAW Glass Property Constraints, Detailed in Vienna et al. (2022)

Waste Loading Rule	Limit
Slow-cooled glass crystallization constraint	$w_{Al_2O_3} + 0.28 \times \left(w_{Na_2O} + 0.66\, w_{K_2O}\right) \leq 15.800$ wt%
Slow-cooled glass crystallization constraint	$w_{CaO} + 0.528 \times \left(w_{Na_2O} + 0.66 w_{K_2O}\right) < 20.840$ wt%
Melter crystallization constraint	$w_{Al_2O_3} + 0.677 \times w_{SnO_2} + 0.827 w_{ZrO_2} < 16.55$ wt%
Melter crystallization constraint	$w_{SnO_2} < 4.500$ wt%
Lithium target constraint	$w_{Li_2O} < 4.300$ wt%
Zirconia target constraint	$w_{ZrO_2} > 2.000$ wt%
Multi-component model validity constraint	$13.500 \text{ wt\%} < w_{Na_2O} + 0.66 w_{K_2O} + 2.07 w_{Li_2O} < 27.018$ wt%
Multi-component model validity constraint	$w_{SiO_2} + 1.697 w_{Al_2O_3} < 61.600$ wt%
Property	**Limit**
Melter SO_3 tolerance	$w_{SO_3}(wt\%, \text{ before retention}) < w_{SO_3}^{MT}$ (wt%)
Product consistency test (PCT)-Na response	$\widehat{PCT}_{Na}^{NL}(\text{g/m}^2) < 2$
PCT-B response	$\widehat{PCT}_{B}^{NL}(\text{g/m}^2) < 2$
Vapor hydration test (VHT) pass/fail probability score	$P(g) < 0.190$
Viscosity at 1150 °C	$20 < \eta_{1150}(\text{P}) < 80$
Electrical conductivity at 1150 °C	$0.12 < EC_{1150}(\text{S/cm}) < 0.59$
K-3 [(a)] neck corrosion at 1208 °C	$k_{1208}(\text{inch}) \leq 0.04$

(a) K-3 is Monofrax K-3 refractory material.

In addition, specific components are subject to minimum and maximum concentrations within the glass. These can be seen in Table 3.2, which is taken from Lu et al. (2021).

Table 3.2. Minimum and Maximum Limits on Specific Glass Components (mass fraction, g)

Component	Range	
Al_2O_3	0.035	$\leq g_{Al_2O_3} \leq 0.1475$
B_2O_3	0.06	$\leq g_{B_2O_3} \leq 0.1383$
CaO	g_{CaO}	≤ 0.1278
Cl	g_{Cl}	≤ 0.0117
Cr_2O_3	$g_{Cr_2O_3}$	≤ 0.0063
F	g_F	≤ 0.013
Fe_2O_3	$g_{Fe_2O_3}$	≤ 0.1198
K_2O	g_{K_2O}	≤ 0.059
Li_2O	g_{Li_2O}	≤ 0.043
MgO	g_{MgO}	≤ 0.0502
Na_2O	0.0247	$\leq g_{Na_2O} \leq 0.2657$
SO_3	g_{SO_3}	≤ 0.0163
P_2O_5	$g_{P_2O_5}$	≤ 0.0403
SiO_2	0.3352	$\leq g_{SiO_2} \leq 0.5226$
TiO_2	g_{TiO_2}	≤ 0.0501
V_2O_5	$g_{V_2O_5}$	≤ 0.0409
ZnO	g_{ZnO}	≤ 0.0582
ZrO_2	0.02	$\leq g_{ZrO_2} \leq 0.0675$

3.1.2 Property Model Prediction Uncertainties

A set of uncertainties in property measurement and prediction must be accounted for while determining glass compositions that will satisfy property constraints with a specified confidence. Different confidence intervals are used for the constrained properties; each are applied at a 90% confidence level (CL%). The various confidence intervals and their explanations, taken from Vienna and Kim (2014), can be found in Table 3.3.

Table 3.3. Prediction Uncertainty Interval Types and Equation Forms

Property	Interval	Equation[(a)]
PCT	SUCI	See Section 3.1.2.1
VHT	UCI	$z_{\alpha/2}\sqrt{\mathrm{g}^{\mathrm{T}}(\mathrm{G}^{\mathrm{T}}\mathrm{VG})^{-1}\mathrm{g}}$
Viscosity	TSCI	$t_{1-\frac{\alpha}{2},n-p}\sqrt{M\mathrm{g}^{\mathrm{T}}(\mathrm{G}^{\mathrm{T}}\mathrm{G})^{-1}\mathrm{g}}$
Electrical Conductivity	TSCI	$t_{1-\frac{\alpha}{2},n-p}\sqrt{M\mathrm{g}^{\mathrm{T}}(\mathrm{G}^{\mathrm{T}}\mathrm{G})^{-1}\mathrm{g}}$
Melter SO_3 Tolerance	UCI	$t_{1-\alpha,n-p}\sqrt{M\mathrm{d}^{\mathrm{T}}(\mathrm{D}^{\mathrm{T}}\mathrm{D})^{-1}\mathrm{d}}$
K-3 Neck Corrosion	UCI	$t_{1-\alpha,n-p}\sqrt{M\mathrm{g}^{\mathrm{T}}(\mathrm{G}^{\mathrm{T}}\mathrm{G})^{-1}\mathrm{g}}$

(a) $z_{\alpha/2}$ = standard normal distribution with upper α/2 confidence interval; $t_{1-\alpha}$ and $t_{1-\alpha/2}$ represent the one-sided and two-sided 100(1-α) percentile of the Student's t-distribution with n-p degrees of freedom; g is the glass composition with the superscript 'T' representing a matrix transpose; $(G^TVG)^{-1}$, $(G^TG)^{-1}$, and $(D^TD)^{-1}$ all represent variance-covariance matrices of their respective models.

SUCI = simultaneous upper confidence interval; UCI = upper confidence interval; TSCI = two-sided confidence interval

3.1.2.1 Product Consistency Test Uncertainty

The SUCI for $ln\left(PCT_j^{NL}\right)$ is a special case. The model recommended by Vienna et al. (2021) is a bias-corrected partial quadratic mixture model (bcPQM) given by:

$$\ln\left(PCT_j^{NL}\right) = \begin{cases} \mathbf{g}^{\mathrm{T}}\mathbf{b} \text{ if} & \mathbf{g}^{\mathrm{T}}\mathbf{b} \le C \\ \mathbf{g}^{\mathrm{T}}\mathbf{b} + (\mathbf{g}^{\mathrm{T}}\mathbf{b} - C)(S_0 + \Delta S) \text{ if} & \mathbf{g}^{\mathrm{T}}\mathbf{b} > C \end{cases} \tag{3.1}$$

where:
- $\mathbf{g}$ = composition of the example glass formatted to match the terms in the model
- T = indicates vector transpose
- $\mathbf{b}$ = vector of coefficients for the model
- C = bias correction cutoff
- S_0 = initial bias correction slope
- ΔS = change in slope

Since $\mathbf{b}$, C, S_0, and ΔS are all uncertain values, the errors are propagated. Eq. (3.1) is expanded to:

$$\ln\left(PCT_j^{NL}\right) = \mathbf{g}^{\mathrm{T}}\mathbf{b} + \mathbf{g}^{\mathrm{T}}\mathbf{b} \cdot S_0 + \mathbf{g}^{\mathrm{T}}\mathbf{b} \cdot \Delta S - C \cdot S_0 - C \cdot \Delta S \tag{3.2}$$

Propagating the variances ($V_T = SD_T^2$) yields:

$$\begin{aligned} X = (\mathbf{g}^{\mathbf{T}}\mathbf{b})^2 v_{S_0} + s_0^2 v_{\mathbf{g}^{\mathbf{T}}\mathbf{b}} - v_{S_0} v_{\mathbf{g}^{\mathbf{T}}\mathbf{b}} + (\mathbf{g}^{\mathbf{T}}\mathbf{b})^2 v_{\Delta s} + \\ \Delta s^2 v_{\mathbf{g}^{\mathbf{T}}\mathbf{b}} - v_{\Delta s} v_{\mathbf{g}^{\mathbf{T}}\mathbf{b}} + c^2 v_{S_0} + S_0^2 v_c - v_c v_{S_0} + \Delta s^2 v_c + c^2 v_{\Delta S} - v_c v_{\Delta S} \end{aligned} \tag{3.3}$$

where:
- v_C = square of the standard error of C
- v_{S_0} = square of the standard error of S_0
- $v_{\Delta S}$ = square of the standard error of ΔS

Although the form of the bias correction yields a continuous prediction across the cutoff (C) with no step function change, the variance does demonstrate a step function change. The variance is therefore smoothed using a sigmoid function at the cutoff value $PCT_j^{NL} = C$:

$$\hat{V}_{\ln\left(\widehat{PCT_j^{NL}}\right)} = v_g T_b + \frac{X}{1 + e^{-k\left(\mathbf{g}^{\mathrm{T}}\mathbf{b} - C\right)}} \tag{3.4}$$

where: X = defined in Eq. (3.3)
k = smoothing factor for sigmoid function
$v_{\mathbf{g}^{\mathrm{T}}\mathbf{b}}$ = variance of $\mathbf{g}^{\mathrm{T}}\mathbf{b}$

Finally, the SUCI for PCT is given by:

$$SUCI_{\ln\left(\widehat{PCT_j^{NL}}\right)} = \ln\left(PCT_j^{NL}\right) + \sqrt{qF_{1-\alpha}(q, n-q)} \cdot \widehat{SD}\left(\widehat{PCT_j^{NL}}\right)^2 \tag{3.5}$$

3.1.2.2 Process and Composition Uncertainties

An additional set of uncertainties arises from sampling and process-volume transfers. The GFA considers six sources of uncertainties: CRV mixing and sampling, component concentration analyses, MFPV level measurement, GFC component concentration, GFC mass, and retention factor. Eq. (3.6) [taken from Kim and Vienna (2012)] gives the MFPV batch glass composition mass balance for concentration of each component i (g_i).

$$g_i = \frac{\left[c_i^{LAW} V^{LAW} f_i + \sum_{k=1}^{n^{GFCs}} g_{ik}^{oxide\,inGFC} M_k^{GFCin\,MFPV}\right] v_i}{\sum_{i=1}^{noxides}\left[c_i^{LAW} V^{LAW} f_i + \sum_{k=1}^{n^{GFCs}} g_{ik}^{oxide\,inGFC} M_k^{GFCin\,MFPV}\right] v_i} \tag{3.6}$$

where: g_i = mass fraction of i^{th} oxide in glass (g/g)
c_i^{LAW} = concentration of the i^{th} component measured in samples from the CRV before transfer to the MFPV (mg/L)
V^{LAW} = volume of LAW transferred in a batch to the MFPV (L)
f_i = a conversion factor from element mg to oxide kg (kg/mg) (Appendix F Table F.3)
$g_{ik}^{oxide\,inGFC}$ = mass fraction of the i^{th} oxide in the k^{th} GFC (g/g)
$M_k^{GFCin\,MFPV}$ = mass of the k^{th} GFC in the MFPV batch (kg)
n^{GFCs} = number of GFCs added to the MFPV batch
v_i = fraction of i^{th} oxide retained in the glass (g/g), i.e., the retention factor

The values for c_i^{LAW} are calculated as a normally distributed Monte Carlo simulation with a minimum of 10,000 instances, with the mean taken to be the measured values for composition in the CRV, and the standard deviation of c_i^{LAW} (s_i^{cLAW}) is described by Eq. (3.7).

$$s_i^{cLAW} = \frac{\sqrt{\left(c_i^{LAW} RSD_i^{Analysis}\right)^2 + \left(c_i^{LAW} RSD_i^{\frac{mix}{samp}}\right)^2}}{\sqrt{n^{samps}}} \tag{3.7}$$

The values for $RSD_i^{Analysis}$ are listed in Appendix A, Table A.2, while the values for $RSD_i^{mix/samp}$ are all 1.47% (Kim and Vienna 2012). The number of samples, n^{samps}, is assumed to be three.

V^{LAW}, or volume of LAW transferred from the CRV to the MFPV, is calculated as a normally distributed Monte Carlo simulation with a minimum of 10,000 instances. The mean is the measured transfer volume, while the standard deviation, with calculations described in Appendix D of Kim and Vienna (2012), is 447.2 L.

The GFC oxide compositions represented by $g_{ik}^{oxide\ in GFC}$ are calculated using the beta distributed Program Evaluation and Review Technique [beta-(PERT)] to generate Monte Carlo simulations with a minimum of 10,000 instances. The minimum, maximum, and most-likely values for calculating the distribution are listed in Appendix F, Table F.1.

The GFC mass transfers $M_k^{GFC\ in\ MFPV}$ for each GFC are calculated as normally distributed Monte Carlo simulations with a minimum of 10,000 instances. The mean is taken to be the nominally measured value, while the standard deviation is calculated to be 0.1039 kg for mass transfers greater than 41.6 kg, and 0.0520 kg for mass transfers less than 41.6 kg.

The natural logarithm of the melter decontamination (or retention) factor, $\ln\left[\frac{1}{1-\nu_i}\right]$, is calculated as a beta-PERT distributed Monte Carlo simulation with a minimum of 10,000 instances. The minimum, maximum, and most likely values for this can be found in Appendix F, Table F.2. Note that the values reported in this table are expressed as percentages and need to be converted to fractions by dividing them by 100 for use in calculations. The natural log equation needs to be solved for ν_i before it can be substituted into the equation for g_i.

3.2 Glass Formulation Optimality Criteria

The Preliminary Enhanced LAW GFA uses waste loading as the optimality criteria for the optimization scheme. As MATLAB's "fmincon" function is a minimization scheme, the code attempts to minimize the negative of waste loading, which maximizes the absolute value.

As optimization occurs, glass property values and prediction uncertainties are calculated based on the composition of the glass, formed by the combination of waste and GFCs in their respective percentages of the total glass. The property values and prediction uncertainties in combination with the composition uncertainties are compared to each property limit as the function attempts to find the highest waste loading value without exceeding the limits. Due to software constraints, the Monte Carlo simulations used to determine composition uncertainties cannot calculate simultaneously with the optimization scheme.

Therefore, an iterative approach is taken to calculating the composition uncertainties. Following each optimization run, the glass composition is used to calculate the composition uncertainties to be used for the next run. This process continues until the difference in all composition uncertainties between the previous and current runs is less than 3%.

3.2.1 Enhanced LAW Correlation Rules

In addition to the waste loading, the informational version of the algorithm contains additional optimality criteria in the form of a set of equations referred to as the Enhanced LAW Correlation (ELC) rules which are described in Muller et al. (2019). These rules are not quality-affecting and are not included as part of the quality-assured software. The purpose of these rules is to push the final glass composition closer to

laboratory-scaled melter tested regions. They achieve this by attempting to minimize the Euclidean distance between the concentration of specific components in the glass and their optimal amounts, which are determined by equations which rely on either the sulfur or normalized sodium and potassium concentrations (equation-dependent). This equation can be found in Eq. (3.8) and describes the balance between weighing waste loading and the ELC equations as the optimality criteria. The lowercase *f* is a weight factor which can be varied between zero and one. At zero, full priority is given to waste loading while at one, full priority goes to the distance equations. Values between the two allow the user to weigh the two criteria relative to one another.

$$\big(W \times (1 - f)\big) - (D \times f) \tag{3.8}$$

where: f = weight factor given to the ELC equations
W = waste loading
D = sum of Euclidean distances for each ELC component

4.0 Stepped Process Approach

The Preliminary Enhanced LAW GFA runs through four steps (more details can be found in Kim and Vienna 2012) to ensure the final glass is within the defined limits and constraints with sufficient confidence. The first step is the optimization process, described in Section 3.0. The remaining steps are described below and are summarized in Figure 4.1.

In step 1, the melter feed composition is formulated to determine the target volume of waste transfer from the CRV to the MFPV. Once the glass is formulated and the LAW transfer volume is calculated, the waste is transferred from the CRV to the MFPV. As part of the initial glass formulation process, we calculated the GFC masses and dilution water volume. Additionally, calculations are performed to determine the Curie concentration per cubic meter of Sr-90 and Cs-137, as well as the sum concentration of several other Class-C radionuclides. During step 2, the actual waste transfer volume is used, and the melter feed batch composition is again calculated to determine the mass of each GFC to add to the MFPV batch. The GFCs are weighed and transferred to the MFPV. The MFPV is then analyzed to confirm the batch for process control but not for waste form qualification. During operations, the actual transfer volumes and weights may not match perfectly with those calculated during glass formulation. Therefore, the glass composition, its properties, and uncertainties need to be recalculated based on these actual transfer numbers during step 3. If the glass no longer meets the constraints, trim GFC masses are calculated. If the glass meets the constraints, the batch is transferred to the MFV and production records can be generated based on this final composition.

