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**OWL Models Update and Use for  
TWRS Strategy Development**

**M. Hoza**

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**March 1996**

**Prepared for the U.S. Department of Energy  
under Contract DE-AC06-76RLO 1830**

**Pacific Northwest National Laboratory  
Operated for the U.S. Department of Energy  
by Battelle Memorial Institute**



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Pacific Northwest National Laboratory  
Richland, Washington 99352

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## Summary

This report presents the results of the development work on the Optimal Waste Loading (OWL) models for FY95. Work was focused in four areas, each of which is discussed below.

The OWL glass property models were updated to be consistent with the latest models based on the experimental glass formulation and modeling work. The updated models include property model uncertainty, permitting the optimization to account for this uncertainty in the calculation.

The OWL model architecture was revised to be more modular. The new architecture enables all OWL models to use the same core model files, facilitates integrating OWL with other Hanford models, and enables the use of the Ternary Waste Envelope Assessment Tool (TWEAT) to view the results of all OWL model calculations. The Base, Uncertainty, and Discrete Blend Models have been converted to the new architecture.

The interface to TWEAT was enhanced. The enhancements make it possible to use TWEAT to view the results of any OWL model calculation and to access both OWL and TWEAT from any IBM-compatible or Macintosh-compatible personal computer, or any engineering workstation on the Pacific Northwest Laboratory (PNL) network.

Several simple high-level strategies for blending all Hanford high-level waste were evaluated for a set of tank farm composition data (Lambert and Kim, 1994). Results suggest that, if it is possible to blend all high-level waste to form four blends, the required volume of high-level waste glass will be the same as if all wastes were blended together. An overall processing and blending strategy that should make it possible to achieve the processing and blending to four blends is described. The benefits of such a strategy are:

- Less glass would be required, potentially resulting in a savings of billions of dollars (relative to not blending at all).
- Fewer distinct high-level wastes would result. This would greatly simplify experimental glass and feed rheology work.
- The strategy could provide a reference technical basis for engineering decisions.

The strategy must be rigorously evaluated against other strategies from a system life-cycle cost perspective. An approach for implementing and evaluating the strategy is proposed.

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- Don Larson for his guidance and programmatic support for the development of the OWL models.
- Ross Lambert and Bob Robertus for their efforts in interfacing OWL and TWEAT.
- Trish Redgate for providing the new property and uncertainty model coefficients and explaining how to implement the Fulcher and Arrhenius uncertainty models.

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## 1.0 Introduction

High Level Waste (HLW) at Hanford will be converted to a borosilicate glass for disposal. The glass will need to meet both processability and durability restrictions. The processability conditions will ensure that the glass has properties (viscosity, electrical conductivity, and liquidus temperature) within ranges known to be acceptable for the vitrification process. Durability restrictions will ensure that the resultant glass will meet quantitative criteria for disposal in a repository.

An experimental program, the Composition Variation Study (CVS), is developing property models which correlate physical properties to glass compositions (Hrma, Piepel, et al. 1994). Property models have been developed for the viscosity, electrical conductivity and liquidus temperature of the glass melt, and durability of the glass. The property models are described in the above report. Bounds on property values, limits on the composition of individual components in the glass, and other restrictions are also published in the report.

The Optimal Waste Loading (OWL) models are being developed as a set of tools to aid the waste and glass evaluation and glass design processes. In the most basic implementation, the OWL model will calculate the maximum waste loading and an optimal frit composition such that all constraints on the glass (as identified in the CVS study) are satisfied. The earliest implementation of the OWL models (as described in the 1993 OWL report<sup>(a)</sup>) has been used to identify limiting constraints, evaluate blending strategies, evaluate the effectiveness of pretreatment processes, and to explore the effects of property model uncertainty and Hanford Waste Vitrification Plant (HWVP) recycle on waste loading.

Additional developments were described in the 1994 OWL report<sup>b</sup>. These included verifying and validating the base OWL model, developing and demonstrating an approach for

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<sup>a</sup> Hoza, M. 1993. *Optimal Waste Loading Models for Vitrification of Hanford High-Level Waste*. PHTD-C93.03.01M, Pacific Northwest Laboratory, Richland, Washington.

<sup>b</sup> Hopkins, D.F., M. Hoza and C.A. Lo Presti, 1994. *FY94 Optimal Waste Loading Models Development*. PVTD-C94.02.04D. Pacific Northwest Laboratory, Richland, Washington.

handling waste composition uncertainty in the calculation, and developing a file interface to the Ternary Waste Envelope Assessment Tool (TWEAT)<sup>(a)</sup>

This report addresses the continuation of the development of the OWL models. The objectives of the work described in this report are listed below:

1. *Update the Glass Property Models in OWL.* Incorporate the glass property models and constraints from the most recent CVS report (Hrma, Piepel, et al. 1994). These include temperature dependent models for viscosity and electrical conductivity. This work is described in Section 2.
2. *Convert OWL to the more flexible Process Chemistry Model architecture.* This reduces the need to maintain multiple versions of the core model code to support the different versions of OWL, and will facilitate the use of OWL with related TWRS programs and with tank inventory data. This work is described in Section 3.
3. *Enhance the interface to TWEAT.* The enhanced OWL-TWEAT interface now facilitates the use of TWEAT for visual examination of OWL results, and enables access to both programs from the PNL network. This work is described in Section 4.
4. *Complete a preliminary technical study to determine optimal glass types/formulations, waste pretreatment/retrieval approach and melter systems to assist in establishing program direction.* This study will provide bases for determining approaches for glass formulation and feed preparation strategies. This work is described in Sections 5 and 6.

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<sup>a</sup> Robertus, R.J., and R. Lambert. 1995. *TWEAT '95 User's Documentation Update*. PVTD-C95-02.04B. Pacific Northwest Laboratory, Richland, Washington.

## 2.0 Incorporation of Updated Glass Property and Property Uncertainty Models

Glass property models developed as part of the Composition Variation Study (CVS) are incorporated into OWL as constraints for the optimization calculation (see 1993 OWL report<sup>a</sup>). The FY94 CVS report (Hrma and Piepel et al., 1994) is the most recent report on the results of the study. This section discusses the incorporation of the glass property models, the property model uncertainties, and component bounds from the FY94 CVS report into OWL.

Table 2.1 Glass Property Limits

Property, units	Minimum Property Value	Maximum Property Value
Viscosity, PaS	2	10
Electrical Conductivity, S/m	10	100
Durability (Release rate of boron by PCT), g/m <sup>2</sup>	Not Applicable (N/A)	8.2
Durability (Release rate of lithium by PCT), g/m <sup>2</sup>	N/A	4.8
Durability (Release rate of sodium by PCT), g/m <sup>2</sup>	N/A	6.6
Liquidus Temperature, °C Clinopyroxene	N/A	1050
Liquidus Temperature, °C Spinel	N/A	1050
Liquidus Temperature, °C Zr-containing crystals	N/A	1050

<sup>a</sup> Hoza, M. 1993. *Optimal Waste Loading Models for Vitrification of Hanford High-Level Waste*. PHTD-C93.03.01M, Pacific Northwest Laboratory, Richland, Washington.

## 2.1 Property Models

The property models for viscosity and electrical conductivity of the melt and durability of the glass were updated in the OWL model; property models were added for liquidus temperature of the glass. Only a brief discussion on each of the models will be presented below. For more information on each of these models, refer to the FY94 CVS report. The default limits on the properties (which are consistent with the CVS Qualified Composition Region) are given in Table 2.1. The limits can easily be changed in the HL\_Constraints.ip file before performing a calculation run. The OWL model file containing the property model coefficients is listed in Appendix A.

### 2.1.1 Viscosity

The nonlinear viscosity model in OWL was replaced by a Fulcher viscosity model. The predicted viscosity is calculated as shown in equation (1)

$$\ln \eta = \sum_{i=1}^{10} A_i x_i + \sum_{i=1}^{10} B_i x_i / (T - \sum_{i=1}^{10} T_i x_i) \quad (1)$$

where  $A_i$ ,  $B_i$ , and  $T_i$  are empirical Fulcher model coefficients,  $x_i$  are the mass fractions of the ten components included in the glass property models, and  $T$  is the melter temperature in degrees C.

### 2.1.2 Electrical Conductivity

The nonlinear electrical conductivity model was replaced by an Arrhenius electrical conductivity model. The predicted electrical conductivity  $\epsilon$  is calculated as shown in equation (2)

$$\ln \epsilon = \sum_{i=1}^{10} A_i x_i + \sum_{i=1}^{10} B_i x_i / T \quad (2)$$

where  $A_i$  and  $B_i$  are empirical Arrhenius model coefficients,  $x_i$  are the mass fractions of the ten components included in the glass property models, and  $T$  is the melter temperature in Kelvin.

### 2.1.3 Durability

The calculation of Materials Characterization Center (MCC-1) test durability has been dropped; Product Consistency Test (PCT) durabilities for boron, lithium, and sodium are

now calculated using the updated property model coefficients given in Appendix A. PCT durabilities (actually normalized elemental releases) are calculated using second order models, as shown in equation (3).

$$\ln r = \sum_{i=1}^{10} A_i x_i + \sum_{i=1}^{10} \sum_{j>1}^{10} B_{ij} x_i x_j \quad (3)$$

where  $A_i$  and  $B_{ij}$  are empirical first and second order model coefficients, respectively, and  $x_i$  are the mass fractions of the ten components included in the glass property models.

#### 2.1.4 Liquidus Temperatures

Linear liquidus temperature models for clinopyroxene, spinel, and Zr-containing species have been added to OWL. The calculation for each is as shown in equation (4)

$$T_L = \sum_{i=1}^{10} A_i x_i \quad (4)$$

where  $A_i$  are empirical first order model coefficients, and  $x_i$  are the mass fractions of the ten components included in the glass property models.

## 2.2 Single Component Bounds

With the exception the upper bound on  $Al_2O_3$  (which increased from 0.15 to 0.17), all single component bounds are unchanged from those used in OWL '94. The default component bounds currently used in OWL are given in Tables 2.2 and 2.3. These bounds are consistent with the CVS Qualified Composition Region. Component bounds are specified in the file HL\_Constraints.ip, and can be modified, if desired, for a particular calculation.

**Table 2.2 Upper and Lower Limits on the Mass Fractions of the Ten CVS Components**

Lower Limit	Component	Upper Limit
0.42	SiO <sub>2</sub>	0.57
0.05	B <sub>2</sub> O <sub>3</sub>	0.20
0.05	Na <sub>2</sub> O	0.20
0.01	Li <sub>2</sub> O	0.07
0	CaO	0.10
0	MgO	0.08
0.02	Fe <sub>2</sub> O <sub>3</sub>	0.15
0	Al <sub>2</sub> O <sub>3</sub>	0.17
0	ZrO <sub>2</sub>	0.13
0.01	Other	0.10

**Table 2.3 Upper Limits on Mass Fractions of Solubility Components**

Solubility Component	Upper Limit
Cr <sub>2</sub> O <sub>3</sub>	0.005
F	0.017
P <sub>2</sub> O <sub>5</sub>	0.01
SO <sub>3</sub>	0.005
Noble Metals (Rh <sub>2</sub> O <sub>3</sub> + PdO + Ru <sub>2</sub> O <sub>3</sub> )	0.025

## 2.4 Property Uncertainty Models

The approach used to account for property model uncertainty in OWL calculations was described in the FY93 OWL report. In that approach the size of the feasible region is reduced by the uncertainties in the property models. The property value constraint (with uncertainty) can then be expressed as equation (5)

$$\ln(\text{MinVal}) + \text{Uncert} \leq \text{CalculatedPropertyValue} \leq \ln(\text{MaxVal}) - \text{Uncert} \quad (5)$$

where

MinVal = the minimum acceptable value of the property

MaxVal = the maximum acceptable value of the property.

For each property, the uncertainty in a constraint for a particular composition can be expressed as in equation (6)

$$\text{Uncert} = M[\mathbf{x}^T \mathbf{S} \mathbf{x}]^{0.5} \quad (6)$$

where

M = multiplier, which is usually the upper 95th percentile of a t-distribution [ $t_{.95}(n-p)$ ], where n is the number of data points used to fit the model and p is the number of fitted parameters (coefficients) in the model

x = glass composition vector expanded in the form of the model

x<sup>T</sup> = transpose of glass composition vector expanded in the form of the model

S = covariance matrix of the estimated parameters (coefficients).

To calculate Uncert for all but the linear (liquidus temperature) models, the glass composition vector must be expanded. For durability models, the composition vector is augmented by second-order terms. For example, if there are two second-order terms,  $x_1^2$  and  $x_2x_4$ , the usual composition vector ( $x_1, \dots, x_{10}$ ) becomes ( $x_1, \dots, x_{10}, x_1^2, x_2x_4$ ). For the Fulcher viscosity model and Arrhenius electrical conductivity model, the composition vector is more complex. For the Fulcher viscosity model, the composition vector becomes (equation (7))

$$[x_1, \dots, x_{10}, \frac{\partial \ln \eta}{\partial B_1}, \dots, \frac{\partial \ln \eta}{\partial B_{10}}, \frac{\partial \ln \eta}{\partial T_1}, \dots, \frac{\partial \ln \eta}{\partial T_{10}}] \quad (7)$$

while the Arrhenius composition vector becomes (equation (8))

$$[x_1, \dots, x_{10}, \frac{\partial \ln \epsilon}{\partial B_1}, \dots, \frac{\partial \ln \epsilon}{\partial B_{10}}] \quad (8)$$

The covariance matrices for all property models are given in Appendix B.

### 3.0 Updating OWL Model Architecture

The previous OWL architecture (see FY93 OWL report) used common input files for the various OWL models (Base, Base with property model uncertainty, Base with Recycle, Discrete Blend Model), but different core model files. This made it necessary to maintain multiple copies of the same information, and did not support combinations of the models (say blend model with uncertainty). In the new model architecture, based on the Process Chemistry Model architecture (see Appendix A in FY94 OWL report), all models work from the same core files and combinations of the models are supported. A model is built at run time by assembling the appropriate model segments into a single model file. The set of files needed for each of the models is given in Table 3.1. For a given model, files that are specific to that model appear only in that model's column. Files that are used by multiple models are shown in rows that span multiple columns.

Conversion to the new architecture facilitated the updating of the glass property models and enables the use of TWEAT to view the results of any OWL model calculation. The new architecture will also facilitate the development of data filters (<HL\_OWL-HLV.flit> in the table above) for interfacing OWL with other Hanford models and the ability to use tank inventory data (rather than pretreated high-level waste compositions) for a calculation.

The Base, Model Uncertainty, and Discrete Blend versions are implemented; the Recycle model has not yet been converted to the new architecture.

