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Preliminary Enhanced LAW Glass Formulation Algorithm

November 2019

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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

Abstract

This report summarizes the Preliminary Enhanced LAW Glass Formulation Algorithm, its background information, and the calculations it performs.

The Preliminary Enhanced LAW Glass Formulation Algorithm is a tool that has been developed in MATLAB to formulate glass at a given a waste composition, while attempting to maximize waste loading. It is intended for use at the Hanford Waste Treatment and Immobilization Plant, where nuclear waste will be vitrified into glass. The formulated glass is required to meet several processing and product quality constraints. In addition, calculations must account for associated uncertainties in constraint prediction and measurement. The algorithm also allows for the ability to hold glass compositions closer to tested regions in order to increase confidence in the output. The algorithm adheres to PNNL nuclear quality assurance procedures and has been through rigorous validation and verification testing.

Acknowledgments

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The authors gratefully acknowledge the financial support provided by the U.S. Department of Energy Office of River Protection Waste Treatment and Immobilization Plant Project managed by Tom Fletcher, with technical oversight by Albert Kruger.

The authors thank Charmayne Lonergan (PNNL) for her technical review, Matt Wilburn (PNNL) for his editorial review, and Hans Brandal and Veronica Perez (PNNL) for programmatic support during the conduct of this work.

Quality Assurance

This work was performed in accordance with the Pacific Northwest National Laboratory (PNNL) Nuclear Quality Assurance Program (NQAP). The NQAP complies with the United States Department of Energy Order 414.1D, Quality Assurance, and 10 CFR 830 Subpart A, Quality Assurance Requirements. The NQAP uses 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 and Subpart 2.7, “Quality Assurance Requirements for Computer Software for Nuclear Facility Applications”.

The NQAP works in conjunction with PNNL’s laboratory-level Quality Management Program, which is based upon the requirements as defined in the United States Department of Energy (DOE) Order 414.1D, Quality Assurance, and 10 CFR 830, Nuclear Safety Management, Subpart A, “Quality Assurance Requirements”.

This work emphasized demonstrating proof of principle with the intent of solving a specific problem or meeting a practical need. The information associated with this report may be used to support design input.

Acronyms and Abbreviations

CI	confidence interval
CL%	confidence level percent
CRV	concentrate receipt vessel
DFLAW	Direct Feed Low-Activity Waste
DOE	U.S. Department of Energy
FIO	for information only
GFC	glass-forming chemical
GUI	graphical user interface
HLW	high-level waste
ILAW	immobilized low-activity waste
LAB	Analytical Laboratory
LAW	low-activity waste
MFPV	melter feed preparation vessel
MFV	melter feed vessel
MRQ	minimum reportable quantity
NQAP	Nuclear Quality Assurance Program
PCT	product consistency test
PERT	Program Evaluation and Review Technique
RSD	relative standard deviation
SCI	simultaneous confidence interval
SCP	software control package
V&V	validation and verification
VHT	vapor hydration test
WTP	Hanford Waste Treatment and Immobilization Plant

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1.0 Background

The United States Department of Energy (DOE) is responsible for managing the legacy nuclear waste stored at the Hanford Site. To facilitate treatment, the waste will be separated into a low-activity waste fraction and a high-level waste (HLW) fraction, each of which has different methods and constraints surrounding its processing. The LAW portion will be treated in advance of completion of the whole plant, through the Direct-Feed, Low-Activity Waste (DFLAW) process which will use the WTP's Low-Activity Waste Facility (LAW), the Analytical Laboratory (LAB) and the supporting facilities that run the plant.

Treatment is to occur at Hanford Site's Waste Treatment and Immobilization Plant (WTP) where, following a pre-treatment process, the separated wastes will be mixed with glass-forming chemicals (GFCs), heated, and poured into canisters or containers where it will cool into a glass.

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 which need to be shipped and stored. This decreases the length of the treatment campaign, which reduces cost.

The purpose of the Preliminary Enhanced LAW Glass Formulation Algorithm, developed by Pacific Northwest National Laboratory (PNNL), is to computationally formulate LAW glass compositions given a waste composition and specific parameters, 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 Immobilized Low-Activity Waste (ILAW) Formulation Algorithm Description (Kim and Vienna 2012). However, differing from this document, it uses the processing and product quality conditions described in Vienna et al. 2016. Additionally, the algorithm has weighted parameters which force glass compositions closer to tested regions. These are described in Muller et al. 2017.

2.0 Process Description

The Preliminary Enhanced LAW Glass Formulation Algorithm follows all the assumptions used in Kim and Vienna 2012 for volume transfers and composition analysis. Waste compositions are assumed to be analyzed for all components in the CRV, with three grab samples used for analysis. This means that only two composition inputs are used for glass formulation: CRV waste composition and GFC additions. The GFC compositions and composition uncertainties are specified by the vendor. GFC additions are the same as those specified in Kim and Vienna 2012, except Rutile has been added as an additional option. The GFC additions to the waste are used to obtain the necessary composition of the final glass waste form to allow it to meet 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.

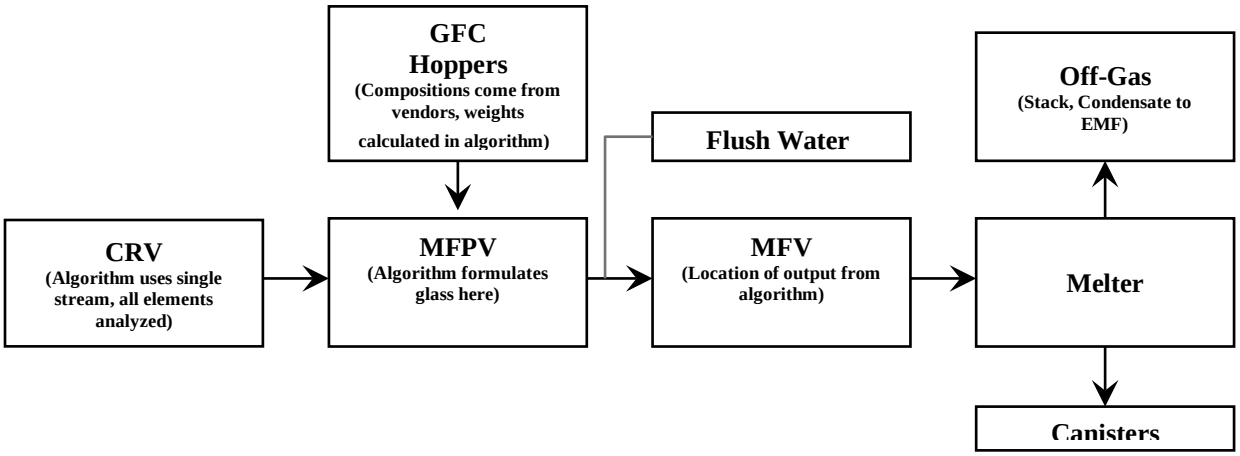

Figure 2.1. Visual depiction of how the glass formulation method used by the Preliminary Enhanced LAW Glass Formulation Algorithm associates with plant operations.

The off-gas system captures varying amounts of specific waste components which evaporate during melter operations, as indicated by the retention factors found in Appendix B, Table B.1. During plant operations, the evaporate bottoms are drained from the Effluent Management Facility (EMF) for reintroduction into the CRV. The EMF is not modeled in the algorithm as it only computes single-stream calculations based on analysis in the CRV. The specific retention factors used in the algorithm are assumptions and may change in the future.

It is assumed that after the retention factor is applied, the remainder of the waste-GFC combination is retained in the glass. No other components are removed after optimization.

3.0 Calculations

This section summarizes the calculations used in the Preliminary Enhanced LAW Glass Formulation Algorithm. For a detailed description of all the equations used, see the *Preliminary ILAW Formulation Algorithm Description, 24590-LAW-RPT-RT04-0003, Rev. 1* (Kim and Vienna 2012).

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 in order 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 Gervasio et al. 2017 can be found in Table 3.1. Additionally, the model coefficients used to predict each of these properties can be found in Appendix D.

Table 3.1. LAW Glass Property Constraints

Waste Loading Rules	Limit
Alkali content	$w_{Na_2O} + 0.66 w_{K_2O} \leq 24$ wt%
Alkali and sulfur content	$w_{Na_2O} + 0.66 w_{K_2O} \leq 33.94 - 11.69 w_{SO_3}$, wt%
Sulfur content	$w_{SO_3} \leq 1.5$ wt%
Halide content	$g_{SO_3} \leq 0.01825 - 0.4936 \times \left(1.761 g_{Cl} + 2.971 g_{Cr_2O_3} - 0.1608 g_{P_2O_5}\right)$
Property	**Limit**
Salt, SO_3 concentration	$w_{SO_3} \leq w_{SO_3}^{Limit}$
Combined zirconia, tin, and alumina constraint	$g_{ZrO_2} + g_{SnO_2} + g_{Al_2O_3} \leq 0.17$
Alkali minus sum of zirconia, tin, and lime constraint	$g_{Na_2O} + 0.66 g_{K_2O} + 2.07 g_{Li_2O} - g_{ZrO_2} - g_{SnO_2} - g_{CaO} \leq 0.15$
PCT response	ln[PCT *NL*, g/L] ≤ 1.386
VHT response	ln[VHT *D*, μm] ≤ 6.116
Viscosity at 1150°C	$1.386 \leq \ln[\eta_{1150}, \text{Pa·s}] \leq 1.792$
K-3 neck corrosion at 1208°C	$\ln[k_{1208}, \text{in}] \leq -3.2189$

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 Gervasio et al. 2017.

Table 3.2. Minimum and maximum limits on specific glass components.

Component	Min	Max
Al_2O_3	0.0553	0.1370
B_2O_3	0.0600	0.1370
CaO	0	0.1060
Cl	0	0.0117
Cr_2O_3	0	0.0100
Fe_2O_3	0	0.0997
K_2O	0	0.0589
Li_2O	0	0.0503
MgO	0	0.0350
Na_2O	0.0248	0.2600
P_2O_5	0	0.0340
SiO_2	0.2983	0.5020
SnO_2	0	0.0501
TiO_2	0	0.0341
V_2O_5	0	0.0401
ZnO	0	0.0540
ZrO_2	0	0.0675

3.1.2 Property Model Prediction Uncertainties

A set of uncertainties surrounding the property models, referred to as prediction uncertainties, must be accounted for while determining glass compositions. Specifically, two different confidence level percent (CL%) methods are used. For the product consistency test (PCT), vapor hydration test (VHT), and K-3 neck corrosion models, which only have upper limits, the model uncertainty half-width for a CL% upper simultaneous confidence interval (SCI) is used (Vienna and Kim 2012). Meanwhile, for the viscosity model, which has both upper and lower limits, the model uncertainty half-width for a CL% two-sided confidence interval (CI) is used.

For models requiring only the upper CI, Eq. (3.1) is used to determine the prediction uncertainty:

$$U_{SCI}^{pred} = \sqrt{ps^2 F_{1-\alpha(\mathrm{p,\ n\text{-}p})} \mathbf{x}^T \left(\mathbf{X}^T \mathbf{X}\right)^{-1} \mathbf{x}} \tag{3.1}$$

For models requiring a two-sided CI, Eq. (3.2) is used for model prediction uncertainty:

$$U_{CI}^{pred} = t_{1-\alpha(n-p)} \sqrt{s^2 \mathbf{x}^T \left(\mathbf{X}^T \mathbf{X}\right)^{-1} \mathbf{x}} \tag{3.2}$$

where:
- n = number of data points used to fit the model
- s = root mean squared error of the model
- F = 1-α quantile of the F-distribution
- t = 1-α quantile of the t-distribution
- α = the confidence level, 90% for all ILAW models
- p = number of model terms
- **x** = glass composition vector represented in model terms
- **X** = matrix of glass compositions used in fitting the model

The preceding equations summarize the prediction uncertainty equations found in Vienna and Kim 2012, and were pulled from Gervasio et al. 2017. The matrices containing the glass compositions used in fitting the model (**X**) can be found in Appendix E.