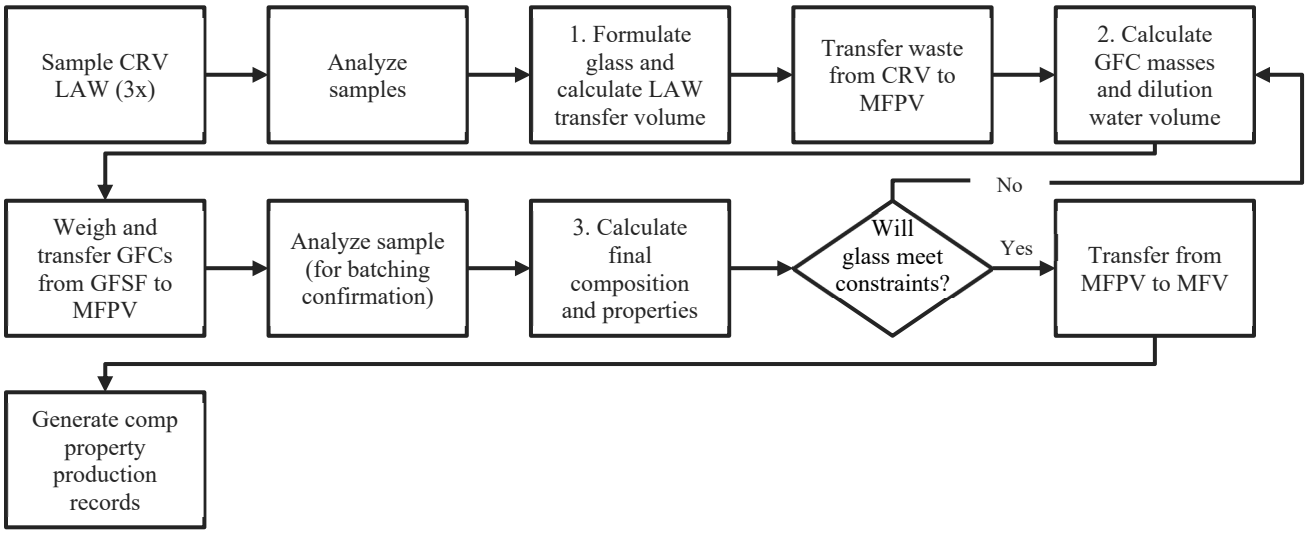

Figure 4.1. Flowchart Model Describing Post-Optimization Steps Taken in the Algorithm

5.0 Technical Layout of the MATLAB Script

This section can be used as a reference when editing or examining the MATLAB script or running the program. Detailed line-by-line comments can be found within the script itself.

5.1 Startup and Program Inputs

The beginning of the Preliminary Enhanced LAW GFA contains startup commands, various user-defined inputs, constants, and technical information. All technical and scientific information used in the script is read-in through .csv files organized by folder. Table 5.1 lists these file names and their associated contents.

Table 5.1. Algorithm Folder Structure and File Description

File/Folder Name			Description
Main Folder	Preliminary_Enhanced_LAW_Glass_Formulation_Algorithm.exe		Main executable file
	splash.png		Image file the .exe file uses for the startup splash screen
	WasteComp.csv		Waste compositions
	Folder: GFC	BulkDensity.csv	Individual GFC bulk density values
		GFC_Compositions.csv	Individual GFC composition values
		HopperID.csv	Hopper ID for each GFC
		HopperParameters.csv	Hopper parameters associated with each ID (weight capacity, volume)
		MinMaxMLgGFC.csv	Minimum, maximum, and most likely values for each GFC, for PERT calculation
		ParticleDensity.csv	Particle density for each GFC
	Folder: Misc.	ClassC_Limit.csv	File containing radionuclide concentration limits
		Constants.csv	File containing constants used by the script, such as imperial-to-metric conversion factors
		conversion_nonrad.csv	Conversion factor from mL(component)/L(waste) to g(oxide)/100g(waste) for nonradioactive components
		conversion_rad.csv	Conversion factor from mL(component)/L(waste) to g(oxide)/100g(waste) for radioactive components
		MinMaxComponents.csv	The minimum and maximum values for each oxide component, in g(oxide)/100g(waste)
		MinMaxMLvi.csv	Minimum, maximum, and most likely values for each component, for PERT calculation
		MRQ.csv	The minimum reportable quantities for each waste component
		OptSeeds.csv	File containing the different seed values for optimization
		Retention.csv	Retention factors for each glass component
		Retention_rad.csv	Retention factors for rad components

File/Folder Name			Description
	Folder: Models	RSD_analytical.csv	Analytical relative standard deviation for each waste component
		RSD_mixsamp.csv	Mixing/sampling relative standard deviation for each waste component
		MultiComponentConstraints.csv	Multicomponent constraints
		Prop_EC_High.csv	Electrical conductivity model and its upper limit
		Prop_EC_Low.csv	Electrical conductivity model and its lower limit
		Prop_K3.csv	K-3 corrosion model and its constraint
		Prop_PCT_B.csv	PCT-B (boron) model and its constraint
		Prop_PCT_Na.csv	PCT-Na (sodium) model
		Prop_Sulfur.csv	Sulfur tolerance model
		Prop_VHT.csv	VHT model
		Prop_Visc_High.csv	Viscosity model and its upper limit
		Prop_Visc_Low.csv	Viscosity model and its lower limit
	Folder: Steps	conversion_nonrad_step4.csv	Conversion factors for non-rad components used in step 4
		Step2.csv	Assumed input values for step 2, for testing purposes only
		Step3.csv	Assumed input values for step 3, for testing purposes only
		Step4Heel	Assumed heel input for step 4, for testing purposes only
		Step4Measured	Assumed composition input for step 4, for testing purposes only
	Folder: VarCovar	VarCovar_EC_High.csv	Electrical conductivity variance/covariance matrix
		VarCovar_EC_Low.csv	Electrical conductivity variance/covariance matrix
		VarCovar_K3.csv	K-3 corrosion variance/covariance matrix
		VarCovar_PCT_B.csv	PCT-B variance/covariance matrix
		VarCovar_PCT_Na.csv	PCT-Na variance/covariance matrix
		VarCovar_Sulfur.csv	Sulfur tolerance variance/covariance matrix
		VarCovar_VHT.csv	VHT variance/covariance matrix
		VarCovar_Visc_High.csv	Viscosity variance/covariance matrix
		VarCovar_Visc_Low.csv	Viscosity variance/covariance matrix

The file “WasteComp.csv” is particularly important to the user. The “WasteComp.csv” file contains the waste compositions, read in mg/L, by element for non-radionuclides, while radionuclides are in mCi/L.

When the script reads the “WasteComp.csv” file, it uses that data and the “conversion_nonrad.csv” and “conversion_rad.csv” files to convert element concentration into oxide concentration for each analyte. The selected waste cluster is converted from milligrams of waste component per liter of waste (mg/L) to grams of oxide per 100 grams of waste (g/100g), or oxide weight percentage in waste using the f_i values found in Appendix F, Table F.3.

Next, retention factors, property models, and limits are read into the script and assigned individual variables.

The GFC bulk density constants, hopper numbers and volumes, and weight capacities are defined next. This information is used later to compute uncertainties related to the GFC transfer weights and volumes used to calculate composition uncertainty.

All the values related to GFC compositions, weights, volumes, and other relevant information related to composition uncertainty calculation are read from files in the "GFC" folder.

This section sets up information used in the Monte Carlo calculations during the optimization routine and computes Monte Carlo values for parameters not affected by waste loading or glass composition. These include component concentration in waste, component concentration in GFC, and melter decontamination (retention) factor. Regardless of the final glass composition, the uncertainties surrounding the compositions of the GFCs and the waste remain the same.

5.2 Software Use and Graphical User Interface

The algorithm has been compiled into a standalone executable file that allows its users to run the program without the MATLAB software and without a MATLAB software license. This enables users who lack experience with MATLAB to use the algorithm without having to navigate the program. The algorithm does require the MATLAB Runtime Library R2020b (v9.9) to be installed, available for free from MATLAB's publisher MathWorks.

Another feature is the addition of a graphical user interface (GUI). The algorithm contains many variables and features that can be modified to simulate how changing specific parameters can affect the outcome of the program. Examples include the ability to select different combinations of GFCs or turn uncertainties off. Reading these parameters from a text-based configuration file can be complicated, particularly without an in-depth knowledge of how the coding and algorithm work. Therefore, the GUI provides a medium through which users can more easily understand the parameters they are changing. Screenshots of the GUI can be seen in Figure 5.1 and Figure 5.2.

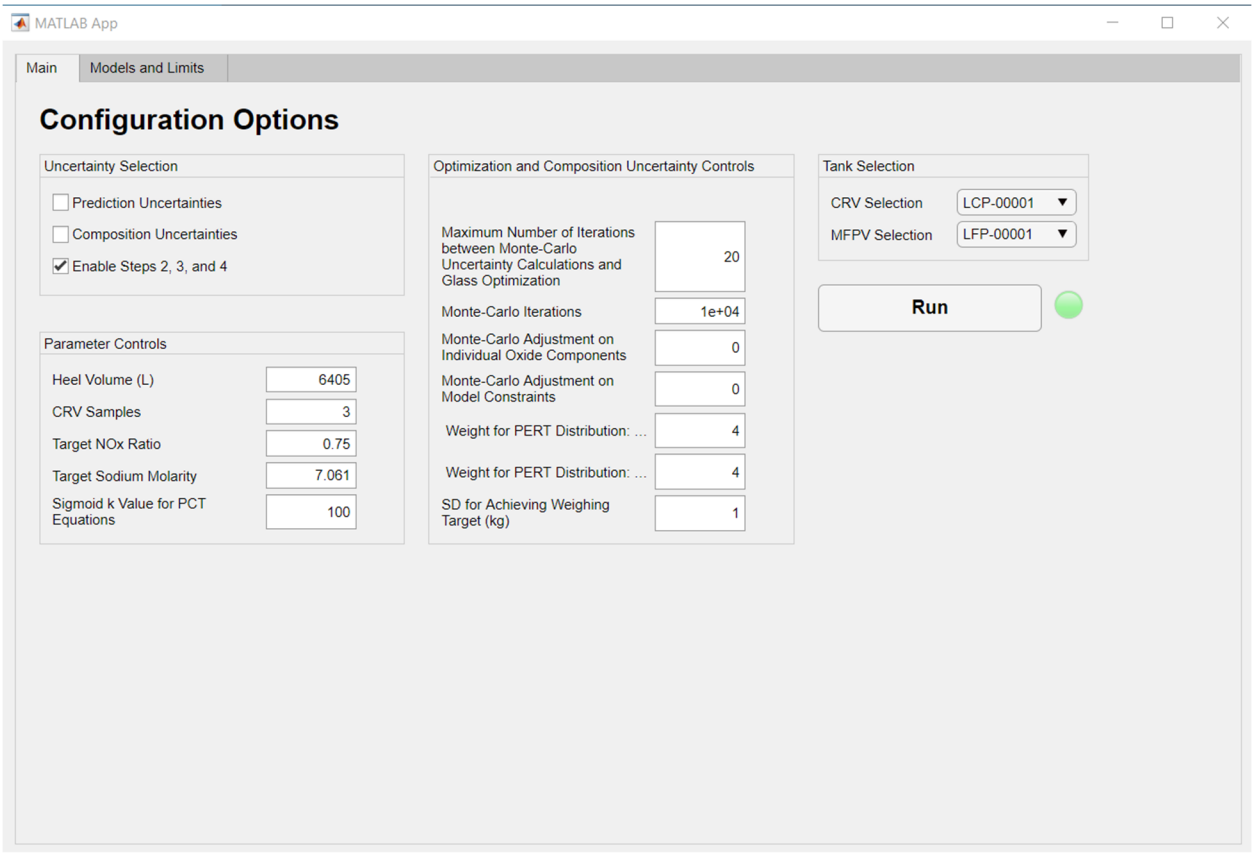

Figure 5.1. GUI Configuration Options Main Tab

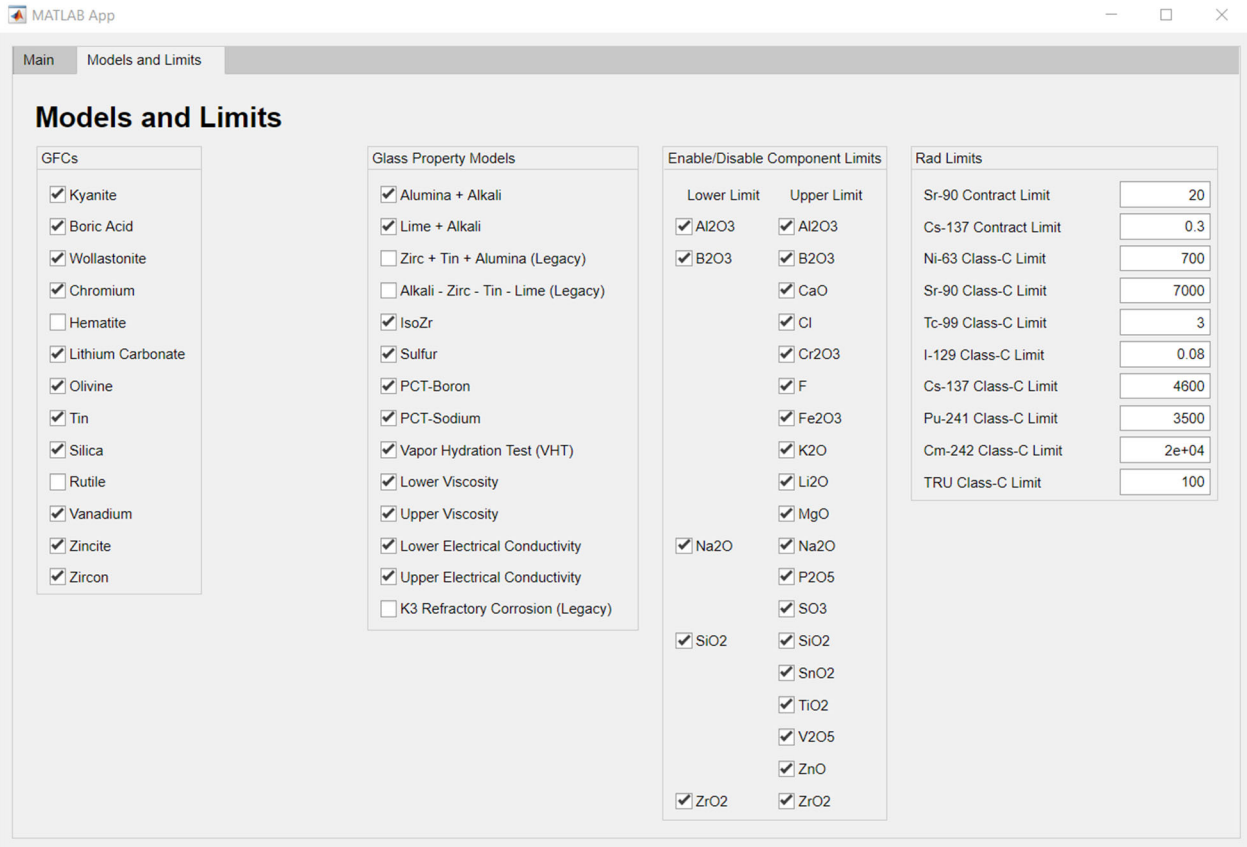

Figure 5.2. GUI Property Models, Limits, and GFCs Tab

6.0 NQAP Validation and Verification

The Preliminary Enhanced LAW GFA was developed in accordance with PNNL's NQAP procedures and has undergone validation and verification processes. A software control package was completed to document the review process for the validation and verification.

A qualified independent technical reviewer completed a full review of the code to establish its accuracy. Also, a calculation check was performed that compared the results from the GFA to the results from another independently developed code that performs the same set of calculations. For this task, we used a script developed in Python by the independent reviewer that performs the exact same set of calculations as the MATLAB script.

Ten waste compositions were chosen that represent the range of waste compositions present on the Hanford Site (e.g., extremes in Na:K, Na:Cl, Na:S, Na:P). These compositions can be found in Appendix B, Table B.1. Appendix A, Table A.2 summarizes the analytical and mixing/sampling uncertainties in relative standard deviation used in this study, which were adopted from Kim and Vienna (2012).

The differing approaches to optimization methods among different software tools in addition to the reliance of Monte Carlo schemes on random number generation prevent exact results from being obtained when comparing two different algorithms. We determined that waste loading results from the two algorithms must match within one relative percent difference. The comparisons were made using (a) prediction uncertainties only, (b) both prediction and composition uncertainties, and (c) both uncertainties while constricting the limits of all constraints and properties by 1%. The results are summarized in Table 6.1.

Table 6.1. Results from Software Control Package Testing Comparison. WL is waste loading.