Table 3.1. OWL Model Files for Revised Model Architecture

Base	Model Uncert	Recycle	Discrete Blend
GAMS_run_options.mdl			
HL_Set_Definition.mdl			
wastcomp.prn			
*HL_Variable_Definition.mdl			
*HL_Input_Parameters.ip			
*User_Params			
			HL_OptBlnd_Params.ip
*HL_Glass_Model.mdl			
		*HL_Covar.mdl	
		*HL_Recyc.mdl	
*HL_Vit_Core.mdl			

<sup>a</sup> Files marked with an asterisk are also used for overall (Process Chemistry) models

*HL_Vit_Base_Adj.mdl			
	*HL_Vit_Uncert_Adj.mdl		
		*HL_Vit_Recycle_Adj.mdl	
			*HL_Vit_OptBlnd_Adj.mdl
<HL_Mdl_Decl.mdl*> <sup>b</sup>			
*HL_Constraints.ip			
*HL_Frit_Component_Bounds.ip			
*HL_Initial_Values.ip <sup>c</sup>			*HL_Init_Val_OptBlnd.ip
* <HL_OWL-HLV.flit> <sup>d</sup>			
<HL_CalcSpec.mdl>			HL_CalcOptBl.mdl
HL_Waste_Input_report.mdl			
*HL_Solve_NLP.mdl			*HL_Solve_MINLP.mdl
*HL_Postprocessor.mdl			
*LoopEnd.mdl for loop calculations			

<sup>a</sup> Declares model and lists equations to be used in model; equations used depend on capabilities selected

<sup>b</sup> <filename.mdl> indicates that multiple versions of this file exist; appropriate version is used

<sup>c</sup> For multiple items on the same line, only one can be selected

<sup>d</sup> Conversion depends on data source (OWL .prn file, Aspen file, Speedup file, etc.)

## **4.0 OWL Interface with TWEAT**

Two improvements were made to the OWL part of the OWL-TWEAT interface. First, the OWL output file writer has been folded into the new architecture so the file can now be written for all OWL calculations. Previously, only the Base OWL model could write a TWEAT file.

Second, the options for using OWL and TWEAT together have been expanded. TWEAT can now be run in a Mac emulator on the Sun workstation where OWL resides. This makes it possible to access both OWL and TWEAT over the PNL network from a Windows PC, a Mac, or an engineering workstation.

## 5.0 Overall Tank Blending Scenario Analyses

This section presents the results of an analysis of several blending scenarios for all of Hanford's high-level tank waste. Such scenarios could form the basis for an overall processing strategy for Hanford tank waste. These results suggest that it should be possible to develop a processing strategy capable of achieving Total Blend performance. Such a strategy is described in Section 6.

### 5.1 Overview of Previous Blending Work

This analysis builds on the results of two previous blending studies, the FY93 Blend report<sup>a</sup>, and the FY94 Blend Report<sup>b</sup>. The FY93 report described three basic blending models (Total Blend, Continuous Blend, and Discrete Blend) and the results of some blending calculations for small waste sets. It was determined that blending could substantially reduce the volume of glass required to vitrify high-level waste, and that the Total Blend (combining all high-level waste into a single blend) produced the minimum volume of glass. The FY94 report examined the effect of blend size (the number of tanks per blend), methods for solving the Discrete Blending problem, and heuristic strategies for formulating discrete blends. A summary of the key aspects of blending behavior is given in Appendix C. More detail can be found in the referenced reports.

### 5.2 Basis for Blend Analyses

The scenarios considered in this report are based on data and scenarios used in the Feed Processability Assessment Report (Lambert and Kim, 1994). The calculations described below were based on the fourteen waste streams (primarily by tank farm—A, AX, B, BX, BY, CC, S (5.27% Cr<sub>2</sub>O<sub>3</sub>)<sup>c</sup>, SX (14.5% Cr<sub>2</sub>O<sub>3</sub>), T, TX, TY, U, DSSF, DST) used by Lambert & Kim. The waste composition file is given in Appendix D. (For information on the pretreatment and other assumptions leading to these compositions, see Lambert and Kim's report). Following Lambert and Kim, the P<sub>2</sub>O<sub>5</sub> limit was raised to 3% (mass fraction in the glass). The Cr<sub>2</sub>O<sub>3</sub> limit used was 0.5%. The same constraints were used for all calculations,

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<sup>a</sup> Hoza, M. and J.G.H. Geeting. 1993. *Blending Analysis Using the Optimal Waste Loading Model*. TWRSP-93-058. Prepared for the Westinghouse Hanford Company by Pacific Northwest Laboratory, Richland, Washington.

<sup>b</sup> Hoza, M. 1994. *Study of Potential Blending Strategies for Immobilization of Hanford High-Level Waste*. TWRSP-94-087. Prepared for the Westinghouse Hanford Company by Pacific Northwest Laboratory, Richland, Washington.

<sup>c</sup> The adjusted Cr<sub>2</sub>O<sub>3</sub> compositions of Lambert and Kim were used.

except Lambert and Kim's tank farm blends (which used different constraints for different waste types).

There were several reasons for selecting this set of waste data for the calculations here:

- Waste composition data by tank farm are generally considered to be more reliable than tank by tank data,
- Compositions for the high-level portions of those wastes were available, and
- Results could be compared with those of Lambert and Kim.

### 5.3 Blending Scenario Results

Several simple blending scenarios were evaluated and compared based on the waste composition data in Lambert and Kim. Table 5.1 summarizes the calculated results; each of the cases is described in the following sections.

**Table 5.1. Blend Scenario Analysis Results**

Blend Scenario	Total Glass Required (million kg)	RunCode
Tank Farm Blends (as determined by Lambert and Kim)	61	N/A
Cr-Metered Blend	43.4	L&K11
Discrete Blend by farm	37.6	L&K08
Discrete Blend by "tank"	31.4	L&K10
Total Blend	31.4	L&K02

#### 5.3.1 Tank Farm Blends

For the tank farm blends, Lambert and Kim estimated maximum reasonable glass waste loadings for each of the tank farms. They modified the constraints for each waste type as they felt appropriate based on Kim's glass formulation expertise.

### 5.3.2 Cr-Metered Blends

For the Cr-metered blends, the high-Cr waste in the S and SX farms was optimally distributed among the remaining 12 farms. This offered an improvement over the tank farm blends, but was not as effective as the discrete blends. There are two reasons for this. First, the discrete blend cases result in four blends; as the FY94 Blend Report showed, blending was more effective with more tanks per blend. Second, the waste was distributed based on one component of a 15-component vector. In many cases, before enough high-Cr waste could be added to a farm to get to the Cr limit, the limit on another component was reached. Since Cr is the limiting component for the Total Blend, all blends must have Cr as the limiting constraint to achieve Total Blend performance. *This phenomenon will limit the effectiveness of all heuristic blending strategies which make blending decisions based on a single component.*

### 5.3.3 Discrete Blend by Farm

For the discrete blend by farm, the fourteen tank farm blends were optimally combined to form four blends using the OWL Discrete Blend Model. This strategy benefits from optimal blending and the formation of only four blends, but is limited because the high-Cr S and SX farm wastes can each go to only one blend. Thus, only two of the blends are limited by Cr. The optimal blending combinations for this case are

- (B, BY, SX),
- (A, BX, C, S, T),
- (AX, U, DST), and
- (TX, TY, DSSF).

### 5.3.4 Discrete Blend by "Tank"

This case is an approximation of blending by tank rather than of blended farms. Each farm was divided into "equivalent tanks", each with the same composition. Each farm had the same number of "equivalent tanks" as the number of actual tanks in that farm. Four blends were optimally formed with wastes from the 177 equivalent tanks; the total glass required was the same as for the Total Blend. The optimal assignments are given in Table 5.2. It is likely that other tank assignments could be found that would also provide Total Blend performance.

Tables 5.3 to 5.6 provide the calculated results for each blend. These results include the compositions of the blend, frit, and glass, waste loading, and mass of glass required. The calculated frit and glass compositions are not unique. The upper limit on  $\text{Cr}_2\text{O}_3$  is the binding constraint for all four blends.

The overall results suggest that a processing and blending strategy, such as the one outlined in section 6, should be able to achieve Total Blend performance. Of course, this analysis was done with "equivalent tanks" and would need to be

**Table 5.2 Optimal Assignments for Discrete Blend by "Tank"**

Farm	Total Tanks	Tanks to Blend 1	Tanks to Blend 2	Tanks to Blend 3	Tanks to Blend 4
A	6	2	1	2	1
AX	4	0	2	0	2
B	16	0	0	16	0
BX	12	0	0	0	12
BY	12	0	3	9	0
C	16	1	2	10	3
S	12	2	7	3	0
SX	15	1	1	7	6
T	16	0	4	1	11
TX	18	3	4	0	11
TY	6	1	2	1	2
U	16	16	0	0	0
DSSF	28	28	0	0	0
DST	28	0	14	0	14

repeated with actual tank compositions and masses. Other considerations, such as safety, logistics, and chemical compatibility, would certainly need to be factored into the process of developing a retrieval sequence consistent with optimal blend results. A process for accommodating necessary considerations is presented in Section 6.

### 5.3.5 Total Blend

The Total Blend case involves combining all waste into a single blend, then determining the required glass for that blend. The Total Blend is logistically impossible, but it serves as a useful reference case against which to compare other strategies, since it produces the minimum possible amount of glass.

Table 5.3 Calculated Results for Blend 1

BLEND B1 Compositions (Mass Fractions)

Component	Blend	Frit	Glass
SiO2	0.1498	0.6620	0.4200
B2O3	0.0000	0.2380	0.1256
Na2O	0.3473	0.0000	0.1641
Li2O	0.0000	0.0569	0.0300
CaO	0.0046	0.0000	0.0022
MgO	0.0000	0.0000	0.0000
Fe2O3	0.0874	0.0000	0.0413
Al2O3	0.1523	0.0431	0.0947
ZrO2	0.0191	0.0000	0.0090
OTHER	0.2394	0.0000	0.1131
CR2O3	0.0106	0.0000	0.0050
F	0.0016	0.0000	0.0007
P2O5	0.0175	0.0000	0.0083
SO3	0.0030	0.0000	0.0014
NOBMET	0.0000	0.0000	0.0000

Mass (kg) of Waste Oxide in Blend 1569167.90

Mass Fraction of Waste in High-Level Glass 0.472

Number of High-Level Glass Logs Required 885.6

Mass (kg) Glass Required 3321067.7

Calculated Glass Properties

Property	Value	Lower Limit	Upper Limit
Viscosity, PaS	3.56	2.0	10.0
Electrical Conductivity, S/m	44.98	10.0	100.0
Release of Boron by MCC, g/m2	26.85		9999.0
Release of Boron by PCT, g/m2	2.00		8.2
Release of Li by PCT, g/m2	1.39		4.8
Release of Na by PCT, g/m2	1.00		6.6
Liq T - Clinopyroxene, deg C	801.49		1050.0
Liq T - Spinel, deg C	878.55		1050.0
Liq T - Zr-contg Xstals, deg C	723.21		1050.0

Table 5.4 Calculated Results for Blend 2

BLEND B2 Compositions (Mass Fractions)

Component	Blend	Frit	Glass
SIO2	0.0723	0.6025	0.4368
B2O3	0.0011	0.1173	0.0810
NA2O	0.3511	0.1454	0.2097
LI2O	0.0000	0.0436	0.0300
CAO	0.0142	0.0000	0.0044
MGO	0.0007	0.0000	0.0002
FE2O3	0.0923	0.0000	0.0289
AL2O3	0.1180	0.0912	0.0995
ZRO2	0.1100	0.0000	0.0344
OTHER	0.2403	0.0000	0.0751
CR2O3	0.0160	0.0000	0.0050
F	0.0062	0.0000	0.0019
P2O5	0.0339	0.0000	0.0106
SO3	0.0037	0.0000	0.0012
NOBMET	0.0002	0.0000	0.0001

Mass (kg) of Waste Oxide in Blend 2546010.40

Mass Fraction of Waste in High-Level Glass 0.313

Number of High-Level Glass Logs Required 2172.0

Mass (kg) Glass Required 8144888.8

Calculated Glass Properties

Property	Value	Lower Limit	Upper Limit
Viscosity, PaS	4.47	2.0	10.0
Electrical Conductivity, S/m	60.15	10.0	100.0
Release of Boron by MCC, g/m2	21.59		9999.0
Release of Boron by PCT, g/m2	1.58		8.2
Release of Li by PCT, g/m2	1.00		4.8
Release of Na by PCT, g/m2	1.00		6.6
Liq T - Clinopyroxene, deg C	791.65		1050.0
Liq T - Spinel, deg C	834.92		1050.0
Liq T - Zr-contg Xstals, deg C	770.35		1050.0

Table 5.5 Calculated Results for Blend 3

BLEND B3 Compositions (Mass Fractions)

Component	Blend	Frit	Glass
SiO2	0.0324	0.7215	0.5168
B2O3	0.0000	0.0711	0.0500
Na2O	0.3358	0.1438	0.2008
Li2O	0.0000	0.0427	0.0300
CaO	0.0326	0.0000	0.0097
MgO	0.0000	0.0000	0.0000
Fe2O3	0.1127	0.0209	0.0482
Al2O3	0.0906	0.0000	0.0269
ZrO2	0.0516	0.0000	0.0153
OTHER	0.3443	0.0000	0.1023
Cr2O3	0.0168	0.0000	0.0050
F	0.0068	0.0000	0.0020
P2O5	0.0574	0.0000	0.0171
SO3	0.0023	0.0000	0.0007
NOBMET	0.0000	0.0000	0.0000

Mass (kg) of Waste Oxide in Blend 3486148.20

Mass Fraction of Waste in High-Level Glass 0.297

Number of High-Level Glass Logs Required 3129.5

Mass (kg) Glass Required 1.1736E+7

Calculated Glass Properties

Property	Value	Lower Limit	Upper Limit
Viscosity, PaS	4.47	2.0	10.0
Electrical Conductivity, S/m	56.53	10.0	100.0
Release of Boron by MCC, g/m2	24.72		9999.0
Release of Boron by PCT, g/m2	6.45		8.2
Release of Li by PCT, g/m2	4.80		4.8
Release of Na by PCT, g/m2	4.79		6.6
Liq T - Clinopyroxene, deg C	799.70		1050.0
Liq T - Spinel, deg C	827.18		1050.0
Liq T - Zr-contg Xstals, deg C	677.09		1050.0

Table 5.6 Calculated Results for Blend 4

BLEND B4 Compositions (Mass Fractions)

Component	Blend	Frit	Glass
SIO2	0.1231	0.8105	0.4200
B2O3	0.0006	0.1150	0.0500
NA2O	0.3385	0.0000	0.1923
LI2O	0.0000	0.0694	0.0300
CAO	0.0059	0.0000	0.0034
MGO	0.0003	0.0000	0.0002
FE2O3	0.0793	0.0000	0.0450
AL2O3	0.1243	0.0050	0.0728
ZRO2	0.0580	0.0000	0.0330
OTHER	0.2699	0.0000	0.1533
CR2O3	0.0088	0.0000	0.0050
F	0.0043	0.0000	0.0024
P2O5	0.0516	0.0000	0.0293
SO3	0.0037	0.0000	0.0021
NOBMET	0.0001	0.0000	0.0000

Mass (kg) of Waste Oxide in Blend 4690973.50

Mass Fraction of Waste in High-Level Glass 0.568

Number of High-Level Glass Logs Required 2201.9

Mass (kg) Glass Required 8256975.6

Calculated Glass Properties

Property	Value	Lower Limit	Upper Limit
Viscosity, PaS	4.20	2.0	10.0
Electrical Conductivity, S/m	60.65	10.0	100.0
Release of Boron by MCC, g/m2	24.91		9999.0
Release of Boron by PCT, g/m2	2.41		8.2
Release of Li by PCT, g/m2	1.62		4.8
Release of Na by PCT, g/m2	1.47		6.6
Liq T - Clinopyroxene, deg C	856.33		1050.0
Liq T - Spinel, deg C	863.55		1050.0
Liq T - Zr-contg Xstals, deg C	759.75		1050.0

## 6.0 Proposed Retrieval, Processing, and Blending Strategy

This section presents an overall processing strategy for Hanford tank waste and an approach for developing and evaluating candidate processing strategies. The processing strategy addresses retrieval, pretreatment, and vitrification of high-level and low-level waste. It uses a comprehensive blending approach based on three years of waste blending analysis work to greatly reduce the number of high-level waste feed streams and to achieve a minimal volume of high-level waste glass with sufficient flexibility to meet safety, processing, and logistics constraints.

