Final Report- Enhanced LAW Glass Property- Composition Models- Phase 1 VSL-13R2940-1, Rev. 0, dated 9/27/2013

Prepared for the U.S. Department of Energy
Assistant Secretary for Environmental Management

**P.O. Box 450
Richland, Washington 99352**

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Date Published
September 2013

Prepared for the U.S. Department of Energy
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The logo for the Office of River Protection features a stylized, wavy grey background behind the text "Office of River Protection" in a bold, black, sans-serif font.

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APPROVED

By Shauna Adams at 9:38 am, Nov 13, 2013

Release Approval

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VSL-13R2940-1

Final Report

Enhanced LAW Glass Property-Composition Models – Phase 1

prepared by

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Richland, WA**

September 3, 2013

Rev. 0, 9/27/13

*The Catholic University of America
Vitreous State Laboratory*

*Enhanced LAW Glass Property-Composition Models - Phase I
Final Report, VSL-13R2940-1, Rev. 0*

Document Title: Enhanced LAW Glass Property-Composition Models – Phase 1

**Document Number
and Revision:** VSL-13R2940-1, Rev. 0

Issue Date: 09/27/2013

Performing Organizations: Vitreous State Laboratory, The Catholic University of America

Test Plan: Enhanced LAW Glass Property-Composition Models, VSL-12T2780-1, Rev. 0

This report describes the results of testing specified by the above Test Plan. The work was performed in compliance with the quality assurance requirements specified in the Test Plan. Results required by the Test Plan are reported. The test results and this report have been reviewed for correctness, technical adequacy, completeness, and accuracy.

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List of Abbreviations

ANL-LRM	Argonne National Laboratory – Low Activity Reference Material
ASTM	American Society for Testing and Materials
BNI	Bechtel National, Inc.
CCC	Canister Centerline Cooling
DCP-AES	Direct Current Plasma - Atomic Emission Spectroscopy
DOE	Department of Energy
EC	Electrical Conductivity
HLW	High Level Waste
ID	Identification
IHLW	Immobilized High Level Waste
ILAW	Immobilized Low Activity Waste
LAW	Low Activity Waste
MRS	Mixture Response Surface
NIST	National Institute of Standards and Technology
ORP	Office of River Protection
PCT	Product Consistency Test
PNNL	Pacific Northwest National Laboratory
PQM	Partial Quadratic Mixture
QA	Quality Assurance
RCRA	Resource Conservation and Recovery Act
RMSE	Root Mean Squared Error
RPM	Revolutions Per Minute
RPP	River Protection Project
RS	Response Surface
RSD	Relative Standard Deviation
SEM	Scanning Electron Microscopy
SEM/EDS	Scanning Electron Microscopy/Energy Dispersive X-Ray Spectroscopy
SRL-EA	Savannah River Laboratory-Environmental Assessment (Glass)
SRTC	Savannah River Technology Center
TCLP	Toxicity Characteristic Leaching Procedure
VHT	Vapor Hydration Test
VSL	Vitreous State Laboratory
WTP	Hanford Tank Waste Treatment and Immobilization Plant
XRF	X-Ray Fluorescence

SECTION 1.0 INTRODUCTION

1.1 Background

About 50 million gallons of high-level mixed waste is currently stored in underground tanks at the United States Department of Energy's (DOE's) Hanford site in the State of Washington. The Hanford Tank Waste Treatment and Immobilization Plant (WTP) will provide DOE's Office of River Protection (ORP) with a means of treating this waste by vitrification for subsequent disposal. The tank waste will be separated into low- and high-activity waste fractions, which will then be vitrified respectively into Immobilized Low Activity Waste (ILAW) and Immobilized High Level Waste (IHLW) products. The ILAW product will be disposed in an engineered facility on the Hanford site while the IHLW product is designed for acceptance into a national geological disposal facility for high-level nuclear waste.

The ILAW and IHLW products must meet a variety of requirements with respect to protection of the environment before they can be accepted for disposal. Glass property-composition models will be used to control the vitrification process at the WTP to ensure that the glass meets product quality and processability requirements. The quality and the validity ranges of the property-composition models and the supporting database will greatly influence waste treatment operations, including the waste loading that is achievable in the glass for each waste composition. The current baseline models for operation of the WTP were developed under the Bechtel National, Inc. (BNI) WTP contract [1 - 4]. These models were based on LAW and HLW glass property data over a range of compositions that was guided primarily by the WTP contract and the specific set of tanks specified therein. While these models should be adequate for commissioning of the facility and processing of the specified tanks, it is likely that refinements and extensions or augmentations of these models will be required to process the balance of the tank waste inventory. Furthermore, the WTP contract includes requirements for minimum waste loadings that are generally rather modest, such that significantly higher loadings than those in the current baseline are likely achievable. However, in order to achieve these higher waste loadings, new models will be required to support the optimized operation of the WTP.

Since the development of the baseline WTP models, ORP has directed a program of work to examine various approaches for optimization of the performance of the WTP, including increasing the waste loadings in the LAW and HLW glass products [5 – 21]. As a result, a significant amount of new data has been collected that can be used for improvement of the baseline models. As seen in the present report, inclusion of the new data in the development of new property-composition models is beneficial in expanding the composition ranges over which they are valid as well as the quality of the models. The first step in this process is the collection of the relevant data in a database and maintenance of that database as additional data are collected. As was the case with the baseline WTP models [1 – 4], the data must meet the necessary quality assurance requirements if they are to support models that can be used in the WTP facility.

Results from ILAW glass testing and baseline model development were presented in 2007 [1]. That report describes the data, model development, model validation, and model uncertainty results for each of the glass properties that the WTP plans to control using glass property models. LAW models were developed for Product Consistency Test (PCT) responses, Vapor Hydration Test (VHT) response, melt viscosity, and melt electrical conductivity. The VHT model was subsequently expanded and the results were presented in 2008 [2].

As noted above, ORP is investigating optimization of the WTP, which includes increasing the glass waste loadings while maintaining acceptable properties with respect to processing and product quality. In that work, new higher-loading LAW formulations were developed that meet all of the WTP contract requirements [5-12]. However, these formulations fall outside the composition range of the current baseline WTP property-composition models.

The WTP models are used to control glass compositions for LAW vitrification at Hanford. These models are based on data from crucible scale tests to large scale LAW Pilot Melter tests, providing high confidence in the models and glass compositions selected for waste processing. However, these models are based on the glass property-composition data collected under the BNI contract, which have much lower waste loadings than compositions subsequently developed for ORP for LAW processing. To utilize the advantages of the new higher waste loading formulations for LAW processing at the WTP, the LAW glass property-composition models need to be updated to incorporate these new compositions. This report documents the progress of the program that ORP has started to incorporate the new higher waste loading LAW glass data into the models.

Developing property-composition models using all available data collected under the appropriate quality assurance programs for LAW glasses will be beneficial in expanding the valid composition ranges as well as quality of the models. The glass property data applicable to the Hanford LAW include the WTP baseline data collected under the BNI contract, the data for higher waste loading glasses collected under the ORP contract, glass property data collected under the DOE-EM technology development program, and relevant available data from other DOE sites.

The present report describes work to develop extended glass property-composition databases for WTP LAW glasses that include all of the data that were used in the development of the WTP baseline models, all of the data collected subsequently as part of the studies performed for ORP, and relevant glass property-composition data collected under the appropriate quality assurance programs available from other DOE sites. The longer-term objective of this multi-year task is to develop new glass property-composition models for PCT, VHT, viscosity and electrical conductivity to control glass compositions for LAW vitrification at Hanford. Development of Toxicity Characteristic Leaching Procedure (TCLP) models are not planned due to the very low concentrations of Resource Conservation and Recovery Act (RCRA) elements in the LAW streams. The bounding approach for TCLP response developed and documented in a previous report [22] is expected to be sufficient.

The WTP baseline models were evaluated against the extended datasets in terms of range of validity and prediction performance. The results were used to identify composition spaces where data gaps existed and needed to be filled by new compositions to be tested. A large composition matrix of 816 glass compositions was developed for this purpose. From this large composition matrix, 50 compositions were initially selected to occupy under-populated regions in the composition space, and subsequently reduced to 20 compositions that were judged to be most effective in filling the data gaps. Crucible melts of these 20 glass compositions were prepared and tested for the properties of interest. Finally, all of the glass property data available were used in the development of enhanced models that cover a larger composition space. The results and the status of the enhanced LAW glass property-composition models development is presented in this report.

1.2 Objectives

The objectives of this work are aimed at the development of enhanced LAW property-composition models that expand the composition region covered by the models. The models of interest include PCT, VHT, viscosity and electrical conductivity. This is planned as a multi-year effort that will be performed in phases with the objectives listed below for the current phase.