3.1.3 Process and Composition Uncertainties

An additional set of uncertainties arises from sampling and process volume transfers. The algorithm considers five sources of uncertainties from the following: composition from sampling of the CRV, volume of LAW transferred from the CRV to the MFPV, composition of the GFCs, GFC mass transfer to the MFPV, and uncertainty surrounding the retention factor. These are combined in Eq. (3.3) (taken from Gervasio et al. 2017) to generate *i* instances of potential glass compositions, each represented by g_i.

$$g_i = \frac{\left[c_i^{LAW} V^{LAW} f_i + \sum_{k=1}^{n^{GFCs}} g_{ik}^{oxide\,in GFC} M_k^{GFC\,in\,MFPV} \right] v_i}{\sum_{i=1}^{n\,oxides} \left[c_i^{LAW} V^{LAW} f_i + \sum_{k=1}^{n^{GFCs}} g_{ik}^{oxide\,in GFC} M_k^{GFC\,in\,MFPV} \right] v_i} \tag{3.3}$$

where:
- g_i = mass fraction of ith oxide in glass (g/g)
- c_i^{LAW} = concentration of the ith component measured in samples from the CRV prior to 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)
- $g_{ik}^{oxide\,in GFC}$ = mass fraction of the ith oxide in the kth GFC (g/g)
- $M_k^{GFC\,in\,MFPV}$ = mass of the kth GFC in the MFPV batch (kg)
- n^{GFCs} = number of GFCs added to the MFPV batch
- v_i = fraction of ith 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. (3.4).

$$s_i^{cLAW} = \frac{\sqrt{\left(c_i^{LAW} RSD_i^{Analysis} \right)^2 + \left(c_i^{LAW} RSD_i^{mix/samp} \right)^2}}{\sqrt{n^{samps}}} \tag{3.4}$$

The values for $RSD_i^{Analysis}$ are listed in Appendix B, Table B.2, while the values for $RSD_i^{mix/samp}$ are all 1.47% (Gervasio et al. 2017). The number of samples, n^{samps}, is taken 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 as program evaluation and review beta-(PERT) distributed 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 log of the melter decontamination (or retention) factor $\ln\left[\frac{1}{1-v_i}\right]$ 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 numbers 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 v_i before it can be substituted into the equation for g_i.

3.2 Enhanced LAW Glass Correlation – Phase 3 Equations

Another set of parameters used by the Preliminary Enhanced LAW Glass Formulation Algorithm is the Enhanced LAW Glass Correlation – Phase 3 fitted equations which are described in Muller et al. 2017. These equations represent data from laboratory testing which has been fit to relate the compositions of glasses which have met the various property constraints described in 3.1.1. The equations compare Sulfur and Alkali concentrations in the waste to model-relevant oxides in order to determine their final concentrations in the glass. Alkali concentration in waste is calculated via the following equation:

$$\mathrm{ALK}=\mathrm{Na2O\ (wt\%)}+0.66\mathrm{K2O\ (wt\%)} \tag{3.5}$$

The equations describing the calculations for each oxide can be found in Appendix A.

3.3 Glass Formulation Optimality Criteria

The Preliminary Enhanced LAW Glass Formulation Algorithm allows for the user to choose between two different optimality criteria. These can be seen in the following equation:

$$\text{Target Value} = Dw - W(1-w) \tag{3.6}$$

In the equation, *D* represents the root difference of squares difference between oxide concentrations in glass for selected components and their corresponding ideal distances calculated based on the Enhanced LAW Glass Correlation – Phase 3 Equations (Muller et al. 2017). The variable *W* represents waste loading, or the total percentage of waste in the final glass composition. The variable *w* is a weighting factor between *D* and *W*. A *w* value of 0 represents full optimization based around waste loading with no effect from the line rules. Validation and verification testing has allowed for the user to use values of *w* between 0 and 0.25, or up to 25% effect from line rules. We have been unable to validate results about w=0.25.

4.0 Technical Layout of the Script

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

4.1 Startup and Program Inputs

The beginning of the algorithm contains startup commands, various user-defined inputs, constants, and technical information. Much of the information, such as the data contained in the appendices of this report, is read from a control spreadsheet (EWG69801_SCP006_Inputs_v1.xlsx), which contains all the data the script needs to optimize a glass composition.

There is a graphical user interface (GUI) type tab in the spreadsheet that allows the user to specify parameters such as the optimality criteria weight, change the optimization seed value, turn uncertainties and property limits on or off, and change selected variables such as the MFPV heel volume or target NO_x molar ratio.

The script then reads waste compositions from the "WasteClusters" tab in the Excel control spreadsheet, as well as the array to convert element concentration into oxide concentration for each analyte. The selected waste cluster is converted from mg/L of waste to grams of oxide per 100 grams of waste, or oxide weight percent in waste using the f_i value found in Appendix F, Table F.3.

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

4.2 GFC Compositions, Weights, and Volumes

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

Additionally, the GFC compositions are read from the control spreadsheet and assigned to individual variables within the script.

4.3 Monte Carlo Parameters

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.

4.4 Line Rule Calculations and Optimization Setup

The initial line rules based on sulfur and alkali in waste are computed next, using the equations found in Appendix A. These are used in the first optimization run, provided $w \neq 0$.

The script pre-allocates arrays for each of the composition uncertainty values and specifies the options for optimization based on user input from the control spreadsheet.

5.0 NQAP Validation and Verification

The Preliminary Enhanced LAW Glass Formulation Algorithm was developed following Nuclear Quality Assurance Program (NQAP) procedures and has undergone the validation and verification (V&V) process defined under NQAP-IP-0303 to ensure it meets the required qualifications. A software control package (SCP) was completed to document the review process for the V&V.

A qualified independent technical reviewer completed a full review of the code to ensure its accuracy. Additionally, a calculation check was performed that compared the results from the algorithm to the results from another independently developed algorithm that performs the same set of calculations. For this task, we used the ILAW Calculation Spreadsheet, a spreadsheet associated with and used to perform the calculations found in Kim and Vienna, 2012, updated with the coefficients found in Vienna et al. 2016. This spreadsheet can be found in the NQAP software control package EWG69801-SCP006 Rev0.

Due to the nature of optimization methods, combined with the use of a Monte Carlo scheme to calculate composition uncertainties, it is impossible to achieve exact results when comparing two different algorithms. We made the determination that waste loading results and the value for D [see Eq. (3.1)] from the two algorithms must compare to within 1 relative percent difference. The comparisons were made with weighting factors of $w = 0$ and $w = 0.25$. The results are summarized in Table 5.1, which is taken directly from the software control package 69801EWG-SCP-006-STRFa.Rev0.

Table 5.1. Results from Software Control Package (SCP) Testing Comparison

Test Batch Number	Matlab D	Matlab WL	Excel D	Excel WL	RPD D	RPD WL	RESULT
w=0							
1	-0.2905816	0.2905816	-0.28904	0.289038	-0.53%	-0.53%	PASS
2	-0.295527188	0.295527188	-0.29721	0.297211	0.57%	0.57%	PASS
3	-0.293125192	0.293125192	-0.29521	0.295206	0.70%	0.70%	PASS
4	-0.285064476	0.285064476	-0.2s8563	0.285631	0.20%	0.20%	PASS
5	-0.285218476	0.285218476	-0.28688	0.286883	0.58%	0.58%	PASS
6	-0.288152276	0.288152276	-0.29053	0.290533	0.82%	0.82%	PASS
7	-0.277523622	0.277523622	-0.2788	0.278798	0.46%	0.46%	PASS
8	-0.211056261	0.211056261	-0.21186	0.211861	0.38%	0.38%	PASS
9	-0.190685014	0.190685014	-0.19211	0.192112	0.74%	0.74%	PASS
10	-0.242362493	0.242362493	-0.24293	0.242931	0.23%	0.23%	PASS
w=0.25							
1	-0.200438896	0.279968463	-0.20145	0.281087	0.50%	0.40%	PASS
2	-0.206426401	0.286187301	-0.20725	0.287733	0.40%	0.54%	PASS
3	-0.20553775	0.286781513	-0.20595	0.287853	0.20%	0.37%	PASS
4	-0.202133782	0.28332939	-0.20261	0.284193	0.23%	0.30%	PASS
5	-0.199332663	0.279159958	-0.20038	0.280839	0.52%	0.60%	PASS
6	-0.202116742	0.280352985	-0.20249	0.282187	0.19%	0.65%	PASS
7	-0.194936455	0.275121649	-0.1954	0.276074	0.24%	0.34%	PASS
8	-0.150417332	0.21548984	-0.15057	0.215703	0.10%	0.10%	PASS

9	-0.129034972	0.189026025	-0.12941	0.190449	0.29%	0.75%	PASS
10	-0.167463846	0.241972633	-0.16826	0.242989	0.47%	0.42%	PASS

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

6.0 Results Summary and Future Work

The Preliminary Enhanced LAW Glass Formulation Algorithm functions as intended, allowing the user to maximize waste loading while being able to implement line rules intended to bring glass compositions closer to tested results. A set of 10 different waste compositions were used to test the algorithm where it developed a glass composition for each, and the waste loading was maximized while meeting all optimization criteria and constraints. The results matched testing from the ILAW Calculation Spreadsheet, and the line rules were authorized for values of *w* up to 0.25.

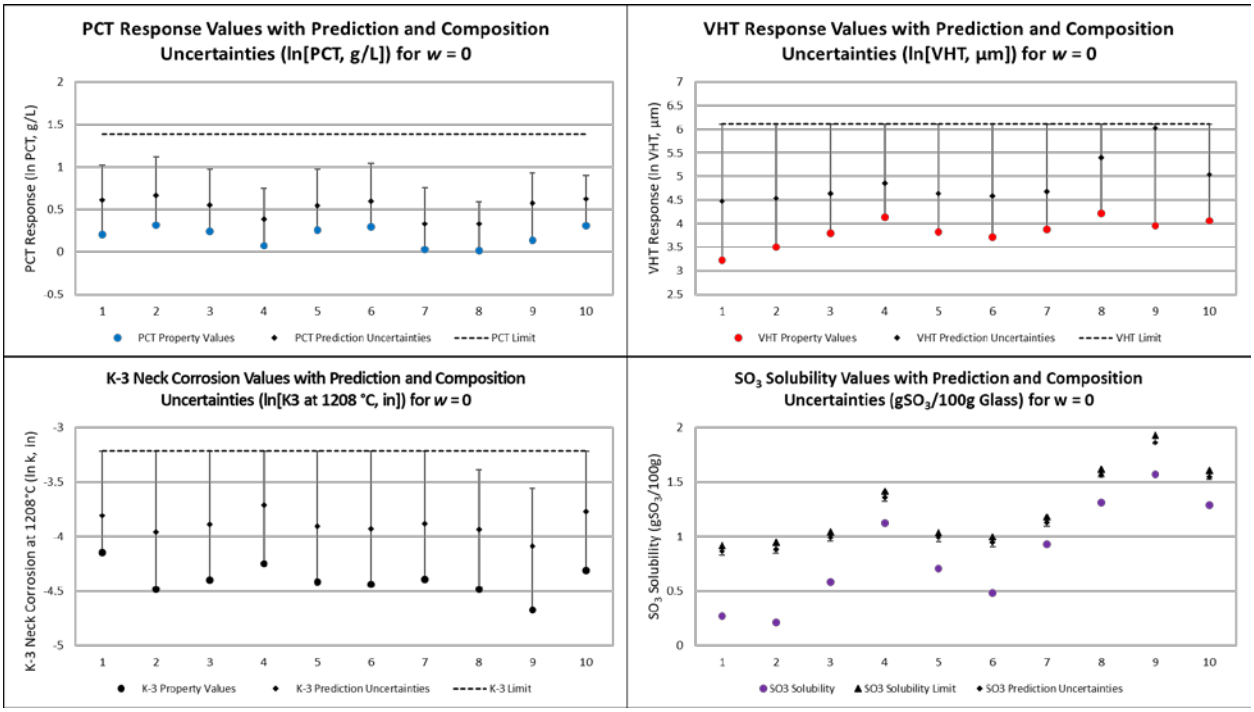

Figure 6.1. Property Constraints and Uncertainties for the 10 Tested Batches at *w* = 0.