The discussion is presented in the next three sections. The motivation for the strategy and the benefits from its implementation are discussed in the first section; a description of the strategy is presented in the following section. Finally, an approach for developing and evaluating candidate strategies is presented.

### 6.1 Motivation for Processing Strategy

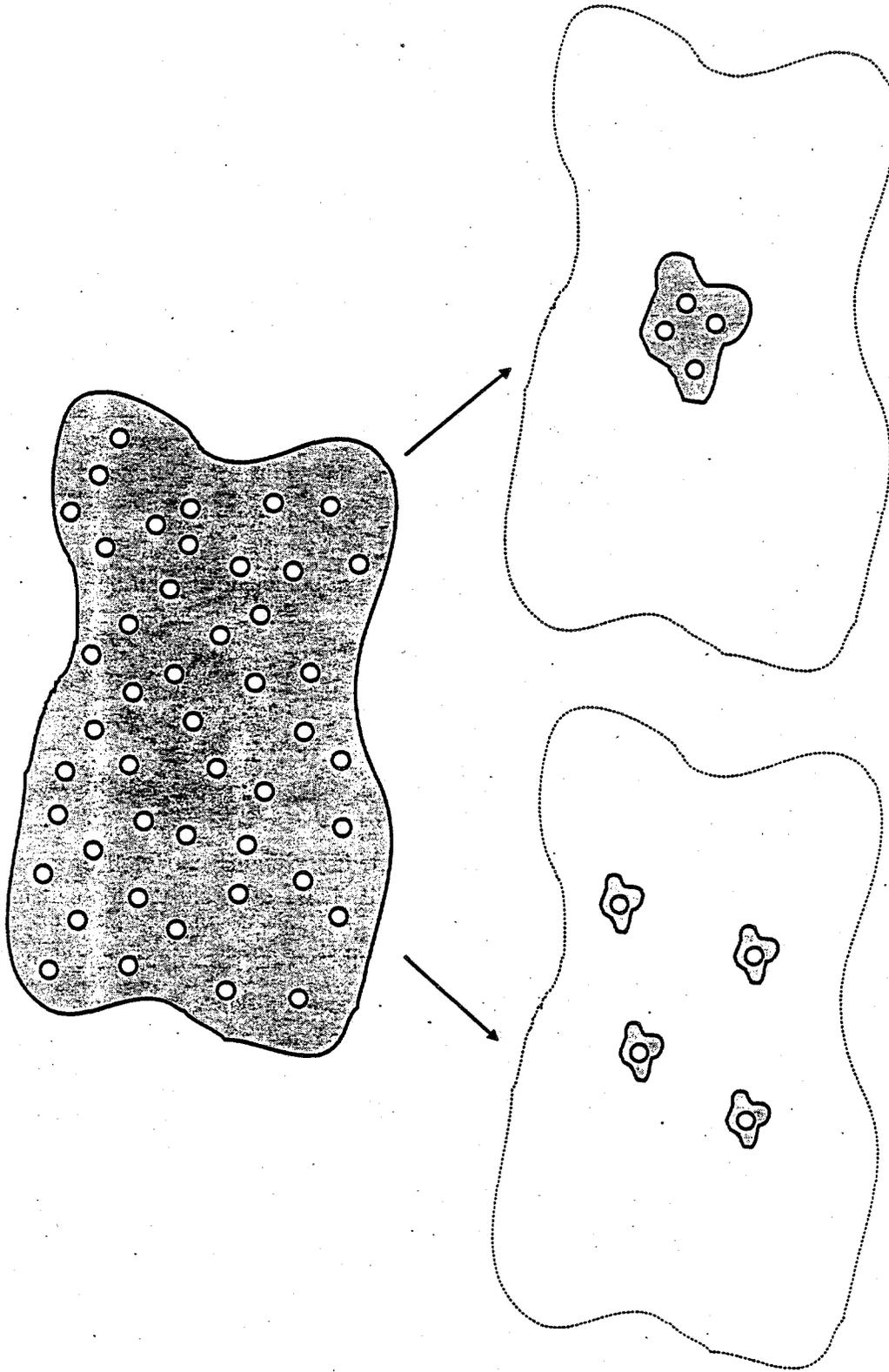
A processing strategy making effective use of waste blending has several compelling advantages:

- The strategy can potentially reduce the number of glass logs required for high-level waste to the Total Blend number, while still meeting all safety, processing, and logistics constraints. The Total Blend number of logs is the minimum number that can be achieved and could be as much as 25<sup>a</sup>-50<sup>b</sup>% less than the number of logs required if no blending were done.
- The strategy can reduce the number of feeds to HLW vitrification to a handful (about four to six). Rather than having to deal with a large number of waste compositions in a large composition space (see Figure 6.1), a much smaller number of waste compositions would be targeted. These compositions could be determined such that the overall volume of waste glass is minimal, resulting in a small number of distinct compositions, each with its associated uncertainty, or such that the final waste compositions are clustered in a single composition region (near the Total Blend composition).

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<sup>a</sup>In the FY94 blending study (report TWRSP-94-087), the blending of 87 tanks for which compositions were available was examined. For those tanks, vitrifying a blend of all tanks required 25.3% fewer logs than vitrifying each waste separately.

<sup>b</sup> In Section 4 of this report, a reduction of almost 50% was achieved relative to blending and vitrifying by tank farm.



Perform blend optimization to produce a small number of distinct HL waste feeds clustered around the Total Blend composition

Perform blend optimization to produce a small number of distinct HL waste feeds such that the overall number of glass logs is minimized

**Figure 6.1** HL Waste Composition Space Comparison - Current vs Two Optimal Blending Strategies

Reducing the number of high-level waste feeds offers several advantages:

- Glass formulation and feed rheology experimental work can focus on a small number of targeted compositions, avoiding the need to try to model either a large number of compositions or any composition within a large composition region. Behavior within the targeted regions could be better understood and more effectively modeled.
  - The number of distinct glasses that need to be qualified would be reduced.
  - Since there would be far fewer waste feeds to deal with, sampling and chemical analysis could be used to a greater extent to reduce the uncertainty in waste feed compositions.
- The strategy can provide a firm technical basis for making TWRS decisions from a system life cycle cost perspective. It can help identify:
  - which components should be targeted for removal in pretreatment (which are most cost effective)?
  - what retrieval/processing facilities/designs are most constraining to implementation of a comprehensive processing strategy (transfer lines, lag storage, new tanks, retrieval annexes)? Which upgrades would be most cost effective?

## 6.2 Description of Processing Strategy

The proposed processing strategy uses extensive optimized blending to reduce the number of high-level waste feeds and minimize the volume of high-level glass produced. Blending of low-level wastes is also addressed.

The strategy is depicted in Figure 6.2. As tanks are retrieved and pretreated, the high-level portions would be collected in HL-Waste holding tanks. For the purpose of illustration sixteen tanks are shown. All the high-level waste produced during a certain time interval would end up in a single HL-Waste holding tank. It would contain the high-level portions of all the tanks retrieved and processed during that time interval.

Assume for the moment that all sixteen tanks are available for blending. One could then perform a discrete blending optimization that would produce (for this example) four HL-Feed Blends. This optimization could be performed such that it would either result in the minimal volume of glass (likely to be the Total-Blend amount) or a set of wastes clustered in composition around the Total Blend composition (which may or may not achieve Total Blend performance).

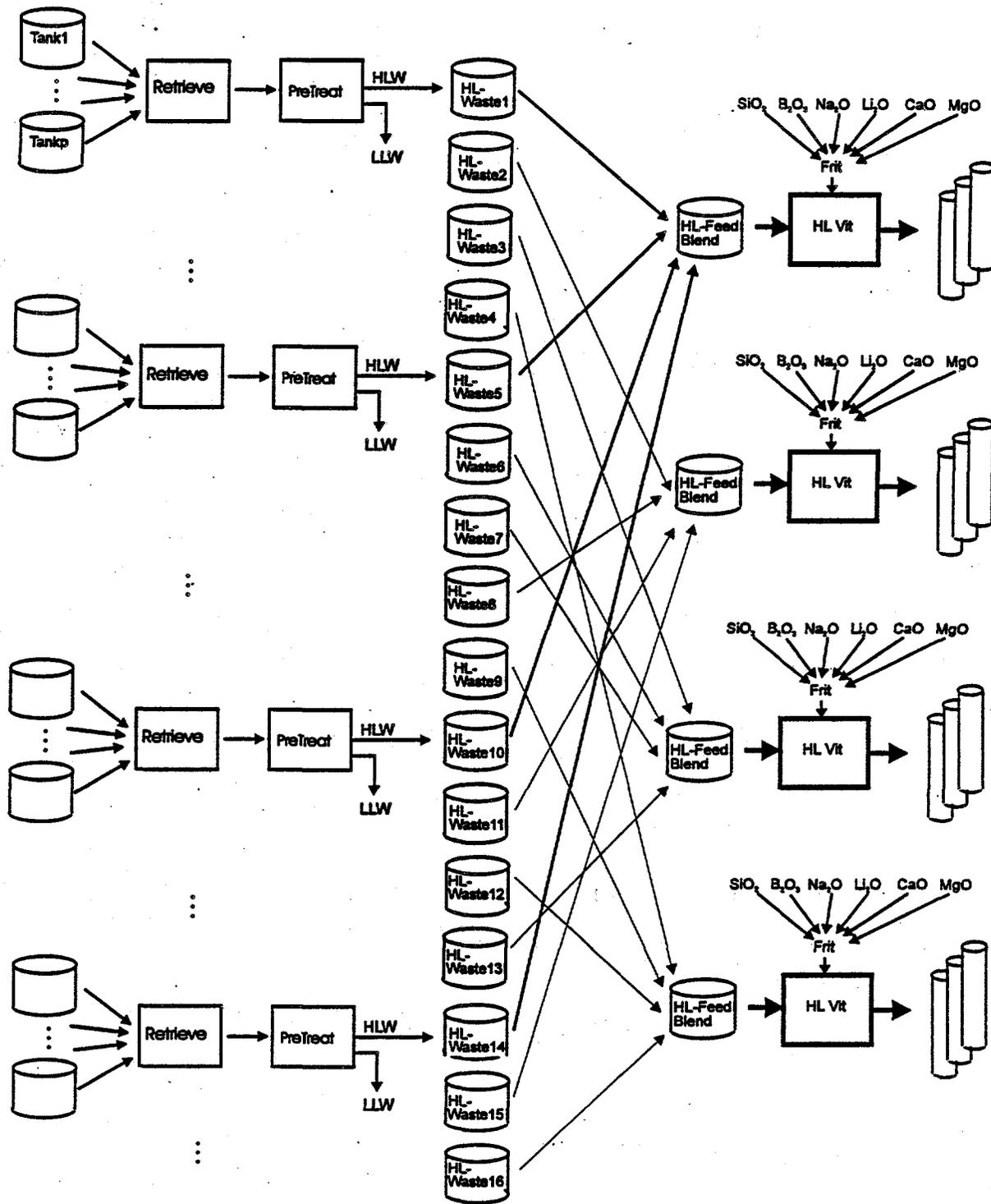


Figure 6.2 Schematic Representative of Proposed TWRS Processing Strategy

Of course, not all the wastes will be available at the same time. But this analysis can help schedule tank retrieval such that the necessary wastes are available. Note the bold lines leading to the first HL-Feed Blend tank. Having identified that these HL-Waste tanks are optimally blended to form the first HL-Feed Blend, one could then identify which Hanford waste tanks went into each of the HL-Waste tanks. Those Hanford waste tanks would be retrieved and processed first. One would proceed similarly for each of the HL-Feed Blends. The methods for assigning tanks to one of the sixteen HL-Waste groups is discussed in the next section.

But what about low-level waste? Where does it fit into the strategy? Since the volume of low-level waste is much greater than that of high-level waste, one is not able to collect LLW for later blending. Rather, one should use the incidental blending encountered in retrieving and processing tanks to achieve LLW blending objectives. Once the tanks are assigned to a retrieval group, the ordering within the group could be determined to meet low-level blending objectives. If, however, most low-level waste is limited by  $\text{Na}_2\text{O}$ , there may not be as much motivation for blending low-level wastes.

### **6.3 Description of Implementation and Evaluation Strategy**

The issue addressed in this section is how to formulate and evaluate specific implementations of the strategy such that the objectives of the strategy, as well as safety, logistics, and programmatic objectives are met. The process is iterative and consists of the following steps:

(iterate on 1-5 until done)

1. Specify the number of HL-Blend tanks and the number of HL-Feed Blends.
2. Assign each tank to one of the HL-Blend groups, distributing them so each tank group has about the same mass or the same number of tanks. This can be done manually or using a rule-based expert system. Initial assignments may use general rules of thumb (e.g., divide each tank farm into at least three groups); subsequent assignments can be based on knowledge about how well previous assignments met system objectives.
3. Use the OWL Tank Waste Blending Model to calculate the performance of the system as defined and optimize the formation of the HL Feed blends from the HL-Blends. If the performance of the system for the collection of tank groups is unacceptable, repeat step 2 to obtain new groups. Calculated glass formulations could be examined with TWEAT to ensure sufficient operational flexibility.
4. If the system provides acceptable performance (target: Total Blend), develop retrieval sequences consistent with appropriate safety, scheduling, chemical compatibility, and other considerations (including low-level waste blending).

Swapping tanks between HL-Blend groups that feed the same HL Feed blend is acceptable. This assignment could be done manually, or using an expert system.

5. Use WHC tank processing logistics models to test the sequences developed in steps 1-4. If processing problems are found, repeat steps 2-4. If necessary, repeat steps 1-4. Processing problems could result from assumptions or decisions which limit processing flexibility. This analysis could suggest revisiting some of those decisions.

When this process is successfully completed, one will have determined a processing and blending architecture, a retrieval sequence, compositions of a small number of high-level waste feeds to be vitrified, and calculated glass volumes for those compositions. This specific strategy can then serve as the basis for engineering and experimental development.

## 7.0 Conclusions and Recommendations

This report presented the results of OWL development and analysis work in FY 95. The following were addressed:

- *Upgrade of OWL property models.* The models are now consistent with the latest CVS report property and uncertainty models.
- *Upgrade of OWL model architecture.* The modular architecture uses core model files for all models, has a single file interface to TWEAT for all models, facilitates interoperability with other Hanford models, and provides a mechanism for use of site tank characterization data.
- *Analysis of high-level blending approaches.* Several simple approaches were evaluated, one of which achieved Total Blend performance.
- *Presentation of an overall Hanford processing and blending strategy.* The strategy could minimize the required high-level waste glass volume, greatly reduce the number of distinct high-level wastes to be vitrified, and provide a consistent technical basis for making system-wide decisions.