- Incorporate property- composition data from the new glasses into the database.
- Assess the database and identify composition spaces in the database that need augmentation.
- Develop statistically-designed composition matrices to cover the composition regions identified in the above analysis.
- Prepare crucible melts of glass compositions from the statistically-designed composition matrix and measure the properties of interest.
- Incorporate the above property-composition data into the database.
- Assess existing models against the complete dataset and, as necessary, start development of new models.

SECTION 2.0

DESCRIPTION OF LAW GLASS PROPERTY DATA

The WTP databases used in the development of earlier LAW glass property-composition models (PCT, VHT, electrical conductivity, and viscosity) [1] include data from statistically designed¹ composition matrices to cover the LAW glass composition regions of interest as well as data from actively designed glass formulations that were developed with the objective of meeting WTP specified processing and product quality requirements. Data for 271 glasses were collected in the WTP database. These include glasses that were prepared at crucible scale, glass samples from melter tests at various scales, and glasses made from actual LAW samples.

The ORP glass property-composition data set that contains data from 207 glasses (referred to as ORP-LAW glasses) nearly doubles the total number of LAW glass data available for modeling. All of the ORP-LAW glasses were actively designed since they were developed with the objective of exploring the extent to which waste loadings could be increased over the WTP baseline. Table 2.1 provides a comparison of the number of glasses and composition ranges for the WTP baseline datasets and the ORP-LAW datasets for each of the glass properties. Property data from the twenty glasses prepared and characterized under the present work scope also are included in ORP-LAW datasets.

The target compositions of the WTP-LAW and ORP-LAW glasses for the main glass constituents and the minor components have been provided in previous reports [1, 21]. Compositions used in modeling were normalized to 100% with XRF measured SO₃ values, following the data structure selected for the WTP baseline data [1]. Major glass components were used as design variables while the minor glass components were combined in an “Others” term. Two additions to the major components in the ORP-LAW compositions are tin oxide and vanadium oxide, which are constituents in many of the ORP-LAW glasses but were not present in any of the WTP baseline glasses. Tin oxide was added to improve VHT performance, especially at high sodium concentrations [23, 24], while vanadium oxide was added to improve sulfate incorporation [6-12, 25-32].

In the following sections, the various studies from which the two sets of glass data were generated are summarized and the compositional space is assessed to identify gaps in the database that would require augmentation. References to the corresponding glass development reports and/or melter test reports for the data have been provided earlier [1, 21]. The property data that were collected from each set of glasses are also identified.

¹ “Statistically designed” refers to a set of glass compositions designed using statistical experimental design methods to cover a composition space. “Actively designed” refers to glasses developed to meet certain specified requirements such as a glass composition to treat a LAW tank waste stream that has to meet all product quality and processing requirements. In this approach, information from characterization of one set of glasses is used to guide formulation of future glass compositions, with little or no intent to cover a composition space.

2.1 WTP- LAW Glasses

The following sections provide short descriptions of 283 glasses divided into groups of glasses for which data on some or all of the properties were collected to create the WTP-LAW glass property databases in 2006 [1]. Target compositions and references to the corresponding test matrix development reports and/or data summary reports for all these glasses are provided in the earlier model report [1]. These glasses can be divided into four categories:

- The first group, which represents a little over half of the glasses, includes the actively designed glass formulations that were developed with the specific objective of meeting the WTP specified glass properties for the three contractual LAW envelopes, Envelope A, B, and C. By definition, these formulations are clustered in compositional domains defined by the waste envelopes.
- Next, representing about a quarter of the glasses, are formulations from two statistically designed composition matrices to cover the LAW glass composition regions of interest.
- To these were added a smaller third group of glasses derived from a correlation that employs waste composition information to determine the appropriate waste loading, glass composition, and amounts and types of glass former additives [33]. By design, these glass formulations remain correlated by the selection of additives, which are directly linked to Na₂O, K₂O, and SO₃ levels in any potential LAW Hanford waste, and were intended to validate the design of a mathematical form that can be used in flow-sheet modeling.
- The dataset also includes nine radioactive glasses prepared at the crucible scale from actual tank waste samples taken from seven underground storage tanks at the Hanford site. Only PCT measurements are available for these glasses, which were formulated to be directly comparable to specific non-radioactive simulant samples from the first group of actively designed glasses.
- Finally, the dataset contains 24 VHT measurements on 12 glass compositions [2] that were conducted to augment the VHT data used in the development of the WTP baseline VHT model [1].

2.1.1 Actively Designed WTP Glasses

Out of the 271 WTP-LAW glasses in the modeling dataset [1], 156 are actively designed glasses formulated and tested at VSL from 1998 to 2006 during Part B1 and subsequent BNI contract phases. By virtue of being "actively" rather than "statistically" designed, compositional correlations are expected in the data. Because of the contractual waste definition, originally subdivided into three envelopes (A, B and C), these compositions were designed to support the development of glass formulations for each of these waste envelopes defined in the contract [34] in terms of the molar ratios of various species to sodium. The primary source of tank waste compositional data were a BNI test specification [35], the Best Basis Inventory (2001) [36], and subsequent revisions to the tank waste compositions (TFCOUP Rev. 2, Rev. 3 and Rev. 3A) [37-39].

39]. The glass compositions are named according to the waste type for LAW Envelope A (LAWA41 to LAWA136), LAW Envelope B (LAWB30 to LAWB96), and LAW Envelope C (LAWC12 to LAWC33). The dataset also includes five glass remelts (LAWA88R1, LAWA93R1, LAWA128R1, LAWA129R1, and LAWC31R1) prepared because the initial crucible melts did not yield sufficient glass sample to perform all of the property measurements. Among this set are crucible and melter glasses that follow the evolutions in the waste definition by sub-dividing the three waste envelopes into LAW Sub-Envelopes A1, A2, A3, B1, B2, C1, and C2. The target glass compositions proposed to treat these LAW wastes were prepared and tested for nominal glass formulations (the sample names are A1-AN105R2 for A1, A2-AP101 and A88-AP101R1 for A2, A3-AN104 for A3, B1-AZ101 for B1, C1-AN107 and C22AN107 for C1, and AN102C35 for C2), at $\pm 15\%$ variation in the blending of waste and glass former additives (A88Si+15, A88Si-15, C22Si+15 and C22Si-15) and formulations at $\frac{1}{4}$, $\frac{1}{2}$, and $\frac{3}{4}$ composition changeovers of the melt pool from the glass compositions for one tank waste to another (A1C1-1, A1C1-2, A1C1-3, A2B1-1, A2B1-2, A2B1-3, A3C2-1, A3C2-2, A3C2-3). The set also includes glass samples from melter tests conducted at three different melter scales:

- DuraMelter 100 (WVF-G-21B and WVM-G-142C for Sub-Envelope A2, A100G115A, WVB-G-124B and WVR-G-127A for Sub-Envelope A3, WVJ-G-109D for Sub-Envelope B1 and WVH-G-57B for Sub-Envelope C2)
- DuraMelter 1200 (12U-G-86A for Sub-Envelope A1 and 12S-G-85C for Sub-Envelope C1)
- LAW Pilot Melter (GTSD-1126 for Sub-Envelope B1 and GTSD-1437 for Sub-Envelope C2).

Glass samples subjected to Canister Centerline Cooling (CCC) heat treatment were also included in the WTP-LAW database (A100CC, C100GCC and PLTC35CCC).

Finally, eight simulant crucible glasses based on composition analysis of actual waste samples at Pacific Northwest National Laboratory (PNNL) and Savannah River Technology Center (SRTC) were prepared at VSL from slurry feeds made by mixing waste simulants with glass forming additives. The crucible melts were prepared and subjected to CCC heat treatment before characterization (LA44PNCC, PNLA126CC, LA137SRCCC, LB83PNCC, LB83CCC-1, LA126CCC, LA44CCCR2, and LB88CCC). Two simulant glass samples prepared at SRTC (AN-102 Surr LC Melter, and AZ-102 Surr) are also included in this set.

2.1.2 Statistically Designed WTP Glasses

LAWM1 to LAWM56 are the first 56 glass formulations that were statistically designed using a total of 13 LAW glass components chosen as design variables (Al_2O_3 , B_2O_3 , CaO , Fe_2O_3 , K_2O , Li_2O , MgO , Na_2O , SO_3 , SiO_2 , TiO_2 , ZnO , and ZrO_2), along with 4 minor components detrimental to waste loading in LAW glasses (Cl , Cr_2O_3 , F , and P_2O_5), and an “Others” component comprising all remaining minor glass components.