Test Batch Number	MATLAB WL%	Python WL%	RPD WL%	Result
Results for Prediction Uncertainties Only				
1	0.30966674	0.30966679	0.000%	Pass
2	0.31276376	0.31276378	0.000%	Pass
3	0.31165535	0.31165536	0.000%	Pass
4	0.29828131	0.29828135	0.000%	Pass
5	0.30426264	0.30426265	0.000%	Pass
6	0.30585192	0.30585193	0.000%	Pass
7	0.29699072	0.29699074	0.000%	Pass
8	0.22952015	0.22952018	0.000%	Pass
9	0.18377069	0.1837707	0.000%	Pass
10	0.25653579	0.25653582	0.000%	Pass
Results for Prediction and Composition Uncertainties				
1	0.289939801	0.289531799	0.141%	Pass
2	0.290071615	0.289940302	0.045%	Pass
3	0.288620607	0.288863792	0.084%	Pass
4	0.283909588	0.283936942	0.010%	Pass
5	0.282485038	0.282415616	0.025%	Pass
6	0.283822794	0.283859954	0.013%	Pass
7	0.277660361	0.277536330	0.045%	Pass
8	0.221018514	0.220926974	0.041%	Pass
9	0.174946367	0.175086246	0.080%	Pass
10	0.244799096	0.244646890	0.062%	Pass
Results for Prediction and Composition Uncertainties with a 1% Limit Adjustment				
1	0.28880787	0.28877274	0.012%	Pass
2	0.28871368	0.28903418	0.111%	Pass
3	0.28768556	0.28787658	0.066%	Pass
4	0.28180671	0.28157534	0.082%	Pass
5	0.28126123	0.28115021	0.039%	Pass
6	0.28249314	0.2820144	0.170%	Pass
7	0.27621573	0.27655722	0.124%	Pass
8	0.21768264	0.21766567	0.008%	Pass
9	0.17314259	0.17309639	0.027%	Pass
10	0.24278305	0.24239478	0.160%	Pass

7.0 Results Summary and Future Work

The Preliminary Enhanced LAW GFA functions as intended, allowing the user to maximize waste loading in the final waste glass while ensuring the processing constraints are maintained. A set of 10 different waste compositions were used to test the algorithm, which developed a glass composition for each, and the waste loading was maximized while satisfying all optimization criteria and constraints. The results matched testing from an independently developed Python script.

Figure 7.1 provides a visual representation of how the optimization scheme can use the maximum amount of leeway to adjust the glass such that the limiting property models are right at their limits, while accounting for prediction and composition uncertainties. This supports maximum waste loading. Figure 7.1 includes error bars that represent the prediction and composition uncertainties surrounding each property. The property values are represented by the data points, the prediction uncertainties by the narrower error regions, and the composition uncertainties by the outer error regions.

Potential updates to the algorithm coding include integrating a set of correlation rules like those found in Rev. 0 of the software and expanding the algorithm to include more of the LAW process, such as introducing EMF product into the CRV as a separate waste stream and modeling tanks at the front of the process.

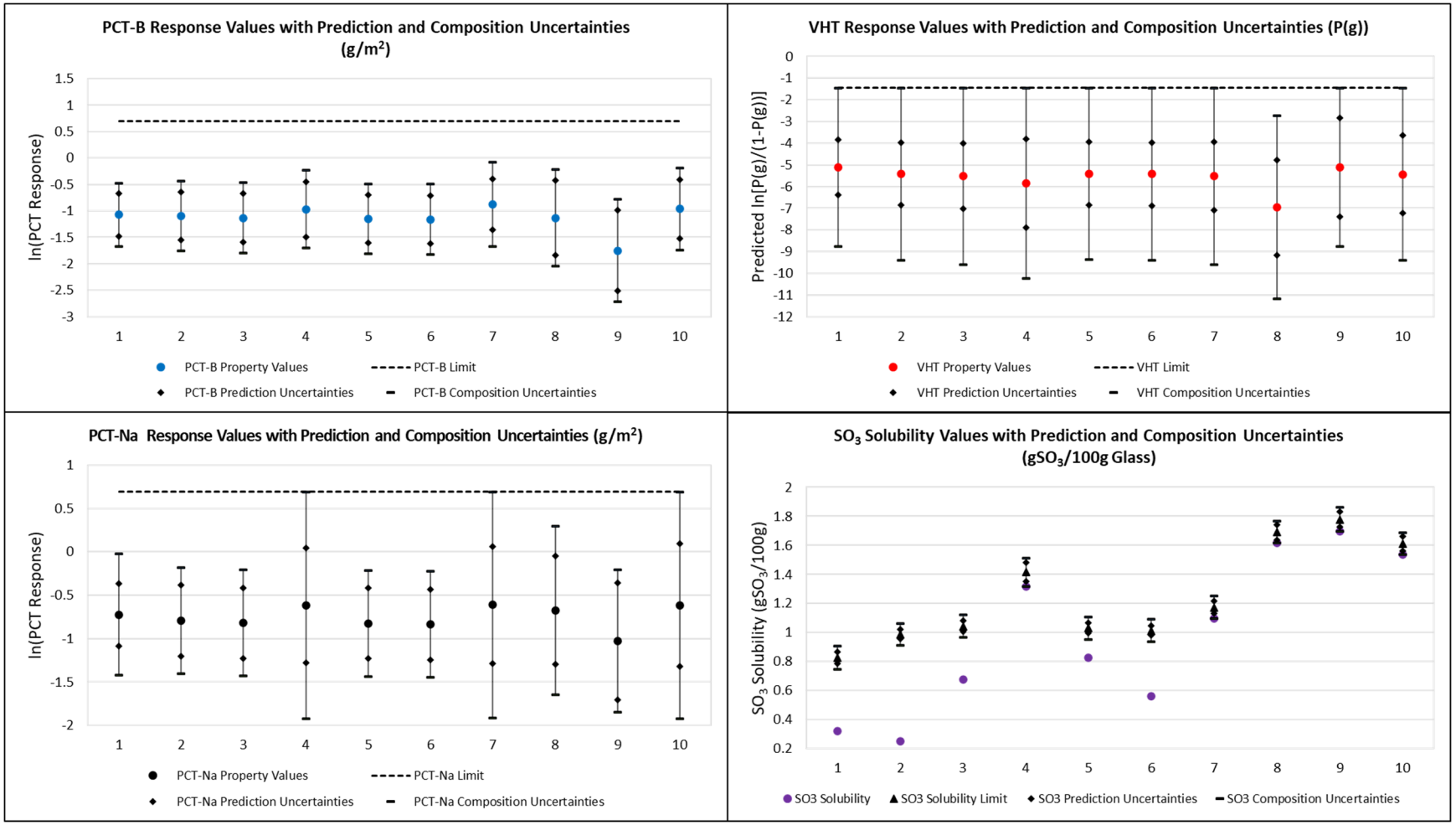

Figure 7.1. Property Constraints and Uncertainties for the 10 Tested Batches. Inner error bars represent prediction uncertainties, while outer error bars represent composition uncertainties.

8.0 References

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Appendix A – Component Retention Factors, Minimum Reportable Quantities, and Relative Standard Deviations

This appendix contains tables of the retention factors, minimum reportable quantities, and relative standard deviations (RSDs) for each of the glass oxide components (see Kim and Vienna 2012[1]).

Table A.1. Retention Factors Used to Calculate Ratios of Components Remaining after Removal of Evaporate Bottoms

Glass Oxide	Retention Factor	Glass Oxide	Retention Factor	Glass Oxide	Retention Factor
Ac_2O_3	99.721%	HgO	0.000%	RuO_2	97.803%
Ag_2O	97.803%	I	50.961%	SO_3	84.032%
Al_2O_3	99.888%	K_2O	96.423%	Sb_2O_3	77.121%
Am_2O_3	97.803%	La_2O_3	99.721%	SeO_2	77.121%
As_2O_5	77.121%	Li_2O	99.601%	SiO_2	99.926%
B_2O_3	98.968%	MgO	99.984%	Sm_2O_3	99.721%
BaO	99.721%	MnO	99.721%	SnO_2	99.721%
BeO	99.721%	MoO_3	97.803%	SrO	99.721%
Bi_2O_3	97.803%	Na_2O	99.136%	Ta_2O_5	99.721%
CaO	99.892%	Nb_2O_5	99.721%	Tc_2O_7	43.049%
CdO	99.721%	Nd_2O_3	99.721%	TeO_2	77.121%
Ce_2O_3	99.721%	NiO	99.187%	ThO_2	99.721%
Cl	54.407%	NpO_2	99.721%	TiO_2	99.752%
Cm_2O_3	99.721%	P_2O_5	99.169%	Tl_2O	77.121%
CoO	99.721%	Pa_2O_5	99.721%	UO_3	99.721%
Cr_2O_3	95.261%	PbO	98.796%	V_2O_5	97.803%
Cs_2O	87.902%	PdO	99.721%	WO_3	99.721%
CuO	99.721%	Pr_2O_3	99.721%	Y_2O_3	99.721%
Eu_2O_3	99.721%	PuO_2	99.721%	ZnO	99.773%
F	72.984%	RaO	77.121%	ZrO_2	99.982%
Fe_2O_3	99.848%	Rb_2O	97.803%	—	—
Gd_2O_3	99.721%	Rh_2O_3	99.721%	—	—

[1] Kim DS and JD Vienna. 2012. *Preliminary ILAW Formulation Algorithm Description*, *24590-LAW-RPT-RT-04-0003, Rev. 1*. ORP-56321, River Protection Project, Hanford Waste Treatment and Immobilization Plant, Richland, WA. https://www.osti.gov/servlets/purl/1110191

Table A.2. Minimum Reportable Quantities and RSDs for Composition Uncertainties

Element/ Isotope	Minimum Reportable Quantity (mg/L)	High %RSD (Analytical)	Low %RSD (Analytical)	Mixing/Sampling RSD
Ac	—	—	—	—
Ag	0.2	20%	5%	1.47%
Al	18	5%	5%	1.47%
Am	—	—	—	—
As	2.8	25%	10%	1.47%
B	0.4	25%	10%	1.47%
Ba	0.4	15%	5%	1.47%
Be	0.03	25%	5%	1.47%
Bi	0.9	15%	10%	1.47%
Ca	2	15%	5%	1.47%
Cd	0.06	10%	5%	1.47%
Ce	2	25%	10%	1.47%
Cl	19	10%	10%	1.47%
Cm	—	—	—	—
Co	0.1	25%	10%	1.47%
Cr	0.7	5%	5%	1.47%
Cs	0.1	15%	10%	1.47%
Cu	2	25%	10v	1.47%
Eu	—	—	—	—
F	19	10%	10%	1.47%
Fe	2	5%	5%	1.47%
Gd	1	15%	5%	1.47%
Hg	0.001	10%	5%	1.47%
I	—	—	—	—
K	10	5%	5%	1.47%
La	0.6	10%	5%	1.47%
Li	0.3	15%	5%	1.47%
Mg	9	25%	10%	1.47%
Mn	2	15%	5%	1.47%
Mo	3	10%	5%	1.47%
Na	200	10%	10%	1.47%
Nb	—	—	—	—
Nd	1	15%	5%	1.47%
Ni	7	10%	5%	1.47%
Np	—	—	—	—
P	12	15%	10%	1.47%
Pa	—	—	—	—
Pb	0.9	15%	15%	1.47%
Pd	1	15%	15%	1.47%
Pr	1	15%	10%	1.47%

Element/ Isotope	Minimum Reportable Quantity (mg/L)	High %RSD (Analytical)	Low %RSD (Analytical)	Mixing/Sampling RSD
Pu	—	—	—	—
Ra	—	—	—	—
Rb	10	25%	15%	1.47%
Rh	0.004	20%	5%	1.47%
Ru	0.02	25%	5%	1.47%
S	10	10%	5%	1.47%
Sb	0.3	25%	10%	1.47%
Se	4	25%	10%	1.47%
Si	4	15%	5%	1.47%
Sm	—	—	—	—
Sn	—	—	—	—
Sr	0.01	5%	5%	1.47%
Ta	0.2	15%	5%	1.47%
Tc	—	—	—	—
Te	1	25%	10%	1.47%
Th	2	25%	10%	1.47%
Ti	0.07	25%	5%	1.47%
Tl	0.02	25%	10%	1.47%
U	1	15%	5%	1.47%
V	0.07	15%	5%	1.47%
W	0.2	15%	5%	1.47%
Y	0.6	25%	5%	1.47%
Zn	4	25%	5%	1.47%
Zr	2	15%	5%	1.47%
NO_2	—	—	—	—
NO_3	—	—	—	—
TOC	—	—	—	—
^{59}Ni	7.98×10^{-7}	10%	10%	1.47%
^{60}Co	1.13×10^{-5}	5%	5%	1.47%
^{63}Ni	5.74×10^{-2}	10%	10%	1.47%
^{79}Se	6.97×10^{-5}	15%	10%	1.47%
^{90}Sr	1.39×10^{-6}	5%	5%	1.47%
^{90}Y	—	0%	0%	1.47%
^{93m}Nb	2.39×10^{-4}	15%	10%	1.47%
^{93}Zr	2.52×10^{-6}	10%	10%	1.47%
^{99}Tc	1.71×10^{-6}	10%	10%	1.47%
^{106}Ru	2.01×10^{-3}	15%	10%	1.47%
^{113m}Cd	4.62×10^{-5}	25%	10%	1.47%
^{125}Sb	3.11×10^{-4}	25%	5%	1.47%
^{126}Sn	5.68×10^{-6}	20%	15%	1.47%
^{129}I	1.77×10^{-4}	15%	10%	1.47%
^{134}Cs	4.53×10^{-6}	25%	10%	1.47%

Element/ Isotope	Minimum Reportable Quantity (mg/L)	High %RSD (Analytical)	Low %RSD (Analytical)	Mixing/Sampling RSD
^{137m}Ba	—	0%	0%	1.47%
^{137}Cs	1.73×10^{-6}	15%	5%	1.47%
^{151}Sm	5.26×10^{-1}	20%	10%	1.47%
^{152}Eu	1.74×10^{-6}	5%	5%	1.47%
^{154}Eu	2.70×10^{-6}	5%	5%	1.47%
^{155}Eu	4.76×10^{-5}	5%	5%	1.47%
^{226}Ra	9.89×10^{-7}	25%	10%	1.47%
^{227}Ac	7.23×10^{-7}	50%	10%	1.47%
^{228}Ra	2.73×10^{-3}	50%	25%	1.47%
^{229}Th	6.38×10^{-4}	50%	50%	1.47%
^{231}Pa	1.42×10^{-4}	50%	50%	1.47%
^{232}Th	3.29×10^{-10}	25%	10%	1.47%
^{232}U	6.62×10^{-8}	25%	5%	1.47%
^{233}U	9.63×10^{-7}	10%	5%	1.47%
^{234}U	6.22×10^{-6}	5%	5%	1.47%
^{235}U	2.16×10^{-07}	10%	5%	1.47%
^{236}U	6.47×10^{-08}	10%	5%	1.47%
^{237}Np	7.05×10^{-07}	10%	5%	1.47%
^{238}Pu	1.71×10^{-07}	5%	5%	1.47%
^{238}U	6.72×10^{-9}	10%	10%	1.47%
^{239}Pu	6.20×10^{-8}	5%	5%	1.47%
^{240}Pu	2.27×10^{-9}	10%	10%	1.47%
^{241}Am	3.43×10^{-6}	10%	10%	1.47%
^{241}Pu	1.03×10^{-7}	15%	15%	1.47%
^{242}Cm	3.31×10^{-6}	10%	10%	1.47%
^{242}Pu	3.95×10^{-11}	10%	10%	1.47%
^{243}Am	3.99×10^{-8}	15%	15%	1.47%
^{243}Cm	9.81×10^{-7}	15%	15%	1.47%
^{244}Cm	2.43×10^{-6}	15%	15%	1.47%

Appendix B – Waste Compositions Used for Testing

Table B.1. Waste Compositions by Element in mg/L, with Radionuclides in mCi/L, Analyzed by the Preliminary Enhanced LAW Glass Formulation Algorithm