Future development work should address the following:

- Adapt OWL to more closely mimic the approach a glass chemist uses in formulating glasses.
- Adapt OWL for use in formulating glasses for a high-temperature melter.
- Develop a version of OWL for low-level glass formulation.
- Complete the development of the interface to tank inventory data. This would include upgrading the simple pretreatment module from the Process Chemistry Model.
- Complete the development of the interfaces to related Hanford models, such as the Aspen pretreatment model and the Arena logistics model.

## 8.0 References

Hrma, P.R., G.F. Piepel, et al. 1994. *Property/Composition Relationships for Hanford High-Level Waste Glasses Melting at 1150 C.* PNL-10359, Volumes 1 and 2, Pacific Northwest Laboratory, Richland, Washington.

Lambert, S.L., D.S. Kim, et al. 1994. *Tank Waste Remediation System High-Level Waste Feed Processability Assessment Report.* WHC-SP-1143, Westinghouse Hanford Company, Richland, Washington.

## **APPENDIX A**

### **Glass Property Model Coefficients**

## Appendix A

### Glass Property Model Coefficients

#### \* Viscosity Model Coefficients

AVHL(HLI) Linear ( $A_1$ ) coefficients of viscosity model

/ SiO <sub>2</sub>	-10.5899
B <sub>2</sub> O <sub>3</sub>	-24.4127
Na <sub>2</sub> O	2.0200
Li <sub>2</sub> O	5.4558
CaO	3.9535
MgO	5.3088
Fe <sub>2</sub> O <sub>3</sub>	-13.6326
Al <sub>2</sub> O <sub>3</sub>	1.4998
ZrO <sub>2</sub>	-0.3590
Other	-2.3815 /

BVHL(HLI)  $B_1$  coefficients of viscosity model

/ SiO <sub>2</sub>	19236.3263
B <sub>2</sub> O <sub>3</sub>	15922.8410
Na <sub>2</sub> O	-12965.4177
Li <sub>2</sub> O	-39177.2042
CaO	-18671.4525
MgO	-11943.9611
Fe <sub>2</sub> O <sub>3</sub>	14559.3344
Al <sub>2</sub> O <sub>3</sub>	9524.4388
ZrO <sub>2</sub>	4618.1457
Other	1710.2061 /

TVHL(HLI)  $T_1$  coefficients of viscosity model

/ SiO <sub>2</sub>	76.1127
B <sub>2</sub> O <sub>3</sub>	263.4849
Na <sub>2</sub> O	425.7163
Li <sub>2</sub> O	474.4299
CaO	1065.8248
MgO	752.2421
Fe <sub>2</sub> O <sub>3</sub>	43.6384
Al <sub>2</sub> O <sub>3</sub>	178.5252

ZrO2	540.5086
Other	270.7406 /

\* Electrical Conductivity Model Coefficients

AEHL(HLI) Linear (A) coefficients of electrical conductivity model

/ SIO2	8.112232
B2O3	12.816943
NA2O	6.054906
LI2O	7.473173
CAO	14.408770
MGO	10.390290
FE2O3	9.940459
AL2O3	7.138001
ZRO2	7.934310
OTHER	18.114167 /

BEHL(HLI) Coefficients of  $x_i/T$  terms of Arrhenius electrical conductivity model

/ SIO2	-10283
B2O3	-15135
NA2O	7089.475578
LI2O	22484
CAO	-18769
MGO	-13414
FE2O3	-10608
AL2O3	-8227.180158
ZRO2	-9723.860686
OTHER	-20653 /

\* Durability Model Coefficients, MCC-1, Boron

ADMBHL(HLI) Linear (A<sub>i</sub>) coefficients of Durability (MCC)  
model (for Boron)

/ SiO <sub>2</sub>	-1.566678
B <sub>2</sub> O <sub>3</sub>	15.884339
Na <sub>2</sub> O	11.442222
Li <sub>2</sub> O	13.358676
CaO	-39.786596
MgO	13.631246
Fe <sub>2</sub> O <sub>3</sub>	6.32358
Al <sub>2</sub> O <sub>3</sub>	-8.841645
ZrO <sub>2</sub>	-1.26597
Other	5.459963 /

BDMBHL(HLI,HLJ) Cross term coefficients of Durability  
(MCC) model (for Boron)

BDMBHL(HLI, HLJ) = 0;  
BDMBHL('Al<sub>2</sub>O<sub>3</sub>', 'Al<sub>2</sub>O<sub>3</sub>') = 69.05324;  
BDMBHL('B<sub>2</sub>O<sub>3</sub>', 'Al<sub>2</sub>O<sub>3</sub>') = -80.041445;  
BDMBHL('SiO<sub>2</sub>', 'CaO') = 70.192224;  
BDMBHL('CaO', 'CaO') = 111.801884;  
BDMBHL('Na<sub>2</sub>O', 'MgO') = -58.424388;

\* Durability Model Coefficients, PCT, Boron

ADPBHL(HLI) Linear (A<sub>i</sub>) coefficients of Durability (PCT)  
model (for Boron)

/ SiO <sub>2</sub>	-4.379969
B <sub>2</sub> O <sub>3</sub>	-3.080004
Na <sub>2</sub> O	21.440509
Li <sub>2</sub> O	24.173993
CaO	14.06971
MgO	-49.728818
Fe <sub>2</sub> O <sub>3</sub>	-1.311381
Al <sub>2</sub> O <sub>3</sub>	-39.578233
ZrO <sub>2</sub>	-11.416302
Other	4.208259 /

BDPBHL(HLI,HLJ) Cross term coefficients of Durability  
(PCT) model for Boron

BDPBHL(HLI, HLJ) = 0;  
BDPBHL('Al<sub>2</sub>O<sub>3</sub>', 'Al<sub>2</sub>O<sub>3</sub>') = 104.218254;  
BDPBHL('B<sub>2</sub>O<sub>3</sub>', 'B<sub>2</sub>O<sub>3</sub>') = 76.658177;  
BDPBHL('SiO<sub>2</sub>', 'MgO') = 117.171887;  
BDPBHL('Na<sub>2</sub>O', 'CaO') = -120.88413;  
BDPBHL('B<sub>2</sub>O<sub>3</sub>', 'CaO') = -91.140649;  
BDPBHL('MgO', 'ZrO<sub>2</sub>') = 122.085204;

\* Durability Model Coefficients, PCT, Lithium

ADPLHL(HLI) Linear (A) coefficients of Durability (PCT)  
model (for Li)

/ SiO2	-2.951747
B2O3	-5.82881
Na2O	18.742069
Li2O	18.904144
CaO	14.066675
MgO	14.47951
Fe2O3	-5.631035
Al2O3	-31.380797
ZrO2	-10.211191
Other	2.652327 /

BDPLHL(HLI,HLJ) Cross term coefficients of Durability  
(PCT) model for Li

BDPLHL(HLI, HLJ) = 0;  
BDPLHL('Al2O3', 'Al2O3') = 94.025208;  
BDPLHL('B2O3', 'B2O3') = 76.945946;  
BDPLHL('MgO', 'Al2O3') = -134.707636;  
BDPLHL('B2O3', 'CaO') = -94.6921;  
BDPLHL('Na2O', 'CaO') = -81.928013;  
BDPLHL('Na2O', 'Al2O3') = -43.351121;  
BDPLHL('Fe2O3', 'Al2O3') = 75.988423;

\* Durability Model Coefficients, PCT, Sodium

ADPNHL(HLI) Linear (A) coefficients of Durability (PCT)  
model (for Na)

/ SiO2	-2.57681
B2O3	-10.546234
Na2O	15.284061
Li2O	4.552893
CaO	7.532897
MgO	-30.228288
Fe2O3	-1.307042
Al2O3	-34.646706
ZrO2	-9.216464
Other	2.496056 /

BDPNHL(HLI,HLJ) Cross term coefficients of Durability  
(PCT) model for Na

BDPNHL(HLI, HLJ) = 0;  
BDPNHL('SiO2', 'MgO') = 75.062121;  
BDPNHL('B2O3', 'CaO') = -77.102749;  
BDPNHL('Na2O', 'Li2O') = 126.135743;  
BDPNHL('B2O3', 'B2O3') = 98.286041;  
BDPNHL('Li2O', 'MgO') = 133.332409;  
BDPNHL('Al2O3', 'Al2O3') = 81.617476;

\* Linear Liquidus Temperature Model coefficients

ATLClHL(HLI) Linear ( $A_i$ ) coefficients of liquidus temp  
model for clinopyroxene

/ SiO <sub>2</sub>	955.648709
B <sub>2</sub> O <sub>3</sub>	314.718016
Na <sub>2</sub> O	38.828095
Li <sub>2</sub> O	-207.052312
CaO	1372.437773
MgO	2387.619243
Fe <sub>2</sub> O <sub>3</sub>	1506.687256
Al <sub>2</sub> O <sub>3</sub>	1319.781389
ZrO <sub>2</sub>	1844.501017
Other	1357.404454 /

ATLSpHL(HLI) Linear ( $A_i$ ) coefficients of liquidus temp  
model for spinel

/ SiO <sub>2</sub>	989.305474
B <sub>2</sub> O <sub>3</sub>	666.419006
Na <sub>2</sub> O	3.772076
Li <sub>2</sub> O	-128.772539
CaO	1366.211045
MgO	2830.582448
Fe <sub>2</sub> O <sub>3</sub>	2256.001202
Al <sub>2</sub> O <sub>3</sub>	1735.02572
ZrO <sub>2</sub>	928.109425
Other	1005.555325 /

ATLZrHL(HLI) Linear ( $A_i$ ) coefficients of liquidus temp  
model for Zr-containing crystals

/ SiO <sub>2</sub>	753.776337
B <sub>2</sub> O <sub>3</sub>	1095.830409
Na <sub>2</sub> O	74.313813
Li <sub>2</sub> O	-956.393494
CaO	886.76338
MgO	2458.467726
Fe <sub>2</sub> O <sub>3</sub>	1461.039068
Al <sub>2</sub> O <sub>3</sub>	1138.061069
ZrO <sub>2</sub>	4541.994125
Other	657.994105 /

## **APPENDIX B**

### **Covariance Matrices for OWL Uncertain Model**

## Appendix B

### Covariance Matrices for OWL Uncertainty Model

```
*-----*
* Module Name:  HL_Covar.FY95NL.mdl
*
* Description:
*  Declares and defines parameters for uncertainty model calculations
*
* Original Author:  Mark Hoza
* Date Created:    1994/08/19
*
* Modification History
*
* date      author  description
* 94/12/07  MH V1.0 - original version, based on
*                               CVS-II, Phase 2 (FY93 report)
* 94/12/07  MH V1.1 - based on F95 property models
*
* Comments:
*  covariance matrices for nonlinear glass property models,
*
*-----*
```

```
* Declare and define parameters for uncertainty calculation
```

#### SCALARS

```
SDVHL  std dev (sqrt variance) of viscosity model
CIVHL  95% confidence interval multiplier viscosity for model
/1.646407/
CBVHL  95% confidence band multiplier for viscosity model
/6.364486/
UMltVHL Uncertainty multiplier (= CI or CB) assigned at runtime

SDEHL  std dev (sqrt variance) of E-Cond model
/0.159812/
CIEHL  95% confidence interval multiplier for E-Cond model
/1.648166/
CBEHL  95% confidence band multiplier for E-Cond model
/5.36027425/
UMltEHL Uncertainty multiplier (= CI or CB) assigned at runtime

SDDMBHL  std dev (sqrt variance) of DMB model           /0.316670/
CIDMBHL  95% confidence interval multiplier for DMB model /1.660391/
```

CBDMBHL 95% confidence band multiplier for DMB model /4.883219/  
 UMltDMBHL Uncertainty multiplier (= CI or CB) assigned at runtime

SDDPBHL std dev (sqrt variance) of DPB model /0.51050/  
 CIDPBHL 95% confidence interval multiplier for DPB model /1.659219/  
 CBDPBHL 95% confidence band multiplier for DPB model  
 /5.11187451/  
 UMltDPBHL Uncertainty multiplier (= CI or CB) assigned at runtime

SDDPLHL std dev (sqrt variance) of DPL model /0.430615/  
 CIDPLHL 95% confidence interval multiplier for DPL model /1.659356/  
 CBDPLHL 95% confidence band multiplier for DPL model  
 /5.09036423/  
 UMltDPLHL Uncertainty multiplier (= CI or CB) assigned at runtime

SDDPNHL std dev (sqrt variance) of DPN model /0.439760/  
 CIDPNHL 95% confidence interval multiplier for DPN model /1.659219/  
 CBDPNHL 95% confidence band multiplier for DPN model  
 /5.0141081/  
 UMltDPNHL Uncertainty multiplier (= CI or CB) assigned at runtime

SDTLC1HL std dev (sqrt variance) of TL-C1 model  
 /17.667/  
 CITLC1HL 95% confidence interval multiplier for TL-C1 model /1.734/  
 CBTLC1HL 95% confidence band multiplier for TL-C1 model /4.446/  
 UMltTLC1HL Uncertainty multiplier (= CI or CB) assigned at runtime

SDTLSpHL std dev (sqrt variance) of TL-Sp model  
 /50.648/  
 CITLSpHL 95% confidence interval multiplier for TL-Sp model /1.729/  
 CBTLSpHL 95% confidence band multiplier for TL-Sp model /4.422/  
 UMltTLSpHL Uncertainty multiplier (= CI or CB) assigned at runtime

SDTLZrHL std dev (sqrt variance) of TL-Zr model  
 /51.650/  
 CITLZrHL 95% confidence interval multiplier for TL-Zr model /1.782/  
 CBTLZrHL 95% confidence band multiplier for TL-Zr model /4.677/  
 UMltTLZrHL Uncertainty multiplier (= CI or CB) assigned at runtime

TABLE CovarVHL(EXTDHLI,EXTDHLJ) Covar matrix for viscosity for Fulcher model

	SiO2	B2O3	Na2O	Li2O
SiO2	1.45	-1.77	-1.11	-3.19
B2O3	-1.77	5.44	1.33	3.99
Na2O	-1.11	1.33	6.27	1.21
Li2O	-3.19	3.99	1.21	28.44
CaO	-0.95	-0.51	-1.17	0.67
MgO	-1.34	0.69	-0.4	2.46
Fe2O3	-1.71	0.46	0.6	1.99
Al2O3	-0.27	-0.87	-2.99	-3.53
ZrO2	-0.74	0.35	-1.32	-5.07
Other	-1.23	0.57	-1.64	-1.03
SiO2TS	-1623.82	1940.71	1181.677	3504.86
B2O3TS	1953.2	-6059.14	-1532.758	-4321.55
Na2OTS	1251.12	-1470.25	-6904.259	-1178.44
Li2OTS	3581.96	-4333.24	-968.43	-31806.81
CaOTS	1072.31	699.29	1441.571	-600.24
MgOTS	1516	-666.54	482.642	-2419.01
Fe2O3TS	1874.37	-474.39	-689.163	-2193.94
Al2O3TS	278.55	979.48	3370.684	3755.13
ZrO2TS	794.34	-264.74	1475.635	5806.68
OtherTS	1336.84	-592.46	1950.806	1227.74
SiO2BXTSQ	37.02	-45.44	-28.23	-80.09
B2O3BXTSQ	-45.35	136.93	33.97	102.06
Na2OBXTSQ	-29.12	34.97	162.63	30.36
Li2OBXTSQ	-81.52	106.36	27.62	734.16
CaOBXTSQ	-23.71	-15.99	-32.26	7.12
MgOBXTSQ	-34.47	14.5	-9.69	55.47
Fe2O3BXTSQ	-43.01	10.75	16.19	50.06
Al2O3BXTSQ	-5.63	-21.69	-77.87	-92.96
ZrO2BXTSQ	-16.89	5.96	-34.61	-139.08
OtherBXTSQ	-30.26	14.44	-41.22	-27.75