LAWM57 to LAWM76 are 20 additional glass compositions, also from a statistically-designed test matrix, selected with the primary objective of augmenting the LAW VHT data set available for modeling, particularly near the contractual limit of 50 g/m²/day. For this second set, Na₂O and K₂O ranges were set beyond the upper bounds of the earlier set and increased from 22 wt% for Na₂O and 4 wt% for K₂O to 23 wt% Na₂O and 5.4 wt% K₂O.

2.1.3 LAW Correlation and High Cr₂O₃, P₂O₅ Glasses

A set of 25 glasses (LAWE2H to LAWE15) were formulated using a set of empirical relationships that define waste loadings and the concentrations of glass former additives for LAW wastes as a function of the molar ratio of sulfate to sodium (SO₄/Na). These relationships together define the LAW Correlation designed by VSL for WTP LAW [33], which uses a two-step algorithm to calculate glass compositions for a given waste stream composition. Na₂O, K₂O and SO₃ concentrations define waste loading limits. The concentrations of the additives CaO, Li₂O and MgO vary with this waste loading, while the other six additives are kept at fixed concentrations (Al₂O₃, B₂O₃, Fe₂O₃, TiO₂, ZnO, ZrO₂) and the SiO₂ concentration is calculated such that the glass composition in wt% sums to 100. As thus defined, compositional correlations are necessarily present in this set of compositions. This dataset includes property data from glasses derived from the correlation, but with increased Cr₂O₃ (from 0.35 to 1.4 wt%) and P₂O₅ (1.3 to 2.4 wt%) concentrations, as well as from the high Cr and P glasses subjected to CCC heat treatment.

2.1.4 Actual LAW Glasses

The results of the PCT on nine glasses made from actual radioactive waste samples prepared at PNNL or SRTC under WTP contracts were included in the WTP baseline database for development of the two PCT property-composition models. Actual radioactive waste supernatant samples from seven underground storage tanks at the Hanford site were processed to remove most of the radioactivity according to the WTP flow-sheet. These steps included dilution, removal of ⁹⁰Sr/TRU by precipitation, ultrafiltration to remove entrained solids, ion exchange to remove ¹³⁷Cs and ⁹⁹Tc, and evaporation to re-concentrate the waste samples to the recommended level for vitrification, as required by the applicable waste envelope. Chemical analyses of these pretreated waste products were performed at PNNL or SRTC and provided to VSL, where glass formulations were developed and tested to identify suitable glass compositions for vitrification testing of the actual wastes. VSL then provided the crucible melt formulations to SRTC or PNNL where the actual tests (glass melting and PCT) were performed.

The tank waste samples were each selected to be representative of a different LAW waste Sub-Envelope or minor variations, leading to the following nine samples:

- AN-103 Actual is a glass sample prepared at SRTC from an actual Tank 241-AN-103 waste sample [40] using VSL formulation LAWA44 and represents LAW Sub-Envelope A1.

- AW-101 Actual is a glass sample prepared at PNNL from an actual Tank 241-AW-101 waste sample [41] using VSL formulation LAWA88 for LAW Sub-Envelope A2. Differences in the measured potassium concentration in the waste, however, led to a revision of the glass composition selected for waste vitrification to VSL formulation LAWA170 [42].
- AP-101 Actual is a glass sample prepared at PNNL from an actual Tank 241-AP-101 waste sample [43] using VSL formulation LAWA126 for LAW Sub-Envelope A2.
- AZ-101 Actual is a glass sample prepared at PNNL from an actual Tank 241-AZ-101 waste sample [44] using VSL formulation LAWB83 for LAW Sub-Envelope B1.
- AN-107 Actual (LAWC15) is a glass sample prepared at PNNL from an actual Tank 241-AN-107 waste sample [41] using VSL formulation LAWC15 for LAW Sub-Envelope C1.
- AZ-102 Actual and AZ-102 Actual CCC are glass samples prepared at SRTC from an actual Tank 241-AZ-102 waste sample [45], quenched and container centerline-cooled, respectively, using VSL formulation LAWB88 for LAW Sub-Envelope B2. A non-radioactive simulant of this glass was prepared in parallel at SRTC, as mentioned earlier in Section 2.1.1.
- AN-102 Actual and AN-102 Actual LC Melter are glass samples prepared at SRTC from an actual Tank 241-AN-102 waste sample, at crucible-scale [46] and in the small-scale crucible-type melter system, respectively [47], using VSL formulation LAWC21 for LAW Sub-Envelope C2. The SRTC melter system was first tested with a simulant of AN-102 waste, leading to glass AN-102 Surr LC Melter.

Of the nine glasses in this subset, all nine have PCT data. No other property measurements were conducted on these glasses.

2.1.5 Glasses to Augment VHT Data

A set of 10 new high alkali glasses were prepared in 2008 to augment the VHT data set in the region of high VHT alteration [2]. Replicate VHT measurements were conducted on all of these glasses to determine the variability inherent in the VHT method. A total of 21 VHT alteration rate measurements were conducted using the 10 new LAW high alkali glasses. In addition to the 21 VHT data, three other VHT test results that became available after the previous model development work was completed are also included in the WTP dataset: glass LAWC21 and two replicates of LAWA137.

2.2 ORP-LAW Glasses

The following sections provide brief descriptions of the 207 glasses prepared and characterized under ORP contracts between 2004 and 2010. The early work for ORP focused on increasing the sulfate loading in LAW glasses (first 54 glasses), while the later work was directed towards increasing overall waste loading in LAW glasses (153 glasses).

2.2.1 ORP-LAW Glasses Designed to Improve Sulfate Loading

Efforts to improve sulfate loading in glasses for LAW Envelopes A, B and C (focusing on tank waste compositions for AN-105, AZ-102 and AN-102, respectively) were conducted between 2004 and 2006 and led to the formulation and testing of the first fifty-four glasses included in the ORP-LAW dataset. These studies [7-9] also introduced vanadium oxide, in the range of 0.94 to 2.00 wt%, as a new glass former additive based on previous work that had suggested its beneficial effects on improving sulfate incorporation [6-12, 25-32]. Small additions of chromium oxide (0.5 wt%) were also included in these formulations in an effort to limit K-3 refractory corrosion.

This dataset also includes eight glasses from melter tests that were conducted on the DM100 melter system:

- WVV-G-11A (based on LAWA161), EWV-G-89B, EWV-G-93B and EWV-G-108B (based on LAWA187), DWV-G-123C (based on LAWB99), and WVY-G-95A (based on LAWC100).
- EWV89BCCC and EWV93BCCC are samples from the melter tests above that were heat-treated according to the LAW CCC temperature profile.

Several replicates are also included in the dataset for PCT (four replicates of melter glass WVY-G-95A) and VHT (duplicate tests of LAWA161 and LAWA187). Discussion of these and all other replicates is provided in Section 5. LAWC100R1 is a replicate sample of glass formulation LAWC100 for which the chemical composition revealed an unacceptable deviation from target; for this reason, LAWC100R1 is included in the ORP-LAW dataset and LAWC100 was discarded.

2.2.2 ORP-LAW Glasses Designed to Improve Overall Waste Loading

The ORP-LAW glass dataset includes 153 LAW glasses developed and tested at VSL for ORP from 2007 to 2010, the details of which are given below. The waste compositions covered in these tests include the full range of Na and S concentrations expected in Hanford LAW. For convenience, the LAW compositions were divided into seven regions based on the three primary waste constituents: sodium, sulfur, and potassium. These region were labeled from A to F, with Region A being the high Na, low S portion of the LAW compositions, Region F being the low

Na, high S portion, and the rest lying in between. In addition, LAW with high Na and K was labeled Region G. As can be seen in Figure 2.1, the design of glass compositions based on compositional regions yield sets of glasses clustered in each composition region.

Forty glasses in this set were tested to support the development of glass formulations in Region A for tank waste AN-105 [10-12], for which the primary source of tank waste compositional data was that given in a WTP Test Specification [35] and included a 2.5 % increase in sodium concentration to account for sodium additions in pretreatment [36]. The primary objective of this effort was to develop glass formulations that could accommodate higher concentrations of Na₂O. Because of the low sulfate concentration in this waste stream, high sulfate loading in the glass was not a primary objective for these glass formulations during the early part of the work. However, the work was later expanded to increase loading of sulfate as well as sodium, thus expanding the applicability of these formulations to a broader range of tank wastes. The glass formulations developed for Region A accommodates from about 0.3 wt% SO₃ and 25 wt% Na₂O to 1 wt% SO₃ and 25 wt% Na₂O. These formulations also include additions of chromium (up to 0.5 wt% Cr₂O₃) and tin (up to 5 wt% SnO₂) as new glass former additives, as well as higher concentrations of zirconium (up to 6 wt% ZrO₂). Moderate amounts of vanadium (less than 1 wt% V₂O₅) were also tested in these glasses. Three glass formulations from Region A were selected and used in subsequent DM10 melter tests. Glass samples from the melter tests include R10-G-155A (based on ORPLA15), Y10-G-146C (based on ORPLA20), and J10-G-24B (based on ORPLA38-1). The compositions of these replicates and near-replicates are further discussed in Section 5.