Figure 6.1 and Figure 6.2 provide visual representations of how the optimization scheme can use the maximum amount of leeway to change the glass such that the property models are right at the limit, while accounting for prediction and composition uncertainties. These plots are taken from the calculation control package EWG-CCP-121. This ensures that maximum waste loading is achieved. In Figure 6.1 and Figure 6.2, error bars are displayed, representing the prediction and composition uncertainties surrounding each property. The property values are represented by the data points, the prediction uncertainties by the closer error regions, and the composition uncertainties by the further error regions.

Planned updates to this software include updating all property models and adding a model for electrical conductivity, as the models are developed. Additionally, the input file will be reworked such that only waste compositions will be read out of the Excel file. The other variables and information contained in the Excel inputs file will be moved to a text file for faster access during code execution. In addition, several hard-coded variables in the code will be moved to the text file so that they can be changed at will without revising the SCP.

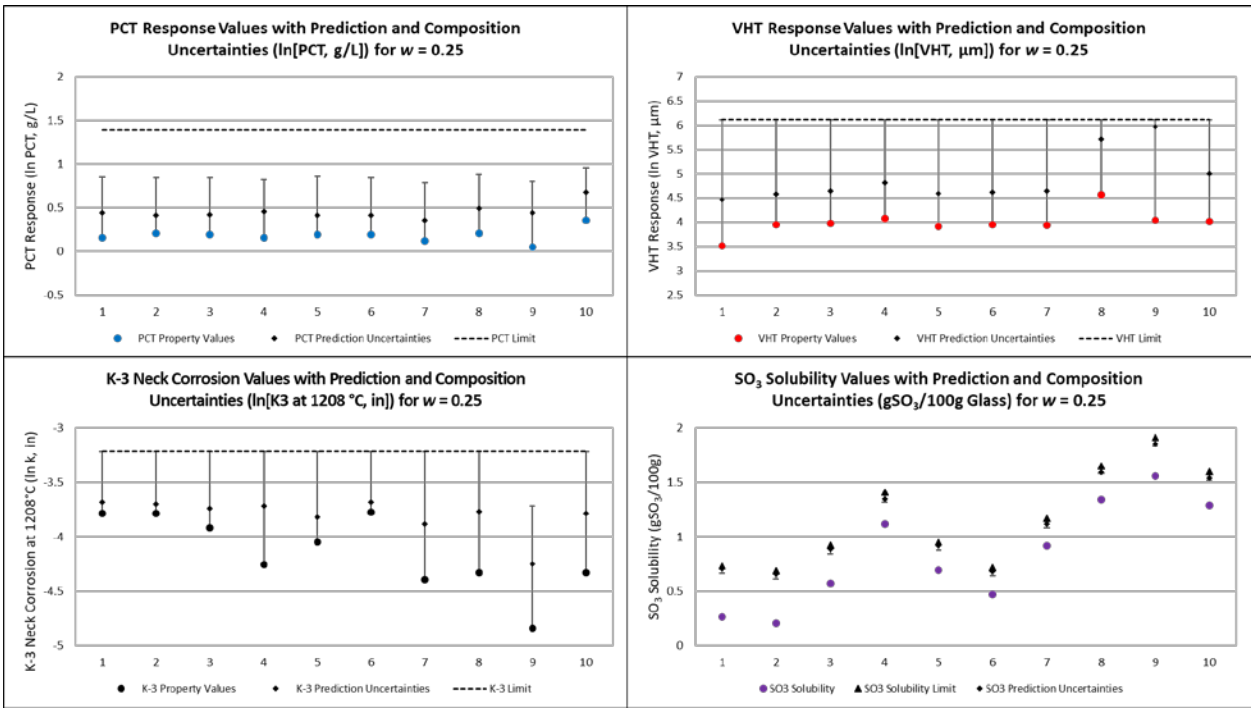

Figure 6.2. Property Constraints and Uncertainties for the 10 Tested Batches at $w = 0.25$.

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Appendix A – ORLEC Phase 3 Line Rules

This appendix contains the ORLEC Phase 3 Line Rules used to compute the distance from the "ideal" glass. Equations come from Muller et al. 2017.[1]

$$\begin{cases} \text{For Alk} < 21.33\% \rightarrow Al_2O_3 = 7.6\% \\ \text{For } 21.33\% < \text{Alk} < \dfrac{20.1702363}{0.83311}\% \rightarrow Al_2O_3 = [(0.83311 * \text{Alk}) - 10.1702363]\% \\ \text{For Alk} > \dfrac{20.1702363}{0.83311}\% \rightarrow Al_2O_3 = 10\% \end{cases}$$

$$B_2O_3 = 11\%$$

$$\begin{cases} For\ Alk < 24.13\% \rightarrow CaO = [(-0.03158 * Alk^2) + (0.48261 * Alk) + 8.69229]\% \\ For\ Alk \geq 24.13\% \rightarrow CaO = 1.95\% \end{cases}$$

$$\begin{cases} \text{For } SO_3 \leq \dfrac{11.39264}{11.96568}\% \rightarrow CaO = 1.95\% \\ \text{For } SO_3 > \dfrac{11.39264}{11.96568}\% \rightarrow CaO = [(11.96568 * SO_3) - 9.44264]\% \end{cases}$$

$$\begin{cases} \text{For } SO3 < \dfrac{0.54898}{0.47627}\% \rightarrow Cr_2O_3 = [(-0.47627 * SO_3) + 0.62898]\% \\ \text{For } SO3 \geq \dfrac{0.54898}{0.47627}\% \rightarrow Cr_2O_3 = 0.08\% \end{cases}$$

$$\begin{cases} \text{For } SO_3 \leq \dfrac{0.12}{1.3}\% \rightarrow Fe_2O_3 = 1\% \\ \text{For } \dfrac{0.12}{1.3}\% < SO_3 < \dfrac{0.92}{1.3}\% \rightarrow Fe_2O_3 = [(-1.3 * SO_3) + 1.12]\,\% \\ \text{For } SO_3 \geq \dfrac{0.92}{1.3}\% \rightarrow Fe_2O_3 = 0.2\% \end{cases}$$

$$\begin{cases} For\ Alk < 22.33 \rightarrow Li_2O = (-0.02529 * Alk^2) + (0.56462 * Alk) + 0.002360281 \\ For\ Alk \geq 22.33 \rightarrow Li_2O = 0 \end{cases}$$

$$\begin{cases} \text{For } SO_3 \leq \dfrac{7.95682}{7.17157}\% \rightarrow Li_2O = 0\% \\ \text{For } SO_3 > \dfrac{7.95682}{7.17157}\% \rightarrow Li_2O = [(7.17157 * SO_3) - 7.95682]\% \end{cases}$$

$$MgO = 1\%$$

$$\begin{cases} \text{For Alk} \leq 23.33\% \rightarrow SnO_2 = 0\% \\ \text{For Alk} > 23.33\% \rightarrow SnO_2 = [\text{Alk} - 23.33]\% \end{cases}$$

[1] Muller IS, KS Matlack, and IL Pegg. 2017. *Enhanced LAW Glass Correlation – Phase 3 Report Rev. 1*. VSL-17R4230-1, Vitreous State Laboratory, The Catholic University of America, Washington D.C.

$$\begin{cases} \text{For } SO_3 \le \dfrac{0.13167}{1.325}\% \rightarrow TiO_2 = 1\% \\ \text{For } \dfrac{0.13167}{1.325}\% < SO_3 < \dfrac{1.13167}{1.325}\% \rightarrow TiO_2 = [(-1.325 * SO_3) + 1.13167]\% \\ \text{For } SO_3 > \dfrac{1.13167}{1.325}\% \rightarrow TiO_2 = 0\% \end{cases}$$

$$\begin{cases} \text{For } SO_3 \le 0.4\% \rightarrow V_2O_5 = 0\% \\ \text{For } 0.4\% < SO_4 < \dfrac{7}{5}\% \rightarrow V_2O_5 = [(-2.5 * (SO_3)^2) + (7 * SO_3) - 2.4]\% \\ \text{For } SO_3 \ge \dfrac{7}{5}\% \rightarrow V_2O_5 = 2.5\% \end{cases}$$

$$ZnO = 3\%$$

$$\begin{cases} \text{For Alk} < 21.8\% \rightarrow ZrO_2 = 3.5\% \\ \text{For Alk} \ge 21.8\% \rightarrow ZrO_2 = [\text{Alk} - 18.3]\% \end{cases}$$

$$SiO_2 = [100 - (Al_2O_3 + B_2O_3 + CaO + Cr_2O_3 + Fe_2O_3 + Li_2O + MgO + SnO_2 + TiO_2 + V_2O_5 + ZnO + ZrO_2)]$$

Appendix B – Tables

This appendix contains tables for 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 B.1. Retention Factors Used to Calculate Remaining Ratios of Components after Removal of Evaporate Bottoms

Glass Oxide	Retention Factor	Glass Oxide	Retention Factor	Glass Oxide	Retention Factor
Ac2O3	99.721%	HgO	0.000%	RuO2	97.803%
Ag2O	97.803%	I	50.961%	SO3	84.032%
Al2O3	99.888%	K2O	96.423%	Sb2O3	77.121%
Am2O3	97.803%	La2O3	99.721%	SeO2	77.121%
As2O5	77.121%	Li2O	99.601%	SiO2	99.926%
B2O3	98.968%	MgO	99.984%	Sm2O3	99.721%
BaO	99.721%	MnO	99.721%	SnO2	99.721%
BeO	99.721%	MoO3	97.803%	SrO	99.721%
Bi2O3	97.803%	Na2O	99.136%	Ta2O5	99.721%
CaO	99.892%	Nb2O5	99.721%	Tc2O7	43.049%
CdO	99.721%	Nd2O3	99.721%	TeO2	77.121%
Ce2O3	99.721%	NiO	99.187%	ThO2	99.721%
Cl	54.407%	NpO2	99.721%	TiO2	99.752%
Cm2O3	99.721%	P2O5	99.169%	Tl2O	77.121%
CoO	99.721%	Pa2O5	99.721%	UO3	99.721%
Cr2O3	95.261%	PbO	98.796%	V2O5	97.803%
Cs2O	87.902%	PdO	99.721%	WO3	99.721%
CuO	99.721%	Pr2O3	99.721%	Y2O3	99.721%
Eu2O3	99.721%	PuO2	99.721%	ZnO	99.773%
F	72.984%	RaO	77.121%	ZrO2	99.982%
Fe2O3	99.848%	Rb2O	97.803%		
Gd2O3	99.721%	Rh2O3	99.721%		

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

	MRQ 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%

[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.