Batch ID	1	2	3	4	5	6	7	8	9	10
Ac	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ag	5.70E-01	2.29E+00	2.07E-01	9.75E-02	7.19E-02	1.16E-01	1.06E-01	9.66E-02	5.77E-02	4.56E-02
Al	1.36E+04	2.02E+04	1.53E+04	1.03E+04	1.15E+04	1.37E+04	8.75E+03	7.56E+03	7.66E+03	7.66E+03
Am	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
As	1.33E+00	6.86E+00	6.17E-01	3.75E-01	3.13E-01	5.66E-01	4.44E-01	3.74E-01	2.05E-01	1.60E-01
B	2.67E+01	1.78E+02	2.39E+02	2.90E+02	3.30E+02	4.15E+02	2.24E+02	1.77E+02	2.31E+02	2.34E+02
Ba	2.93E-01	7.95E-01	3.37E-01	2.09E-01	9.01E-02	1.10E-01	1.85E-01	1.77E-01	1.00E-01	7.78E-02
Be	1.14E+00	3.50E-01	4.59E-02	2.45E-02	1.05E-02	1.49E-02	1.90E-02	1.78E-02	1.00E-02	8.08E-03
Bi	2.16E+00	6.50E+00	4.59E+00	3.98E+01	4.10E+00	5.48E+00	3.35E+00	3.69E+00	4.53E+00	2.93E+00
Ca	7.69E+00	4.15E+01	6.86E+01	1.77E+02	6.93E+01	6.84E+01	6.18E+01	6.16E+01	5.35E+01	5.13E+01
Cd	1.77E+00	1.38E+00	3.95E+00	1.35E+00	2.75E-01	4.41E-01	4.18E-01	3.72E-01	2.02E-01	2.74E-01
Ce	6.86E-02	1.02E+01	2.53E+00	1.64E+00	2.03E+00	3.55E+00	9.91E-01	6.02E-01	3.79E+00	1.28E+01
Cl	2.01E+03	5.06E+03	3.36E+03	2.40E+03	3.56E+03	4.34E+03	3.00E+03	2.27E+03	1.88E+03	1.95E+03
Cm	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Co	5.80E-01	1.17E+00	2.16E-01	3.61E-01	2.12E-01	2.79E-01	2.23E-01	2.43E-01	2.52E-01	1.15E-01
Cr	1.57E+02	8.75E+02	1.18E+03	7.14E+02	3.01E+03	3.77E+03	1.54E+03	5.72E+02	2.93E+02	5.13E+02
Cs	1.43E-03	1.83E-03	5.64E-04	3.49E-04	4.80E-04	5.29E-04	4.29E-04	7.89E-04	1.21E-03	5.77E-04
Cu	1.42E+00	1.24E+00	3.42E-01	1.10E-01	7.20E-02	1.23E-01	1.15E-01	1.00E-01	5.06E-02	6.56E-02
Eu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
F	1.66E+03	3.02E+03	2.95E+03	4.83E+03	1.67E+03	1.51E+03	2.06E+03	1.29E+04	2.56E+04	9.34E+03
Fe	6.58E+00	4.45E+01	1.12E+02	1.32E+02	9.33E+01	1.07E+02	8.99E+01	7.41E+01	5.13E+01	8.23E+01
Gd	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Hg	7.12E-02	1.91E+00	2.30E+00	3.91E+00	8.10E-01	1.72E+00	9.26E-01	4.45E-01	2.57E-01	8.19E-01
I	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
K	2.88E+04	5.32E+03	8.62E+02	6.52E+02	6.09E+02	5.50E+02	6.87E+02	2.53E+03	4.56E+03	1.69E+03
La	1.83E-01	4.95E-01	6.05E-02	4.04E-02	3.44E-02	8.55E-02	1.26E-02	3.19E-03	2.41E-03	8.77E-03
Li	2.96E-01	5.41E+00	3.82E+01	8.16E+01	8.64E+01	7.52E+01	3.84E+01	6.46E+01	7.03E+01	6.03E+01
Mg	2.42E+00	8.79E+00	6.35E-01	3.71E-01	3.32E-01	5.81E-01	4.18E-01	3.65E-01	2.11E-01	1.73E-01
Mn	1.16E+00	1.47E+01	2.24E+01	6.11E+00	6.68E+00	9.39E+00	6.19E+00	4.51E+00	2.46E+00	5.63E+00
Mo	1.29E+01	2.16E+01	1.52E+00	5.48E-01	5.23E-01	9.11E-01	6.70E-01	5.92E-01	3.65E-01	3.08E-01
Na	1.50E+05	1.78E+05	1.68E+05	1.56E+05	1.65E+05	1.73E+05	1.55E+05	1.63E+05	1.74E+05	1.53E+05

Batch ID	1	2	3	4	5	6	7	8	9	10
Nb	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Nd	2.25E+00	8.13E+00	5.85E-01	3.55E-01	2.37E-01	3.65E-01	3.85E-01	3.52E-01	1.99E-01	1.62E-01
Ni	1.33E+01	1.36E+01	1.12E+01	2.41E+01	1.04E+01	1.20E+01	9.08E+00	6.01E+00	3.30E+00	5.63E+00
Np	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
P	9.90E+02	1.29E+03	3.20E+03	8.80E+03	2.39E+03	2.00E+03	3.48E+03	3.15E+03	2.96E+03	4.54E+03
Pa	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Pb	1.90E+01	2.44E+01	7.68E+00	1.16E+01	1.29E+01	1.62E+01	9.59E+00	5.95E+00	3.82E+00	3.30E+00
Pd	1.63E+01	3.40E-01	4.42E-01	4.02E-02	2.57E-01	6.55E-01	7.64E-02	1.05E-03	1.81E-04	5.77E-02
Pr	1.87E-02	1.03E-01	2.46E-03	2.14E-04	1.07E-01	2.73E-01	3.13E-02	1.84E-05	1.40E-06	1.72E-04
Pu	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Ra	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Rb	3.40E+00	1.17E-01	3.28E-03	3.18E-04	5.91E-03	1.51E-02	1.77E-03	9.67E-06	1.53E-06	3.88E-04
Rh	6.67E+00	3.21E-01	1.20E-01	1.10E-02	3.05E-02	7.77E-02	9.24E-03	2.76E-04	4.85E-05	1.53E-02
Ru	2.66E+01	7.82E-01	2.13E-02	1.63E-02	2.45E-01	6.24E-01	7.19E-02	5.06E-04	4.99E-04	2.42E-03
S	1.20E+03	1.04E+03	2.65E+03	5.17E+03	3.17E+03	2.24E+03	4.01E+03	8.28E+03	1.25E+04	6.63E+03
Sb	6.80E-02	7.56E+00	1.54E+00	5.30E-01	2.44E+00	3.36E+00	1.61E+00	7.53E-01	4.33E-01	3.08E-01
Se	2.38E+00	1.58E+01	1.26E+01	6.96E+00	1.07E+01	1.31E+01	1.09E+01	8.08E+00	4.88E+00	3.37E+00
Si	1.60E+02	4.08E+02	1.05E+03	1.71E+03	5.39E+02	6.90E+02	3.62E+02	3.93E+02	4.94E+02	3.49E+02
Sm	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sn	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Sr	6.41E-02	2.33E+00	1.37E+01	1.93E+01	4.70E+00	3.86E+00	4.31E+00	3.61E+00	3.07E+00	4.01E+00
Ta	8.39E-02	1.72E-01	1.08E-01	9.76E-03	1.19E-01	3.04E-01	3.52E-02	2.60E-04	4.39E-05	1.39E-02
Tc	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Te	2.08E-01	4.18E-01	9.53E-03	7.54E-04	2.30E-01	6.21E-01	9.93E-02	6.07E-04	1.55E-05	2.86E-04
Th	2.91E-01	6.78E+00	1.08E+00	2.46E+00	3.24E-01	6.77E-01	1.66E-01	1.24E-01	1.39E-01	1.08E-01
Ti	1.75E+00	1.10E+01	1.02E+01	1.11E+01	1.49E+01	1.93E+01	1.08E+01	9.57E+00	8.80E+00	7.01E+00
Tl	3.60E-02	6.27E+00	5.93E-01	1.92E-01	2.49E-01	6.55E-01	1.20E-01	1.40E-02	4.64E-03	2.02E-02
U	1.81E+02	5.68E+01	6.13E+01	9.65E+01	2.70E+01	2.82E+01	2.32E+01	3.49E+01	4.84E+01	2.48E+01
V	7.01E-01	4.00E+00	6.22E-01	5.04E-01	5.10E-01	6.95E-01	4.80E-01	4.30E-01	3.30E-01	2.63E-01
W	0.00E+00	2.87E+00	7.60E-02	7.11E-03	3.51E-01	8.97E-01	1.03E-01	2.25E-04	3.32E-05	7.85E-03
Y	1.36E+00	7.21E-01	6.12E-02	5.64E-03	3.95E-02	1.00E-01	1.22E-02	7.08E-04	3.39E-04	7.85E-03
Zn	8.76E+00	3.49E+01	3.37E+01	3.57E+01	4.79E+01	6.26E+01	3.47E+01	3.06E+01	2.80E+01	2.23E+01
Zr	6.06E+00	6.10E+01	5.10E+00	4.51E+00	5.14E+00	5.23E+00	4.52E+00	8.30E+00	1.27E+01	5.99E+00
NO_2	3.82E+04	2.25E+04	9.66E+03	2.70E+04	3.81E+04	3.35E+04	3.76E+04	3.59E+04	3.29E+04	3.15E+04
NO_3	1.02E+05	1.01E+05	1.52E+05	1.64E+05	1.42E+05	1.17E+05	1.78E+05	1.57E+05	1.14E+05	1.83E+05
TOC	1.61E+03	1.43E+03	5.87E+02	6.79E+02	6.53E+02	6.12E+02	9.32E+02	1.19E+03	1.30E+03	8.99E+02
^{59}Ni	2.61E-04	2.82E-04	4.70E-04	5.12E-04	5.47E-04	4.00E-04	6.96E-04	5.81E-04	3.64E-04	7.68E-04

Batch ID	1	2	3	4	5	6	7	8	9	10
^{60}Co	3.93E-04	1.10E-04	3.48E-05	1.76E-05	7.56E-06	6.94E-06	9.27E-06	7.35E-06	3.60E-06	7.84E-06
^{63}Ni	2.20E-02	2.16E-02	3.50E-02	3.89E-02	3.99E-02	2.89E-02	5.10E-02	4.25E-02	2.64E-02	5.57E-02
^{79}Se	4.19E-04	1.96E-03	1.23E-03	8.62E-04	8.74E-04	7.61E-04	1.10E-03	1.42E-03	1.62E-03	1.24E-03
^{90}Sr	7.85E-01	8.21E-01	9.69E-01	1.02E+00	9.05E-01	9.12E-01	8.19E-01	9.08E-01	1.11E+00	8.62E-01
^{90}Y	7.81E-01	6.70E-01	6.74E-01	7.98E-01	7.40E-01	7.43E-01	6.92E-01	8.37E-01	1.05E+00	8.21E-01
^{93m}Nb	1.36E-02	6.31E-03	1.69E-03	1.26E-03	9.48E-04	1.04E-03	1.13E-03	1.34E-03	1.44E-03	1.13E-03
^{93}Zr	1.48E-02	6.49E-03	1.77E-03	1.42E-03	1.09E-03	1.09E-03	1.32E-03	1.49E-03	1.54E-03	1.36E-03
^{99}Tc	4.87E-02	1.00E-01	5.09E-02	4.08E-02	6.38E-02	7.27E-02	5.72E-02	6.38E-02	8.12E-02	5.06E-02
^{106}Ru	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
^{113m}Cd	6.84E-03	3.10E-03	5.02E-04	4.64E-04	4.54E-04	3.89E-04	5.35E-04	4.92E-04	3.77E-04	5.09E-04
^{125}Sb	6.31E-05	2.29E-05	5.91E-07	1.09E-07	4.82E-08	1.09E-07	2.85E-08	3.21E-08	4.20E-08	1.80E-08
^{126}Sn	2.11E-03	3.45E-03	4.82E-04	3.71E-04	2.78E-04	3.15E-04	2.99E-04	2.44E-04	1.64E-04	2.01E-04
^{129}I	1.22E-04	1.20E-04	5.15E-05	3.69E-05	4.79E-05	4.95E-05	4.87E-05	5.46E-05	6.27E-05	4.82E-05
^{134}Cs	2.48E-08	4.30E-10	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
^{137m}Ba	1.95E-02	2.18E-02	6.17E-03	3.41E-03	4.17E-03	4.64E-03	3.79E-03	6.84E-03	1.04E-02	4.91E-03
^{137}Cs	2.06E-02	2.31E-02	6.48E-03	3.65E-03	4.52E-03	5.07E-03	4.05E-03	7.26E-03	1.09E-02	5.21E-03
^{151}Sm	2.10E+00	1.36E+00	7.77E-02	7.51E-02	7.18E-02	1.11E-01	6.38E-02	4.50E-02	2.51E-02	3.96E-02
^{152}Eu	1.64E-04	1.01E-04	3.48E-06	2.32E-06	2.96E-06	6.25E-06	1.67E-06	8.78E-07	5.20E-07	6.97E-07
^{154}Eu	1.80E-03	2.78E-03	1.29E-04	1.00E-04	3.67E-05	6.07E-05	3.25E-05	2.36E-05	1.30E-05	1.77E-05
^{155}Eu	9.19E-04	2.21E-04	9.47E-06	5.56E-06	1.99E-06	4.01E-06	1.29E-06	7.59E-07	3.81E-07	5.50E-07
^{226}Ra	2.50E-08	2.19E-08	3.18E-09	4.51E-09	5.09E-09	4.77E-09	5.81E-09	5.52E-09	4.62E-09	5.63E-09
^{227}Ac	1.16E-05	4.70E-06	1.67E-06	1.45E-06	5.18E-07	6.90E-07	3.85E-07	8.50E-07	1.48E-06	5.97E-07
^{228}Ra	1.37E-09	7.49E-07	1.98E-07	7.80E-07	4.62E-08	9.65E-08	5.73E-08	5.46E-08	4.12E-08	2.79E-08
^{229}Th	1.04E-08	4.84E-07	2.53E-08	5.78E-08	4.91E-09	1.16E-08	2.33E-09	2.16E-09	3.08E-09	1.82E-09
^{231}Pa	2.75E-05	8.94E-06	3.44E-06	2.61E-06	9.98E-07	1.17E-06	9.01E-07	1.57E-06	2.38E-06	1.15E-06
^{232}Th	3.11E-08	7.36E-07	1.12E-07	2.63E-07	2.61E-08	6.19E-08	1.14E-08	7.56E-09	9.69E-09	7.43E-09
^{232}U	4.45E-07	8.63E-07	3.69E-07	4.20E-07	1.56E-07	1.49E-07	1.28E-07	2.12E-07	3.03E-07	1.73E-07
^{233}U	4.04E-05	5.21E-05	3.00E-05	3.55E-05	1.54E-05	1.55E-05	1.19E-05	1.86E-05	2.63E-05	1.53E-05
^{234}U	7.23E-05	2.11E-05	1.99E-05	3.28E-05	9.59E-06	9.76E-06	8.32E-06	1.37E-05	1.97E-05	9.35E-06
^{235}U	2.90E-06	8.44E-07	8.50E-07	1.42E-06	4.03E-07	4.13E-07	3.49E-07	5.56E-07	7.91E-07	3.85E-07
^{236}U	3.37E-06	9.28E-07	3.79E-07	5.37E-07	2.39E-07	2.07E-07	2.26E-07	6.57E-07	1.13E-06	3.81E-07
^{237}Np	8.75E-05	5.61E-05	4.07E-05	3.52E-05	2.24E-05	2.14E-05	2.61E-05	2.54E-05	2.21E-05	2.90E-05
^{238}Pu	3.78E-05	6.54E-05	2.67E-05	1.23E-04	7.59E-05	7.88E-05	6.37E-05	5.14E-05	4.55E-05	4.56E-05
^{238}U	6.04E-05	1.89E-05	2.05E-05	3.22E-05	9.01E-06	9.43E-06	7.74E-06	1.17E-05	1.61E-05	8.26E-06
^{239}Pu	2.03E-04	1.39E-03	7.92E-04	5.34E-03	1.50E-03	1.26E-03	2.07E-03	1.91E-03	1.36E-03	1.70E-03
^{240}Pu	1.53E-04	3.29E-04	1.56E-04	9.72E-04	3.15E-04	2.64E-04	4.24E-04	3.99E-04	3.01E-04	3.51E-04
^{241}Am	1.89E-04	9.38E-03	1.76E-03	6.11E-03	6.21E-03	1.03E-02	3.24E-03	1.48E-03	1.17E-03	1.27E-03

Batch ID	1	2	3	4	5	6	7	8	9	10
^{241}Pu	7.29E-04	1.42E-03	2.51E-04	1.42E-03	3.86E-04	3.16E-04	4.74E-04	5.34E-04	5.24E-04	4.32E-04
^{242}Cm	3.24E-07	1.58E-05	1.51E-05	5.25E-05	3.75E-05	4.13E-05	3.43E-05	2.32E-05	1.25E-05	1.58E-05
^{242}Pu	1.25E-08	2.87E-08	7.81E-09	5.96E-08	2.05E-08	1.71E-08	2.60E-08	2.64E-08	2.35E-08	2.33E-08
^{243}Am	1.09E-07	3.96E-06	1.07E-06	2.56E-06	4.38E-06	8.36E-06	2.06E-06	8.47E-07	7.02E-07	7.23E-07
^{243}Cm	1.38E-08	9.75E-07	6.26E-07	1.74E-06	6.58E-07	7.64E-07	5.85E-07	3.95E-07	2.18E-07	2.95E-07
^{244}Cm	2.65E-07	1.66E-05	1.02E-05	2.67E-05	9.26E-06	1.08E-05	8.22E-06	5.55E-06	3.02E-06	4.07E-06

Appendix C – Model Terms

This appendix provides the model terms and statistics used to calculate glass properties needed for formulation (see Vienna et al. 2021[1]).