Eighteen glasses in the intermediate Regions B, C, and D, identified as ORPLB1 to ORPLB4, ORPLC1 to ORPLC5, and ORPLD1 to ORPLD9 were formulated using similar strategies to address waste streams with increasing concentrations of sulfate. These apply to LAW from tanks such as AN-107, AN-104, and AN-102 in which the SO₄/Na ratios may be as high as 2.11×10^{-2} . In these formulations, sodium varies from 21 to 25 wt%, while SO₃ ranges from 0.5 to 1.2 wt%. In view of the higher sulfate levels, additions of vanadium in the range of 1 to 2 wt% as V₂O₅ were used. Five DM10 melter glasses based on these formulations were subjected to PCT and VHT: S10-G-45A (based on ORPLB4), S10-G-101B (based on ORPLC5), T10-G-16A (based on ORPLD1), Z10-G-60C and 10A-G-53C (based on ORPLD6).

Since increased sulfate incorporation was the primary objective for these formulations, many of these formulations were remelted with an excess of sodium sulfate, this excess amounting to 4 wt% SO₃ if all of it were retained in the glass. Such glasses were prepared for the ORPLA, ORPLB, OPRLC, and ORPLD series of glasses and are identified by the addition of an “S4” at the end of the sample name. In addition, the effect of the increased sulfate on VHT alteration rate was assessed through 29 near-replicate glasses, as discussed in Section 5.

Further increases in sulfate to the maximum levels expected in LAW streams (Regions E and F) were studied in the twenty six formulations identified as ORPLE1 to ORPLE12 and ORPLF1 to ORPLF14, for LAW from tanks AZ-101 and AZ-102, respectively. To accommodate wastes in which SO₄/Na ratios may be as high as 4.85×10^{-2} , the glasses were formulated at lower waste loadings, corresponding to sodium contents ranging from 11 to 20 wt% and with the addition of lithium (up to 5 wt% Li₂O) to improve sulfate incorporation.

Some of these formulations were also produced in DM10 melter tests and subjected to PCT and VHT: Q10-G-134A (based on ORPLE12), Z10-G-122B (based on ORLF7-low SO₃), and Z10-G-153B (based on ORLF7-high SO₃).

Region G glass formulation development was focused on LAW for which the primary challenge is the combined effect of both high sodium and potassium, as is the case for Hanford tank AP-101 (71.67 wt% Na₂O + 19.61 wt% K₂O on a waste oxide basis). Twenty nine glasses were formulated in which the waste loading was varied such that Na₂O loadings in the glasses increased from 18.5 wt% to 21.5 wt% (and K₂O from 5 to 5.75 wt%). Iron oxide was eliminated from the additives blend to make room for additional tin oxide and zirconia, with ZrO₂ + SnO₂ exceeding 10 wt% in the glass. Two glass samples produced in DM10 tests from these formulations are 10A-G-43B (based on ORPLG9) and I10-G-135A (based on ORPLG27). The glass samples from the melter runs were subjected to PCT and VHT and the results are compared with those from the crucible melts of the corresponding target formulations in Section 5.

2.3 Summary of Combined LAW Glass Property-Composition Dataset

The 283 glasses in the WTP-LAW dataset include 271 glasses used in the development of the WTP LAW glass property-composition models and 12 glasses prepared and characterized to augment the WTP VHT dataset. The WTP-LAW dataset contains data from both simulated and actual WTP-LAW glasses, as discussed above, including some remelts. Of these, 264 glasses have data on PCT boron (PCT-B), PCT sodium (PCT-Na), and PCT silicon (PCT-Si) releases, 181 glasses have VHT data, many in replicates, and 181 simulated glasses have melt viscosity and melt electrical conductivity data, as summarized in Table 2.2. PCT was the only property measured on the actual radioactive glass samples.

For the ORP work, initial characterization of the glass samples was limited to the properties that were expected to be most challenging so that further characterization would be conducted only on those samples that passed the initial screening. Of the 207 ORP-LAW glasses, 171 have PCT data, 203 have VHT data, and 122 have viscosity and electrical conductivity data, as summarized in Table 2.3.

In comparison to the WTP datasets on which the baseline models were developed, these additional data represent an increase of 70%, 123%, and 31% in the data available for the PCT, VHT and viscosity-electrical conductivity models, respectively. As shown in Figure 2.2, the additional data expand the compositional range for Al₂O₃, CaO, MgO, Na₂O, SiO₂, and ZrO₂, increase the measured SO₃ content, and introduce the new components V₂O₅ and SnO₂. Iron is generally much lower in the ORP-LAW data set, with a median value of 0.9 wt% Fe₂O₃ to allow for the increases made in other constituents (both glass formers and waste loading). It is also noted that the broadening of the compositional space may also allow adding back some of the twenty compositions that were identified as outliers in the WTP-LAW glass dataset that was used to generate the baseline models [1]. A re-evaluation of outliers for the combined set of glasses is presented in Section 5.

2.4 Identification of Data Gaps

The baseline WTP LAW glass models were based on data for 271 glasses with compositions illustrated in the scatter-plot matrix shown in Figure 2.3 (green markers). As noted above, this dataset includes both statistically designed and actively designed glasses and therefore the dataset provides reasonably even coverage over the composition range that they span. In contrast, the 207 glasses developed more recently for ORP were all actively designed with the objective of determining the likely limits of waste loadings for the range of expected LAW compositions. Consequently, ORP glasses cover a wider composition range but tend to be less evenly distributed in composition space when compared to the WTP glasses (see for example the clustering in the Na₂O-SO₃ domain depicted in Figure 2.1). In addition, the ORP formulations employ glass components (vanadium and tin oxides) that were not present in the WTP-LAW glasses. These features are also illustrated in Figure 2.3 where the ORP-LAW data are shown as black squares. Green markers of WTP-LAW glasses are found at zero SnO₂ and V₂O₅ and data gaps are clearly evident in the figure. As part of the present work, an initial set of 20 glasses intended to provide a first step in efforts to fill those gaps and to provide a combined dataset that is better suited to building extended glass property models were selected. The compositions of the selected 20 new glasses are shown as red circles in Figure 2.3. The following discussion outlines the design and selection of those glasses.

The approach used to design the 20 new glasses for testing was generally similar to that used in the statistical design of the WTP baseline glasses. A 3-layer matrix was developed by using the Design of Experiments routines of the program JMP (Version 10.0) with the “Mixture Design” option and the “Optimal” type of mixture. Two new components (vanadium and tin oxides) were added to the original 14 for a total of 16 design variables. The 16 design variables included an “Others” component that was the same as that shown in Table 2.1 for ORP-LAW glasses except for the omission of iodine since its retention in glasses produced in crucible melts is extremely low. The ranges for the 16 components for each of the three layers were selected by consideration of the ranges spanned by the combined WTP-LAW and ORP-LAW datasets, with the results listed in Table 2.4, and “Others” listed in Table 2.5. The following additional constraints were also imposed:

$$13.92 \text{ wt\%} < (\text{K}_2\text{O} + \text{Li}_2\text{O} + \text{Na}_2\text{O}) < 27.39 \text{ wt\%}$$

and

$$42.13 \text{ wt\%} < (\text{Al}_2\text{O}_3 + \text{SiO}_2 + \text{ZrO}_2) < 58.87 \text{ wt\%},$$

which were intended to limit the number of glasses with very poor durability, low waste loadings, or high viscosity.

The matrices corresponding to the three layers were run independently. Each one consists of 272 compositions giving a total of 816 designed compositions. Fifty compositions were selected from the 816 design glasses to occupy under-populated regions in composition space, and particularly those due to the expansion provided by the actively designed ORP glasses. This selection was performed manually by searching the 2-D scatter-plots as well as selected 3-D regions including all ternary regions with Sn and V and with emphasis on those with Fe, Li and

K. This set was then reduced to the 20 recommended initial compositions by first eliminating the compositions with total alkali (defined as $ALK = \text{wt\% Na}_2\text{O} + 0.66 \text{ wt\% K}_2\text{O} + 2 \text{ wt\% Li}_2\text{O}$) above 25 wt% in order to reduce the number of glasses that were likely to exhibit complete alteration of the test coupon in the VHT. The compositions of these 20 glasses are listed in Table 2.6; they are plotted as the red circles in Figure 2.3 and in selected 3-D plots in Figures 2.4 to 2.7.