	MRQ mg/L	High %RSD (Analytical)	Low %RSD (Analytical)	Mixing/Sampling RSD
Cl	19	10%	10%	1.47%
Cm	--	--	--	--
Co	19	10%	10%	1.47%
Cr	19	10%	10%	1.47%
Cs	19	10%	10%	1.47%
Cu	19	10%	10%	1.47%
Eu	--	--	--	--
F	19	10%	10%	1.47%
Fe	19	10%	10%	1.47%
Gd	19	10%	10%	1.47%
Hg	19	10%	10%	1.47%
I	--	--	--	--
K	19	10%	10%	1.47%
La	19	10%	10%	1.47%
Li	19	10%	10%	1.47%
Mg	19	10%	10%	1.47%
Mn	19	10%	10%	1.47%
Mo	19	10%	10%	1.47%
Na	19	10%	10%	1.47%
Nb	--	--	--	--
Nd	19	10%	10%	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%
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%

	MRQ mg/L	High %RSD (Analytical)	Low %RSD (Analytical)	Mixing/Sampling RSD
NO2	--	--	--	--
NO3	--	--	--	--
TOC	--	--	--	--
59Ni	7.98E-07	10%	10%	1.47%
60Co	1.13E-05	5%	5%	1.47%
63Ni	5.74E-02	10%	10%	1.47%
79Se	6.97E-05	15%	10%	1.47%
90Sr	1.39E-06	5%	5%	1.47%
90Y	--	0%	0%	1.47%
93mNb	2.39E-04	15%	10%	1.47%
93Zr	2.52E-06	10%	10%	1.47%
99Tc	1.71E-06	10%	10%	1.47%
106Ru	2.01E-03	15%	10%	1.47%
113mCd	4.62E-05	25%	10%	1.47%
125Sb	3.11E-04	25%	5%	1.47%
126Sn	5.68E-06	20%	15%	1.47%
129I	1.77E-04	15%	10%	1.47%
134Cs	4.53E-06	25%	10%	1.47%
137mBa	--	0%	0%	1.47%
137Cs	1.73E-06	15%	5%	1.47%
151Sm	5.26E-01	20%	10%	1.47%
152Eu	1.74E-06	5%	5%	1.47%
154Eu	2.70E-06	5%	5%	1.47%
155Eu	4.76E-05	5%	5%	1.47%
226Ra	9.89E-07	25%	10%	1.47%
227Ac	7.23E-07	50%	10%	1.47%
228Ra	2.73E-03	50%	25%	1.47%
229Th	6.38E-04	50%	50%	1.47%
231Pa	1.42E-04	50%	50%	1.47%
232Th	3.29E-10	25%	10%	1.47%
232U	6.62E-08	25%	5%	1.47%
233U	9.63E-07	10%	5%	1.47%
234U	6.22E-06	5%	5%	1.47%
235U	2.16E-07	10%	5%	1.47%
236U	6.47E-08	10%	5%	1.47%
237Np	7.05E-07	10%	5%	1.47%
238Pu	1.71E-07	5%	5%	1.47%
238U	6.72E-09	10%	10%	1.47%
239Pu	6.20E-08	5%	5%	1.47%
240Pu	2.27E-09	10%	10%	1.47%
241Am	3.43E-06	10%	10%	1.47%
241Pu	1.03E-07	15%	15%	1.47%
242Cm	3.31E-06	10%	10%	1.47%
242Pu	3.95E-11	10%	10%	1.47%
243Am	3.99E-08	15%	15%	1.47%
243Cm	9.81E-07	15%	15%	1.47%
244Cm	2.43E-06	15%	15%	1.47%

Appendix C – Waste Compositions Used for Testing

Table C.1. Waste Compositions in mg/L Analyzed by the Preliminary Enhanced LAW Glass Formulation Algorithm

Vol, L	48661	48661	48661	48661	48661	48661	48661	48661	48661	48661
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	4.77E-01	1.61E+00	1.55E-01	7.82E-02	5.47E-02	8.41E-02	8.56E-02	7.43E-02	4.16E-02	3.73E-02
Al	1.14E+04	1.42E+04	1.15E+04	8.35E+03	8.76E+03	9.94E+03	7.11E+03	5.88E+03	5.58E+03	6.31E+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	1.11E+00	4.82E+00	4.62E-01	3.01E-01	2.38E-01	4.11E-01	3.58E-01	2.88E-01	1.48E-01	1.31E-01
B	1.90E+02	3.08E+02	3.51E+02	5.21E+02	4.21E+02	4.78E+02	3.80E+02	3.65E+02	5.44E+02	6.18E+02
Ba	2.45E-01	5.59E-01	2.52E-01	1.68E-01	6.84E-02	8.00E-02	1.49E-01	1.36E-01	7.20E-02	6.36E-02
Be	9.52E-01	2.46E-01	3.44E-02	1.97E-02	8.00E-03	1.08E-02	1.53E-02	1.37E-02	7.22E-03	6.61E-03
Bi	1.81E+00	4.57E+00	3.43E+00	3.19E+01	3.11E+00	3.98E+00	2.71E+00	2.83E+00	3.26E+00	2.39E+00
Ca	3.57E+01	5.35E+01	7.92E+01	1.96E+02	8.07E+01	7.07E+01	9.34E+01	1.15E+02	1.44E+02	1.17E+02
Cd	1.48E+00	9.73E-01	2.96E+00	1.09E+00	2.09E-01	3.20E-01	3.37E-01	2.86E-01	1.46E-01	2.24E-01
Ce	5.74E-02	7.16E+00	1.89E+00	1.32E+00	1.54E+00	2.58E+00	7.99E-01	4.63E-01	2.73E+00	1.04E+01
Cl	2.52E+03	5.65E+03	3.91E+03	2.91E+03	4.18E+03	4.95E+03	3.67E+03	2.69E+03	2.14E+03	2.40E+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	4.85E-01	8.22E-01	1.61E-01	2.90E-01	1.61E-01	2.03E-01	1.80E-01	1.87E-01	1.81E-01	9.38E-02
Cr	2.95E+02	7.94E+02	1.05E+03	6.37E+02	2.45E+03	2.90E+03	1.35E+03	4.66E+02	2.24E+02	4.44E+02
Cs	1.20E-03	1.29E-03	4.22E-04	2.80E-04	3.64E-04	3.84E-04	3.46E-04	6.07E-04	8.73E-04	4.72E-04
Cu	1.19E+00	8.72E-01	2.56E-01	8.80E-02	5.47E-02	8.95E-02	9.25E-02	7.71E-02	3.64E-02	5.37E-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	1.80E+03	2.86E+03	2.93E+03	5.06E+03	1.68E+03	1.47E+03	2.17E+03	1.31E+04	2.47E+04	9.93E+03
Fe	1.78E+01	3.48E+01	9.31E+01	1.09E+02	8.22E+01	8.17E+01	7.58E+01	6.81E+01	3.98E+01	7.12E+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	5.96E-02	1.34E+00	1.72E+00	3.13E+00	6.15E-01	1.25E+00	7.47E-01	3.42E-01	1.85E-01	6.70E-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	2.50E+04	3.91E+03	6.73E+02	5.45E+02	4.83E+02	4.17E+02	5.77E+02	2.03E+03	3.43E+03	1.43E+03
La	1.53E-01	3.48E-01	4.52E-02	3.24E-02	2.61E-02	6.21E-02	1.01E-02	2.45E-03	1.74E-03	7.18E-03
Li	2.49E-01	3.82E+00	2.87E+01	6.57E+01	6.59E+01	5.49E+01	3.11E+01	1.45E+02	1.91E+02	4.95E+01
Mg	2.52E+00	7.71E+00	2.13E+00	1.34E+00	1.92E+00	2.20E+00	1.28E+00	3.01E-01	1.82E-01	1.29E+00
Mn	9.73E-01	1.03E+01	1.68E+01	4.90E+00	5.08E+00	6.82E+00	4.99E+00	3.47E+00	1.77E+00	4.61E+00
Mo	1.08E+01	1.52E+01	1.14E+00	4.39E-01	3.97E-01	6.61E-01	5.40E-01	4.55E-01	2.63E-01	2.52E-01
Na	1.27E+05	1.27E+05	1.27E+05	1.27E+05	1.27E+05	1.27E+05	1.27E+05	1.27E+05	1.27E+05	1.27E+05
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	1.89E+00	5.72E+00	4.37E-01	2.85E-01	1.80E-01	2.65E-01	3.11E-01	2.71E-01	1.44E-01	1.33E-01
Ni	1.11E+01	9.59E+00	8.35E+00	1.94E+01	7.87E+00	8.73E+00	7.32E+00	4.62E+00	2.38E+00	4.60E+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	8.36E+02	9.16E+02	2.42E+03	7.13E+03	1.84E+03	1.47E+03	2.84E+03	2.44E+03	2.16E+03	3.75E+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	1.59E+01	1.71E+01	5.75E+00	9.32E+00	9.78E+00	1.18E+01	7.74E+00	4.57E+00	2.75E+00	2.70E+00
Pd	1.36E+01	2.39E-01	3.30E-01	3.23E-02	1.95E-01	4.75E-01	6.16E-02	8.03E-04	1.30E-04	4.72E-02
Pr	1.57E-02	7.21E-02	1.84E-03	1.71E-04	8.12E-02	1.98E-01	2.53E-02	1.41E-05	1.01E-06	1.40E-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	2.85E+00	8.19E-02	2.45E-03	2.55E-04	4.49E-03	1.10E-02	1.43E-03	7.44E-06	1.10E-06	3.17E-04
Rh	5.58E+00	2.25E-01	9.01E-02	8.81E-03	2.32E-02	5.64E-02	7.46E-03	2.12E-04	3.49E-05	1.25E-02
Ru	2.23E+01	5.50E-01	1.59E-02	1.31E-02	1.86E-01	4.53E-01	5.80E-02	3.89E-04	3.59E-04	1.98E-03
S	1.18E+03	8.80E+02	2.36E+03	4.90E+03	2.87E+03	1.95E+03	3.82E+03	7.57E+03	1.08E+04	6.39E+03
Sb	5.69E-02	5.31E+00	1.15E+00	4.25E-01	1.86E+00	2.44E+00	1.30E+00	5.79E-01	3.12E-01	2.52E-01
Se	1.99E+00	1.11E+01	9.41E+00	5.58E+00	8.14E+00	9.50E+00	8.77E+00	6.22E+00	3.51E+00	2.75E+00
Si	2.51E+02	4.15E+02	9.02E+02	1.48E+03	5.23E+02	6.24E+02	4.01E+02	4.58E+02	5.81E+02	4.18E+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	8.23E+01	8.81E+01	4.86E+01	3.28E-05	4.05E+01	8.43E+01	2.82E+00	1.42E+01	1.66E+01	1.78E-05
Sr	5.37E-02	1.64E+00	1.02E+01	1.54E+01	3.57E+00	2.80E+00	3.48E+00	2.77E+00	2.21E+00	3.28E+00
Ta	7.02E-02	1.21E-01	8.05E-02	7.83E-03	9.05E-02	2.21E-01	2.84E-02	2.00E-04	3.16E-05	1.13E-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	1.74E-01	2.94E-01	7.13E-03	6.05E-04	1.75E-01	4.51E-01	8.01E-02	4.67E-04	1.12E-05	2.34E-04
Th	2.43E-01	4.77E+00	8.10E-01	1.98E+00	2.46E-01	4.92E-01	1.34E-01	9.52E-02	9.98E-02	8.82E-02
Ti	1.65E+01	2.67E+01	2.20E+01	1.05E+01	2.56E+01	4.03E+01	1.04E+01	2.03E+01	8.85E+00	7.23E+00

Vol, L	48661	48661	48661	48661	48661	48661	48661	48661	48661	48661
Batch ID	1	2	3	4	5	6	7	8	9	10
Tl	3.01E-02	4.41E+00	4.43E-01	1.54E-01	1.89E-01	4.76E-01	9.66E-02	1.08E-02	3.34E-03	1.65E-02
U	1.52E+02	3.99E+01	4.58E+01	7.74E+01	2.05E+01	2.05E+01	1.87E+01	2.69E+01	3.49E+01	2.02E+01
V	2.70E+02	4.50E+02	4.23E+02	4.32E+02	4.18E+02	4.34E+02	4.05E+02	5.66E+02	7.50E+02	4.83E+02
W	0.00E+00	2.02E+00	5.68E-02	5.71E-03	2.67E-01	6.51E-01	8.32E-02	1.73E-04	2.39E-05	6.42E-03
Y	1.14E+00	5.07E-01	4.57E-02	4.53E-03	3.00E-02	7.28E-02	9.87E-03	5.45E-04	2.44E-04	6.42E-03
Zn	7.35E+00	2.46E+01	2.53E+01	2.87E+01	3.65E+01	4.55E+01	2.81E+01	2.36E+01	2.02E+01	1.83E+01
Zr	1.25E+01	5.09E+01	1.14E+01	9.40E+00	1.14E+01	1.16E+01	1.09E+01	1.65E+01	2.26E+01	8.14E+00
NO2	3.20E+04	1.58E+04	7.22E+03	2.16E+04	2.89E+04	2.43E+04	3.04E+04	2.76E+04	2.37E+04	2.57E+04
NO3	8.52E+04	7.07E+04	1.13E+05	1.31E+05	1.08E+05	8.49E+04	1.44E+05	1.21E+05	8.22E+04	1.50E+05
TOC	1.34E+03	1.00E+03	4.39E+02	5.45E+02	4.96E+02	4.44E+02	7.52E+02	9.17E+02	9.35E+02	7.35E+02

Appendix D – Model Terms

This appendix contains the model terms and statistics used to calculate glass properties need for formulation (see Vienna et al. 2016[1]).