Table C.1. Product Consistency Test (PCT)-B Model Terms and Statistics

Component	ln(PCT-B), g/m^2
Al_2O_3	−29.5323
B_2O_3	5.9849
CaO	8.3534
Fe_2O_3	0.9519
K_2O	6.7807
Li_2O	24.2726
MgO	13.8911
Na_2O	8.674
SiO_2	−4.4655
SnO_2	−7.6174
TiO_2	−8.6853
V_2O_5	9.6149
ZnO	−2.0873
ZrO_2	0.4532
Others	0.0176
$Al_2O_3 \times Al_2O_3$	121.296
$Al_2O_3 \times Li_2O$	−156.1213
CaO × CaO	−96.9262
CaO × V_2O_5	−147.9209
n	690
p	19
q	22
α	0.9
c	−0.7193
S_0 (initial bias)	1.6836
ΔS (change in slope)	0.5869
V_c (variance from c)	0.0527
V_{S0} (variance from S_0)	0.1893
$V_{\Delta S}$ (variance from ΔS)	0.1585

[1] Vienna JD, A Heredia-Langner, SK Cooley, AE Holmes, DS Kim, and NA Lumetta. 2021. *Glass Property-Composition Models for Support of Hanford WTP LAW Facility Operation*. PNNL-30932, Rev. 1, Pacific Northwest National Laboratory, Richland, WA.

Table C.2. PCT-Na Model Terms and Statistics

PCT-Na Model Terms and Statistics	
Component	ln(PCT-Na, g/m^2)
Al_2O_3	−31.814
B_2O_3	3.2631
CaO	5.5241
Fe_2O_3	−0.0973
K_2O	7.6834
Li_2O	13.4028
MgO	8.8211
Na_2O	6.1643
SiO_2	−3.159
SnO_2	−5.3964
TiO_2	−3.5008
V_2O_5	8.6155
ZnO	−1.1891
ZrO_2	−0.4027
Others	0.7336
$Al_2O_3 \times Al_2O_3$	85.1327
CaO × CaO	−41.0621
CaO × V_2O_5	−106.4057
$Al_2O_3 \times Na_2O$	44.4157
n	690
p	19
q	22
α	0.9
c	−0.5891
sO	1.9108
Ds	0.9457
Vc	0.0421
VsO	0.2086
VDs	0.2373

Table C.3. Vapor Hydration Test (VHT) Model Terms and Statistics

VHT Model Terms and Statistics	
Component	VHT Pass/Fail Term
Al_2O_3	−33.2908
B_2O_3	−10.2672
CaO	−57.3456
F	47.6668
K_2O	97.7116
Li_2O	435.0046
MgO	30.6084
Na_2O	108.6944
P_2O_5	−42.4271
SiO_2	−34.1488
SnO_2	−59.3127
TiO_2	−72.6017
V_2O_5	20.7981
ZnO	−48.7954
ZrO_2	−102.701
Others	−20.9574
$Li_2O \times Na_2O$	−983.3257
$TiO_2 \times ZrO_2$	−1488.983
$Li_2O \times Li_2O$	−2124.0889
n	686
p	19
α	0.9

Table C.4. K-3 Corrosion Model Terms and Statistics

K-3 Corrosion Model Terms and Statistics	
Term	k_{1208} (ln[inch])
Al_2O_3	−33.3105
B_2O_3	−12.0828
CaO	−0.6772
Cr_2O_3	−101.3429
K_2O	4.8322
Li_2O	64.3499
Na_2O	54.7839
SiO_2	−4.2539
V_2O_5	−27.1194
ZrO_2	−20.5035
Others	−11.0123
$Li_2O \times Li_2O$	−438.1673
$Na_2O \times SiO_2$	−84.6857
n	333
p	13
α	0.9

Table C.5. Sulfur Model Terms and Statistics

Sulfur Solubility Model Terms and Statistics	
Term	Melter SO_3 Tolerance, wt%
Al_2O_3	−2.5573
B_2O_3	3.0315
CaO	4.8032
Cl	−17.7273
Li_2O	19.3989
Na_2O	3.0912
P_2O_5	2.1968
SiO_2	0.2258
V_2O_5	6.2143
Others	−1.2757
LiNa	−77.5811
n	576
p	11
α	0.9

Table C.6. Viscosity Model Terms and Statistics

Viscosity Model Terms and Statistics	
Term	$\ln(\eta_{1150})^{(a)}$, (P)
Al_2O_3	10.4974
B_2O_3	−5.4755
CaO	−4.671
Cr_2O_3	−6.4633
F	−13.1106
Fe_2O_3	2.2898
K_2O	−2.0094
Li_2O	−53.786
MgO	-0.5599
Na_2O	−10.3153
P_2O_5	11.2378
SiO_2	12.1422
SnO_2	7.6387
TiO_2	−0.3143
V_2O_5	−1.1041
ZnO	−0.96
ZrO_2	9.7255
Others	10.8166
AlNa	28.5242
LiLi	265.7235
LiNa	80.3767
n	534
p	21
α	0.9

(a) Viscosity at 1150 °C

Table C.7. Electrical Conductivity Model Terms and Statistics

Electrical Conductivity Model Terms and Statistics	
Term	$\ln(EC_{1150})$[(a)], (S/cm)
Al_2O_3	−4.4821
B_2O_3	−3.7135
CaO	−4.279
K_2O	−1.4916
Li_2O	34.1609
MgO	−4.5173
Na_2O	14.4633
SiO_2	−3.9157
SnO_2	−5.3792
V_2O_5	−2.8106
Others	−2.4484
LiNa	−136.2023
NaNa	−19.7143
n	526
p	13
α	0.9

(a) Electrical conductivity at 1150 °C

Appendix D – Enhanced LAW Correlation Rules

This appendix provides the Enhanced LAW Correlation (ELC) rules found in Muller et al. (2019). Alkali content (ALK) is defined as the following:

$$\mathrm{ALK}=\mathrm{Na_2O\ (wt\%)}+0.66\times\mathrm{K_2O\ (wt\%)}$$

The equations for B_2O_3, MgO, and ZnO are constant:

$$\mathrm{B_2O_3}=11.0\ \mathrm{wt\%}$$

$$\mathrm{MgO}=1.0\ \mathrm{wt\%}$$

$$\mathrm{ZnO}=3.0\ \mathrm{wt\%}$$

The other components are written as functions of ALK and SO_3 as follows:

- **Al_2O_3**

  $\mathrm{For\ ALK} < 21.3\ \mathrm{wt\%},\ \mathrm{Al_2O_3\ (wt\%)} = 7.6$

  $\mathrm{For\ ALK} \geq 21.3\ \mathrm{wt\%},\ \mathrm{Al_2O_3\ (wt\%)} = (0.465 \times \mathrm{ALK})$ - 2.3

- **CaO**

  $\mathrm{For\ SO_3} \leq 0.95\ \mathrm{wt\%},\ \mathrm{CaO\ (wt\%)} = 1.95$

  $\mathrm{For\ SO_3} > 0.95\ \mathrm{wt\%},\ \mathrm{CaO\ (wt\%)} = (12 \times \mathrm{SO_3})$ - 9.5

  Or as a function of ALK:

  $\mathrm{For\ SO_3} > 0.95\ \mathrm{wt\%},\ \mathrm{CaO\ (wt\%)} = \left(\text{-}0.0432 \times \mathrm{ALK}^2\right) + (0.88065 \times \mathrm{ALK}) + 5.3851$

- **Cr_2O_3**

  $\mathrm{For\ 0} \leq \mathrm{SO_3} \leq 0.1\ \mathrm{wt\%},\ \mathrm{Cr_2O_3\ (wt\%)} = 0.58$

  $\mathrm{For\ 0.1} \leq \mathrm{SO_3} \leq 1.14\ \mathrm{wt\%},\ \mathrm{Cr_2O_3\ (wt\%)} = 0.63 - (0.48 \times \mathrm{SO_3})$

  $\mathrm{For\ SO_3} > 1.14\ \mathrm{wt\%},\ \mathrm{Cr_2O_3}$ is not added

- **Fe_2O_3**

  $\mathrm{For\ 0} \leq \mathrm{SO_3} \leq 0.1\ \mathrm{wt\%},\ \mathrm{Fe_2O_3\ (wt\%)} = 1.0$

  $\mathrm{For\ 0.1} \leq \mathrm{SO_3} \leq 0.7\ \mathrm{wt\%},\ \mathrm{Fe_2O_3\ (wt\%)} = 1.133 - (1.33 \times \mathrm{SO_3})$

  $\mathrm{For\ SO_3} > 0.7\ \mathrm{wt\%},\ \mathrm{Fe_2O_3}$ is not added

- **Li_2O**

For $SO_3 \leq 1.1$ wt%, Li_2O is not added

For $SO_3 > 1.1$ wt%, Li_2O (wt%) $= (7.2 \times SO_3) - 8$

Or as a function of ALK:

For $SO_3 > 1.1$ wt%, Li_2O (wt%) $= \left(-0.01846 \times ALK^2\right) + (0.257065 \times ALK) + 3.35652$

- **TiO_2**

  For $0 \leq SO_3 \leq 0.1$ wt%, TiO_2 (wt%) $= 1.0$

  For $0.1 \leq SO_3 \leq 0.85$ wt%, TiO_2 (wt%) $= 1.133 - (1.33 \times SO_3)$

  For $SO_3 > 0.85$ wt%, TiO_2 is not added

- **V_2O_5**

  For $0.17 \leq SO_3 \leq 1.08$ wt%, V_2O_5 (wt%) $= \left(-1.8 \times (SO_3)^2\right) + (5 \times SO_3) - 0.8$

  For $SO_3 > 1.08$ wt%, V_2O_5 (wt%) $= 2.50$

  For $SO_3 < 0.17$ wt%, V_2O_5 is not added

- **SnO_2**

  For $K_2O \leq 0.5$ wt% and ALK ≤ 23.33 wt%, SnO_2 is not added

  For $K_2O \leq 0.5$ wt% and ALK > 23.33 wt%, SnO_2 (wt%) $=$ ALK - 23.33

  For $K_2O > 0.5$ wt% and all ALK, SnO_2 (wt%) $= Na_2O + (0.895 \times K_2O) - 23.33$

- **ZrO_2**

  For $K_2O \leq 0.5$ wt% and ALK ≤ 22.3 wt%, ZrO_2 (wt%) $= 3.5$

  For $K_2O \leq 0.5$ wt% and ALK > 22.3 wt%, ZrO_2 (wt%) $=$ ALK - 18.8

  For $K_2O > 0.5$ wt% and all ALK, $ZrO_2 = 3.5 + Na_2O + (0.75 \times K_2O) - 22.3$

Appendix E – Glass Variance-Covariance Matrices

Source for Glass Variance-Covariance Matrices: see Vienna et al. 2021.[1]

Table E.1. Variance/Covariance Matrix for Product Consistency Test-B Model

Component	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SiO_2	SnO_2	TiO_2	V_2O_5	ZnO	ZrO_2	Others	Al_2O_3×Al_2O_3	Al_2O_3×Li_2O	CaO×CaO	CaO×V_2O_5
Al_2O_3	25.471817	-1.20772	-4.344667	-0.076427	-0.427823	2.856344	0.130499	-0.958991	-1.111311	0.20737	-1.170801	0.7375	-0.826343	-2.140986	-0.331007	-149.682999	-48.978214	32.22759	-20.884699
B_2O_3	-1.20772	0.697856	0.005962	0.011418	0.003054	-0.512135	-0.081662	-0.017313	-0.032632	0.126531	0.202408	-0.398197	-0.047286	0.092205	-0.02822	6.487049	5.142475	-0.407089	6.920648
CaO	-4.344667	0.005962	4.964385	-0.088406	0.221486	-1.2736	0.12636	0.148251	0.01722	0.469206	1.437434	0.448745	-0.234892	0.459892	-0.100705	24.607478	18.441405	-38.86732	-3.638362
Fe_2O_3	-0.076427	0.011418	-0.088406	0.646984	-0.050309	0.08973	-0.071668	0.029905	-0.073566	0.135234	-0.608554	0.104262	0.116763	0.164718	0.12885	0.923354	-1.312134	0.986919	0.930814
K_2O	-0.427823	0.003054	0.221486	-0.050309	0.984784	0.528137	-0.035621	0.096838	-0.029786	-0.443486	-0.192072	0.352062	-0.058413	-0.182075	0.041243	2.71041	-1.564051	-1.020915	-6.658844
Li_2O	2.856344	-0.512135	-1.2736	0.08973	0.528137	10.885676	-0.335643	0.558165	-0.384757	-0.217229	-0.551289	-0.770961	0.122506	-1.155193	-0.233332	-9.458567	-106.902332	6.883273	6.439389
MgO	0.130499	-0.081662	0.12636	-0.071668	-0.035621	-0.335643	2.978226	0.134684	-0.094235	-0.256211	-0.811255	0.222723	-0.20585	-0.039685	-0.248036	-1.829832	1.744186	0.091046	-5.477255
Na_2O	-0.958991	-0.017313	0.148251	0.029905	0.096838	0.558165	0.134684	0.314099	-0.050958	-0.192114	-0.051501	-0.023112	0.082996	-0.109206	-0.14142	4.615579	3.082478	-0.699715	-2.826332
SiO_2	-1.111311	-0.032632	0.01722	-0.073566	-0.029786	-0.384757	-0.094235	-0.050958	0.154299	0.00164	-0.078868	-0.052427	-0.164134	0.055001	-0.024807	6.822777	1.957565	-0.320979	1.872214
SnO_2	0.20737	0.126531	0.469206	0.135234	-0.443486	-0.217229	-0.256211	-0.192114	0.00164	2.035562	0.510089	-0.663133	0.106165	-0.168246	-0.24741	-0.437623	-5.696826	-4.077822	9.774779
TiO_2	-1.170801	0.202408	1.437434	-0.608554	-0.192072	-0.551289	-0.811255	-0.051501	-0.078868	0.510089	5.182647	0.328957	-0.203718	0.508594	0.28237	6.90359	7.14573	-10.259386	2.247095
V_2O_5	0.7375	-0.398197	0.448745	0.104262	0.352062	-0.770961	0.222723	-0.023112	-0.052427	-0.663133	0.328957	6.834246	-0.071665	0.248785	-0.262637	-7.268965	3.548646	4.083478	-86.880557
ZnO	-0.826343	-0.047286	-0.234892	0.116763	-0.058413	0.122506	-0.20585	0.082996	-0.164134	0.106165	-0.203718	-0.071665	3.211062	-0.059927	-0.048268	5.010206	-2.099436	1.319312	5.352353
ZrO_2	-2.140986	0.092205	0.459892	0.164718	-0.182075	-1.155193	-0.039685	-0.109206	0.055001	-0.168246	0.508594	0.248785	-0.059927	1.640204	0.21525	11.451765	12.054899	-2.770333	-0.272737
Others	-0.331007	-0.02822	-0.100705	0.12885	0.041243	-0.233332	-0.248036	-0.14142	-0.024807	-0.24741	0.28237	-0.262637	-0.048268	0.21525	3.353813	2.067308	0.719613	0.175947	-0.13776
Al_2O_3×Al_2O_3	-149.682999	6.487049	24.607478	0.923354	2.71041	-9.458567	-1.829832	4.615579	6.822777	-0.437623	6.90359	-7.268965	5.010206	11.451765	2.067308	912.792737	160.712087	-188.874767	176.148561
Al_2O_3×Li_2O	-48.978214	5.142475	18.441405	-1.312134	-1.564051	-106.902332	1.744186	3.082478	1.957565	-5.696826	7.14573	3.548646	-2.099436	12.054899	0.719613	160.712087	1502.468116	-121.775691	-101.283024
CaO×CaO	32.22759	-0.407089	-38.86732	0.986919	-1.020915	6.883273	0.091046	-0.699715	-0.320979	-4.077822	-10.259386	4.083478	1.319312	-2.770333	0.175947	-188.874767	-121.775691	343.956007	-140.035979
CaO×V_2O_5	-20.884699	6.920648	-3.638362	0.930814	-6.658844	6.439389	-5.477255	-2.826332	1.872214	9.774779	2.247095	-86.880557	5.352353	-0.272737	-0.13776	176.148561	-101.283024	-140.035979	1684.304327

[1] Vienna JD, A Heredia-Langner, SK Cooley, AE Holmes, DS Kim, and NA Lumetta. 2021. *Glass Property-Composition Models for Support of Hanford WTP LAW Facility Operation*. PNNL-30932, Rev. 1, Pacific Northwest National Laboratory, Richland, WA.