The experimental techniques for preparation and testing of these glasses, identified as LORPM1 to LORPM20R1, are described in Section 3 and the results of testing are provided in Section 4.

SECTION 3.0 EXPERIMENTAL METHODS

The experimental procedures used in the preparation and characterization of the 20 new simulated LAW glasses are presented in this section. The following subsections discuss the preparation of glass batches, crucible glass melting, glass composition analysis, normalization of target glass compositions with measured SO_3 values, and test procedures for PCT, VHT, electrical conductivity, and viscosity.

3.1 Glass Batching and Preparation

Glass preparation began with a batching sheet that provided information on the required starting materials and their weights. The information included the chemicals needed, identification of the chemicals according to vendors and catalog numbers with the associated purity, and the amounts necessary to produce 450 g of glass. Chemicals (reagent grade or higher purity) were weighed and batched according to the batching sheets. The information found in the batching sheets, including actual weights of chemicals used and their associated purities, can be used to calculate the composition of the glasses. The batching chemicals were determined such that the calculated compositions equaled the target compositions given in Table 2.6.

A blender was used to mix and homogenize the starting materials before they were loaded into platinum-gold crucibles (Pt-Au) that were engraved with individual identification numbers. The crucible melts were prepared in a random order. After batching was completed, the loaded platinum-gold crucibles were placed inside a Deltech DT-28 (or DT-29) furnace with a Eurotherm 2404 temperature controller. The glasses were melted for 75 minutes at 1200°C. Mixing of the melt was accomplished mechanically using a platinum stirrer, beginning 15 minutes after the furnace temperature reached the target and continuing for the next 60 minutes. The molten glass was poured at the end of the melting period onto a graphite plate to cool.

3.2 Analyses of Glass Compositions

The primary method used for glass composition analysis was X-Ray Fluorescence Spectroscopy (XRF) on powdered glass samples. A PANalytical Axios mAX-Advanced wavelength dispersive XRF spectrometer was used for this purpose. The XRF spectrometer was calibrated over a range of glass compositions using standard reference materials traceable to the National Institute of Standards and Technology (NIST), as well as waste glasses such as Argonne National Laboratory – Low Activity Waste Reference Material (ANL-LRM) [48] and Savannah River Laboratory – Environmental Assessment (SRL-EA) glass [49]. XRF analysis provides data for most glass components of interest, except lithium and boron, which are analyzed by Direct Current Plasma - Atomic Emission Spectroscopy (DCP-AES), as described below.

The twenty glass samples were also analyzed by DCP-AES after being subjected to microwave-assisted total acid dissolution in Teflon vessels according to VSL standard operating procedures. Twenty milliliters of a 1:5 mixture of concentrated HF:HNO₃ was diluted to 50 ml and used for the dissolution. This procedure is similar to the ASTM Test Method C1412-99, which also employs a mixture of concentrated HF and HNO₃ in microwave digestion of pulverized glass samples. However, supplemental use of HCl/H₃BO₃ is not included in the VSL procedure because boron is normally one of the analytes. The resulting solutions were analyzed by DCP-AES for all constituents except anionic species such as sulfur and halogens. These results complement those obtained by XRF, specifically for boron and lithium, and confirm the glass concentration of components that exceed the current VSL upper evaluation limit for XRF.

The XRF detection limit for most components is about 0.01 wt%. The accuracy of the analysis is about ± 10 relative percent for major components (> 3.0 wt% in the glass) or 1.0 wt% absolute, whichever is smaller. However, with the exception of volatile components such as SO₃, the batched (target) glass compositions are expected to be more accurate than the analyzed compositions because the batched compositions are derived from simple weighing of pure chemicals. Hence, the target compositions for all major constituents, except SO₃, are believed to provide the best compositional representations of the tested glasses. The principal role of the compositional analyses is, therefore, to confirm the target compositions.

Because SO₃ is a constituent that limits waste loading in LAW glasses and has a tendency to volatilize during glass preparation, the SO₃ concentration to be used in modeling LAW glass properties was of particular interest. Analysis of crucible melts and melter discharge glass samples have shown SO₃ analyzed values to be consistently below target values due to volatilization [28]. For this reason, it was decided during WTP baseline model development that XRF analyzed SO₃ values would better represent the LAW glass composition. Accordingly, XRF measured SO₃ values were collected for modeling.

3.3 Product Consistency Test

The PCT was conducted using 4 g of crushed glass (100-200 mesh, 75-149 μm) placed in 40 ml of test solution (de-ionized water) inside 304L stainless steel vessels. These test conditions result in a ratio of the glass surface area to the solution volume of about 2000 m⁻¹. PCT tests were performed at 90°C for 7 days according to ASTM [50], in accordance with the current WTP contract requirement [34]. All tests were conducted in triplicate, in parallel with the LAW standard glass included in each test set (ANL-LRM [48]). The leachates were sampled after seven days. One milliliter of sampled leachate was mixed with 20 ml of 1M HNO₃ and the resulting solution was analyzed by DCP-AES. Another 3 ml of sampled leachate was used for pH measurement.

In addition to the leachate concentrations, it is convenient and conventional to also consider the normalized leachate concentrations. The normalization is performed by dividing the concentration measured in the leachate for any given component by its fraction in the glass.

Thus, the *normalized concentration* C_i of element i (in g/L) is calculated from the elemental concentration c_i measured in the leachate (in ppm) as:

$$C_i = \frac{c_i}{f_i}, \quad (3.1)$$

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

The surface area of the glass sample tested and the volume of leachant used will also affect the measured leachate concentrations and, therefore, a standard value of their ratio (2000 m^{-1}) is specified in the PCT method [50]. A further normalization for this effect is often considered by dividing the normalized concentration by the ratio of the surface area of glass exposed to the solution volume (S/V , in m^{-1}). The *normalized mass loss* (in g/m^2) is then obtained from

$$L_i = \frac{C_i}{(S/V)}, \quad (3.2)$$

where S/V is the ratio of the glass surface area to the volume of the leachant, which for the standard PCT is nominally 2000 m^{-1} . Assuming this value of S/V , if C_i is expressed in g/L, one need only divide by two to obtain L_i in g/m^2 (because $1 \text{ g/L} = 1000 \text{ g}/\text{m}^3$). Specification 2.2.2.17.2 in the WTP contract [34] sets a limit of $2 \text{ g}/\text{m}^2$ for the normalized mass losses of Na, B, and Si on the PCT for the ILAW product. Thus, the WTP contract limit of a normalized mass loss of less than $2 \text{ g}/\text{m}^2$ corresponds to a normalized concentration of 4 g/L .

3.4 Vapor Hydration Test

The vapor hydration tests were run in Parr series 4700 screw-cap pressure vessels made of 304L stainless steel and having either 22 or 45 ml capacity, in accordance with VSL procedure. Glass coupons were fashioned about 5 to 10 mm square and about 2 mm thick. A hole of approximately 1.6 mm in diameter was drilled near one corner of the coupon to allow it to be suspended from a hanger made of 24 gauge stainless steel wire. Dimensional measurements were made to permit calculation of the area, and the coupon was weighed before and after the VHT on a balance having a resolution of $100 \text{ }\mu\text{g}$. The coupon was suspended vertically from the hanger in the pressure vessel and enough de-ionized water was added to the vessel to saturate the volume at the test temperature of 200°C and to allow for a non-dripping layer covering the coupon. The pressure vessels were flushed with argon, sealed, weighed, and placed in an oven held at 200°C . The temperature was monitored continuously with an independent thermocouple. At the completion of the test, the pressure vessels were removed and immediately partially immersed in an ice/water bath to condense the water vapor near the bottom of the vessel. Once cool, the vessels were weighed and opened, and then the coupons were removed and weighed. If the difference in the mass of the sealed pressure vessel before and after the test indicated a water loss in excess of 50% of the original amount, the test results were discarded. Otherwise, the coupons were examined using low-power optical microscopy and an X-ray diffraction pattern was taken

directly off the surface of the coupon. Next, the coupons were sectioned and the pieces mounted separately to allow for microscopic examination, both of the cross section of the leached coupon and the leached surface itself, and to measure the layer thickness; Scanning Electron Microscopy/Energy Dispersive X-ray Spectroscopy (SEM/EDS; JEOL JSM-35C, equipped with Noran Vantage Integrated EDS or JSM-5910LV, equipped with Oxford Instruments INCAEnergy 300 system) was used for this purpose.

For a layer thickness greater than 100 microns, the layer thickness (which can be uneven), was measured by subtracting the average remaining glass thickness measured at ten points throughout the cross-section of the coupon from the original thickness of the coupon. The altered layer thickness, which (given certain assumptions) relates directly to the mean glass alteration rate over the test interval, was the variable that was used in this report. Thus, the dependence of the altered layer thickness on glass composition was investigated. All of the VHT data used in this report were collected from tests performed at 200°C for a nominal duration of 24 days.