Table D.7.1. PCT Model Terms and Statistics

PCT Model Terms and Statistics	
Model Term	Coefficient
Al_2O_3	-4.7932
B_2O_3	-31.2612
CaO	3.8636
K_2O	-13.5298
Li_2O	-16.6826
MgO	21.4263
Na_2O	-25.2993
P_2O_5	-5.1242
SiO_2	0.3093
SnO_2	-4.4031
TiO_2	-1.7604
ZrO_2	3.8966
Others	6.2375
$B_2O_3 \times B_2O_3$	157.3873
$K_2O \times K_2O$	201.4790
$Al_2O_3 \times Li_2O$	-255.4098
$CaO \times Li_2O$	-128.0130
$Li_2O \times Li_2O$	474.3082
$B_2O_3 \times Na_2O$	81.1682
$K_2O \times Na_2O$	120.3814
$Li_2O \times Na_2O$	391.5456
$Na_2O \times Na_2O$	97.6643
Statistic	Value
# data points	577
Mean of response, ln(g/L)	-0.0313
RMSE	0.3086
R^2	0.8411
R^2_{Adj}	0.8351
R^2_{Pred}	0.8217
R^2_{Val129}	0.5494
R^2_{Val}	0.8230

[1] Vienna JD, GF Piepel, DS Kim, JV Crum, CE Lonergan, BA Stanfill, BJ Riley, SK Cooley, and T Jin. 2016. 2016 Update of Hanford Glass Property Models and Constraints for Use in Estimating the Glass Mass to Be Produced at Hanford by Implementing Current Enhanced Glass Formulation Efforts. PNNL-25835, Pacific Northwest National Laboratory, Richland, WA.

Table D.7.2. VHT Model Terms and Statistics

VHT Model Terms and Statistics	
Model Term	Coefficient
Al_2O_3	-3.1247
B_2O_3	9.0537
CaO	-165.0264
Fe_2O_3	-9.3359
K_2O	-68.6719
Li_2O	308.9919
Na_2O	75.8436
SiO_2	-22.5420
SnO_2	-28.5312
TiO_2	-27.0704
ZrO_2	-48.6944
Others	2.5197
CaO×CaO	452.8308
$Li_2O \times Li_2O$	-3040.2579
$K_2O \times Na_2O$	433.9384
$Li_2O \times Na_2O$	-1273.4629
$CaO \times SiO_2$	267.5427
$K_2O \times K_2O$	724.3290
$Li_2O \times SiO_2$	361.8056
Statistic	Value
# data points	330
Mean of response, ln(D, μm)	4.685
RMSE	0.8329
R^2	0.7400
R^2_{Adj}	0.7249
R^2_{Pred}	0.7041
R^2_{Val}	0.6930

Table D.7.3. K-3 Corrosion Model Terms and Statistics

K-3 Corrosion Model Terms and Statistics	
Model Term	Coefficient
Al_2O_3	-23.696
B_2O_3	-0.965
CaO	6.590
Cr_2O_3	-85.437
Fe_2O_3	-4.315
K_2O	7.997
Li_2O	44.748
MgO	-37.185
Na_2O	20.337
P_2O_5	117.297
SiO_2	-10.103
SnO_2	-38.779
TiO_2	90.238
V_2O_5	-114.733
ZnO	-12.560
ZrO_2	-11.150
Others	-20.952
$Li_2O \times P_2O_5$	-3092.687
$(MgO)^2$	716.072
$Na_2O \times P_2O_5$	-579.772
$Na_2O \times V_2O_5$	335.374
$SiO_2 \times TiO_2$	-241.722
$SnO_2 \times$Others	2880.688
$V_2O_5 \times$ZnO	1028.765
Statistic	Value
# data points	261
RMSE	0.255
R^2	0.905
R^2_{Adj}	0.896
R^2_{Pred}	0.881

Table D.7.4. Sulfur Model Terms and Statistics

Sulfur Model Terms and Statistics	
Model Term	Coefficient
Al_2O_3	-2.0919
B_2O_3	3.044075
CaO	4.442289
Cl	-22.6535
Cr_2O_3	-13.1414
K_2O	0.615785
Li_2O	2.473926
Na_2O	2.897209
P_2O_5	4.606083
SiO_2	0.240729
SnO_2	-1.77533
V_2O_5	7.534548
ZrO_2	-1.87192
Others	-0.28027
$(Li_2O)^2$	260.203
Statistic	Value
# data points	253
Mean value, SO_3 wt%	1.004
RMSE	0.115
R^2	0.891
R^2_{Adj}	0.885
R^2_{Pred}	0.874
R^2_{Val}	0.869

Table D.7.5. Viscosity Model Terms and Statistics

Viscosity Model Terms and Statistics	
Model Term	Coefficient
Al_2O_3	11.67007
B_2O_3	-7.44665
CaO	-7.60545
Fe_2O_3	-0.11082
K_2O	-4.65558
Li_2O	-32.67344
MgO	-4.26291
Na_2O	-9.30809
P_2O_5	7.94147
SiO_2	8.88092
SnO_2	4.73082
TiO_2	-4.93294
V_2O_5	-2.64858
ZnO	-4.51330
ZrO_2	6.91854
Others	2.74032
Statistic	Value
# data points	429
Mean value, $\ln(\eta_{1150}$, Pa.s)	1.4584
RMSE	0.1476
R^2	0.9303
R^2_{Adj}	0.9277
R^2_{Pred}	0.9241

Appendix E – Glass Variance Covariance Matrices

Table E.1. Variance Covariance Matrix for PCT Model

Term	Al2O3	B2O3	CaO	K2O	Li2O	MgO	Na2O	P2O5	SiO2	SnO2	TiO2	ZrO2	Others	B2O3×B2O3	K2O×K2O	Al2O3×Li2O	CaO×Li2O	Li2O×Li2O	B2O3×Na2O	K2O×Na2O	Li2O×Na2O	Na2O×Na2O
Al2O3	1.013	-1.878	0.029	-0.770	-1.828	0.145	-1.113	0.230	0.225	0.230	0.509	0.126	0.164	8.083	-2.792	-20.321	3.973	18.004	1.894	6.609	15.842	2.058
B2O3	-1.878	43.732	-1.333	4.584	-16.823	-1.918	-2.995	-0.700	-2.186	-0.892	-3.374	-2.930	-1.659	-205.279	-8.583	0.909	-11.416	144.499	-29.551	-32.885	57.039	9.398
CaO	0.029	-1.333	0.643	-0.696	-2.126	0.164	-1.236	0.212	0.195	-0.012	0.584	0.315	0.166	5.506	2.965	5.268	-11.690	17.528	2.093	4.922	12.420	3.266
K2O	-0.770	4.584	-0.696	16.850	2.239	-0.335	2.034	0.091	-0.361	-0.326	-3.111	-0.308	-0.801	-23.286	-188.420	-5.355	5.967	-1.464	-3.366	-41.545	-21.732	-5.720
Li2O	-1.828	-16.823	-2.126	2.239	119.479	-3.045	32.741	-1.476	-3.577	-0.853	-2.707	-3.586	-2.344	71.149	-73.657	-98.258	-56.501	-868.660	-4.015	-2.388	-496.237	-84.031
MgO	0.145	-1.918	0.164	-0.335	-3.045	1.551	-1.239	-0.006	0.252	0.042	-0.001	0.332	0.133	7.525	-2.234	1.689	3.631	15.484	4.071	3.680	15.092	2.637
Na2O	-1.113	-2.995	-1.236	2.034	32.741	-1.239	16.396	-1.496	-1.714	-1.015	-2.073	-1.643	-1.319	22.809	-10.069	-21.228	-9.123	-170.604	-21.903	-19.918	-172.718	-41.097
P2O5	0.230	-0.700	0.212	0.091	-1.476	-0.006	-1.496	4.717	0.152	-0.021	0.454	0.302	0.074	0.419	-9.639	-1.736	1.216	9.018	4.736	4.822	10.324	3.354
SiO2	0.225	-2.186	0.195	-0.361	-3.577	0.252	-1.714	0.152	0.388	0.150	0.248	0.328	0.170	8.692	2.024	2.860	1.426	20.205	4.507	2.856	18.164	3.900
SnO2	0.230	-0.892	-0.012	-0.326	-0.853	0.042	-1.015	-0.021	0.150	1.717	0.700	0.049	0.184	2.937	-13.892	-5.292	10.158	-7.227	4.190	4.932	4.261	1.544
TiO2	0.509	-3.374	0.584	-3.111	-2.707	-0.001	-2.073	0.454	0.248	0.700	4.661	0.853	0.112	19.031	23.306	4.040	1.856	1.648	1.840	12.511	21.653	6.343
ZrO2	0.126	-2.930	0.315	-0.308	-3.586	0.332	-1.643	0.302	0.328	0.049	0.853	1.536	0.286	12.508	-4.379	6.631	-0.370	18.409	4.996	3.730	17.297	3.407
Others	0.164	-1.659	0.166	-0.801	-2.344	0.133	-1.319	0.074	0.170	0.184	0.112	0.286	0.587	8.338	4.200	2.760	3.027	6.130	1.760	5.020	13.772	3.676
B2O3×B2O3	8.083	-205.279	5.506	-23.286	71.149	7.525	22.809	0.419	8.692	2.937	19.031	12.508	8.338	1059.776	133.488	36.004	93.718	-713.695	31.511	137.960	-240.895	-40.476
K2O×K2O	-2.792	-8.583	2.965	-188.420	-73.657	-2.234	-10.069	-9.639	2.024	-13.892	23.306	-4.379	4.200	133.488	4116.753	374.910	-42.274	307.374	-69.922	-131.780	337.169	69.399
Al2O3×Li2O	-20.321	0.909	5.268	-5.355	-98.258	1.689	-21.228	-1.736	2.860	-5.292	4.040	6.631	2.760	36.004	374.910	1185.957	-36.162	78.082	7.946	-70.077	128.766	82.532
CaO×Li2O	3.973	-11.416	-11.690	5.967	-56.501	3.631	-9.123	1.216	1.426	10.158	1.856	-0.370	3.027	93.718	-42.274	-36.162	703.693	-77.100	11.620	-24.359	179.508	24.134
Li2O×Li2O	18.004	144.499	17.528	-1.464	-868.660	15.484	-170.604	9.018	20.205	-7.227	1.648	18.409	6.130	-713.695	307.374	78.082	-77.100	9033.259	-5.957	-80.419	3215.376	389.557
B2O3×Na2O	1.894	-29.551	2.093	-3.366	-4.015	4.071	-21.903	4.736	4.507	4.190	1.840	4.996	1.760	31.511	-69.922	7.946	11.620	-5.957	174.187	55.109	48.683	23.286
K2O×Na2O	6.609	-32.885	4.922	-41.545	-2.388	3.680	-19.918	4.822	2.856	4.932	12.511	3.730	5.020	137.960	-131.780	-70.077	-24.359	-80.419	55.109	318.414	130.617	44.618
Li2O×Na2O	15.842	57.039	12.420	-21.732	-496.237	15.092	-172.718	10.324	18.164	4.261	21.653	17.297	13.772	-240.895	337.169	128.766	179.508	3215.376	48.683	130.617	2463.752	455.719
Na2O×Na2O	2.058	9.398	3.266	-5.720	-84.031	2.637	-41.097	3.354	3.900	1.544	6.343	3.407	3.676	-40.476	69.399	82.532	24.134	389.557	23.286	44.618	455.719	114.386