Table E.2. Variance/Covariance Matrix for Product Consistency Test-Na Model

Component	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SiO_2	SnO_2	TiO_2	V_2O_5	ZnO	ZrO_2	Others	Al_2O_3×Al_2O_3	CaO×CaO	CaO×V_2O_5	Al_2O3×Na_2O
Al_2O_3	19.670735	-0.87813	-2.702538	-0.256798	-0.60167	-0.591151	-0.02761	-0.043264	-0.936112	-0.217357	-0.803216	0.421815	-0.786417	-1.323664	-0.409484	-109.232903	19.35096	-19.536014	-9.868312
B_2O_3	-0.87813	0.548792	-0.076026	0.025471	0.026011	-0.104573	-0.056078	-0.07386	-0.0237	0.137293	0.139341	-0.323719	-0.027149	0.033242	-0.007352	4.238075	0.332357	5.832578	0.805614
CaO	-2.702538	-0.076026	3.896607	-0.117397	0.104581	-0.024157	0.02072	0.327242	-0.043919	0.349539	1.071276	0.267969	-0.187489	0.271802	-0.165936	20.032505	-31.079851	-1.930647	-3.73575
Fe_2O_3	-0.256798	0.025471	-0.117397	0.549966	0.007417	0.020785	-0.017928	-0.114327	-0.034115	0.149468	-0.466985	0.144107	0.106099	0.127637	0.142299	-0.32864	1.368604	0.671311	2.171553
K_2O	-0.60167	0.026011	0.104581	0.007417	0.851005	0.367415	0.024952	-0.113206	0.00933	-0.293792	-0.133721	0.353019	-0.028948	-0.15271	0.089567	0.659912	0.046705	-5.373786	2.991749
Li_2O	-0.591151	-0.104573	-0.024157	0.020785	0.367415	2.633428	-0.143	0.524006	-0.181426	-0.45722	-0.0373	-0.403854	-0.012197	-0.250449	-0.114551	0.662194	-0.83137	-0.531194	1.484695
MgO	-0.02761	-0.056078	0.02072	-0.017928	0.024952	-0.143	2.411566	-0.045657	-0.051923	-0.151167	-0.638324	0.239032	-0.146655	-0.054843	-0.156232	-2.84443	0.887187	-4.282112	2.324207
Na_2O	-0.043264	-0.07386	0.327242	-0.114327	-0.113206	0.524006	-0.045657	0.800773	-0.135249	-0.325132	-0.101428	-0.250625	0.012403	-0.058826	-0.27021	8.074418	-3.02143	-2.091657	-8.603005
SiO_2	-0.936112	-0.0237	-0.043919	-0.034115	0.00933	-0.181426	-0.051923	-0.135249	0.135838	0.038021	-0.061292	-0.005944	-0.118652	0.02301	0.00395	4.482021	0.303902	1.607184	1.412275
SnO_2	-0.217357	0.137293	0.349539	0.149468	-0.293792	-0.45722	-0.151167	-0.325132	0.038021	1.656836	0.441273	-0.449356	0.094169	-0.109826	-0.137684	-1.252711	-2.74768	7.413039	2.828242
TiO_2	-0.803216	0.139341	1.071276	-0.466985	-0.133721	-0.0373	-0.638324	-0.101428	-0.061292	0.441273	4.121145	0.306567	-0.146301	0.3582	0.226455	4.493527	-7.623558	2.146839	0.729139
V_2O_5	0.421815	-0.323719	0.267969	0.144107	0.353019	-0.403854	0.239032	-0.250625	-0.005944	-0.449356	0.306567	5.62614	-0.021968	0.162855	-0.171296	-7.979264	4.204437	-69.083049	3.440518
ZnO	-0.786417	-0.027149	-0.187489	0.106099	-0.028948	-0.012197	-0.146655	0.012403	-0.118652	0.094169	-0.146301	-0.021968	2.561625	-0.037479	-0.022086	3.733824	1.15259	4.123675	0.884438
ZrO_2	-1.323664	0.033242	0.271802	0.127637	-0.15271	-0.250449	-0.054843	-0.058826	0.02301	-0.109826	0.3582	0.162855	-0.037479	1.232209	0.149132	8.427631	-1.672206	0.464629	-0.75434
Others	-0.409484	-0.007352	-0.165936	0.142299	0.089567	-0.114551	-0.156232	-0.27021	0.00395	-0.137684	0.226455	-0.171296	-0.022086	0.149132	2.718699	0.183102	1.04329	-0.005333	2.427738
Al_2O_3×Al_2O_3	-109.232903	4.238075	20.032505	-0.32864	0.659912	0.662194	-2.84443	8.074418	4.482021	-1.252711	4.493527	-7.979264	3.733824	8.427631	0.183102	750.132224	-162.068997	150.269482	-72.455364
CaO×CaO	19.35096	0.332357	-31.079851	1.368604	0.046705	-0.83137	0.887187	-3.02143	0.303902	-2.74768	-7.623558	4.204437	1.15259	-1.672206	1.04329	-162.068997	280.225444	-118.071928	41.532013
CaO×V_2O_5	-19.536014	5.832578	-1.930647	0.671311	-5.373786	-0.531194	-4.282112	-2.091657	1.607184	7.413039	2.146839	-69.083049	4.123675	0.464629	-0.005333	150.269482	-118.071928	1335.67195	0.287181
Al_2O_3×Na_2O	-9.868312	0.805614	-3.73575	2.171553	2.991749	1.484695	2.324207	-8.603005	1.412275	2.828242	0.729139	3.440518	0.884438	-0.75434	2.427738	-72.455364	41.532013	0.287181	133.226339

Table E.3. Variance/Covariance Matrix for Vapor Hydration Test Model

Component	Al_2O_3	B_2O_3	CaO	F	K_2O	Li_2O	MgO	Na_2O	P_2O_5	SiO_2	SnO_2	TiO_2	V_2O_5	ZnO	ZrO_2	Others	$Li_2O \times Na_2O$	$TiO_2 \times ZrO_2$	$Li_2O \times Li_2O$
Al_2O_3	61.853735	-7.995062	11.994068	-26.224535	-18.268189	-402.107228	-3.913059	-50.704214	49.006524	12.518598	17.591088	108.221307	-3.542689	-3.818794	27.436951	9.241988	1316.070399	-1350.943215	3168.018611
B_2O_3	-7.995062	46.318296	3.117576	27.882688	-6.693278	-93.341664	-2.220724	-10.803966	-4.436338	-3.571706	8.661558	38.812779	-11.524668	-24.696057	17.637137	4.130961	290.74816	-956.595328	647.424934
CaO	11.994068	3.117576	66.078419	-12.679472	-56.193683	-455.858446	10.59062	-67.368698	17.160778	19.213611	40.306765	74.584688	-23.210599	20.541658	72.398328	10.658384	1187.761355	721.774789	3329.92608
F	-26.224535	27.882688	-12.679472	8919.670394	44.645687	1237.6379	66.077648	109.538919	-2803.354614	-41.288235	-50.774622	-313.777454	-234.024886	-110.68935	-121.138054	-104.030176	-3872.860693	6463.05467	-12695.90214
K_2O	-18.268189	-6.693278	-56.193683	44.645687	131.808032	554.660152	-10.653396	102.720522	-65.103318	-33.576814	-71.404937	-77.742128	31.680709	-53.702022	-102.829243	-27.739303	-1166.521691	-802.111211	-4305.328516
Li_2O	-402.107228	-93.341664	-455.858446	1237.6379	554.660152	17886.05642	-485.020189	977.665269	9.022222	-363.634872	-410.46055	-1785.636655	-73.947152	419.183968	-594.314068	-52.086287	-53811.96148	21130.36377	-199028.462
MgO	-3.913059	-2.220724	10.59062	66.077648	-10.653396	-485.020189	352.839596	-10.130859	35.983715	2.184334	-0.664785	-240.100302	-27.189419	-38.948076	-12.777566	9.854105	1367.670724	2903.072101	4643.348867
Na_2O	-50.704214	-10.803966	-67.368698	109.538919	102.720522	977.665269	-10.130859	145.694467	-73.802189	-44.976646	-70.80866	-119.583465	3.066306	-40.531242	-126.280873	-35.248093	-2625.879428	527.549794	-7578.547971
P_2O_5	49.006524	-4.436338	17.160778	-2803.354614	-65.103318	9.022222	35.983715	-73.802189	2420.179474	10.977073	4.786175	137.321538	-57.577241	-26.724807	125.267503	68.198556	289.865719	-1297.710941	-5386.851469
SiO_2	12.518598	-3.571706	19.213611	-41.288235	-33.576814	-363.634872	2.184334	-44.976646	10.977073	21.405482	16.303868	5.235819	-2.356876	-6.292719	19.803919	-1.797571	874.765044	690.450911	3553.404158
SnO_2	17.591088	8.661558	40.306765	-50.774622	-71.404937	-410.46055	-0.664785	-70.80866	4.786175	16.303868	171.471306	27.988348	13.714619	47.384932	44.005541	50.036521	883.360276	1450.644484	2403.915485
TiO_2	108.221307	38.812779	74.584688	-313.777454	-77.742128	-1785.636655	-240.100302	-119.583465	137.321538	5.235819	27.988348	2547.506704	-15.872043	-73.590286	347.777258	-153.848532	8197.672255	-42761.873	10840.09357
V_2O_5	-3.542689	-11.524668	-23.210599	-234.024886	31.680709	-73.947152	-27.189419	3.066306	-57.577241	-2.356876	13.714619	-15.872043	230.266027	16.884889	-10.329896	18.207349	-29.773818	1169.128215	882.703566
ZnO	-3.818794	-24.696057	20.541658	-110.68935	-53.702022	419.183968	-38.948076	-40.531242	-26.724807	-6.292719	47.384932	-73.590286	16.884889	393.341135	53.822375	25.544746	-1974.023596	682.042188	-5287.589919
ZrO_2	27.436951	17.637137	72.398328	-121.138054	-102.829243	-594.314068	-12.777566	-126.280873	125.267503	19.803919	44.005541	347.777258	-10.329896	53.822375	256.135473	61.77767	2178.867193	-5973.986292	1641.327386
Others	9.241988	4.130961	10.658384	-104.030176	-27.739303	-52.086287	9.854105	-35.248093	68.198556	-1.797571	50.036521	-153.848532	18.207349	25.544746	61.77767	130.179622	375.195976	-55.05741	-1587.016141
$Li_2O \times Na_2O$	1316.070399	290.74816	1187.761355	-3872.860693	-1166.521691	-53811.96148	1367.670724	-2625.879428	289.865719	874.765044	883.360276	8197.672255	-29.773818	-1974.023596	2178.867193	375.195976	204039.2859	-136648.8206	489992.9971
$TiO_2 \times ZrO_2$	-1350.943215	-956.595328	721.774789	6463.05467	-802.111211	21130.36377	2903.072101	527.549794	-1297.710941	690.450911	1450.644484	-42761.873	1169.128215	682.042188	-5973.986292	-55.05741	-136648.8206	1194858.927	-97934.14614
$Li_2O \times Li_2O$	3168.018611	647.424934	3329.92608	-12695.90214	-4305.328516	-199028.462	4643.348867	-7578.547971	-5386.851469	3553.404158	2403.915485	10840.09357	882.703566	-5287.589919	1641.327386	-1587.016141	489992.9971	-97934.14614	2794365.342

Table E.4. Variance/Covariance Matrix for K-3 Neck Corrosion Model

Comp	Al_2O_3	B_2O_3	CaO	Cr_2O_3	K_2O	Li_2O	Na_2O	SiO_2	V_2O_5	ZrO_2	Others	$Li_2O \times Li_2O$	$Na_2O \times SiO_2$
Al_2O_3	3.573147	1.51997	1.516088	3.246322	0.772305	-2.515171	-7.987438	-1.889312	0.253034	2.145784	1.712778	60.388215	19.666766
B_2O_3	1.51997	2.357941	0.938047	3.479048	0.388767	-0.899775	-5.44148	-1.681855	0.137742	1.649922	1.354328	45.375048	14.402735
CaO	1.516088	0.938047	2.094815	0.769452	0.667521	-2.870531	-5.483996	-1.532965	0.03803	2.117489	1.468916	71.699047	14.594724
Cr_2O_3	3.246322	3.479048	0.769452	106.220365	-3.511597	-2.447411	-10.651697	-2.258378	-0.169643	-1.185556	4.200548	-45.335949	24.097781
K_2O	0.772305	0.388767	0.667521	-3.511597	1.791339	-0.193112	-2.032416	-0.605337	-0.178361	0.752612	0.147252	29.579515	5.617009
Li_2O	-2.515171	-0.899775	-2.870531	-2.447411	-0.193112	24.233045	8.299026	0.902785	-3.315438	-3.316944	-1.72865	-379.754076	-16.764174
Na_2O	-7.987438	-5.44148	-5.483996	-10.651697	-2.032416	8.299026	24.832372	6.235704	-1.65107	-8.167206	-5.775041	-220.734103	-63.532158
SiO_2	-1.889312	-1.681855	-1.532965	-2.258378	-0.605337	0.902785	6.235704	1.946707	-0.134198	-2.05128	-1.702693	-62.902963	-17.144585
V_2O_5	0.253034	0.137742	0.03803	-0.169643	-0.178361	-3.315438	-1.65107	-0.134198	5.617225	1.572596	0.909986	13.760979	2.242051
ZrO_2	2.145784	1.649922	2.117489	-1.185556	0.752612	-3.316944	-8.167206	-2.05128	1.572596	5.729554	2.202219	52.41448	19.58427
Others	1.712778	1.354328	1.468916	4.200548	0.147252	-1.72865	-5.775041	-1.702693	0.909986	2.202219	2.00943	46.172721	15.050488
$Li_2O \times Li_2O$	60.388215	45.375048	71.699047	-45.335949	29.579515	-379.754076	-220.734103	-62.902963	13.760979	52.41448	46.172721	10449.37597	624.494574
$Na_2O \times SiO_2$	19.666766	14.402735	14.594724	24.097781	5.617009	-16.764174	-63.532158	-17.144585	2.242051	19.58427	15.050488	624.494574	168.489058

Table E.5. Variance/Covariance Matrix for Sulfur Model

Comp	Al_2O_3	B_2O_3	CaO	Cl	Li_2O	Na_2O	P_2O_5	SiO_2	V_2O_5	Others	$Li_2O \times Na_2O$
Al_2O_3	0.106166	-0.023641	-0.006321	-0.042622	-0.116415	-0.03756	0.003878	0.005365	-0.019318	-0.001282	0.3993
B_2O_3	-0.023641	0.098671	-0.008139	-0.137443	0.00774	0.000059	0.056206	-0.019151	-0.002605	0.007102	-0.151396
CaO	-0.006321	-0.008139	0.053655	-0.045479	-0.024439	0.005047	0.03128	-0.008033	-0.002969	0.009788	0.060851
Cl	-0.042622	-0.137443	-0.045479	7.365518	-0.082514	-0.14965	-1.533789	0.077818	0.222002	-0.061961	1.280449
Li_2O	-0.116415	0.00774	-0.024439	-0.082514	1.628478	0.191322	0.116498	-0.067394	0.009706	-0.026574	-9.128442
Na_2O	-0.03756	0.000059	0.005047	-0.14965	0.191322	0.048268	0.046391	-0.015836	-0.01683	0.000936	-0.703963
P_2O_5	0.003878	0.056206	0.03128	-1.533789	0.116498	0.046391	3.884548	-0.030861	-0.109986	-0.012867	-1.458618
SiO_2	0.005365	-0.019151	-0.008033	0.077818	-0.067394	-0.015836	-0.030861	0.017306	-0.000056	-0.010683	0.242571
V_2O_5	-0.019318	-0.002605	-0.002969	0.222002	0.009706	-0.01683	-0.109986	-0.000056	0.394144	0.010043	-0.664261
Others	-0.001282	0.007102	0.009788	-0.061961	-0.026574	0.000936	-0.012867	-0.010683	0.010043	0.030772	0.169424
$Li_2O \times Na_2O$	0.3993	-0.151396	0.060851	1.280449	-9.128442	-0.703963	-1.458618	0.242571	-0.664261	0.169424	71.38192