WTP Contract Specification 2 [34] requires that the VHT alteration rate determined from tests of seven days or longer duration be below 50 g/m²/day. If it is assumed that the altered layer density is not appreciably different from that of the glass, the mean glass alteration rate over the test interval (r in g/m²/d) is related to the measured altered layer thickness D in microns by

$$r = \rho D/t, \quad (3.3)$$

where ρ is the glass density in g/cm³ and t is the test duration. Under this assumption, for a typical glass density of 2.65 g/cm³, a layer thickness of 453 microns in a 24-day VHT would correspond to a mean glass alteration rate of 50 g/m²/day.

Although in some previous VHT modeling work the test duration was included as a modeling variable [51], the VHT modeling work in this report is similar to that in the preceding reports [1, 52] in that modeling is restricted to VHT results obtained at a single test duration (24 days) because all of the more recent data have been collected at this test duration.

3.5 Electrical Conductivity

The electrical conductivity (abbreviated as “EC” in the following sections) of LAW glasses was determined by measuring the impedance of the glass melt at temperatures around 950, 1050, 1150 and 1250°C as a function of AC frequency using a calibrated platinum-rhodium electrode probe attached to a Hewlett-Packard model 4194A impedance analyzer. The collected impedance data were analyzed to obtain the DC electrical conductivity. The probe (analyzer along with the crucible to assure that the geometry is replicated) was calibrated and checked periodically using NIST traceable standard reference materials.

The current WTP requirement is that glass melt EC be in the range of 0.1 to 0.7 Siemens/cm at 1100 - 1200 °C [53].

3.6 Viscosity

The melt viscosity (η) of each glass was measured using a Brookfield viscometer with a platinum-rhodium spindle and crucible. The relative torque of a rotating spindle immersed in molten glass was measured as a function of rotational velocity (revolutions per minute (RPM)) at temperatures around 950, 1050, 1150 and 1250°C. The viscosity of the molten glass was then calculated from the collected data of torque versus RPM. The equipment was calibrated using viscosity standard oils and checked periodically using a NIST traceable standard reference glass.

Per current WTP requirements, glass melts should satisfy the viscosity limits of 10 to 150 poise at 1100 °C, with the preferred range being 40-80 poise at 1150°C [53].

SECTION 4.0

PREPARATION AND TESTING OF NEW GLASSES

This section describes the preparation of 20 new ORP-LAW glasses (LORPM glasses) and the property measurements on these glasses. Section 4.1 describes the preparation and analyses of the glasses. Section 4.2 provides the PCT, VHT, EC, and viscosity results for these glasses, along with an assessment of the measured properties and how they fit into the combined LAW glass property-composition data set.

4.1 Preparation and Analysis of Twenty LORPM Glasses

The target and analyzed compositions of the 20 ORPLM glasses are given in Table 4.1. Preparation and analysis of the glasses followed the methods described in Section 3. As is evident from Table 4.1, the target and analyzed compositions show good agreement. XRF analyses of all major constituents (> 3.0 wt% in the glass) are within 10 relative percent of target for all but three cases: in LORPM5 and LORPM8R1, SnO_2 is low (-12 % and -19% relative deviations, respectively); in LORPM18, ZrO_2 is low (-17%). However, in LORPM5 and LORPM18, DCP analysis showed the measured values to be much closer to target for SnO_2 and ZrO_2 ; XRF analysis deviations can in this case be potentially due to possible interferences, particularly for high concentrations of the two new additives SnO_2 and V_2O_5 . In contrast, LORPM8R1 showed a consistent deviation from target for SnO_2 in both XRF and DCP analyses.

Evaluation of the as-melted glass for possible secondary phases by SEM (Figures 4.1 and 4.2) showed clusters of elongated tin oxide crystals amounting to 2 vol%, which would likely account for the SnO_2 deficiency in the glass analysis. A similar observation was made on the glass remaining after melt viscosity and electrical conductivity measurements, explaining the difficulties experienced in these measurements (see Section 4.2.3). In combination with 1 vol% zinc chromite that was also observed in this glass, it is possible that the glass properties may be affected, which would suggest considering LORPM8R1 as an outlier for property modeling. Optical and SEM evaluations were conducted on all LORPM glass samples to assess homogeneity. Two samples at the highest ZrO_2 concentration and lowest alkali content, LORPM13 and LORPM2R1, were found to contain 2.1 and 1.5 vol% zirconium oxide crystals in clusters. ZrO_2 clusters display a pattern similar to feldspar exsolution, indicating that the solubility limit of ZrO_2 in this melt is exceeded. However, no discrepancy in glass composition was detected from either XRF or DCP analyses of these glasses. It is nonetheless important to note that the ZrO_2 range may have been expanded to too high a value and the limit defined by $(\text{Al}_2\text{O}_3 + \text{SiO}_2 + \text{ZrO}_2) < 58.87$ wt% may need to be reduced to a lower value in the selection of additional glasses for testing.

4.2 Properties of the New LORPM Glasses

4.2.1 Product Consistency Test

The PCT-B, PCT-Na, and PCT-Si releases are given in Table 4.2 for the 20 new LORPM glasses. The PCT releases vary from 0.264 g/L (0.132 g/m²) to 3.573 g/L (1.786g/m²) for PCT-B, 0.200 g/L (0.100 g/m²) to 4.094 g/L (2.047 g/m²) for PCT-Na, and 0.105 g/L (0.053 g/m²) to 0.721 g/L (0.360 g/m²) for PCT-Si. The normalized PCT mass loss for Si remains well below the PCT contract limit of 2 g/m² and is always less than mass losses for Na and B for all twenty glasses, as was the case with all other WTP and ORP glasses [1, 21]. As before, therefore, no model is developed for PCT-Si since: (i) if the B and Na mass losses are below the PCT limit, so too will be the Si mass loss, and (ii) the Si mass loss does not exceed the PCT limit over the expanded composition region of interest.

The WTP contract limit was exceeded only for glass LORPM10R1 and then only for PCT-Na. This glass was designed at the combined lowest concentration of Al₂O₃ (3.5 wt%), SnO₂, and ZrO₂ (both zero). All other LORPM glasses show relatively low leaching, for which the observed sodium and boron releases are generally congruent, as can be seen in Figure 4.3. The data are well distributed between values of 0.1 and 1.0 g/m². A high PCT-Na value that exceeds the WTP contract limit [34] where sodium leaching exceeds that of boron (2.05 versus 1.79 g/m²) is observed only with glass sample LORPM10R1. This is unusual for a low sodium glass, but it has the highest calcium and potassium and the lowest aluminum and zirconium concentrations. A similar situation has been observed previously with a higher sodium glass of a statistically designed WTP composition, LAWM13, and may point to a compositional leaching domain where more data are needed.

The PCT leachate pH values for the 20 LORPM glasses range from 9.0 (LORPM13) to 11.8 (LORPM10R1). This compares well with the range of pH values from both previous sets: the WTP-LAW glasses ranging in pH from 9 to 12.5 and the ORP-LAW glasses from 10.5 to 12.5, and generally higher, as expected, with higher alkali content. The leachate pH is an indicator of the glass-water reaction since alkali ion exchange tends to rapidly increase the pH from neutral to basic. Leachate pH is also a factor in determining the rate and path of subsequent phases of the leaching reaction since as the pH increases, the rate of hydrolysis of the silicate matrix increases. Finally, the stability of alteration phases can depend on the solution pH. Conversely, certain glass constituents, such as boron, tend to buffer the solution and moderate the pH increase. It is, therefore, instructive to examine the relationships between the measured leachate pH values, the glass composition, and PCT releases. PCT boron release as a function of leachate pH is shown in Figure 4.4 for the previous ORP-LAW glasses and the 20 LORPM glasses, along with the contractual limit of 2.0 g/m². The boron release increases with pH in both cases, but the relationship is markedly non-linear for the ORP-LAW glasses, reflecting the combined effects of high sodium and potassium with high magnesium, specifically investigated in a set of ORP glasses. This non-linear effect is not observed when the MgO concentration is capped at 5.0 wt%, as can be seen by the red markers of LORPM glasses. Nonetheless, LORPM10R1 has a pH value that is noticeably above the trend among the LORPM glasses, indicating a possible model outlier, potentially due to the combined effects of Mg and Ca. In this

case, PCT leachate concentrations could be related to a more advanced, multiphase stage of leaching driven by the growth of secondary phases containing magnesium and calcium.