+	ZrO2	Other	SiO2TS	B2O3TS
SiO2	0.74	-1.23	-1623.82	1953.2
B2O3	0.35	0.57	1940.71	-6059.14
Na2O	-1.32	-1.64	1181.677	-1532.758
Li2O	-5.07	-1.03	3504.86	-4321.55
CaO	0.9	1.8	1019.95	689.39
MgO	1	0.49	1481.09	-717.47
Fe2O3	1.42	2.09	1884.94	-480.46
Al2O3	3.78	2.23	293.47	990.36
ZrO2	12.09	1.24	793.12	-321.07
Other	1.24	11.91	1324.03	614.99
SiO2TS	793.12	1324.03	1870487.98	-2174808.43
B2O3TS	-321.07	614.99	-2174808.43	6911647.08
Na2OTS	1457.88	1901.55	-1388107.47	1722995.12
Li2OTS	5798.06	1280.68	-4071108.37	4741411.64
CaOTS	-986.33	-1936	-1209626.91	-940971.25
MgOTS	-1199.84	-372.21	-1748998.88	683758.94
Fe2O3TS	-1648.22	-2341.06	-2118947.65	510127.5
Al2O3TS	-4186.48	-2509.76	-325935.74	-1167359.69
ZrO2TS	-13426.36	-1295.28	-899635.65	182513.69
OtherTS	-1307.52	-13322.3	-1492336.93	617096.84
SiO2BXTSQ	-17.33	-30.39	-42964.92	51327.42
B2O3BXTSQ	6.45	13.75	51167.27	-157858.67
Na2OBXTSQ	-34.7	-40.85	32294.28	-41286.95
Li2OBXTSQ	-136.6	-26.78	92896.34	-117217.92
CaOBXTSQ	23.33	47.92	26659.23	21781.69
MgOBXTSQ	26.44	13.38	39980.28	-14841.29
Fe2O3BXTSQ	36.45	49.53	49308.93	-11629.71
Al2O3BXTSQ	97.46	53.88	6797.28	26412.27
ZrO2BXTSQ	309.22	26.9	19467.74	-3795.57
OtherBXTSQ	26.72	304.11	34100.16	-15015.37

+	Na2OTS	Li2OTS	CaOTS	MgOTS
SiO2	1251.12	3581.96	1072.31	1516
B2O3	-1470.25	-4333.24	699.29	-666.54
Na2O	-6904.259	-968.43	1441.571	482.642
Li2O	-1178.44	-31806.81	-600.24	-2419.01
CaO	1316.77	-648.9	-22092.26	-6190.94
MgO	461.52	-2630.74	-6020.58	-19211.27
Fe2O3	-617.24	-2071.51	-1055.19	-713.01
Al2O3	3347.69	3730.45	920.15	-575.42
ZrO2	1457.88	5798.06	-986.33	-1199.84
Other	1901.55	1280.68	-1936	-372.21
SiO2TS	-1388107.47	-4071108.37	-1209626.91	1748998.88
B2O3TS	1722995.12	4741411.64	-940971.25	63758.94
Na2OTS	7790388.71	1041302.59	-1570877.07	-521394.29
Li2OTS	1041302.59	36672881.49	749332.21	2653888.85
CaOTS	-1570877.07	749332.21	25095263.86	7269517.5
MgOTS	-521394.29	2653888.85	7269517.5	22309878.08
Fe2O3TS	691677.59	2216637.63	885876.72	859413.23
Al2O3TS	-3852812.44	-4105376.92	-1283815.55	612756.37
ZrO2TS	-1645121.84	-6742289.24	1168402.71	1470012.6
OtherTS	-2283900.18	-1561222.23	2227184.63	236061.19
SiO2BXTSQ	33225.89	93419.68	27070.84	41289.25
B2O3BXTSQ	-38991.58	-113766.42	22649.44	-13225.27
Na2OBXTSQ	-184403.04	-26731.62	36542.24	11132.09
Li2OBXTSQ	-29387.2	-852861.31	-6440.79	-62242.1
CaOBXTSQ	35800.4	-8811.1	-580349.24	-163290.15
MgOBXTSQ	11070.14	-59974.41	-159628.25	-518474.1
Fe2O3BXTSQ	-16433.39	-50806.84	-26620.04	-24041.44
Al2O3BXTSQ	89785.44	103196.32	27159.95	-19324.8
ZrO2BXTSQ	38988.31	162696.87	-26551.46	-34711.93
OtherBXTSQ	49026.19	36824.08	-53676.12	-10773.44

+	Fe2O3TS	Al2O3TS	ZrO2TS	OtherTS
SiO2	1874.37	278.55	794.34	1336.84
B2O3	-474.39	979.48	-264.74	-592.46
Na2O	-689.163	3370.684	1475.635	1950.806
Li2O	-2193.94	3755.13	5806.68	1227.74
CaO	-1029.44	977.41	-1033.44	-2033.51
MgO	-663.22	-632.92	-1138.93	-381.11
Fe2O3	-8656.58	-2065.53	-1655.27	-2319.48
Al2O3	-2026.5	-8229.95	-4168.48	-2538.29
ZrO2	-1648.22	-4186.48	-13426.36	-1307.52
Other	-2341.06	-2509.76	-1295.28	-13322.3
SiO2TS	-2118947.65	-325935.74	-899635.65	-1492336.93
B2O3TS	510127.5	-1167359.69	182513.69	617096.84
Na2OTS	691677.59	-3852812.44	-1645121.84	-2283900.13
Li2OTS	2216637.63	-4105376.92	-6742289.24	-1561222.2
CaOTS	885876.72	-1283815.55	1168402.71	2227184.6
MgOTS	859413.23	612756.37	1470012.6	236061.19
Fe2O3TS	10149083.9	2411446.29	2011910.12	2649988.1
Al2O3TS	2411446.29	9481972.9	4767106.17	2957260.6
ZrO2TS	2011910.12	4767106.17	15321751.33	1440152.9
OtherTS	2649988.14	2957260.69	1440152.97	15383114.9
SiO2BXTSQ	49439.22	7099.13	19976.02	34650.96
B2O3BXTSQ	-11805.12	26602.73	-3027.62	-13763.3
Na2OBXTSQ	-18573.07	90478.07	39658.12	49832.71
Li2OBXTSQ	-53145.48	102443.7	160340.07	34072.41
CaOBXTSQ	-25885.54	27953.9	-27669.97	-55325.37
MgOBXTSQ	-24628.35	-18751.15	-33334.75	-10527.49
Fe2O3BXTSQ	-232468.32	-55002.63	-45702.66	-56713.15
Al2O3BXTSQ	-53845.9	-223612.39	-112462.34	-64708.02
ZrO2BXTSQ	-44892.45	-112013.32	-356977.2	-30563.03
OtherBXTSQ	-58149.36	-64063.98	-29990.83	-355966.18

+	SiO2BXTSQ	B2O3BXTSQ	Na2OBXTSQ	Li2OBXTSQ
SiO2	37.02	-45.35	-29.12	-81.52
B2O3	-45.44	136.93	34.97	106.36
Na2O	-28.23	33.97	162.63	27.62
Li2O	-80.09	102.06	30.36	734.16
CaO	-22.98	-17.28	-29.5	6.82
MgO	-34.82	13.83	-9.13	62.68
Fe2O3	-43.37	11.24	16.4	49.12
Al2O3	-6.12	-22.01	-78.18	-92.27
ZrO2	-17.33	6.45	-34.7	-136.6
Other	-30.39	13.75	-40.85	-26.78
SiO2TS	-42964.92	51167.27	32294.28	92896.34
B2O3TS	51327.42	-157858.67	-41286.95	-117217.92
Na2OTS	33225.89	-38991.58	-184403.04	-29387.2
Li2OTS	93419.68	-113766.42	-26731.62	-852861.31
CaOTS	27070.84	22649.44	36542.24	-6440.79
MgOTS	41289.25	-13225.27	11132.09	-62242.1
Fe2O3TS	49439.22	-11805.12	-18573.07	-53145.48
Al2O3TS	7099.13	26602.73	90478.07	102443.7
ZrO2TS	19976.02	-3027.62	39658.12	160340.07
OtherTS	34650.96	-13763.3	49832.71	34072.41
SiO2BXTSQ	1005.1	-1215.99	-790.49	-2176.16
B2O3BXTSQ	-1215.99	3671.299	37.09	2800.1
Na2OBXTSQ	-790.49	937.09	4433.55	786.69
Li2OBXTSQ	-2176.16	2800.1	786.69	20228.3
CaOBXTSQ	-610.09	-543.73	-822.37	-4.22
MgOBXTSQ	-967.02	275.13	-222.64	1451.27
Fe2O3BXTSQ	-1167.51	275.21	430.64	1201.38
Al2O3BXTSQ	-157.43	-622.6	-2131.18	-2592.13
ZrO2BXTSQ	-445.95	47.49	-948.37	-3894.65
OtherBXTSQ	-810.17	326.5	-1071.82	-819.03

+	CaOBXTSQ	MgOBXTSQ	Fe2O3BXTSQ	Al2O3BXTSQ
SiO2	-23.71	-34.47	-43.01	-5.63
B2O3	-15.99	14.5	10.75	-21.69
Na2O	-32.26	-9.69	16.19	-77.87
Li2O	7.12	55.47	50.06	-92.96
CaO	507.49	135.11	29.31	-19.82
MgO	134.03	440.94	18.37	18.95
Fe2O3	29.28	20.02	195.48	44.92
Al2O3	-19.61	16.8	45.17	191.84
ZrO2	23.33	26.44	36.45	97.46
Other	47.92	13.38	49.53	53.88
SiO2TS	26659.23	39980.28	49308.93	6797.28
B2O3TS	21781.69	-14841.29	-11629.71	26412.27
Na2OTS	35800.4	11070.14	-16433.39	89785.44
Li2OTS	-8811.1	-59974.41	-50806.84	103196.32
CaOTS	-580349.24	-159628.25	-26620.04	27159.95
MgOTS	-163290.15	-518474.1	-24041.44	-19324.8
Fe2O3TS	-25885.54	-24628.35	-232468.32	-53845.9
Al2O3TS	27953.9	-18751.15	-55002.63	-223612.39
ZrO2TS	-27669.97	-33334.75	-45702.66	-112462.34
OtherTS	-55325.37	-10527.49	-56713.15	-64708.02
SiO2BXTSQ	-610.09	-967.02	-1167.51	-157.43
B2O3BXTSQ	-543.73	275.13	275.21	-622.66
Na2OBXTSQ	-822.37	-222.64	430.64	-2131.18
Li2OBXTSQ	-4.22	1451.27	201.38	-2592.13
CaOBXTSQ	13615.6	3661.25	713.75	-598.43
MgOBXTSQ	3661.25	12314.43	.664.7	563.74
Fe2O3BXTSQ	713.75	664.79	5442.47	1272.93
Al2O3BXTSQ	-598.43	563.74	1272.93	5371.77
ZrO2BXTSQ	639.94	821.29	1051.39	2697.92
OtherBXTSQ	1342.32	359.5	1260.59	1434.92

+	ZrO2BXTSQ	OtherBXTSQ
SiO2	-16.89	-30.26
B2O3	5.96	14.44
Na2O	-34.61	-41.22
Li2O	-139.08	-27.75
CaO	23.53	48.93
MgO	26.22	13.91
Fe2O3	35.91	50.27
Al2O3	96.58	53.93
ZrO2	309.22	26.72
Other	26.9	304.11
SiO2TS	19467.74	34100.16
B2O3TS	-3795.57	-15015.37
Na2OTS	38988.31	49026.19
Li2OTS	162696.87	36824.08
CaOTS	-26551.46	-53676.12
MgOTS	-34711.93	-10773.44
Fe2O3TS	-44892.45	-58149.36
Al2O3TS	-112013.32	-64063.98
ZrO2TS	-356977.2	-29990.83
OtherTS	-30563.03	-355966.18
SiO2BXTSQ	-445.95	-810.17
B2O3BXTSQ	47.49	326.5
Na2OBXTSQ	-948.37	-1071.82
Li2OBXTSQ	-3894.65	-819.03
CaOBXTSQ	639.94	1342.32
MgOBXTSQ	821.29	359.5
Fe2O3BXTSQ	1051.39	1260.59
Al2O3BXTSQ	2697.92	1434.92
ZrO2BXTSQ	8461.59	654.17
OtherBXTSQ	654.17	8411.84

TABLE XtXIEHL(EXTDHLI,EXTDHLJ) (XtX)-1 matrix for e-conductivity for Arrhenius model

	SIO2	B2O3	NA2O	LI2O
SIO2	28.092975637	-20.45039003	-29.84457112	-42.81692192
B2O3	-20.45039003	98.201107298	13.388919134	-0.731121548
NA2O	-29.84457112	13.388919134	136.58485143	55.311274387
LI2O	-42.81692192	-0.731121548	55.311274387	530.3180915
CAO	-4.986749218	-34.25345149	-18.04318818	-26.54016321
MGO	-20.02243047	-11.8316473	-1.545640131	11.766394373
FE2O3	-35.97951226	1.1701434315	2.1687742523	-29.21573563
AL2O3	-23.18396659	-17.45734375	-38.07137382	-70.58656158
ZRO2	-23.51812887	2.3132710911	-29.00100872	-66.18703145
OTHER	-40.39062298	6.6252635466	0.4230065669	-10.38519723
SIO2T	-37860.79547	27503.05649	40617.778907	57973.781349
B2O3T	27583.03275	-132113.1317	-18715.1158	523.09514684
NA2OT	40502.851538	-18458.48681	-184878.6846	-76381.23859
LI2OT	57885.236937	1149.5861836	-76872.23545	-719254.6829
CAOT	5995.1796458	47173.254651	24530.71252	38722.584613
MGOT	26451.291556	16724.344163	1972.4283066	-12734.89674
FE2O3T	48126.772416	-424.953368	-2390.797548	42050.139166
AL2O3T	31121.301095	23724.703355	51750.813024	96622.375673
ZRO2T	31197.940079	-2829.739527	40043.03838	92435.255467
OTHERT	54491.86345	-9859.427878	-418.326177	13881.736414