Table E.2. Variance Covariance Matrix for VHT Model

Term	Al2O3	B2O3	CaO	Fe2O3	K2O	Li2O	Na2O	SiO2	SnO2	TiO2	ZrO2	Others	CaO*CaO	Li2O*Li2O	K2O*Na2O	Li2O*Na2O	CaO*SiO2	K2O*K2O	Li2O*SiO2
Al2O3	12.746	0.717	-44.230	5.183	1.344	-113.697	-2.794	-2.544	6.346	9.709	2.318	2.947	52.426	485.601	-17.296	280.223	103.449	90.626	107.165
B2O3	0.717	10.804	-40.807	3.351	-6.163	0.816	0.844	-3.543	5.031	0.519	3.699	0.975	76.321	-102.487	24.771	-63.066	81.805	32.649	23.555
CaO	-44.230	-40.807	617.498	-37.925	-29.592	312.852	-24.581	38.237	-43.182	-28.746	-12.014	-29.643	-795.889	-1514.524	116.451	-626.993	-1368.016	-280.083	-349.151
Fe2O3	5.183	3.351	-37.925	12.907	-2.946	-60.692	0.104	-3.717	7.813	-7.885	5.458	3.207	70.259	157.710	1.496	119.081	83.080	86.574	81.063
K2O	1.344	-6.163	-29.592	-2.946	414.284	-676.601	-3.878	1.107	6.921	-33.011	10.215	0.378	3.334	2956.842	-1435.935	1635.399	95.804	-2562.025	694.912
Li2O	-113.697	0.816	312.852	-60.692	-676.601	5618.445	66.341	20.844	-95.659	-150.804	-131.107	-71.612	-1081.111	-26761.881	3310.805	-12174.931	-673.883	178.923	-6401.233
Na2O	-2.794	0.844	-24.581	0.104	-3.878	66.341	10.316	-4.120	-2.805	3.097	-6.046	-1.016	47.683	-656.006	23.449	-246.026	45.487	71.573	34.983
SiO2	-2.544	-3.543	38.237	-3.717	1.107	20.844	-4.120	4.451	-2.990	-6.681	-1.574	-2.421	-52.270	111.298	-23.053	24.855	-84.717	-5.993	-82.258
SnO2	6.346	5.031	-43.182	7.813	6.921	-95.659	-2.805	-2.990	24.829	10.163	4.776	2.651	88.206	203.569	-31.182	201.058	96.865	-53.258	105.113
TiO2	9.709	0.519	-28.746	-7.885	-33.011	-150.804	3.097	-6.681	10.163	97.242	9.776	2.336	108.370	85.139	159.999	135.046	60.480	123.403	324.192
ZrO2	2.318	3.699	-12.014	5.458	10.215	-131.107	-6.046	-1.574	4.776	9.776	23.459	3.287	70.999	480.686	-25.555	220.229	19.980	-143.365	162.848
Others	2.947	0.975	-29.643	3.207	0.378	-71.612	-1.016	-2.421	2.651	2.336	3.287	9.340	20.976	376.337	20.973	147.949	71.223	-48.571	72.778
CaO×CaO	52.426	76.321	-795.889	70.259	3.334	-1081.111	47.683	-52.270	88.206	108.370	70.999	20.976	4832.705	-6889.248	-160.396	131.261	759.346	1345.902	3164.818
Li2O×Li2O	485.601	-102.487	-1514.524	157.710	2956.842	-26761.881	-656.006	111.298	203.569	85.139	480.686	376.337	-6889.248	282652.050	-14440.190	81168.356	6545.537	-7117.321	7483.857
K2O×Na2O	-17.296	24.771	116.451	1.496	-1435.935	3310.805	23.449	-23.053	-31.182	159.999	-25.555	20.973	-160.396	-14440.190	8228.991	-9463.356	-318.559	-1617.293	-2859.521
Li2O×Na2O	280.223	-63.066	-626.993	119.081	1635.399	-12174.931	-246.026	24.855	201.058	135.046	220.229	147.949	131.261	81168.356	-9463.356	40141.239	1899.236	3175.249	6950.847
CaO×SiO2	103.449	81.805	-1368.016	83.080	95.804	-673.883	45.487	-84.717	96.865	60.480	19.980	71.223	759.346	6545.537	-318.559	1899.236	3327.562	229.069	201.205
K2O×K2O	90.626	32.649	-280.083	86.574	-2562.025	178.923	71.573	-5.993	-53.258	123.403	-143.365	-48.571	1345.902	-7117.321	-1617.293	3175.249	229.069	53642.927	-465.127
Li2O×SiO2	107.165	23.555	-349.151	81.063	694.912	-6401.233	34.983	-82.258	105.113	324.192	162.848	72.778	3164.818	7483.857	-2859.521	6950.847	201.205	-465.127	12262.160

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

Term	Al2O3	B2O3	CaO	Cr2O3	Fe2O3	K2O	Li2O	MgO	Na2O	P2O5	SiO2	SnO2	TiO2	V2O5	ZnO	ZrO2	Others	MgO× MgO	Li2O× P2O5	Na2O× P2O5	SiO2× TiO2	Na2O× V2O5	V2O5× ZnO	SnO2× Others
Al2O3	1.221	-0.076	-0.082	-0.432	-0.073	0.075	-1.502	0.440	-0.656	-2.757	0.158	0.098	-4.742	-1.721	-0.812	0.314	-0.210	-19.572	31.342	15.318	11.589	-0.516	58.617	-13.609
B2O3	-0.076	1.634	-0.467	-1.029	0.271	0.002	1.278	0.725	0.138	2.296	-0.417	0.963	-5.864	1.702	-0.572	0.429	-1.142	-30.149	-49.941	-8.486	15.447	-6.467	5.696	-10.627
CaO	-0.082	-0.467	1.236	1.175	0.344	0.196	-1.160	-2.311	-0.047	-2.030	0.053	-0.500	3.213	-4.153	-0.378	0.171	-0.488	72.567	41.805	10.578	-5.992	12.383	31.957	61.119
Cr2O3	-0.432	-1.029	1.175	180.761	-0.767	-0.305	-5.593	9.739	-1.802	69.659	0.300	-45.505	32.021	-2.782	0.863	0.079	5.351	-212.958	-1323.156	-336.205	-58.112	58.465	-1015.350	2492.961
Fe2O3	-0.073	0.271	0.344	-0.767	1.186	-0.391	-0.148	-0.617	-0.031	0.060	-0.218	2.578	0.517	0.472	0.030	0.791	-0.417	8.466	-0.755	-2.979	-0.301	-1.819	33.108	-127.001
K2O	0.075	0.002	0.196	-0.305	-0.391	2.108	1.849	1.052	0.259	4.698	-0.265	-5.018	-5.856	-3.661	-0.474	0.220	0.293	-12.704	-71.499	-23.250	15.266	13.324	22.216	445.272
Li2O	-1.502	1.278	-1.160	-5.593	-0.148	1.849	14.460	5.020	3.130	47.110	-1.705	0.612	-18.963	-2.385	0.081	-0.687	0.359	-162.457	-816.760	-215.811	48.105	20.218	-95.077	-13.422
MgO	0.440	0.725	-2.311	9.739	-0.617	1.052	5.020	86.686	-0.888	4.598	-1.238	9.502	-15.994	-1.703	-4.967	1.202	5.059	-2274.683	-124.851	-34.090	36.928	11.249	40.756	-481.985
Na2O	-0.656	0.138	-0.047	-1.802	-0.031	0.259	3.130	-0.888	1.022	9.533	-0.414	0.784	-4.854	1.612	0.502	-0.557	-0.020	40.549	-146.074	-45.412	12.234	-2.293	-47.241	-77.863
P2O5	-2.757	2.296	-2.030	69.659	0.060	4.698	47.110	4.598	9.533	1812.446	-5.886	-56.662	-122.566	17.484	6.576	-1.182	3.621	-679.942	-32061.469	-8471.361	313.660	-35.652	-651.416	5159.127
SiO2	0.158	-0.417	0.053	0.300	-0.218	-0.265	-1.705	-1.238	-0.414	-5.886	0.412	-0.497	6.776	-1.564	-0.375	-0.290	0.008	27.046	94.924	26.834	-17.521	3.347	27.199	10.981
SnO2	0.098	0.963	-0.500	-45.505	2.578	-5.018	0.612	9.502	0.784	-56.662	-0.497	80.005	-0.388	1.492	-1.509	-3.294	0.380	-129.183	1082.934	229.969	4.599	-20.404	578.491	-6561.121
TiO2	-4.742	-5.864	3.213	32.021	0.517	-5.856	-18.963	-15.994	-4.854	-122.566	6.776	-0.388	520.421	-58.847	-2.967	-11.124	-1.491	599.431	2025.336	531.455	-1283.638	191.836	506.500	-245.139
V2O5	-1.721	1.702	-4.153	-2.782	0.472	-3.661	-2.385	-1.703	1.612	17.484	-1.564	1.492	-58.847	257.351	18.625	-2.686	3.743	154.743	-318.970	-64.224	131.245	-528.481	-5083.903	329.670
ZnO	-0.812	-0.572	-0.378	0.863	0.030	-0.474	0.081	-4.967	0.502	6.576	-0.375	-1.509	-2.967	18.625	8.062	-0.739	1.908	84.784	-31.510	-36.443	5.454	-27.096	-445.202	202.217
ZrO2	0.314	0.429	0.171	0.079	0.791	0.220	-0.687	1.202	-0.557	-1.182	-0.290	-3.294	-11.124	-2.686	-0.739	4.107	-0.885	-54.482	-9.059	16.961	27.173	-4.968	115.730	182.968
Others	-0.210	-1.142	-0.488	5.351	-0.417	0.293	0.359	5.059	-0.020	3.621	0.008	0.380	-1.491	3.743	1.908	-0.885	5.645	-107.767	-50.172	-27.485	3.880	-2.301	-108.316	9.504
MgO× MgO	-19.572	-30.149	72.567	-212.958	8.466	-12.704	-162.457	-2274.683	40.549	-679.942	27.046	-129.183	599.431	154.743	84.784	-54.482	-107.767	69459.709	12166.362	3361.524	-1396.751	-1132.268	2754.270	124.032
Li2O× P2O5	31.342	-49.941	41.805	-1323.156	-0.755	-71.499	-816.760	-124.851	-146.074	-32061.469	94.924	1082.934	2025.336	-318.970	-31.510	-9.059	-50.172	12166.362	593929.474	148142.141	-5190.311	991.599	10515.689	-97200.545
Na2O× P2O5	15.318	-8.486	10.578	-336.205	-2.979	-23.250	-215.811	-34.090	-45.412	-8471.361	26.834	229.969	531.455	-64.224	-36.443	16.961	-27.485	3361.524	148142.141	40472.588	-1359.444	93.011	2031.022	-21807.393
SiO2× TiO2	11.589	15.447	-5.992	-58.112	-0.301	15.266	48.105	36.928	12.234	313.660	-17.521	4.599	-1283.638	131.245	5.454	27.173	3.880	-1396.751	-5190.311	-1359.444	3192.268	-446.287	-962.560	460.891
Na2O× V2O5	-0.516	-6.467	12.383	58.465	-1.819	13.324	20.218	11.249	-2.293	-35.652	3.347	-20.404	191.836	-528.481	-27.096	-4.968	-2.301	-1132.268	991.599	93.011	-446.287	1902.362	4583.929	1098.163
V2O5× ZnO	58.617	5.696	31.957	-1015.350	33.108	22.216	-95.077	40.756	-47.241	-651.416	27.199	578.491	506.500	-5083.903	-445.202	115.730	-108.316	2754.270	10515.689	2031.022	-962.560	4583.929	155520.756	-50357.458
SnO2× Others	-13.609	-10.627	61.119	2492.961	-127.001	445.272	-13.422	-481.985	-77.863	5159.127	10.981	-6561.121	-245.139	329.670	202.217	182.968	9.504	124.032	-97200.545	-21807.393	460.891	1098.163	-50357.458	615219.982