PCT boron and sodium release for the LORPM glasses are compared to the corresponding results for the WTP and ORP glasses as a function of alkali concentration in the glasses in Figure 4.5. In the figure, the alkali concentration is expressed as the wt% summation of $\text{Na}_2\text{O} + 0.6\text{K}_2\text{O} + 2\text{Li}_2\text{O}$, and is referred to as “Alk” in the following sections. A clear increasing trend of PCT boron and sodium releases is observed as the alkali oxide content increases. This is expected because alkalis are the essential contributors in the inter-diffusion during the first stage of leaching. In this stage (Stage I), ion exchange between glass network-modifying cations and protons from the leaching solution takes place. The term ‘reactive diffusion’ has also been used to describe the combined effects of water diffusion into the glass, alkali ion exchange, and the resulting reorganization of the glass network leading to concomitant release of boron. The second stage (Stage II), when the initial forward rate is established, consists of both ion exchange and hydrolysis reactions. During the next stage, as the glass-water reaction proceeds and the concentration of glass components (particularly silicic acid) increases in solution, the rate of dissolution decreases (Stage III). For LAW glasses however, under alkaline conditions, it has been observed that ion exchange becomes the dominant process controlling the glass leaching mechanism under these near-saturated conditions. Dissolution may continue at a relatively constant residual rate (Stage IV) consistent with a process controlled by diffusion through the hydrated surface layer. Among the new glasses, higher than expected PCT releases on the basis of alkali content are observed in glasses LORPM10R1 and LORPM6 (Figure 4.5). These glasses contain the glass composition matrix design maximum of 12.24 wt% CaO as well as high MgO concentrations (4.11 and 4.50 wt%). In these glasses, Ca^{2+} and Mg^{2+} compete unfavorably as cations in the gel created as a result of the ‘reactive diffusion’ and favor the formation of detrimental secondary phases that develop at the glass-leaching solution interface (phyllosilicates). Although these two glasses appear to be outliers to the general trend of PCT releases as a function of alkali content, their contribution is nevertheless important in the development of glass property-composition models and in defining the acceptable limits of these components in LAW glass.

4.2.2 Vapor Hydration Test

The VHT alteration depths (in μm) and alteration rates (in $\text{g}/\text{m}^2/\text{d}$) are given in Table 4.3 for the 20 LORPM glasses. In these tests, the VHT alteration depths and rates vary from undetectable to 777 μm (85.8 $\text{g}/\text{m}^2/\text{day}$). This range excludes the results for glass LORPM17R1 that was found to be fully altered at the end of the 24-day test period.

As was previously demonstrated for WTP-LAW and ORP-LAW glasses, finding general trends for VHT alteration rate as a function of glass composition are more challenging than with PCT data. This is essentially due to the fact that VHT is designed to assess a late-stage feature of alteration and one that involves a period of incubation. For instance, a time period of 24 days at 200 °C appears to be below the incubation threshold for corrosion in glass LORPM6 for which no alteration is detected even at 2000X magnification. In this case, an estimated alteration depth of less than 0.05 μm was used based on the resolution of the microscope.

Figure 4.6 shows the VHT alteration rates as a function of the alkali oxide concentration for the 20 LORPM glasses, along with data for the previous 203 ORP-LAW glasses [21] and the 171 WTP-LAW glasses [1]. The WTP baseline model for VHT was based on the data from the 171 WTP-LAW glasses. As was discussed in past model analyses, a noticeable effect related to the alkali content shown in this figure is a threshold at around 23 wt% “Alk” beyond which VHT alteration depths increase rapidly. Thus, it is apparent from the combined data that the glasses are significantly more likely to fail the contract VHT contract requirement when the “Alk” content is higher than 23 wt%. This behavior is broadly consistent with expectations from a glass structure perspective, where alkali oxides act as modifiers in breaking up the glass network structure and glass network former oxides act to strengthen it. Glasses with a more highly polymerized network, which results from having more network former oxides and less alkali oxides, tend to be more durable; LORPM6 is a good example of this type of glass. There are, however, multiple glasses falling out of the general trend, particularly among the LORPM set: glasses LORPM1, LORPM4, LORPM8R1, and LORPM13. The high VHT alteration rates shown by LORPM1 and LORPM4 are probably due to the absence of ZrO_2 in these compositions. Their compositions, which have varying concentrations of Al_2O_3 , SiO_2 , SnO_2 and alkalis, are therefore expected to provide valuable additions for model development. Crystallization observed in LORPM8R1 and LORPM13 indicate that these glasses may need to be excluded from the modeling dataset.

4.2.3 Melt Electrical Conductivity and Melt Viscosity

As described in Section 3.5, electrical conductivity was generally measured at four temperatures for each LORPM glass. The electrical conductivity versus temperature values are given in Table 4.4 for the 20 LORPM glasses. Each row of Table 4.4 provides the electrical conductivity data for a given glass at four temperatures. There are four columns corresponding to the four temperatures at which electrical conductivity data were measured for each glass. The current WTP requirement for glass melt electrical conductivity is that it be within 0.1 to 0.7 S/cm in the temperature range of 1100 to 1200°C [53]. Among the measurements taken in this temperature range, electrical conductivity values were acceptable for all glasses, ranging from 0.166 to 0.675 S/cm.

As described in Section 3.6, viscosity was generally measured at four temperatures for each LAW glass. The viscosity values and measurement temperatures are given in Table 4.5 for eighteen of the twenty LORPM glasses. Measurements on glass samples LORPM8R1 and LORPM13 revealed non-Newtonian behavior at all four measurement temperatures and high torque values indicative of crystallization. These two glasses were, therefore, excluded from the dataset for viscosity modeling. Each row of Table 4.5 provides the viscosity data for a given glass at four temperatures. There are four columns of data for each glass corresponding to the four temperatures at which viscosity data were measured.

Glasses LORPM5, LORPM9, and LORPM11 had viscosities exceeding the recommended WTP upper limit of 150 poise at 1100°C [53], with interpolated values of 293, 153 and 249 poise, respectively. On the other hand, none of the viscosity values interpolated at 1100°C, ranging from 11 to 293 poise, fell below the WTP lower limit of 10 poise at 1100°C.

Figure 4.7 and 4.8 show the distribution of temperature values at which electrical conductivity and viscosity were measured for each LORPM glass melt, respectively. These figures show that the measurements were taken at temperatures close to the four nominal values (950, 1050, 1150, and 1250°C).

SECTION 5.0 LAW GLASS DATA SET AND MODELING

PCT, VHT, electrical conductivity, and viscosity data for the combined WTP-LAW, ORP-LAW, and LORPM glasses are presented and discussed in this section. The performance of the baseline WTP LAW property-composition models as applied to the combined dataset is also discussed. In total, there are now 512 LAW glasses with data for at least one of the four properties, as well as many replicates, as discussed below. More than half of these glasses (282) have data for all four properties.

The ranges (minimum and maximum values) for LAW glass components in the modeling dataset for each property discussed below were selected as the rounded values of the minimums and maximums of mass fraction for each component, as given in Table 5.6. Minimum mass fraction values were rounded down to the nearest third decimal place (nearest 0.1 wt%). Maximum mass fraction values were rounded up to the nearest third decimal place (nearest 0.1 wt%). The only exception made to reduce the composition range was to limit MgO to 5.1 wt% in order to exclude glasses that may favor augite crystallization [1] and show very high leach rates, which are unlikely to be used for waste processing at the WTP.

The previously recommended WTP baseline LAW model forms and coefficient estimates that were developed [1] are given in Tables 5.1 to 5.5 for PCT-B, PCT-Na, VHT, electrical conductivity, and viscosity, respectively. The WTP baseline models were used as the starting points for the preliminary model work with the combined dataset described in the following sections.

In the subsections below, the status of model development using the combined dataset for each property is presented and discussed. Summaries of the modeling parameters and performance of the various models that were studied for each property are compiled in tables in each subsection. The statistical terms that are used in modeling are described in Appendix C of the WTP baseline model report [1] and are given below for convenience.

n = the number of data points used to fit the model,

p = the number of parameters (coefficients) in the model form estimated via regression on the data,

y_i = the measured property value (in the present case, the natural logarithm of the measured property value) for the i^{th} data point,

$\hat{y}_i$ = the predicted property value (in the present case, the natural logarithm of the predicted property value) for the i^{th} data point using the model fitted to all n data points,

$\bar{y}$ = the average (mean) of the n measured property values (in the present case, the average of the natural logarithm of the measured property values).