+	CAO	MGO	FE2O3	AL2O3
SIO2	-4.986749218	-20.02243047	-35.97951226	-23.18396659
B2O3	-34.25345149	-11.8316473	1.1701434315	-17.45734375
NA2O	-18.04318818	-1.545640131	2.1687742523	-38.07137382
LI2O	-26.54016321	11.766394373	-29.21573563	-70.58656158
CAO	317.65526608	97.783369763	-43.54684485	13.508844253
MGO	97.783369763	388.16391146	-7.008590807	18.674264402
FE2O3	-43.54684485	-7.008590807	198.64556098	90.186896086
AL2O3	13.508844253	18.674264402	90.186896086	174.82681363
ZRO2	2.4829211437	-12.79878641	64.863442981	103.5199129
OTHER	26.56790329	9.9874667161	54.273151565	44.50542219
SIO2T	5773.7526739	26529.575558	48016.429502	31053.349132
B2O3T	47439.851166	16600.677992	-329.4988369	23908.189628
NA2OT	24995.233168	2027.948815	-2070.153742	51660.919489
LI2OT	40326.696617	-13222.15303	42907.721279	96720.003927
CAOT	-427333.283	-131540.4662	61382.639394	-18392.31355
MGOT	-131257.6583	-521997.1338	7960.9014822	-24371.74392
FE2O3T	61444.706721	7965.1251207	-268773.571	-122707.9603
AL2O3T	-18877.40706	-24450.08528	-123079.6132	-235961.6059
ZRO2T	-4998.637803	17305.990575	-89062.0384	-139727.7733
OTHERT	-35557.0191	-11591.57169	-73096.78018	-60091.03931

+	ZRO2	OTHER	SIO2T	B203T
SIO2	-23.51812887	-40.39062298	-37860.79547	27583.03275
B203	2.3132710911	6.6252635466	27503.05649	-132113.1317
NA20	-29.00100872	0.4230065669	40617.778907	-18715.1158
LI20	-66.18703145	-10.38519723	57973.781349	523.09514684
CAO	2.4829211437	26.56790329	5773.7526739	47439.851166
MGO	-12.79878641	9.9874667161	26529.575558	16600.677992
FE203	64.863442981	54.273151565	48016.429502	-329.4988369
AL203	103.5199129	44.50542219	31053.349132	23908.189628
ZRO2	255.16510207	19.997363614	31269.275856	-2785.293069
OTHER	19.997363614	313.59463685	54347.145394	-9621.912498
SIO2T	31269.275856	54347.145394	51445874.836	-37457678
B203T	-2785.293069	-9621.912498	-37457678	179149283.03
NA20T	39867.937675	-416.6076008	-55566186.41	26063878.806
LI20T	91868.365386	14346.412016	-79315954.33	-303172.3355
CAOT	-4760.023603	-34704.31884	-7019489.964	-65460681.27
MGOT	17181.878318	-11229.47761	-35395029.29	-23510977.71
FE203T	-88933.1939	-72668.95107	-64735263.39	-994534.5394
AL203T	-139666.6431	-60196.21059	-41865014.96	-32867774.02
ZRO2T	-344912.5756	-24655.63452	-41691554.7	3170082.758
OTHERT	-24699.04842	-424017.7718	-73761132.2	14190099.93

+	NA20T	LI20T	CAOT	MGOT
SIO2	40502.851538	57885.236937	5995.1796458	26451.291556
B203	-18458.48681	1149.5861836	47173.254651	16724.344163
NA20	-184878.6846	-76872.23545	24530.71252	1972.4283066
LI20	-76381.23859	-719254.6829	38722.584613	-12734.89674
CAO	24995.233168	40326.696617	-427333.283	-131257.6583
MGO	2027.948815	-13222.15303	-131540.4662	-521997.1338
FE203	-2070.153742	42907.721279	61382.639394	7960.9014822
AL203	51660.919489	96720.003927	-18392.31355	-24371.74392
ZRO2	39867.937675	91868.365386	-4760.023603	17181.878318
OTHER	-416.6076008	14346.412016	-34704.31884	-11229.47761
SIO2T	-55566186.41	-79315954.33	-7019489.964	-35395029.29
B203T	26063878.806	-303172.3355	-65460681.27	-23510977.71
NA20T	252022294.84	107244444.88	-34000826.46	-2556276.204
LI20T	107244444.88	984263828.86	-57859271.82	14068316.934
CAOT	-34000826.46	-57859271.82	579397752.47	177846534.47
MGOT	-2556276.204	14068316.934	177846534.47	707510770.6
FE203T	2114285.8744	-61405019.61	-86775503.2	-8673485.43
AL203T	-70845615.38	-133806529.1	25529310.349	32157352.831
ZRO2T	-55476684.1	-129480357.9	8602902.44	-22973931.8
OTHERT	312521.81771	-19693647.14	46556005.505	12644634.017

+	FE2O3T	AL2O3T	ZRO2T	OTHERT
SIO2	48126.772416	31121.301095	31197.940079	54491.86345
B2O3	-424.953368	23724.703355	-2829.739527	-9859.427878
NA2O	-2390.797548	51750.813024	40043.03838	-418.326177
LI2O	42050.139166	96622.375673	92435.255467	13881.736414
CAO	61444.706721	-18877.40706	-4998.637803	-35557.0191
MGO	7965.1251207	-24450.08528	17305.990575	-11591.57169
FE2O3	-268773.571	-123079.6132	-89062.0384	-73096.78018
AL2O3	-122707.9603	-235961.6059	-139727.7733	-60091.03931
ZRO2	-88933.1939	-139666.6431	-344912.5756	-24699.04842
OTHER	-72668.95107	-60196.21059	-24655.63452	-424017.7718
SIO2T	-64735263.39	-41865014.96	-41691554.7	-73761132.2
B2O3T	-994534.5394	-32867774.02	3170082.758	14190099.93
NA2OT	2114285.8744	-70845615.38	-55476684.1	312521.81771
LI2OT	-61405019.61	-133806529.1	-129480357.9	-19693647.14
CAOT	-86775503.2	25529310.349	8602902.44	46556005.505
MGOT	-8673485.43	32157352.831	-22973931.8	12644634.017
FE2O3T	366510680.24	168475443.08	122779753.52	98302517.384
AL2O3T	168475443.08	320836573.79	189945701.25	81958155.025
ZRO2T	122779753.52	189945701.25	469761449.43	30513863.347
OTHERT	98302517.384	81958155.025	30513863.347	577571620.37

+	FE2O3T	AL2O3T	ZRO2T	OTHERT
SIO2	48126.772416	31121.301095	31197.940079	54491.86345
B2O3	-424.953368	23724.703355	-2829.739527	-9859.427878
NA2O	-2390.797548	51750.813024	40043.03838	-418.326177
LI2O	42050.139166	96622.375673	92435.255467	13881.736414
CAO	61444.706721	-18877.40706	-4998.637803	-35557.0191
MGO	7965.1251207	-24450.08528	17305.990575	-11591.57169
FE2O3	-268773.571	-123079.6132	-89062.0384	-73096.78018
AL2O3	-122707.9603	-235961.6059	-139727.7733	-60091.03931
ZRO2	-88933.1939	-139666.6431	-344912.5756	-24699.04842
OTHER	-72668.95107	-60196.21059	-24655.63452	-424017.7718
SIO2T	-64735263.39	-41865014.96	-41691554.7	-73761132.2
B2O3T	-994534.5394	-32867774.02	3170082.758	14190099.93
NA2OT	2114285.8744	-70845615.38	-55476684.1	312521.81771
LI2OT	-61405019.61	-133806529.1	-129480357.9	-19693647.14
CAOT	-86775503.2	25529310.349	8602902.44	46556005.505
MGOT	-8673485.43	32157352.831	-22973931.8	12644634.017
FE2O3T	366510680.24	168475443.08	122779753.52	98302517.384
AL2O3T	168475443.08	320836573.79	189945701.25	81958155.025
ZRO2T	122779753.52	189945701.25	469761449.43	30513863.347
OTHERT	98302517.384	81958155.025	30513863.347	577571620.37

TABLE XtXIDMBHL(EXTDHLI,EXTDHLJ) (XtX)-1 matrix for durability  
(MCC-boron) for nonlinear model #2

	SiO2	B2O3	Na2O	Li2O
SiO2	2.314064663	-2.567515849	-1.771611935	-2.561434172
B2O3	-2.567515849	10.71497223	1.473221063	2.339172608
Na2O	-1.771611935	1.473221063	6.219445806	2.44182813
Li2O	-2.561434172	2.339172608	2.44182813	20.16526667
CaO	26.46779357	-32.4780005	-28.08068877	-19.0218942
MgO	-4.621367402	4.739153063	11.70361801	0.497095844
Fe2O3	-3.077346797	1.157586987	0.450833189	0.487725242
Al2O3	-6.878955353	5.639016069	0.300902747	0.722554656
ZrO2	-2.349999326	-0.400164019	-0.922679166	-1.357398579
Other	-2.902207371	0.877441567	0.867908464	-0.416554977
Al-Al	14.3212684	26.89477895	-0.677318881	-8.331236891
B-Al	21.03765703	-99.12010223	-11.23479144	-16.30610978
Si-Ca	-47.39513486	54.26224737	44.79058176	23.80475054
Ca-Ca	-49.28761271	61.49939443	75.81297115	103.7089561
Na-Mg	33.82429991	-29.80865457	-101.7866964	7.99652033
+	CaO	MgO	Fe2O3	Al2O3
SiO2	26.46779357	-4.621367402	-3.077346797	-6.878955353
B2O3	-32.4780005	4.739153063	1.157586987	5.639016069
Na2O	-28.08068877	11.70361801	0.450833189	0.300902747
Li2O	-19.0218942	0.497095844	0.487725242	0.722554656
CaO	872.3260644	-64.09891273	-32.88776077	-76.54009227
MgO	-64.09891273	88.58653901	1.123643603	12.67576193
Fe2O3	-32.88776077	1.123643603	10.20858926	10.04432011
Al2O3	-76.54009227	12.67576193	10.04432011	73.88617604
ZrO2	-28.02483877	-1.464186316	5.132571595	13.11785888
Other	-40.21538439	5.154499767	4.536849074	5.913500941
Al-Al	197.3003113	8.503161686	-20.90361449	-287.06573
B-Al	148.05194	-116.8313284	-4.034016994	-122.2937233
Si-Ca	-1382.468593	96.2518223	65.39292431	77.32248522
Ca-Ca	-2379.406614	236.2378923	12.9549973	453.5621028
Na-Mg	470.5883961	-669.8169964	-17.11029614	-144.8299367

+	ZrO2	Other	Al-Al	B-Al
SiO2	-2.349999326	-2.902207371	14.3212684	21.03765703
B2O3	-0.400164019	0.877441567	26.89477895	-99.12010223
Na2O	-0.922679166	0.867908464	-0.677318881	-11.23479144
Li2O	-1.357398579	-0.416554977	-8.331236891	-16.30610978
CaO	-28.02483877	-40.21538439	197.3003113	148.05194
MgO	-1.464186316	5.154499767	8.503161686	-116.8313284
Fe2O3	5.132571595	4.536849074	-20.90361449	-4.034016994
Al2O3	13.11785888	5.913500941	-287.06573	-122.2937233
ZrO2	11.94311208	4.274619069	-42.38187181	6.872282194
Other	4.274619069	13.69620004	-5.117178736	-2.175757773
Al-Al	-42.38187181	-5.117178736	1809.610947	-334.6593283
B-Al	6.872282194	-2.175757773	-334.6593283	1632.793525
Si-Ca	48.94437502	74.33336672	-7.151483437	-191.0198921
Ca-Ca	55.6998415	60.43354069	-2317.265377	-512.3589475
Na-Mg	5.547174186	-39.61447776	130.9912636	980.0419586

+	Si-Ca	Ca-Ca	Na-Mg
SiO2	-47.39513486	-49.28761271	33.82429991
B2O3	54.26224737	61.49939443	-29.80865457
Na2O	44.79058176	75.81297115	-101.7866964
Li2O	23.80475054	103.7089561	7.99652033
CaO	-1382.468593	-2379.406614	470.5883961
MgO	96.2518223	236.2378923	-669.8169964
Fe2O3	65.39292431	12.9549973	-17.11029614
Al2O3	77.32248522	453.5621028	-144.8299367
ZrO2	48.94437502	55.6998415	5.547174186
Other	74.33336672	60.43354069	-39.61447776
Al-Al	-7.151483437	-2317.265377	130.9912636
B-Al	-191.0198921	-512.3589475	980.0419586
Si-Ca	2604.289121	1612.802646	-640.5928249
Ca-Ca	1612.802646	19091.96369	-1813.18914
Na-Mg	-640.5928249	-1813.18914	6102.573843

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TABLE XtXIDPBHL(EXTDHLI,EXTDHLJ) (XtX)-1 matrix for durability  
(PCT-boron) for nonlinear model #2

	SiO2	B2O3	Na2O	Li2O
SiO2	2.025550884	-7.843010848	-1.562174282	-1.913845956
B2O3	-7.843010848	127.8551399	-1.261880635	-5.180156274
Na2O	-1.562174282	-1.261880635	5.94779636	1.830160416
Li2O	-1.913845956	-5.180156274	1.830160416	19.09379344
CaO	-6.59561083	21.70992183	11.40082643	-1.82019211
MgO	19.25282102	30.72195842	-20.77907722	-22.80114134
Fe2O3	-1.534072076	-7.516684861	0.931118217	1.293958744
Al2O3	-1.892548876	-27.58090618	0.036920525	-0.115705094
ZrO2	-1.245873556	-6.253772782	-0.751966856	-0.96649532
Other	-1.174535075	-9.680005944	0.891645591	-0.297383019
Al-Al	6.93690327	97.49400521	-1.647320414	-8.368937137
B-B	26.99830679	-532.0267433	9.64052991	29.64755549
Si-Mg	-41.75692287	-50.19434372	40.68731289	48.06547044
Na-Ca	28.09694493	-66.87147098	-93.75751826	31.86606391
B-Ca	27.86959893	-135.8101192	-16.07544596	-0.769622011
Mg-Zr	8.281956107	-77.33066002	28.20141261	7.755535044
+				
	CaO	MgO	Fe2O3	Al2O3
SiO2	-6.59561083	19.25282102	-1.534072076	-1.892548876
B2O3	21.70992183	30.72195842	-7.516684861	-27.58090618
Na2O	11.40082643	-20.77907722	0.931118217	0.036920525
Li2O	-1.82019211	-22.80114134	1.293958744	-0.115705094
CaO	115.1578768	-67.34134888	0.703049152	1.789123177
MgO	-67.34134888	876.3750037	-31.12045298	-61.26012455
Fe2O3	0.703049152	-31.12045298	7.862091853	6.477262323
Al2O3	1.789123177	-61.26012455	6.477262323	46.28727524
ZrO2	-0.468398989	-24.84589195	3.573483554	8.319855446
Other	2.993947196	-32.08430603	2.627512902	4.37552871
Al-Al	-3.591889695	168.6777909	-13.67189244	-222.4100746
B-B	-51.76801936	-215.9954617	35.12236785	125.5023829
Si-Mg	142.3246379	-1734.934184	64.06431548	121.4895207
Na-Ca	-550.2177318	335.7556505	-14.71741661	1.559706673
B-Ca	-450.6970826	273.7154942	4.464014376	-24.63415157
Mg-Zr	53.64645037	-468.6686934	-30.71135618	28.44779876