Table E.4. Variance Covariance Matrix for Sulfur Model

Term	Al2O3	B2O3	CaO	Cl	Cr2O3	K2O	Li2O	Na2O	P2O5	SiO2	SnO2	V2O5	ZrO2	Others	Li2OxLi2O
Al2O3	0.228	-0.04	-0.05	-0.0483	-0.392	0.021	-0.063	-0.0754	0.0049	0.00593	0.044	-0.0206	0.02127	0.00042	-1.156
B2O3	-0.038	0.165	-0.03	-0.6468	-0.225	-0.003	-0.013	0.02625	0.0808	-0.0371	0.055	0.01019	0.01786	0.01591	0.9863
CaO	-0.045	-0.03	0.17	-0.2871	0.181	-0.037	-0.328	0.00582	0.1068	-0.01581	0.123	-0.0888	0.04882	0.03159	4.4471
Cl	-0.048	-0.65	-0.29	19.6498	6.2705	0.824	3.6138	-0.5416	-1.489	0.243986	-0.26	1.5278	-0.8566	-0.114	-58.96
Cr2O3	-0.392	-0.23	0.181	6.27046	26.834	-0.365	-1.181	-0.3685	-0.996	0.231613	-3	-1.1946	-0.7319	-0.0177	0.8038
K2O	0.021	-0	-0.04	0.82383	-0.365	0.341	0.4523	0.01943	-0.18	-0.02992	-0.1	0.20537	-0.0582	0.03152	-4.118
Li2O	-0.063	-0.01	-0.33	3.61376	-1.181	0.452	5.1086	0.16011	-0.599	-0.11048	0.078	0.3264	-0.1426	0.14457	-81.36
Na2O	-0.075	0.026	0.006	-0.5416	-0.369	0.019	0.1601	0.09633	-9E-04	-0.03053	-0	-0.0406	-0.0434	0.01919	0.9899
P2O5	0.0049	0.081	0.107	-1.4887	-0.996	-0.18	-0.599	-0.0009	2.7017	-0.03085	0.215	-0.2128	0.21784	-0.0254	8.9113
SiO2	0.0059	-0.04	-0.02	0.24399	0.2316	-0.03	-0.11	-0.0305	-0.031	0.038062	-0.05	-0.0134	-0.0591	-0.0445	0.2602
SnO2	0.0443	0.055	0.123	-0.2615	-2.998	-0.099	0.0777	-0.0022	0.2146	-0.05104	1.279	0.27211	-0.0925	0.08384	-0.689
V2O5	-0.021	0.01	-0.09	1.5278	-1.195	0.205	0.3264	-0.0406	-0.213	-0.01344	0.272	1.04019	-0.023	0.04337	-2.685
ZrO2	0.0213	0.018	0.049	-0.8566	-0.732	-0.058	-0.143	-0.0434	0.2178	-0.05906	-0.09	-0.023	0.68582	0.07489	0.5904
Others	0.0004	0.016	0.032	-0.114	-0.018	0.032	0.1446	0.01919	-0.025	-0.04455	0.084	0.04337	0.07489	0.0931	-1.661
Li2OxLi2O	-1.156	0.986	4.447	-58.956	0.8038	-4.118	-81.36	0.9899	8.9113	0.260196	-0.69	-2.6847	0.5904	-1.6606	1623.9

Table E.5. Variance Covariance Matrix for Viscosity Model

Term	Al2O3	B2O3	CaO	Fe2O3	K2O	Li2O	MgO	Na2O	P2O5	SiO2	SnO2	TiO2	V2O5	ZnO	ZrO2	Others
Al2O3	0.119	-0.017	-0.014	0.006	-0.006	-0.083	-0.029	-0.041	0.030	0.006	0.024	0.036	0.000	-0.003	-0.017	-0.030
B2O3	-0.017	0.138	-0.002	0.013	0.001	-0.029	-0.017	-0.008	-0.014	-0.023	0.044	0.029	-0.023	-0.016	-0.006	-0.003
CaO	-0.014	-0.002	0.064	0.008	0.012	-0.013	0.019	0.010	0.019	-0.010	0.018	0.034	-0.025	0.001	0.001	-0.033
Fe2O3	0.006	0.013	0.008	0.132	-0.009	-0.010	-0.011	-0.002	-0.007	-0.019	0.045	-0.114	0.017	0.030	0.020	0.102
K2O	-0.006	0.001	0.012	-0.009	0.229	0.075	0.028	0.017	0.058	-0.010	-0.107	-0.094	-0.008	0.001	-0.054	0.030
Li2O	-0.083	-0.029	-0.013	-0.010	0.075	0.616	-0.006	0.153	0.052	-0.048	-0.152	-0.013	-0.162	-0.018	-0.043	-0.096
MgO	-0.029	-0.017	0.019	-0.011	0.028	-0.006	0.568	0.033	-0.049	-0.022	-0.063	-0.178	-0.069	0.009	-0.023	0.043
Na2O	-0.041	-0.008	0.010	-0.002	0.017	0.153	0.033	0.059	0.005	-0.017	-0.044	-0.017	-0.048	0.006	-0.030	-0.059
P2O5	0.030	-0.014	0.019	-0.007	0.058	0.052	-0.049	0.005	1.714	-0.012	-0.110	-0.013	-0.047	-0.010	0.072	-0.298
SiO2	0.006	-0.023	-0.010	-0.019	-0.010	-0.048	-0.022	-0.017	-0.012	0.022	-0.002	-0.022	0.019	-0.045	-0.008	-0.022
SnO2	0.024	0.044	0.018	0.045	-0.107	-0.152	-0.063	-0.044	-0.110	-0.002	0.463	0.122	-0.116	0.043	-0.007	0.007
TiO2	0.036	0.029	0.034	-0.114	-0.094	-0.013	-0.178	-0.017	-0.013	-0.022	0.122	1.025	0.109	-0.003	0.111	-0.093
V2O5	0.000	-0.023	-0.025	0.017	-0.008	-0.162	-0.069	-0.048	-0.047	0.019	-0.116	0.109	0.653	0.048	0.059	-0.095
ZnO	-0.003	-0.016	0.001	0.030	0.001	-0.018	0.009	0.006	-0.010	-0.045	0.043	-0.003	0.048	0.567	-0.003	0.051
ZrO2	-0.017	-0.006	0.001	0.020	-0.054	-0.043	-0.023	-0.030	0.072	-0.008	-0.007	0.111	0.059	-0.003	0.295	-0.018
Others	-0.030	-0.003	-0.033	0.102	0.030	-0.096	0.043	-0.059	-0.298	-0.022	0.007	-0.093	-0.095	0.051	-0.018	1.716

Appendix F – Terms Used for Composition Uncertainty Calculations

Table F.1. Minimum, Maximum, and Most Likely Values for the GFC Compositions

Min	Kyanite	Borax	Boric Acid	Wollastonite	Hematite	Li Carbnt	Olivine	Cr2O3 (e)	Silica	Rutile	Zincite	Zircon	V2O5 (b)	SnO2 (d)
Ac2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Ag2O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Al2O3	0.54	0	0	0.0013	0.0099	0	0.0003	0	0.0004	0	0	0.001	0	0
Am2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
As2O5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
B2O3	0	0.369	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	0
BeO	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Bi2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CaO	0	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	0
Ce2O3	0	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	0
Cm2O3	0	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	0
Cr2O3	0	0	0	0	0	0	0	0.985	0	0	0	0	0	0
Cs2O	0	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	0

Min	Kyanite	Borax	Boric Acid	Wollastonite	Hematite	Li Carbnt	Olivine	Cr2O3 (e)	Silica	Rutile	Zincite	Zircon	V2O5 (b)	SnO2 (d)
Eu2O3	0	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	0
Fe2O3	0.0042	0	0	0.0029	0.9615	0	0.0468	0	0.0001	0	0	0.0006	0	0
Gd2O3	0	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	0
I	0	0	0	0	0	0	0	0	0	0	0	0	0	0
K2O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
La2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Li2O	0	0	0	0	0	0.4	0	0	0	0	0	0	0	0
MgO	0	0	0	0	0.0001	0	0.4634	0	0	0	0	0	0	0
MnO	0	0	0	0.0009	0.0003	0	0	0	0	0	0	0	0	0
MoO3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Na2O	0	0.164	0	0	0	0	0	0	0	0	0	0	0	0
Nb2O5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nd2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NiO	0	0	0	0	0	0	0.0022	0	0	0	0	0	0	0
NpO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
P2O5	0	0	0	0	0.0018	0	0	0	0	0	0	0	0	0
Pa2O5	0	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	0
PdO	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Pr2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PuO2	0	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	0
Rb2O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Rh2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Min	Kyanite	Borax	Boric Acid	Wollastonite	Hematite	Li Carbnt	Olivine	Cr2O3 (e)	Silica	Rutile	Zincite	Zircon	V2O5 (b)	SnO2 (d)
RuO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO3	0	0	0	0	0.0006	0	0	0	0	0	0	0	0	0
Sb2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SeO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SiO2	0.39	0	0	0.48	0.0084	0	0.4085	0	0.992	0	0	0.32	0	0
Sm2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SnO2	0	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	0
Ta2O5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Tc2O7	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TeO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ThO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TiO2	0.005	0	0	0.0001	0	0	0	0	0	0.928	0	0.0007	0	0
Tl2O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
UO3	0	0	0	0	0	0	0	0	0	0	0	0.0003	0	0
V2O5	0	0	0	0	0	0	0	0	0	0	0	0	0.992	0
WO3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Y2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ZnO	0	0	0	0	0	0	0	0	0	0	0.993	0	0	0
ZrO2	0	0	0	0	0	0	0	0	0	0	0	0.65	0	0

Max	Kyanite	Borax	Boric Acid	Wollastonite	Hematite	Li Carbnt	Olivine	Cr2O3 (e)	Silica	Rutile	Zincite	Zircon	V2O5 ©	SnO2 (d)
Ac2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Ag2O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Al2O3	0.6	0	0	0.0027	0.0201	0	0.0078	0	0.004	0.0075	0	0.004	0	0
Am2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
As2O5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
B2O3	0	0.382	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	0
BeO	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Bi2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0.00017
CaO	0.0004	0	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	0.0002	0	0	0
Ce2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Cl	0	0.0007	0	0	0	0.0001	0	0	0	0	0	0	0	0
Cm2O3	0	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	0
Cr2O3	0	0	0	0	0	0.0002	0.0078	0.991	0	0.0075	0	0	0	0
Cs2O	0	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	0

Max	Kyanite	Borax	Boric Acid	Wollastonite	Hematite	Li Carbnt	Olivine	Cr2O3 (e)	Silica	Rutile	Zincite	Zircon	V2O5 ©	SnO2 (d)
Eu2O3	0	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	0
Fe2O3	0.01	0.0001	0	0.0051	0.9785	0.0001	0.1068	0.0003	0.0004	0.025	0.0001	0.0009	0.00057189	0.00021
Gd2O3	0	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	0
I	0	0	0	0	0	0	0	0	0	0	0	0	0	0
K2O	0.0007	0	0	0	0	0.0001	0	0	0.0002	0	0	0	0.00018069	0
La2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Li2O	0	0	0	0	0	0.4044	0	0	0	0	0	0	0	0
MgO	0.0004	0	0	0.001	0.0037	0.0002	0.4934	0	0.0001	0	0	0	0	0
MnO	0	0	0	0.0011	0.0039	0	0	0	0	0	0.0001	0	0	0
MoO3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Na2O	0.0042	0.17	0	0	0	0.0011	0.0004	0	0.0002	0	0	0	0.00033699	0
Nb2O5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nd2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NiO	0	0	0	0	0	0	0.0052	0	0	0	0	0	0	0
NpO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
P2O5	0	0	0	0	0.0054	0	0	0	0	0.0007	0	0	0	0
Pa2O5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PbO	0	0	0	0	0	0	0	0	0	0	0.0001	0	0	0.00054
PdO	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Pr2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PuO2	0	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	0
Rb2O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Rh2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Max	Kyanite	Borax	Boric Acid	Wollastonite	Hematite	Li Carbnt	Olivine	Cr2O3 (e)	Silica	Rutile	Zincite	Zircon	V2O5 ©	SnO2 (d)
RuO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO3	0	0.0005	0.0003	0	0.0009	0.0004	0	0	0	0.0007	0	0	0	0
Sb2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0.00018
SeO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SiO2	0.42	0	0	0.53	0.0186	0	0.4385	0	0.999	0.025	0	0.325	0.00021393	0
Sm2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SnO2	0	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	0
Ta2O5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Tc2O7	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TeO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ThO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TiO2	0.016	0	0	0.0003	0	0	0	0	0.0005	0.936	0	0.0014	0	0
Tl2O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
UO3	0	0	0	0	0	0	0	0	0	0	0	0.0008	0	0
V2O5	0	0	0	0	0	0	0	0	0	0.0075	0	0	0.996	0
WO3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Y2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ZnO	0	0	0	0	0	0	0	0	0	0	0.9999	0	0	0
ZrO2	0	0	0	0	0	0	0	0	0	0.025	0	0.67	0	0