Table E.6. Variance/Covariance Matrix for Viscosity Model

Comp	Al_2O_3	B_2O_3	CaO	Cr_2O_3	F	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	P_2O_5	SiO_2	SnO_2	TiO_2	V_2O_5	ZnO	ZrO_2	Others	$Al_2O_3 \times Na_2O$	$Li_2O \times Li_2O$	$Li_2O \times Na_2O$
Al_2O_3	0.717602	-0.043274	-0.060347	-0.166514	-0.332527	-0.049073	-0.098431	0.063224	-0.070843	0.230974	-0.088181	-0.061862	-0.037026	-0.018061	-0.050998	-0.024184	-0.023604	0.143878	-3.946554	0.584707	-1.641575
B_2O_3	-0.043274	0.084652	0.001822	0.04815	0.077623	0.006009	0.005494	0.028415	-0.008866	-0.013741	-0.001308	-0.010703	0.012435	0.029772	0.003184	-0.017716	-0.007463	-0.070206	0.198512	-0.373448	-0.162145
CaO	-0.060347	0.001822	0.050912	-0.019399	-0.076547	0.007605	0.007499	-0.251668	0.019311	-0.034138	0.020154	0.006128	0.016658	0.037513	-0.007317	0.003673	0.01395	-0.077307	0.380492	2.480365	0.889889
Cr_2O_3	-0.166514	0.04815	-0.019399	12.93498	-2.28797	0.178625	-0.19671	-0.872359	0.292973	-0.19935	-0.682494	0.021969	-0.394182	0.44093	0.185134	0.082567	-0.258016	0.177713	0.94251	1.562524	5.965481
F	-0.332527	0.077623	-0.076547	-2.28797	18.677641	0.061504	-0.102945	1.257702	-0.102957	-0.117396	-2.361222	0.019815	-0.180529	0.050297	-0.254142	-0.165541	0.136009	-0.702338	2.199756	-16.346837	-5.076567
Fe_2O_3	-0.049073	0.006009	0.007605	0.178625	0.061504	0.100173	-0.00576	-0.126897	-0.014068	-0.036323	-0.011642	-0.002271	0.024106	-0.05481	0.037819	0.020076	0.031715	0.086261	0.376149	0.741448	0.57118
K_2O	-0.098431	0.005494	0.007499	-0.19671	-0.102945	-0.00576	0.158651	0.12707	0.011291	-0.019819	0.065013	0.000853	-0.038644	-0.042207	-0.005059	0.006557	-0.028659	0.051037	0.577486	-1.139271	-0.0691
Li_2O	0.063224	0.028415	-0.251668	-0.872359	1.257702	-0.126897	0.12707	10.629705	-0.254035	0.865027	0.007577	-0.279771	-0.102527	-0.093994	-0.14002	-0.209757	-0.41527	-0.281713	-2.331489	-115.320597	-33.700401
MgO	-0.070843	-0.008866	0.019311	0.292973	-0.102957	-0.014068	0.011291	-0.254035	0.450713	-0.020535	-0.033087	-0.002544	-0.043622	-0.091031	-0.013462	0.009093	-0.005341	-0.043339	0.391123	1.884166	1.030654
Na_2O	0.230974	-0.013741	-0.034138	-0.19935	-0.117396	-0.036323	-0.019819	0.865027	-0.020535	0.203073	-0.043448	-0.055053	-0.050926	-0.029896	-0.061521	-0.028741	-0.059891	-0.038186	-1.712168	-6.776355	-3.204304
P_2O_5	-0.088181	-0.001308	0.020154	-0.682494	-2.361222	-0.011642	0.065013	0.007577	-0.033087	-0.043448	1.465013	0.002318	0.021706	0.005911	-0.004509	0.015873	0.036868	0.084534	0.651165	0.2775	0.225991
SiO_2	-0.061862	-0.010703	0.006128	0.021969	0.019815	-0.002271	0.000853	-0.279771	-0.002544	-0.055053	0.002318	0.0259	0.008531	-0.008314	0.012722	-0.024304	0.006307	-0.029918	0.438343	2.432383	0.979568
SnO_2	-0.037026	0.012435	0.016658	-0.394182	-0.180529	0.024106	-0.038644	-0.102527	-0.043622	-0.050926	0.021706	0.008531	0.282608	0.042735	-0.013014	0.034438	0.007684	0.13306	0.299146	-0.308944	0.053712
TiO_2	-0.018061	0.029772	0.037513	0.44093	0.050297	-0.05481	-0.042207	-0.093994	-0.091031	-0.029896	0.005911	-0.008314	0.042735	0.629105	0.080855	-0.006301	0.03039	-0.14743	0.196828	0.577983	0.459827
V_2O_5	-0.050998	0.003184	-0.007317	0.185134	-0.254142	0.037819	-0.005059	-0.14002	-0.013462	-0.061521	-0.004509	0.012722	-0.013014	0.080855	0.347009	0.025636	0.032487	-0.110279	0.402344	0.848683	0.038429
ZnO	-0.024184	-0.017716	0.003673	0.082567	-0.165541	0.020076	0.006557	-0.209757	0.009093	-0.028741	0.015873	-0.024304	0.034438	-0.006301	0.025636	0.471413	0.002238	0.149906	0.173039	0.88528	0.928863
ZrO_2	-0.023604	-0.007463	0.01395	-0.258016	0.136009	0.031715	-0.028659	-0.41527	-0.005341	-0.059891	0.036868	0.006307	0.007684	0.03039	0.032487	0.002238	0.216095	0.076864	0.136196	3.560076	1.455479
Others	0.143878	-0.070206	-0.077307	0.177713	-0.702338	0.086261	0.051037	-0.281713	-0.043339	-0.038186	0.084534	-0.029918	0.13306	-0.14743	-0.110279	0.149906	0.076864	3.302962	-1.099502	0.480692	0.158056
AlNa	-3.946554	0.198512	0.380492	0.94251	2.199756	0.376149	0.577486	-2.331489	0.391123	-1.712168	0.651165	0.438343	0.299146	0.196828	0.402344	0.173039	0.136196	-1.099502	24.643517	12.450573	15.813503
LiLi	0.584707	-0.373448	2.480365	1.562524	-16.346837	0.741448	-1.139271	-115.320597	1.884166	-6.776355	0.2775	2.432383	-0.308944	0.577983	0.848683	0.88528	3.560076	0.480692	12.450573	1480.941397	326.761218
LiNa	-1.641575	-0.162145	0.889889	5.965481	-5.076567	0.57118	-0.0691	-33.700401	1.030654	-3.204304	0.225991	0.979568	0.053712	0.459827	0.038429	0.928863	1.455479	0.158056	15.813503	326.761218	132.241786

Appendix F – Terms Used for Composition Uncertainty Calculations

Table F.1. Minimum, Maximum, Most Likely, and Nominal Values for the Glass-Forming Chemical Compositions. Source: Vienna & Kim (2014)[1]

Minimum	Kyanite	Boric Acid	Wollastonite	Hematite	Li Carbonate	Olivine	Cr_2O_3	Silica	Rutile	Zincite	Zircon	V_2O_5	SnO_2
Ac_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Ag_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
Al_2O_3	0.54	0	0.0013	0.0099	0	0.0003	0	0.0004	0	0	0.001	0	0
Am_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
As_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
B_2O_3	0	0.5625	0	0	0	0	0	0	0	0	0	0	0
BaO	0	0	0	0	0	0	0	0	0	0	0	0	0
BeO	0	0	0	0	0	0	0	0	0	0	0	0	0
Bi_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
CaO	0	0	0.4477	0	0	0	0	0	0	0	0	0	0
CdO	0	0	0	0	0	0	0	0	0	0	0	0	0
Ce_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Cl	0	0	0	0	0	0	0	0	0	0	0	0	0
Cm_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
CoO	0	0	0	0	0	0	0	0	0	0	0	0	0
Cr_2O_3	0	0	0	0	0	0	0.985	0	0	0	0	0	0
Cs_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
CuO	0	0	0	0	0	0	0	0	0	0	0	0	0

[1] Vienna JD and DS Kim. 2014. *Preliminary IHLW Formulation Algorithm Description*. 24590-HLW-RPT-RT-05-001, Rev. 1, River Protection Project, Hanford Waste Treatment and Immobilization Plant, Richland, WA. https://www.osti.gov/servlets/purl/1110191

Table F.1 (cont.)

Minimum	Kyanite	Boric Acid	Wollastonite	Hematite	Li Carbonate	Olivine	Cr_2O_3	Silica	Rutile	Zincite	Zircon	V_2O_5	SnO_2
Eu_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
F	0	0	0	0	0	0	0	0	0	0	0	0	0
Fe_2O_3	0.0042	0	0.0029	0.9615	0	0.0468	0	0.0001	0	0	0.0006	0	0
Gd_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
HgO	0	0	0	0	0	0	0	0	0	0	0	0	0
I	0	0	0	0	0	0	0	0	0	0	0	0	0
K_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
La_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Li_2O	0	0	0	0	0.4	0	0	0	0	0	0	0	0
MgO	0	0	0	0.0001	0	0.4634	0	0	0	0	0	0	0
MnO	0	0	0.0009	0.0003	0	0	0	0	0	0	0	0	0
MoO_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Na_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
Nb_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
Nd_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
NiO	0	0	0	0	0	0.0022	0	0	0	0	0	0	0
NpO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
P_2O_5	0	0	0	0.0018	0	0	0	0	0	0	0	0	0
Pa_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
PbO	0	0	0	0	0	0	0	0	0	0	0	0	0
PdO	0	0	0	0	0	0	0	0	0	0	0	0	0
Pr_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
PuO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
RaO	0	0	0	0	0	0	0	0	0	0	0	0	0
Rb_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
Rh_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0

Table F.1 (cont.)

Minimum	Kyanite	Boric Acid	Wollastonite	Hematite	Li Carbonate	Olivine	Cr_2O_3	Silica	Rutile	Zincite	Zircon	V_2O_5	SnO_2
RuO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
SO_3	0	0	0	0.0006	0	0	0	0	0	0	0	0	0
Sb_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
SeO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
SiO_2	0.39	0	0.48	0.0084	0	0.4085	0	0.992	0	0	0.32	0	0
Sm_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
SnO_2	0	0	0	0	0	0	0	0	0	0	0	0	0.999
SrO	0	0	0	0	0	0	0	0	0	0	0	0	0
Ta_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
Tc_2O_7	0	0	0	0	0	0	0	0	0	0	0	0	0
TeO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
ThO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
TiO_2	0.005	0	0.0001	0	0	0	0	0	0.928	0	0.0007	0	0
Tl_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
UO_3	0	0	0	0	0	0	0	0	0	0	0.0003	0	0
V_2O_5	0	0	0	0	0	0	0	0	0	0	0	0.992	0
WO_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Y_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
ZnO	0	0	0	0	0	0	0	0	0	0.993	0	0	0
ZrO_2	0	0	0	0	0	0	0	0	0	0	0.65	0	0

Table F.1 (cont.)

Maximum	Kyanite	Boric Acid	Wollastonite	Hematite	Li Carbonate	Olivine	Cr_2O_3	Silica	Rutile	Zincite	Zircon	V_2O_5	SnO_2
Ac_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Ag_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
Al_2O_3	0.6	0	0.0027	0.0201	0	0.0078	0	0.004	0.0075	0	0.004	0	0
Am_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
As_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
B_2O_3	0	0.568	0	0	0	0	0	0	0	0	0	0	0
BaO	0	0	0	0	0	0	0	0	0	0	0	0	0
BeO	0	0	0	0	0	0	0	0	0	0	0	0	0
Bi_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0.00017
CaO	0.0004	0	0.5023	0.0008	0.022	0.0003	0	0.0002	0	0	0	0	0
CdO	0	0	0	0	0	0	0	0	0	0.0002	0	0	0
Ce_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Cl	0	0	0	0	0.0001	0	0	0	0	0	0	0	0
Cm_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
CoO	0	0	0	0	0	0	0	0	0	0	0	0	0
Cr_2O_3	0	0	0	0	0.0002	0.0078	0.991	0	0.0075	0	0	0	0
Cs_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
CuO	0	0	0	0	0	0	0	0	0	0	0	0	0

Table F.1 (cont.)

Maximum	Kyanite	Boric Acid	Wollastonite	Hematite	Li Carbonate	Olivine	Cr_2O_3	Silica	Rutile	Zincite	Zircon	V_2O_5	SnO_2
Eu_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
F	0	0	0	0	0	0	0	0	0	0	0	0	0
Fe_2O_3	0.01	0	0.0051	0.9785	0.0001	0.1068	0.0003	0.0004	0.025	0.0001	0.0009	0.00057189	0.00021
Gd_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
HgO	0	0	0	0	0	0	0	0	0	0	0	0	0
I	0	0	0	0	0	0	0	0	0	0	0	0	0
K_2O	0.0007	0	0	0	0.0001	0	0	0.0002	0	0	0	0.00018069	0
La_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Li_2O	0	0	0	0	0.4044	0	0	0	0	0	0	0	0
MgO	0.0004	0	0.001	0.0037	0.0002	0.4934	0	0.0001	0	0	0	0	0
MnO	0	0	0.0011	0.0039	0	0	0	0	0	0.0001	0	0	0
MoO_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Na_2O	0.0042	0	0	0	0.0011	0.0004	0	0.0002	0	0	0	0.00033699	0
Nb_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
Nd_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
NiO	0	0	0	0	0	0.0052	0	0	0	0	0	0	0
NpO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
P_2O_5	0	0	0	0.0054	0	0	0	0	0.0007	0	0	0	0
Pa_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
PbO	0	0	0	0	0	0	0	0	0	0.0001	0	0	0.00054
PdO	0	0	0	0	0	0	0	0	0	0	0	0	0
Pr_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
PuO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
RaO	0	0	0	0	0	0	0	0	0	0	0	0	0
Rb_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
Rh_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0

Table F.1 (cont.)

Maximum	Kyanite	Boric Acid	Wollastonite	Hematite	Li Carbonate	Olivine	Cr_2O_3	Silica	Rutile	Zincite	Zircon	V_2O_5	SnO_2
RuO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
SO_3	0	0.0003	0	0.0009	0.0004	0	0	0	0.0007	0	0	0	0
Sb_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0.00018
SeO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
SiO_2	0.42	0	0.53	0.0186	0	0.4385	0	0.999	0.025	0	0.325	0.00021393	0
Sm_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
SnO_2	0	0	0	0	0	0	0	0	0	0	0	0	0.9999
SrO	0	0	0	0	0	0	0	0	0	0	0	0	0
Ta_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
Tc_2O_7	0	0	0	0	0	0	0	0	0	0	0	0	0
TeO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
ThO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
TiO_2	0.016	0	0.0003	0	0	0	0	0.0005	0.936	0	0.0014	0	0
Tl_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
UO_3	0	0	0	0	0	0	0	0	0	0	0.0008	0	0
V_2O_5	0	0	0	0	0	0	0	0	0.0075	0	0	0.996	0
WO_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Y_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
ZnO	0	0	0	0	0	0	0	0	0	0.9999	0	0	0
ZrO_2	0	0	0	0	0	0	0	0	0.025	0	0.67	0	0

Table F.1 (cont.)

Most Likely	Kyanite	Boric Acid	Wollastonite	Hematite	Li Carbonate	Olivine	Cr_2O_3	Silica	Rutile	Zincite	Zircon	V_2O_5	SnO_2
Ac_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Ag_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
Al_2O_3	0.5703	0	0.002	0.015	0	0.0019	0	0.0014	0.005	0	0.0025	0	0
Am_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
As_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
B_2O_3	0	0.5652	0	0	0	0	0	0	0	0	0	0	0
BaO	0	0	0	0	0	0	0	0	0	0	0	0	0
BeO	0	0	0	0	0	0	0	0	0	0	0	0	0
Bi_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
CaO	0.0003	0	0.475	0.0004	0	0.0002	0	0.0001	0	0	0	0	0
CdO	0	0	0	0	0	0	0	0	0	0.0001	0	0	0
Ce_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Cl	0	0	0	0	0.0001	0	0	0	0	0	0	0	0
Cm_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
CoO	0	0	0	0	0	0	0	0	0	0	0	0	0
Cr_2O_3	0	0	0	0	0.0001	0.0013	0.991	0	0.0016	0	0	0	0
Cs_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
CuO	0	0	0	0	0	0	0	0	0	0	0	0	0

Table F.1 (cont.)

Most Likely	Kyanite	Boric Acid	Wollastonite	Hematite	Li Carbonate	Olivine	Cr_2O_3	Silica	Rutile	Zincite	Zircon	V_2O_5	SnO_2
Eu_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
F	0	0	0	0	0	0	0	0	0	0	0	0	0
Fe_2O_3	0.0078	0	0.004	0.97	0	0.0768	0	0.0002	0.007	0	0.0008	0	0
Gd_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
HgO	0	0	0	0	0	0	0	0	0	0	0	0	0
I	0	0	0	0	0	0	0	0	0	0	0	0	0
K_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
La_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Li_2O	0	0	0	0	0.402	0	0	0	0	0	0	0	0
MgO	0.0001	0	0.001	0.001	0.0001	0.4801	0	0.0001	0	0	0	0	0
MnO	0	0	0.001	0.0012	0	0	0	0	0	0	0	0	0
MoO_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Na_2O	0.0042	0	0	0	0.0008	0.0003	0	0.0002	0	0	0	0	0
Nb_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
Nd_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
NiO	0	0	0	0	0	0.0037	0	0	0	0	0	0	0
NpO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
P_2O_5	0	0	0	0.0027	0	0	0	0	0	0	0	0	0
Pa_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
PbO	0	0	0	0	0	0	0	0	0	0	0	0	0
PdO	0	0	0	0	0	0	0	0	0	0	0	0	0
Pr_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
PuO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
RaO	0	0	0	0	0	0	0	0	0	0	0	0	0
Rb_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
Rh_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0

Table F.1 (cont.)