+	ZrO2	Other	Al-Al	B-B
SiO2	-1.245873556	-1.174535075	6.93690327	26.99830679
B2O3	-6.253772782	-9.680005944	97.49400521	-532.0267433
Na2O	-0.751966856	0.891645591	-1.647320414	9.64052991
Li2O	-0.96649532	-0.297383019	-8.368937137	29.64755549
CaO	-0.468398989	2.993947196	-3.591889695	-51.76801936
MgO	-24.84589195	-32.08430603	168.6777909	-215.9954617
Fe2O3	3.573483554	2.627512902	-13.67189244	35.12236785
Al2O3	8.319855446	4.37552871	-222.4100746	125.5023829
ZrO2	11.58160779	2.633215749	-19.59367803	27.22924089
Other	2.633215749	10.88614124	-4.940595861	43.56515161
Al-Al	-19.59367803	-4.940595861	1264.627734	-467.5838866
B-B	27.22924089	43.56515161	-467.5838866	2309.115685
Si-Mg	58.47901838	65.1233521	-316.7844291	382.0234168
Na-Ca	14.82039264	-19.34766795	-90.94732705	230.6880014
B-Ca	-6.2211561	-3.045051218	153.7446565	242.5974511
Mg-Zr	-132.5914074	1.330568177	-258.1160241	446.0701382

+	Si-Mg	Na-Ca	B-Ca	Mg-Zr
SiO2	-41.75692287	28.09694493	27.86959893	8.281956107
B2O3	-50.19434372	-66.87147098	-135.8101192	-77.33066002
Na2O	40.68731289	-93.75751826	-16.07544596	28.20141261
Li2O	48.06547044	31.86606391	-0.769622011	7.755535044
CaO	142.3246379	-550.2177318	-450.6970826	53.64645037
MgO	-1734.934184	335.7556505	273.7154942	-468.6686934
Fe2O3	64.06431548	-14.71741661	4.464014376	-30.71135618
Al2O3	121.4895207	1.559706673	-24.63415157	28.44779876
ZrO2	58.47901838	14.82039264	-6.2211561	-132.5914074
Other	65.1233521	-19.34766795	-3.045051218	1.330568177
Al-Al	-316.7844291	-90.94732705	153.7446565	-258.1160241
B-B	382.0234168	230.6880014	242.5974511	446.0701382
Si-Mg	3504.721854	-650.9363113	-573.188233	529.2925864
Na-Ca	-650.9363113	4360.052206	957.3737683	-491.1483645
B-Ca	-573.188233	957.3737683	3249.815669	-179.3444639
Mg-Zr	529.2925864	-491.1483645	-179.3444639	7905.832096

TABLE XtXIDPLHL(EXTDHLI,EXTDHLJ) (XtX)-1 matrix for durability  
(PCT-lithium) for nonlinear model #2

	SiO2	B2O3	Na2O	Li2O
SiO2	1.646745679	-7.583744375	-1.759170641	-1.231457367
B2O3	-7.583744375	133.0906284	-3.91693923	-2.842790557
Na2O	-1.759170641	-3.91693923	10.54213579	-0.632359036
Li2O	-1.231457367	-2.842790557	-0.632359036	19.69153179
CaO	-4.686874543	28.95605768	4.878019311	-0.344798638
MgO	-2.132533527	0.641915723	1.679470348	2.637449771
Fe2O3	-0.852619138	-11.36297078	0.535443944	-0.607935849
Al2O3	-2.649619511	-46.93281975	8.781062158	-7.103473818
ZrO2	-0.386923928	-7.582691747	-0.826341235	-1.827387654
Other	-0.340382239	-8.078948004	-0.002798843	-0.999336243
Al-Al	7.382393515	149.6763729	5.337240015	0.371250263
B-B	28.04184358	-547.3552778	14.99319496	19.69296564
Mg-Al	20.7777074	68.28203034	-34.34635283	-28.55514002
B-Ca	19.55015685	-164.5486119	13.41390787	-6.68513554
Na-Ca	20.05962385	-99.86496695	-61.52286717	24.10602745
Na-Al	10.15435433	59.03205868	-89.80537694	36.5740469
Fe-Al	0.459332966	126.4568466	16.91902114	29.52946111
+				
	CaO	MgO	Fe2O3	Al2O3
SiO2	-4.686874543	-2.132533527	-0.852619138	-2.649619511
B2O3	28.95605768	0.641915723	-11.36297078	-46.93281975
Na2O	4.878019311	1.679470348	0.535443944	8.781062158
Li2O	-0.344798638	2.637449771	-0.607935849	-7.103473818
CaO	118.7695968	8.618598835	-5.319001815	-19.32361359
MgO	8.618598835	25.57185623	-0.898747664	8.655104113
Fe2O3	-5.319001815	-0.898747664	11.34031673	19.36772926
Al2O3	-19.32361359	8.655104113	19.36772926	110.6955819
ZrO2	-2.545125592	1.195484115	2.464264187	9.420657356
Other	1.010206668	-0.098465756	0.671700287	-0.371088445
Al-Al	32.37635136	-23.50176981	-69.01515806	-408.7669945
B-B	-83.47630489	-0.212882043	46.59901153	189.9067133
Mg-Al	-81.11871194	-250.3942932	3.257496195	-194.2191505
B-Ca	-464.4720217	-26.28814366	25.56546363	58.46696437
Na-Ca	-567.9370578	-22.68986865	8.941366253	90.53505982
Na-Al	92.97134181	-13.87724934	-6.691177285	-176.5269958
Fe-Al	109.0295292	47.53201651	-162.366204	-442.9661573

+	ZrO2	Other	Al-Al	B-B
SiO2	-0.386923928	-0.340382239	7.382393515	28.04184358
B2O3	-7.582691747	-8.078948004	149.6763729	-547.3552778
Na2O	-0.826341235	-0.002798843	5.337240015	14.99319496
Li2O	-1.827387654	-0.999336243	0.371250263	19.69296564
CaO	-2.545125592	1.010206668	32.37635136	-83.47630489
MgO	1.195484115	-0.098465756	-23.50176981	-0.212882043
Fe2O3	2.464264187	0.671700287	-69.01515806	46.59901153
Al2O3	9.420657356	-0.371088445	-408.7669945	189.9067133
ZrO2	8.207245864	1.283148175	-28.82631721	31.4772274
Other	1.283148175	9.777318748	9.631219823	34.14046863
Al-Al	-28.82631721	9.631219823	2085.24609	-656.4018921
B-B	31.4772274	34.14046863	-656.4018921	2339.953753
Mg-Al	-16.05478862	1.245192103	607.6013841	-323.8175289
B-Ca	2.671814798	5.380746211	45.04882772	367.8969579
Na-Ca	19.21933426	-10.17954949	-212.167184	376.6153296
Na-Al	-2.923620623	3.165569279	-62.07872502	-180.8999145
Fe-Al	-20.61412192	23.40844588	1962.791702	-473.4303576

+	Mg-Al	B-Ca	Na-Ca	Na-Al
SiO2	20.7777074	19.55015685	20.05962385	10.15435433
B2O3	68.28203034	-164.5486119	-99.86496695	59.03205868
Na2O	-34.34635283	13.41390787	-61.52286717	-89.80537694
Li2O	-28.55514002	-6.68513554	24.10602745	36.5740469
CaO	-81.11871194	-464.4720217	-567.9370578	92.97134181
MgO	-250.3942932	-26.28814366	-22.68986865	-13.87724934
Fe2O3	3.257496195	25.56546363	8.941366253	-6.691177285
Al2O3	-194.2191505	58.46696437	90.53505982	-176.5269958
ZrO2	-16.05478862	2.671814798	19.21933426	-2.923620623
Other	1.245192103	5.380746211	-10.17954949	3.165569279
Al-Al	607.6013841	45.04882772	-212.167184	-62.07872502
B-B	-323.8175289	367.8969579	376.6153296	-180.8999145
Mg-Al	4651.390991	236.9166547	457.025043	298.0136091
B-Ca	236.9166547	3307.614678	1027.959568	-426.3891048
Na-Ca	457.025043	1027.959568	4443.202545	-460.5233654
Na-Al	298.0136091	-426.3891048	-460.5233654	1594.347898
Fe-Al	-735.8587514	-303.9119381	-412.8024043	-177.7486993

	+	Fe-Al
SiO2		0.459332966
B2O3		126.4568466
Na2O		16.91902114
Li2O		29.52946111
CaO		109.0295292
MgO		47.53201651
Fe2O3		-162.366204
Al2O3		-442.9661573
ZrO2		-20.61412192
Other		23.40844588
Al-Al		1962.791702
B-B		-473.4303576
Mg-Al		-735.8587514
B-Ca		-303.9119381
Na-Ca		-412.8024043
Na-Al		-177.7486993
Fe-Al		5594.623434

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TABLE XtXIDPNHL (EXTDHLI, EXTDHLJ) (XtX)-1 matrix for durability  
(PCT-sodium) for nonlinear model #2

	SiO2	B2O3	Na2O	Li2O
SiO2	2.300899608	-8.320367668	-3.237253572	-9.228359863
B2O3	-8.320367668	128.3516866	2.871004659	11.0144846
Na2O	-3.237253572	2.871004659	15.77137561	36.54907788
Li2O	-9.228359863	11.0144846	36.54907788	125.2411402
CaO	-2.463821344	11.52977863	-4.130510374	-6.627185171
MgO	15.87314561	31.69100572	-12.55127667	0.918944941
Fe2O3	-1.018396043	-8.639163391	-0.430960462	-3.994556937
Al2O3	-1.003858853	-29.69584476	-5.451990761	-14.50246193
ZrO2	-0.773375912	-8.265858827	-1.939102947	-6.539934833
Other	-0.999675	-10.26379359	-0.177584323	-0.989664741
Si-Mg	-37.56554932	-54.10917021	28.88362792	43.77451174
B-Ca	19.37414525	-114.8943028	20.45017697	29.77743338
Na-Li	57.33726105	-136.7580269	-301.9254992	-866.4937568
B-B	30.59434199	-536.9675887	-16.39751826	-59.82447112
Li-Mg	39.95695379	-34.36756608	-60.13272823	-567.8055285
Al-Al	6.345941937	99.08027183	10.53932864	17.65103761
+				
	CaO	MgO	Fe2O3	Al2O3
SiO2	-2.463821344	15.87314561	-1.018396043	-1.003858853
B2O3	11.52977863	31.69100572	-8.639163391	-29.69584476
Na2O	-4.130510374	-12.55127667	-0.430960462	-5.451990761
Li2O	-6.627185171	0.918944941	-3.994556937	-14.50246193
CaO	47.25692064	-20.14592008	-1.304034205	3.99846044
MgO	-20.14592008	900.8590291	-38.27215918	-56.00300208
Fe2O3	-1.304034205	-38.27215918	8.356142811	6.778119858
Al2O3	3.99846044	-56.00300208	6.778119858	48.88787663
ZrO2	1.723566833	-34.61381962	3.379353536	9.544738848
Other	0.97365606	-27.60878005	2.353587624	4.843394596
Si-Mg	55.98950908	-1711.011537	67.94912083	115.9323948
B-Ca	-336.518108	173.4460369	7.908981959	-33.13736396
Na-Li	94.3284153	-3.470596052	28.63994736	138.5966045
B-B	-13.04847342	-211.6435305	40.99030556	137.2633657
Li-Mg	-63.47512186	-1150.217801	106.7718118	-31.82000693
Al-Al	-22.47472216	120.7127918	-12.81802199	-229.7024533

+	ZrO2	Other	Si-Mg	B-Ca
SiO2	-0.773375912	-0.999675	-37.56554932	19.37414525
B2O3	-8.265858827	-10.26379359	-54.10917021	-114.8943028
Na2O	-1.939102947	-0.177584323	28.88362792	20.45017697
Li2O	-6.539934833	-0.989664741	43.77451174	29.77743338
CaO	1.723566833	0.97365606	55.98950908	-336.518108
MgO	-34.61381962	-27.60878005	-1711.011537	173.4460369
Fe2O3	3.379353536	2.353587624	67.94912083	7.908981959
Al2O3	9.544738848	4.843394596	115.9323948	-33.13736396
ZrO2	9.648457552	2.725212648	68.80220078	-12.61858325
Other	2.725212648	10.96077097	60.0051581	-0.604444691
Si-Mg	68.80220078	60.0051581	3417.414933	-406.1264942
B-Ca	-12.61858325	-0.604444691	-406.1264942	3066.849998
Na-Li	45.7967486	16.54878252	-80.09480365	-400.2546523
B-B	38.92546431	46.13944796	383.4914076	157.6107608
Li-Mg	31.42419857	-43.85033109	780.1633987	272.5683837
Al-Al	-25.02987298	-7.77209024	-283.2072499	201.5992466

+	Na-Li	B-B	Li-Mg	Al-Al
SiO2	57.33726105	30.59434199	39.95695379	6.345941937
B2O3	-136.7580269	-536.9675887	-34.36756608	99.08027183
Na2O	-301.9254992	-16.39751826	-60.13272823	10.53932864
Li2O	-866.4937568	-59.82447112	-567.8055285	17.65103761
CaO	94.3284153	-13.04847342	-63.47512186	-22.47472216
MgO	-3.470596052	-211.6435305	-1150.217801	120.7127918
Fe2O3	28.63994736	40.99030556	106.7718118	-12.81802199
Al2O3	138.5966045	137.2633657	-31.82000693	-229.7024533
ZrO2	45.7967486	38.92546431	31.42419857	-25.02987298
Other	16.54878252	46.13944796	-43.85033109	-7.77209024
Si-Mg	-80.09480365	383.4914076	780.1633987	-283.2072499
B-Ca	-400.2546523	157.6107608	272.5683837	201.5992466
Na-Li	7673.815773	761.0267858	1566.598903	-342.7756346
B-B	761.0267858	2344.158012	208.909845	-478.7471422
Li-Mg	1566.598903	208.909845	18180.16327	557.6640032
Al-Al	-342.7756346	-478.7471422	557.6640032	1290.924507