Most likely	Kyanite	Borax	Boric Acid	Wollastonite	Hematite	Li Carbnt	Olivine	Cr2O3 (e)	Silica	Rutile	Zincite	Zircon	V2O5 (a)	SnO2 (d)
Ac2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Ag2O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Al2O3	0.5703	0	0	0.002	0.015	0	0.0019	0	0.0014	0.005	0	0.0025	0	0
Am2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
As2O5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
B2O3	0	0.375	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	0
BeO	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Bi2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CaO	0.0003	0	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	0.0001	0	0	0
Ce2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Cl	0	0	0	0	0	0.0001	0	0	0	0	0	0	0	0
Cm2O3	0	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	0
Cr2O3	0	0	0	0	0	0.0001	0.0013	0.991	0	0.0016	0	0	0	0
Cs2O	0	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	0

Most likely	Kyanite	Borax	Boric Acid	Wollastonite	Hematite	Li Carbnt	Olivine	Cr2O3 (e)	Silica	Rutile	Zincite	Zircon	V2O5 (a)	SnO2 (d)
Eu2O3	0	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	0
Fe2O3	0.0078	0	0	0.004	0.97	0	0.0768	0	0.0002	0.007	0	0.0008	0	0
Gd2O3	0	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	0
I	0	0	0	0	0	0	0	0	0	0	0	0	0	0
K2O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
La2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Li2O	0	0	0	0	0	0.402	0	0	0	0	0	0	0	0
MgO	0.0001	0	0	0.001	0.001	0.0001	0.4801	0	0.0001	0	0	0	0	0
MnO	0	0	0	0.001	0.0012	0	0	0	0	0	0	0	0	0
MoO3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Na2O	0.0042	0.167	0	0	0	0.0008	0.0003	0	0.0002	0	0	0	0	0
Nb2O5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Nd2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NiO	0	0	0	0	0	0	0.0037	0	0	0	0	0	0	0
NpO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
P2O5	0	0	0	0	0.0027	0	0	0	0	0	0	0	0	0
Pa2O5	0	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	0
PdO	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Pr2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PuO2	0	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	0
Rb2O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Rh2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Most likely	Kyanite	Borax	Boric Acid	Wollastonite	Hematite	Li Carbnt	Olivine	Cr2O3 (e)	Silica	Rutile	Zincite	Zircon	V2O5 (a)	SnO2 (d)
RuO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO3	0	0	0	0	0.0007	0.0003	0	0	0	0	0	0	0	0
Sb2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SeO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SiO2	0.4067	0	0	0.51	0.0135	0	0.4252	0	0.997	0.022	0	0.3225	0	0
Sm2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SnO2	0	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	0
Ta2O5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Tc2O7	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TeO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ThO2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
TiO2	0.0079	0	0	0.0002	0	0	0	0	0.0001	0.932	0	0.001	0	0
Tl2O	0	0	0	0	0	0	0	0	0	0	0	0	0	0
UO3	0	0	0	0	0	0	0	0	0	0	0	0.0004	0	0
V2O5	0	0	0	0	0	0	0	0	0	0.0045	0	0	0.994	0
WO3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Y2O3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ZnO	0	0	0	0	0	0	0	0	0	0	0.999	0	0	0
ZrO2	0	0	0	0	0	0	0	0	0	0.019	0	0.66	0	0

Table F.2. Minimum, Maximum, and Most Likely Values for the Natural Log of Melter Decontamination Factor

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
Ac2O3	2.9601	6.8772	11.1239		MoO3	1.8563	4.194	6.4944		UO3	2.9601	6.8772	11.1239
Ag2O	1.8563	4.194	6.4944		Na2O	3.4874	4.8633	6.4944		V2O5	1.8563	4.194	6.4944
Al2O3	5.0764	7.0814	8.8901		Nb2O5	2.9601	6.8772	11.1239		WO3	2.9601	6.8772	11.1239
Am2O3	1.8563	4.194	6.4944		Nd2O3	2.9601	6.8772	11.1239		Y2O3	2.9601	6.8772	11.1239
As2O5	0.0945	1.5296	4.237		NiO	3.9299	4.7875	6.3835		ZnO	4.7353	6.2383	7.8709
B2O3	3.708	4.5886	5.8519		NpO2	2.9601	6.8772	11.1239		ZrO2	7.2204	8.7143	11.1239
BaO	2.9601	6.8772	11.1239		P2O5	2.9601	5.1381	6.7822					
BeO	2.9601	6.8772	11.1239		Pa2O5	2.9601	6.8772	11.1239					
Bi2O3	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		Pr2O3	2.9601	6.8772	11.1239					
Ce2O3	2.9601	6.8772	11.1239		PuO2	2.9601	6.8772	11.1239					
Cl	0.0979	0.7583	1.9095		RaO	0.0945	1.5296	4.237					
Cm2O3	2.9601	6.8772	11.1239		Rb2O	1.8563	4.194	6.4944					
CoO	2.9601	6.8772	11.1239		Rh2O3	2.9601	6.8772	11.1239					
Cr2O3	1.8563	3.0681	5.3033		RuO2	1.8563	4.194	6.4944					
Cs2O	0.47	2.3609	4.237		SO3	0.6308	1.9694	3.2089					
CuO	2.9601	6.8772	11.1239		Sb2O3	0.0945	1.5296	4.237					
Eu2O3	2.9601	6.8772	11.1239		SeO2	0.0945	1.5296	4.237					
F	0.1179	1.4682	2.4361		SiO2	5.3471	7.5372	9.7527					
Fe2O3	4.9381	6.6712	8.8984		Sm2O3	2.9601	6.8772	11.1239					
Gd2O3	2.9601	6.8772	11.1239		SnO2	2.9601	6.8772	11.1239					
HgO	0	0	0		SrO	2.9601	6.8772	11.1239					
I	0.0945	0.5807	2.266		Ta2O5	2.9601	6.8772	11.1239					
K2O	2.0669	3.3844	5.5607		Tc2O7	0.0953	0.47	1.6094					
La2O3	2.9601	6.8772	11.1239		TeO2	0.0945	1.5296	4.237					
Li2O	3.4689	5.987	7.2894		ThO2	2.9601	6.8772	11.1239					
MgO	7.2464	8.8618	11.0268		TiO2	4.6308	6.1247	8.074					
MnO	2.9601	6.8772	11.1239		Tl2O	0.0945	1.5296	4.237					

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

Element	**Glass oxide**	***fi***		**Radionuclide**	**Glass oxide**	***fi***	***Ai*, Ci/g**
Ac	Ac2O3	NA		59Ni	59NiO	1.2714800	7.982E-02
Ag	Ag2O	1.0741618		60Co	60CoO	1.2669102	1.131E+03
Al	Al2O3	1.8894637		63Ni	63NiO	1.2542412	5.738E+01
Am	Am2O3	NA		79Se	79SeO2	1.4054638	6.969E-02
As	As2O5	1.5338715		90Sr	90SrO	1.1779550	1.388E+02
B	B2O3	3.2198779		90Y	90Y2O3	1.2669393	5.437E+05
Ba	BaO	1.1165059		93mNb	93mNb2O5	1.4305248	2.386E+02
Be	BeO	2.7753081		93Zr	93ZrO2	1.3444224	2.515E-03
Bi	Bi2O3	1.1148390		99Tc	99Tc2O7	1.5661615	1.711E-02
Ca	CaO	1.3992065		106Ru	106RuO2	1.3018755	3.349E+03
Cd	CdO	1.1423295		113mCd	113mCdO	1.1417075	2.311E+02
Ce	Ce2O3	1.1712814		125Sb	125Sb2O3	1.1919928	1.037E+03
Cl	Cl	1.0000000		126Sn	126SnO2	1.2539587	2.839E-02
Cm	Cm2O3	NA		129I	129I	1.0000000	1.768E-04
Co	CoO	1.2714836		134Cs	134Cs2O	1.0596993	1.293E+03
Cr	Cr2O3	1.4615558		137mBa	137mBaO	1.1167839	5.382E+08
Cs	Cs2O	1.0601909		137Cs	137Cs2O	1.0583920	8.655E+01
Cu	CuO	1.2517767		151Sm	151Sm2O3	1.1589344	2.632E+01
Eu	Eu2O3	NA		152Eu	152Eu2O3	1.1578888	1.740E+02
F	F	1.0000000		154Eu	154Eu2O3	1.1558383	2.703E+02
Fe	Fe2O3	1.4297294		155Eu	155Eu2O3	1.1548329	4.762E+02
Gd	Gd2O3	1.1526175		226Ra	226RaO	1.0707860	9.885E-01
Hg	HgO	1.0797617		227Ac	227Ac2O3	1.1057099	7.232E+01
I	I	NA		228Ra	228RaO	1.0701728	2.727E+02
K	K2O	1.2046048		229Th	229ThO2	1.1397132	2.127E-01
La	La2O3	1.1727729		231Pa	231Pa2O5	1.1731267	4.723E-02
Li	Li2O	2.1525285		232Th	232ThO2	1.1379033	1.097E-07
Mg	MgO	1.6582761		232U	232UO3	1.2068558	2.207E+01
Mn	MnO	1.2912262		233U	233UO3	1.2059655	9.633E-03
Mo	MoO3	1.5002939		234U	234UO3	1.2050846	6.217E-03
Na	Na2O	1.3479678		235U	235UO3	1.2042094	2.161E-06
Nb	Nb2O5	NA		236U	236UO3	1.2033426	6.468E-05
Nd	Nd2O3	1.1663831		237Np	237NpO2	1.1349887	7.047E-04

Ni	NiO	1.2725928
Np	NpO2	NA
P	P2O5	2.2913672
Pa	Pa2O5	NA
Pb	PbO	1.0772172
Pd	PdO	1.1503420
Pr	Pr2O3	1.1703179
Pu	PuO2	NA
Ra	RaO	NA
Rb	Rb2O	1.0935990
Rh	Rh2O3	1.2332149
Ru	RuO2	1.3166004
S	SO3	2.4968565
Sb	Sb2O3	1.1971065
Se	SeO2	1.4052533
Si	SiO2	2.1393352
Sm	Sm2O3	NA
Sn	SnO2	NA
Sr	SrO	1.1825999
Ta	Ta2O5	1.2210498
Tc	Tc2O7	NA
Te	TeO2	1.2507743
Th	ThO2	1.1379032
Ti	TiO2	1.6683124
Tl	Tl2O	1.0391407
U	UO3	1.2016486
V	V2O5	1.7851850
W	WO3	1.2610726
Y	Y2O3	1.2699384
Zn	ZnO	1.2446766
Zr	ZrO2	1.3507717

238Pu	238PuO2	1.1344205	1.712E+01
238U	238UO3	1.2016299	3.361E-07
239Pu	239PuO2	1.1338571	6.202E-02
240Pu	240PuO2	1.1332983	2.269E-01
241Am	241Am2O3	1.0995578	3.427E+00
241Pu	241PuO2	1.1327437	1.030E+02
242Cm	242Cm2O3	1.0991457	3.311E+03
242Pu	242PuO2	1.1321942	3.954E-03
243Am	243Am2O3	1.0987369	1.997E-01
243Cm	243Cm2O3	1.0987369	4.903E+01
244Cm	244Cm2O3	1.0983316	8.093E+01

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