Most Likely	Kyanite	Boric Acid	Wollastonite	Hematite	Li Carbonate	Olivine	Cr_2O_3	Silica	Rutile	Zincite	Zircon	V_2O_5	SnO_2
RuO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
SO_3	0	0	0	0.0007	0.0003	0	0	0	0	0	0	0	0
Sb_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
SeO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
SiO_2	0.4067	0	0.51	0.0135	0	0.4252	0	0.997	0.022	0	0.3225	0	0
Sm_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
SnO_2	0	0	0	0	0	0	0	0	0	0	0	0	0.99945
SrO	0	0	0	0	0	0	0	0	0	0	0	0	0
Ta_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
Tc_2O_7	0	0	0	0	0	0	0	0	0	0	0	0	0
TeO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
ThO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
TiO_2	0.0079	0	0.0002	0	0	0	0	0.0001	0.932	0	0.001	0	0
Tl_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
UO_3	0	0	0	0	0	0	0	0	0	0	0.0004	0	0
V_2O_5	0	0	0	0	0	0	0	0	0.0045	0	0	0.994	0
WO_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Y_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
ZnO	0	0	0	0	0	0	0	0	0	0.999	0	0	0
ZrO_2	0	0	0	0	0	0	0	0	0.019	0	0.66	0	0

Table F.1 (cont.)

Nominal	Kyanite	Boric Acid	Wollastonite	Hematite	Li Carbonate	Olivine	Cr_2O_3	Silica	Rutile	Zincite	Zircon	V_2O_5	SnO_2
Ac_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Ag_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
Al_2O_3	0.570223	0	0.002003	0.015	0	0.00261	0	0.001657	0.004584	0	0.002502	0	0
Am_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
As_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
B_2O_3	0	0.565221	0	0	0	0	0	0	0	0	0	0	0
BaO	0	0	0	0	0	0	0	0	0	0	0	0	0
BeO	0	0	0	0	0	0	0	0	0	0	0	0	0
Bi_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	2.83E-05
CaO	0.000267	0	0.475099	0.000399	0.003657	0.000184	0	0.0001	0	0	0	0	0
CdO	0	0	0	0	0	0	0	0	0	0.0001	0	0	0
Ce_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Cl	0	0	0	0	8.32E-05	0	0	0	0	0	0	0	0
Cm_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
CoO	0	0	0	0	0	0	0	0	0	0	0	0	0
Cr_2O_3	0	0	0	0	0.0001	0.002172	0.990223	0	0.002309	0	0	0	0
Cs_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
CuO	0	0	0	0	0	0	0	0	0	0	0	0	0
Eu_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
F	0	0	0	0	0	0	0	0	0	0	0	0	0
Fe_2O_3	0.007568	0	0.004003	0.970057	1.67E-05	0.076858	3.88E-05	0.000217	0.008835	1.66E-05	0.000783	0.000074	0.000035
Gd_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
HgO	0	0	0	0	0	0	0	0	0	0	0	0	0
I	0	0	0	0	0	0	0	0	0	0	0	0	0
K2O	0.000116	0	0	0	1.66E-05	0	0	3.35E-05	0	0	0	2.34E-05	0
La_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Li_2O	0	0	0	0	0.402062	0	0	0	0	0	0	0	0
MgO	0.000133	0	0.000835	0.001299	9.99E-05	0.47949	0	8.33E-05	0	0	0	0	0
MnO	0	0	0.001	0.001499	0	0	0	0	0	1.66E-05	0	0	0
MoO_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Na_2O	0.003495	0	0	0	0.000716	0.000267	0	0.000167	0	0	0	4.36E-05	0
Nb_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
Nd_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
NiO	0	0	0	0	0	0.003704	0	0	0	0	0	0	0
NpO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
P_2O_5	0	0	0	0.002996	0	0	0	0	0.000117	0	0	0	0

Table F.1 (cont.)

Nominal	Kyanite	Boric Acid	Wollastonite	Hematite	Li Carbonate	Olivine	Cr2O3	Silica	Rutile	Zincite	Zircon	V2O5	SnO2
Pa_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
PbO	0	0	0	0	0	0	0	0	0	1.66E-05	0	0	0.00009
PdO	0	0	0	0	0	0	0	0	0	0	0	0	0
Pr_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
PuO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
RaO	0	0	0	0	0	0	0	0	0	0	0	0	0
Rb_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
Rh_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
RuO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
SO_3	0	4.98E-05	0	0.000717	0.000266	0	0	0	0.000117	0	0	0	0
Sb_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0.00003
SeO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
SiO_2	0.406079	0	0.508207	0.013493	0	0.424659	0	0.996506	0.018817	0	0.322526	2.77E-05	0
Sm_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
SnO_2	0	0	0	0	0	0	0	0	0	0	0	0	0.99945
SrO	0	0	0	0	0	0	0	0	0	0	0	0	0
Ta_2O_5	0	0	0	0	0	0	0	0	0	0	0	0	0
Tc_2O_7	0	0	0	0	0	0	0	0	0	0	0	0	0
TeO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
ThO_2	0	0	0	0	0	0	0	0	0	0	0	0	0
TiO_2	0.008769	0	0.0002	0	0	0	0	0.00015	0.932065	0	0.001017	0	0
Tl_2O	0	0	0	0	0	0	0	0	0	0	0	0	0
UO_3	0	0	0	0	0	0	0	0	0	0	0.00045	0	0
V_2O_5	0	0	0	0	0	0	0	0	0.004252	0	0	0.994	0
WO_3	0	0	0	0	0	0	0	0	0	0	0	0	0
Y_2O_3	0	0	0	0	0	0	0	0	0	0	0	0	0
ZnO	0	0	0	0	0	0	0	0	0	0.998145	0	0	0
ZrO_2	0	0	0	0	0	0	0	0	0.016837	0	0.660036	0	0

Table F.2. Minimum, Maximum, and Most Likely Values for the Natural Logarithm of the Melter Decontamination Factor (DF)

Comp	ln(DF), Min	ln(DF), Most likely	ln(DF), Max	Comp	ln(DF), Min	ln(DF), Most likely	ln(DF), Max	Comp	ln(DF), Min	ln(DF), Most likely	ln(DF), Max
Ac_2O_3	2.9601	6.8772	11.1239	MoO_3	1.8563	4.194	6.4944	UO_3	2.9601	6.8772	11.1239
Ag_2O	1.8563	4.194	6.4944	Na_2O	3.4874	4.8633	6.4944	V_2O_5	1.8563	4.194	6.4944
Al_2O_3	5.0764	7.0814	8.8901	Nb_2O_5	2.9601	6.8772	11.1239	WO_3	2.9601	6.8772	11.1239
Am_2O_3	1.8563	4.194	6.4944	Nd_2O_3	2.9601	6.8772	11.1239	Y_2O_3	2.9601	6.8772	11.1239
As_2O_5	0.0945	1.5296	4.237	NiO	3.9299	4.7875	6.3835	ZnO	4.7353	6.2383	7.8709
B_2O_3	3.708	4.5886	5.8519	NpO_2	2.9601	6.8772	11.1239	ZrO_2	7.2204	8.7143	11.1239
BaO	2.9601	6.8772	11.1239	P_2O_5	2.9601	5.1381	6.7822	—	—	—	—
BeO	2.9601	6.8772	11.1239	Pa_2O_5	2.9601	6.8772	11.1239	—	—	—	—
Bi_2O_3	1.8563	4.194	6.4944	PbO	3.2542	4.4716	6.2971	—	—	—	—
CaO	5.2311	7.0825	8.6034	PdO	2.9601	6.8772	11.1239	—	—	—	—
CdO	2.9601	6.8772	11.1239	Pr_2O_3	2.9601	6.8772	11.1239	—	—	—	—
Ce_2O_3	2.9601	6.8772	11.1239	PuO_2	2.9601	6.8772	11.1239	—	—	—	—
Cl	0.0979	0.7583	1.9095	RaO	0.0945	1.5296	4.237	—	—	—	—
Cm_2O_3	2.9601	6.8772	11.1239	Rb_2O	1.8563	4.194	6.4944	—	—	—	—
CoO	2.9601	6.8772	11.1239	Rh_2O_3	2.9601	6.8772	11.1239	—	—	—	—
Cr_2O_3	1.8563	3.0681	5.3033	RuO_2	1.8563	4.194	6.4944	—	—	—	—
Cs_2O	0.47	2.3609	4.237	SO_3	0.6308	1.9694	3.2089	—	—	—	—
CuO	2.9601	6.8772	11.1239	Sb_2O_3	0.0945	1.5296	4.237	—	—	—	—
Eu_2O_3	2.9601	6.8772	11.1239	SeO_2	0.0945	1.5296	4.237	—	—	—	—
F	0.1179	1.4682	2.4361	SiO_2	5.3471	7.5372	9.7527	—	—	—	—
Fe_2O_3	4.9381	6.6712	8.8984	Sm_2O_3	2.9601	6.8772	11.1239	—	—	—	—
Gd_2O_3	2.9601	6.8772	11.1239	SnO_2	2.9601	6.8772	11.1239	—	—	—	—
HgO	0	0	0	SrO	2.9601	6.8772	11.1239	—	—	—	—
I	0.0945	0.5807	2.266	Ta_2O_5	2.9601	6.8772	11.1239	—	—	—	—
K_2O	2.0669	3.3844	5.5607	Tc_2O_7	0.0953	0.47	1.6094	—	—	—	—
La_2O_3	2.9601	6.8772	11.1239	TeO_2	0.0945	1.5296	4.237	—	—	—	—
Li_2O	3.4689	5.987	7.2894	ThO_2	2.9601	6.8772	11.1239	—	—	—	—
MgO	7.2464	8.8618	11.0268	TiO_2	4.6308	6.1247	8.074	—	—	—	—
MnO	2.9601	6.8772	11.1239	Tl_2O	0.0945	1.5296	4.237	—	—	—	—

Table F.3. Oxide Conversion Factors (f_i) for Chemical Elements and Radionuclides and Specific Activities (A_i) for Radionuclides. Source: Table A-1 in Kim and Vienna (2012)

Element	Glass oxide	f_i
Ac	Ac_2O_3	NA
Ag	Ag_2O	1.0741618
Al	Al_2O_3	1.8894637
Am	Am_2O_3	NA
As	As_2O_5	1.5338715
B	B_2O_3	3.2198779
Ba	BaO	1.1165059
Be	BeO	2.7753081
Bi	Bi_2O_3	1.1148390
Ca	CaO	1.3992065
Cd	CdO	1.1423295
Ce	Ce_2O_3	1.1712814
Cl	Cl	1.0000000
Cm	Cm_2O_3	NA
Co	CoO	1.2714836
Cr	Cr_2O_3	1.4615558
Cs	Cs_2O	1.0601909
Cu	CuO	1.2517767
Eu	Eu_2O_3	NA
F	F	1.0000000
Fe	Fe_2O_3	1.4297294
Gd	Gd_2O_3	1.1526175
Hg	HgO	1.0797617
I	I	NA
K	K_2O	1.2046048
La	La_2O_3	1.1727729
Li	Li_2O	2.1525285
Mg	MgO	1.6582761
Mn	MnO	1.2912262
Mo	MoO_3	1.5002939
Na	Na_2O	1.3479678

Radionuclide	Glass oxide	f_i	A_i, Ci/g
^{59}Ni	^{59}NiO	1.2714800	7.982E-02
^{60}Co	^{60}CoO	1.2669102	1.131E+03
^{63}Ni	^{63}NiO	1.2542412	5.738E+01
^{79}Se	$^{79}SeO_2$	1.4054638	6.969E-02
^{90}Sr	^{90}SrO	1.1779550	1.388E+02
^{90}Y	$^{90}Y_2O_3$	1.2669393	5.437E+05
^{93m}Nb	$^{93m}Nb_2O_5$	1.4305248	2.386E+02
^{93}Zr	$^{93}ZrO_2$	1.3444224	2.515E-03
^{99}Tc	$^{99}Tc_2O_7$	1.5661615	1.711E-02
^{106}Ru	$^{106}RuO_2$	1.3018755	3.349E+03
^{113m}Cd	^{113m}CdO	1.1417075	2.311E+02
^{125}Sb	$^{125}Sb_2O_3$	1.1919928	1.037E+03
^{126}Sn	$^{126}SnO_2$	1.2539587	2.839E-02
^{129}I	^{129}I	1.0000000	1.768E-04
^{134}Cs	$^{134}Cs_2O$	1.0596993	1.293E+03
^{137m}Ba	^{137m}BaO	1.1167839	5.382E+08
^{137}Cs	$^{137}Cs_2O$	1.0583920	8.655E+01
^{151}Sm	$^{151}Sm_2O_3$	1.1589344	2.632E+01
^{152}Eu	$^{152}Eu_2O_3$	1.1578888	1.740E+02
^{154}Eu	$^{154}Eu_2O_3$	1.1558383	2.703E+02
^{155}Eu	$^{155}Eu_2O_3$	1.1548329	4.762E+02
^{226}Ra	^{226}RaO	1.0707860	9.885E-01
^{227}Ac	$^{227}Ac_2O_3$	1.1057099	7.232E+01
^{228}Ra	^{228}RaO	1.0701728	2.727E+02
^{229}Th	$^{229}ThO_2$	1.1397132	2.127E-01
^{231}Pa	$^{231}Pa_2O_5$	1.1731267	4.723E-02
^{232}Th	$^{232}ThO_2$	1.1379033	1.097E-07
^{232}U	$^{232}UO_3$	1.2068558	2.207E+01
^{233}U	$^{233}UO_3$	1.2059655	9.633E-03
^{234}U	$^{234}UO_3$	1.2050846	6.217E-03
^{235}U	$^{235}UO_3$	1.2042094	2.161E-06

Element	Glass oxide	f_i
Nb	Nb_2O_5	NA
Nd	Nd_2O_3	1.1663831
Ni	NiO	1.2725928
Np	NpO_2	NA
P	P_2O_5	2.2913672
Pa	Pa_2O_5	NA
Pb	PbO	1.0772172
Pd	PdO	1.1503420
Pr	Pr_2O_3	1.1703179
Pu	PuO_2	NA
Ra	RaO	NA
Rb	Rb_2O	1.0935990
Rh	Rh_2O_3	1.2332149
Ru	RuO_2	1.3166004
S	SO_3	2.4968565
Sb	Sb_2O_3	1.1971065
Se	SeO_2	1.4052533
Si	SiO_2	2.1393352
Sm	Sm_2O_3	NA
Sn	SnO_2	NA
Sr	SrO	1.1825999
Ta	Ta_2O_5	1.2210498
Tc	Tc_2O_7	NA
Te	TeO_2	1.2507743
Th	ThO_2	1.1379032
Ti	TiO_2	1.6683124
Tl	Tl_2O	1.0391407
U	UO_3	1.2016486
V	V_2O_5	1.7851850
W	WO_3	1.2610726
Y	Y_2O_3	1.2699384
Zn	ZnO	1.2446766
Zr	ZrO_2	1.3507717

Radionuclide	Glass oxide	f_i	A_i, Ci/g
^{236}U	$236UO_3$	1.2033426	6.468E-05
^{237}Np	$237NpO_2$	1.1349887	7.047E-04
^{238}Pu	$^{238}PuO_2$	1.1344205	1.712E+01
^{238}U	$^{238}UO_3$	1.2016299	3.361E-07
^{239}Pu	$^{239}PuO_2$	1.1338571	6.202E-02
^{240}Pu	$^{240}PuO_2$	1.1332983	2.269E-01
^{241}Am	$^{241}Am_2O_3$	1.0995578	3.427E+00
^{241}Pu	$^{241}PuO_2$	1.1327437	1.030E+02
^{242}Cm	$^{242}Cm_2O_3$	1.0991457	3.311E+03
^{242}Pu	$^{242}PuO_2$	1.1321942	3.954E-03
^{243}Am	$^{243}Am_2O_3$	1.0987369	1.997E-01
^{243}Cm	$^{243}Cm_2O_3$	1.0987369	4.903E+01
^{244}Cm	$^{244}Cm_2O_3$	1.0983316	8.093E+01

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Pacific Northwest National Laboratory

902 Battelle Boulevard
P.O. Box 999
Richland, WA 99354
1-888-375-PNNL (7665)

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