TABLE XtXITLClHL (EXTDHLI, EXTDHLJ) (XtX)-1 matrix for TL-Cl model

	SiO2	B2O3	Na2O	Li2O
SiO2	15.33694116	2.721480014	-7.731138814	-45.88503111
B2O3	2.721480014	50.73296717	2.866733075	-6.966217531
Na2O	-7.731138814	2.866733075	34.05702884	31.07079651
Li2O	-45.88503111	-6.966217531	31.07079651	329.1377321
CaO	-11.57191558	7.301316248	12.77805795	2.600051286
MgO	-7.632414919	41.11895403	1.185289875	-2.932355674
Fe2O3	-22.45150452	-32.99153855	-21.49480829	30.20928784
Al2O3	-23.5420828	-62.55639216	-13.52783767	17.17381274
ZrO2	-34.68281851	-47.15879835	-6.867038133	155.7116344
Other	-23.31257092	-22.24694916	10.24142926	-24.13308896
+	CaO	MgO	Fe2O3	Al2O3
SiO2	-11.57191558	-7.632414919	-22.45150452	-23.5420828
B2O3	7.301316248	41.11895403	-32.99153855	-62.55639216
Na2O	12.77805795	1.185289875	-21.49480829	-13.52783767
Li2O	2.600051286	-2.932355674	30.20928784	17.17381274
CaO	134.6993369	28.47029814	-16.32258516	-31.90327088
MgO	28.47029814	254.933063	-10.80295375	-95.39176201
Fe2O3	-16.32258516	-10.80295375	115.2773998	109.32833
Al2O3	-31.90327088	-95.39176201	109.32833	190.3615961
ZrO2	-13.79025218	-86.42449712	75.48137845	115.6868622
Other	51.1794025	36.05684615	33.15492967	43.20236887
+	ZrO2	Other		
SiO2	-34.68281851	-23.31257092		
B2O3	-47.15879835	-22.24694916		
Na2O	-6.867038133	10.24142926		
Li2O	155.7116344	-24.13308896		
CaO	-13.79025218	51.1794025		
MgO	-86.42449712	36.05684615		
Fe2O3	75.48137845	33.15492967		
Al2O3	115.6868622	43.20236887		
ZrO2	270.4216398	9.809937389		
Other	9.809937389	157.1526726		

TABLE XtXITLSpHL (EXTDHLI, EXTDHLJ) (XtX)-1 matrix for TL-Sp model

	SiO2	B2O3	Na2O	Li2O
SiO2	12.27477942	-7.244986532	-5.775434397	-25.03994891
B2O3	-7.244986532	39.16857817	2.322680502	59.51403069
Na2O	-5.775434397	2.322680502	51.20981716	20.67566279
Li2O	-25.03994891	59.51403069	20.67566279	297.2932401
CaO	-1.203685605	36.71532139	-10.79003812	145.9593821
MgO	-11.81130782	5.523252651	-3.520013128	-38.85376167
Fe2O3	-20.92691484	-4.343722557	-12.44577308	-19.18007319
Al2O3	-12.61849615	-45.5004805	0.934552666	-92.13203042
ZrO2	-21.18567511	-16.46195008	-4.134106374	11.11271276
Other	-14.21064028	-18.24789444	-32.30456106	-84.04316537
+				
	CaO	MgO	Fe2O3	Al2O3
SiO2	-1.203685605	-11.81130782	-20.92691484	-12.61849615
B2O3	36.71532139	5.523252651	-4.343722557	-45.5004805
Na2O	-10.79003812	-3.520013128	-12.44577308	0.934552666
Li2O	145.9593821	-38.85376167	-19.18007319	-92.13203042
CaO	156.2214885	-17.06746615	-32.63419591	-89.11921951
MgO	-17.06746615	122.9555369	38.69668551	25.89201033
Fe2O3	-32.63419591	38.69668551	76.29678186	58.3693502
Al2O3	-89.11921951	25.89201033	58.3693502	135.8339794
ZrO2	-14.8205397	-9.816356271	39.32146123	61.968641
Other	-71.18238546	26.73836216	60.80501747	62.86905225
+				
	ZrO2	Other		
SiO2	-21.18567511	-14.21064028		
B2O3	-16.46195008	-18.24789444		
Na2O	-4.134106374	-32.30456106		
Li2O	11.11271276	-84.04316537		
CaO	-14.8205397	-71.18238546		
MgO	-9.816356271	26.73836216		
Fe2O3	39.32146123	60.80501747		
Al2O3	61.968641	62.86905225		
ZrO2	153.2981429	54.48047616		
Other	54.48047616	137.1994924		

TABLE XtXITLSpHL (EXTDHLI, EXTDHLJ) (XtX)-1 matrix for TL-Sp model

	SiO2	B2O3	Na2O	Li2O
SiO2	12.27477942	-7.244986532	-5.775434397	-25.03994891
B2O3	-7.244986532	39.16857817	2.322680502	59.51403069
Na2O	-5.775434397	2.322680502	51.20981716	20.67566279
Li2O	-25.03994891	59.51403069	20.67566279	297.2932401
CaO	-1.203685605	36.71532139	-10.79003812	145.9593821
MgO	-11.81130782	5.523252651	-3.520013128	-38.85376167
Fe2O3	-20.92691484	-4.343722557	-12.44577308	-19.18007319
Al2O3	-12.61849615	-45.5004805	0.934552666	-92.13203042
ZrO2	-21.18567511	-16.46195008	-4.134106374	11.11271276
Other	-14.21064028	-18.24789444	-32.30456106	-84.04316537
+	CaO	MgO	Fe2O3	Al2O3
SiO2	-1.203685605	-11.81130782	-20.92691484	-12.61849615
B2O3	36.71532139	5.523252651	-4.343722557	-45.5004805
Na2O	-10.79003812	-3.520013128	-12.44577308	0.934552666
Li2O	145.9593821	-38.85376167	-19.18007319	-92.13203042
CaO	156.2214885	-17.06746615	-32.63419591	-89.11921951
MgO	-17.06746615	122.9555369	38.69668551	25.89201033
Fe2O3	-32.63419591	38.69668551	76.29678186	58.3693502
Al2O3	-89.11921951	25.89201033	58.3693502	135.8339794
ZrO2	-14.8205397	-9.816356271	39.32146123	61.968641
Other	-71.18238546	26.73836216	60.80501747	62.86905225
+	ZrO2	Other		
SiO2	-21.18567511	-14.21064028		
B2O3	-16.46195008	-18.24789444		
Na2O	-4.134106374	-32.30456106		
Li2O	11.11271276	-84.04316537		
CaO	-14.8205397	-71.18238546		
MgO	-9.816356271	26.73836216		
Fe2O3	39.32146123	60.80501747		
Al2O3	61.968641	62.86905225		
ZrO2	153.2981429	54.48047616		
Other	54.48047616	137.1994924		

## **APPENDIX C**

### **Blending Behavior**

#### **Summary from FY94 Blend Report**

# Appendix C

## Blending Behavior Summary from FY94 Blend Report

This appendix summarizes the accumulated understanding of blending, its role, its behavior. It originally appeared in the FY94 Blend report.

### Blending Behavior

#### *Effect of Constraints*

- Blending is most beneficial when the system is tightly constrained by single component or multi-component crystallinity constraints.
- Blending offers little reduction in the number of glass logs when all constraints except glass property constraints are removed.
- Blending wastes with the same binding constraint does *not*<sup>a</sup> reduce the number of glass logs.

#### *Effect of Blend Size*

- The benefit gained from blending increases with the number of wastes in each blend (i.e., for a given waste set, the Total Blend is always best. It is often possible to match Total Blend performance with a small number of optimally formulated blends).

#### *Bounds on Blending Benefit*

- For discrete blending of a waste set, the best blend may be as good as but not better than the Total Blend; the worst blend may be as bad as but not worse than the No Blend case. There may be a wide range of performance among the different blending combinations.

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<sup>a</sup> The word "not" was inadvertently omitted from this sentence in the FY94 Blend report.

- Continuous blending of a waste set will equal the performance of the Total Blend

### **Criteria for Evaluating Blending Strategies**

- Blending strategies can be compared by comparing the total number of glass logs produced by vitrification of a set of tank wastes.
- Blending strategies must be evaluated in the context of the entire waste set:
  - Can form good blends but leave bad balance of wastes (waste complement)
  - Must consider effect of blend selection on total waste set
  - Determine total number of logs for waste set and its complement.
- Comparisons are only valid if the same glass constraints are used for all blending strategies compared

### **Blend Formulation Strategies**

#### *What to Blend When*

- To gain maximum reduction in glass logs required, blend wastes of very different compositions.
- Any blending of wastes done prior to pretreatment ("early") should be of similar wastes to avoid dilution of species to be removed.
- Blend similar wastes prior to pretreatment and dissimilar wastes ( pretreated early blends) after pretreatment.

#### *Techniques for Formulating Blends*

- Based on preliminary results obtained so far, simulated annealing appears to be a very effective mathematical method for formulating blends.
- Experience so far with solving the discrete blending problem with MINLP/DICOPT has been good with very small waste sets. Further experience with the method should enable us to get better results with larger waste sets.
- Random blending MAY work satisfactorily with large sets of tanks and large blend sizes, assuming numerous optimal or near-optimal solutions.
- Blending by retrieval annex and tank farm is recommended only for early blending.
- Alternate formulations of the blending optimization problem may prove useful in formulating blends.

- Formulating blends by distributing masses of limiting components evenly among the blends is a simple strategy that can be performed manually.
- Optimal blends OptiBlends can be produced if the binding constraint for each of the blends is the same as for the Total Blend. This may not be possible for small tank sets and blend sizes; but may be very achievable for larger tank sets and blend sizes.

### **Approaches for Increasing Waste Loading and Reducing Volume of Glass Produced**

There are several approaches one can take to increase the waste loading in the glass and reduce the volume of glass produced.

- *Relax Constraints* - In the OWL calculations, the waste loading is increased until a constraint prevents it from being increased further. If one or more constraints are relaxed or removed, the waste loading can be increased further. Experimental studies may be able to show that some of the more restrictive constraints can be relaxed or removed.
- *Pretreat to Remove Troublesome Species and Reduce Mass of Waste to Be Vitrified* - For those components whose constraints cannot be relaxed or removed, pretreatment methods may be able to substantially reduce their concentration in the waste such that these components are no longer limiting.
- *Blend to Average out Troublesome Species* - Blending can very effectively decrease the amount of vitrified waste glass produced though the extent of the benefit from blending diminishes as constraints are relaxed and troublesome components removed (i.e., by pretreatment).
- *Combination of Above* - All three methods above can provide a benefit. All three should be used in combination to provide the maximum benefit.

### **Caveats**

- Calculated numerical results depend on waste compositions, constraints, and assumed pretreatments - all of which are likely to change

- These results were obtained by studying only high-level waste vitrification. Much of the behavior could be applicable to low-level vitrification. The blending behavior of low-level glass can be examined after experimentally derived glass models become available.
- These results do not address tank farm logistics, safety issues, or processing schedules. (Though the strategy described in Section 6 does address these issues)
- All calculations have assumed perfect blending of wastes uniform in composition

## **Appendix D**

### **Waste Compositions - Tank Farm Blends**

## Appendix D

### Waste Compositions - Tank Farm Blends

(Compositions are listed as mass fractions; OxideMass is given in kg)

	NCAW	ALL	SSTnDST	A
SiO2	0.04020000	0.10000000	0.10000000	0.01480000
B2O3	0.00005730	0.00075400	0.00075400	0.00000000
Na2O	0.21400000	0.25300000	0.25300000	0.17300000
Li2O	0.00000184	0.00000890	0.00000690	0.00000000
CaO	0.00789000	0.02060000	0.02060000	0.00031800
MgO	0.00201000	0.00076600	0.00076500	0.00000000
Fe2O3	0.28100000	0.11000000	0.11000000	0.59600000
Al2O3	0.09010000	0.13000000	0.13000000	0.01480000
ZrO2	0.15100000	0.07080000	0.07080000	0.00035400
Other	0.21374086	0.31407110	0.31407410	0.20072800
Cr2O3	0.00261000	0.00450000	0.00452000	0.00004300
F	0.00096700	0.00558000	0.00555000	0.00003000
P2O5	0.00869000	0.04720000	0.04710000	0.00021700
SO3	0.00653000	0.00314000	0.00341000	0.00411000
NobMet	0.00603000	0.00024100	0.00074500	0.00000000
OxideMass	240000	11800000	10500000	399000
+	AX	B	BX	BY
SiO2	0.00574000	0.00765000	0.21400000	0.05840000
B2O3	0.00000000	0.00000000	0.00000000	0.00000000
Na2O	0.51900000	0.52200000	0.25100000	0.23800000
Li2O	0.00000000	0.00000000	0.00000000	0.00000000
CaO	0.02790000	0.00025300	0.00122000	0.05660000
MgO	0.00000000	0.00000000	0.00000000	0.00000000
Fe2O3	0.23500000	0.07930000	0.05910000	0.09890000
Al2O3	0.01460000	0.01200000	0.23000000	0.12300000
ZrO2	0.00051600	0.00217000	0.00332000	0.00216000
Other	0.19724400	0.37662700	0.24136000	0.42294000
Cr2O3	0.00429000	0.00159000	0.00004270	0.00002780
F	0.00113000	0.00724000	0.00169000	0.00516000
P2O5	0.00023200	0.14200000	0.02560000	0.01820000

SO3	0.00018400	0.00180000	0.00540000	0.00227000
NobMet	0.00000000	0.00000000	0.00000000	0.00000000
OxideMass	65900	1150000	1160000	1200000

+	C	S	SX.	T
SiO2	0.0055900	0.0213000	0.0937000	0.0488000
B2O3	0.0000000	0.0000000	0.0000000	0.0000000
Na2O	0.1040000	0.6930000	0.3390000	0.5600000
Li2O	0.0000000	0.0000000	0.0000000	0.0000000
CaO	0.0939000	0.0000000	0.0124000	0.0000000
MgO	0.0000000	0.0000000	0.0000000	0.0000000
Fe2O3	0.1100000	0.0270000	0.1280000	0.0895000
Al2O3	0.0755000	0.1320000	0.2270000	0.0065500
ZrO2	0.2580000	0.0293000	0.0001240	0.0042300
Other	0.3530100	0.0974000	0.1997760	0.2909200
Cr2O3	0.0000641	0.0072300	0.0392000	0.0002000
F	0.0156000	0.0012200	0.0003770	0.0050200
P2O5	0.0027700	0.0053500	0.0042100	0.1540000
SO3	0.0015700	0.0027800	0.0021900	0.0002540
NobMet	0.0000000	0.0000000	0.0000000	0.0000000
OxideMass	989000	1030000	599000	1430000

+	TX	TY	U	DSSF
SiO2	0.1730000	0.2920000	0.1880000	0.2940000
B2O3	0.0000000	0.0000000	0.0000000	0.0000003
Na2O	0.3010000	0.2230000	0.3990000	0.6600000
Li2O	0.0000000	0.0000000	0.0000000	0.0000000
CaO	0.0001150	0.0000000	0.0000000	0.0082300
MgO	0.0000000	0.0000000	0.0000000	0.0000060
Fe2O3	0.0391000	0.1540000	0.0228000	0.0000200
Al2O3	0.1580000	0.1010000	0.1670000	0.0200000
ZrO2	0.0041000	0.0252000	0.0029600	0.0000000
Other	0.3246850	0.2048000	0.2202400	0.0177437
Cr2O3	0.0000521	0.0003230	0.0019000	0.0002300
F	0.0011800	0.0003700	0.0007010	0.0006510
P2O5	0.0410000	0.0347000	0.0074000	0.0001820
SO3	0.0051000	0.0058700	0.0006480	0.0007270
NobMet	0.0000000	0.0000000	0.0000000	0.0000000
OxideMass	2200000	176000	566000	74400

	DST
+	
SiO2	0.0831000
B2O3	0.0047500
Na2O	0.3200000
Li2O	0.0000613
CaO	0.0079500
MgO	0.0026800
Fe2O3	0.0075000
Al2O3	0.0265000
ZrO2	0.3520000
Other	0.1954587
Cr2O3	0.0039700
F	0.0143000
P2O5	0.0338000
SO3	0.0043400
NobMet	0.0006870
OxideMass	1190000

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