The R^2 statistic is interpreted as the fraction of the variability in the property data (in the present case, natural logarithm of the property data) accounted for by the fitted model and is given by:

$$R^2 = 1 - \frac{\sum_{i=1}^n (\hat{y}_i - y_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (5.1)$$

The $R^2_{Adjusted}$ statistic is interpreted as the adjusted fraction of the variability in the property data (in the present case, natural logarithm of the property data) accounted for by the fitted model and is given below. The adjustment is for the number of parameters (p) and the number of data points (n) used to fit the model.

$$R^2_{Adjusted} = 1 - \frac{\sum_{i=1}^n (\hat{y}_i - y_i)^2 / (n - p)}{\sum_{i=1}^n (y_i - \bar{y})^2 / (n - 1)} \quad (5.2)$$

Generally R^2 statistics take values between 0 and 1. Negative values reflect a poor fitting model, a model that contains more terms than needed to fit the data, or a model fitted to data with one or more very influential data points. More than a minor difference between R^2 and $R^2_{Adjusted}$ indicates that the model may contain more terms than needed to achieve the same goodness of fit.

If the fitted model is adequate, the root mean square error ($RMSE$) provides an estimate of the experimental and measurement uncertainty standard deviation associated with melting glasses and measuring the associated property. $RMSE$ is therefore expected to be comparable to the measured glass preparation and property measurement uncertainty assessed from replicates testing. The statistic $RMSE$ is included as a standard output in the software used in modeling, JMP, and is given by:

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (\hat{y}_i - y_i)^2}{n - p}} \quad (5.3)$$

Press RMSE helps in comparing the performance of multiple models. The residual value of each predicted/measured row is computed in modeling software JMP after dropping that row from the computations. *Press RMSE* is given by:

$$PressRMSE = \sqrt{\frac{\sum_{i=1}^n (\hat{y}_{(i)p} - y_i)^2}{n}} \quad (5.4)$$

where $\hat{y}_{(i)p}$ is the predicted property value for the omitted observation. Models with lower *Press RMSE* are favored.

The *statistical lack-of-fit (LOF) test* checks whether the differences between measured and predicted property values from a fitted model are larger than expected based on the experimental and measurement uncertainty in the data. If the predicted versus measured differences are larger than data uncertainty at a high enough statistical confidence (e.g., greater than 90%), the model is said to have a statistically significant LOF. Replicate data points containing all applicable sources of experimental and measurement uncertainty are required to perform statistical LOF tests.

This process is conducted using a LOF F-test given by:

$$F = \frac{(SSE - SSPE)/(n - p - f)}{SSPE/f} = \frac{\left[\left(\sum_{i=1}^n (\hat{y}_i - y_i)^2 - \sum_{k=1}^K \sum_{j=1}^{m_k} (y_{kj} - \bar{y}_k)^2 \right) / (n - p - f) \right]}{\sum_{k=1}^K \sum_{j=1}^{m_k} (y_{kj} - \bar{y}_k)^2 / f} \quad (5.5)$$

The scatter among the replicates of the measured property (multiple y_i for a single x_i) is calculated to assess the scatter of points around the best fit curve. The scatter around the replicates is pooled into the sum of squares of pure error (SSPE). The sum of square error (SSE) is calculated for all of the model data points. The degree of freedom for SSE is $n-p$; and the degree of freedom for pure error is given by $f = \sum_{k=1}^K (m_k - 1)$, where m_k is the number of replicate data points in the k^{th} replicate set, $k = 1, 2, \dots, K$.

The *p-value* of the F-test (F probability distribution) is used to assess whether the fitted model has a statistically significant LOF for the modeling dataset. The smaller the *LOF p-value*, the greater the indication that the model is inadequate. A threshold *LOF p-value* of 0.05 is traditionally used to assess whether the fitted model has a statistically significant LOF (significant at the 95% confidence level) for the modeling dataset and that a different model might be required.

5.1 PCT-B and PCT-Na Modeling

5.1.1 PCT Dataset

Of the 512 LAW glasses collected and discussed in Sections 2 and 4 above, 455 glasses have data on PCT boron (PCT-B), sodium (PCT-Na), and silicon (PCT-Si) releases. However, since the dataset contains PCT data on four samples of glass WVY-G-95A (WVY-G-95A-1, WVY-G-95A-2, WVY-G-95A-3, and WVY-G-95A-4), the full PCT model dataset has 458 sets of PCT data. For *every one* of these 455 glasses, the normalized PCT mass loss for Si is below the PCT contract limit of 2 g/m². In fact, the Si mass loss only exceeds 1 g/m² (half the limit) in the PCT leachate of the statistically designed WTP-LAW glasses LAWM12 and LAWM55 [54], which are clear PCT model outliers, as discussed below. As observed earlier, the present results also show that: (i) if the B and Na mass losses are below the PCT limit, so too will be the Si mass loss, and (ii) the Si mass loss does not exceed the PCT limit for any of the glasses. For these reasons, Si PCT release is not discussed further and was not used for model development; PCT models were developed only for PCT-B and PCT-Na releases.

As can be seen in Figure 5.1, PCT-Na and PCT-B releases for the 455 LAW glasses are less than the contract limit of 2 g/m² (4.0 g/L) in the majority of the cases, even though all ORP-LAW glasses were designed to extend the composition region toward higher waste loadings. Of the 455 LAW glasses with PCT results, 26 glasses have PCT-B releases greater than 2 g/m² and 19 have PCT-Na releases greater than 2 g/m². More than half of these (16 and 10, respectively) are from a set of ORP-LAW glass formulations investigating the effect of magnesium and most of the others are from the statically designed WTP-LAW matrix glasses (see glass labels in Figure 5.1). As mentioned in the introduction to this section, the high PCT response with high MgO concentrations led to the following considerations:

- Setting a limit on MgO concentration: Glasses with very high MgO content (7 and 10 wt% MgO), which are unlikely to be selected for waste processing at the WTP, were excluded from the model dataset (the model composition region was limited to 5.1 wt% MgO, as previously done for the WTP baseline models).
- MgO concentration in ORPLM glasses: Over half of the ORPLM glasses were selected with MgO concentrations in the range of 3 to 5 wt% so that model terms for the effect of MgO can be improved.

5.1.2 PCT Model Range and Outliers

In the WTP baseline model development, 20 WTP-LAW glasses were excluded from the ILAW PCT modeling dataset. Sixteen of these glasses were excluded as compositional outliers and four were container-centerline-cooled glasses with high Cr₂O₃ content that were considered non-representative. These last four samples were also excluded from the current modeling work, but the expansion of the compositional space allowed the inclusion of 8 of the 16 glasses that were previously excluded.

The identification of the glasses excluded from the PCT modeling dataset and the reasons for their exclusion are provided in Table 5.7. Glasses previously excluded because of high concentrations of Al_2O_3 , B_2O_3 , CaO , K_2O , Fe_2O_3 , TiO_2 , and ZnO were all kept in the dataset used for the present preliminary model development work and their outlier status was reevaluated individually during model development. Similarly, the new glasses LORPM8R1 and LORPM13, which showed about 2 vol% crystallization, were kept in the model dataset and later individually evaluated as possible outliers, as discussed in Section 5.1.4 below. The outlier diagnostics, using Grubbs' test² of the population normality in particular, identified as outliers five statistically designed WTP-LAW glasses, two high sodium and potassium ORP-LAW glasses for which PCT-Na release is greater than 8 g/L, and LORPM13, all of which are listed in Table 5.7.

5.1.3 PCT Validation Set Selection

Model validation was accomplished during the WTP baseline model development by data-splitting, data-partitioning, and by applying the models to calculate the properties of outlying glass compositions. This permitted use of all available data in the modeling dataset for a given property but did not offer an *independent* set of data (not used in model development) that could be used to compare the relative predictive capability of various types of models independently from the model set. Since the dataset has nearly doubled in size, a validation set of 28 samples was reserved for independent validation of the PCT models (PCT-Na and PCT-B releases). To select the validation set, all actively designed glasses were sorted by PCT-Na release and one out of every ten samples was pulled from the dataset. None of the statistically designed glasses were included in the validation set. A final count of 28 validation glasses was considered to be a reasonable compromise between sufficiency for validation and not unduly reducing the size of the modeling dataset. A display of the sample distribution, including outliers and validation set, is shown in Figure 5.2 where the glasses are sorted according to the natural logarithm of the normalized PCT-Na release. A list of the validation glasses is provided in Table 5.8. The selection of glasses with their normalized release for boron and sodium is listed in Table 5.8 in the order of increasing PCT-Na release. The list ends with ORPLG14 with a PCT-Na release of 7 g/L but PCT-B release of 10 g/L, which, at approximately twice the WTP limit of 4 g/L [53], was considered as a model boundary (see Section 5.1.4). The same validation dataset was used for both PCT models and, since sodium and boron leaching is not always congruent, the selection is therefore not as evenly distributed for boron in the lower section of Figure 5.2.

5.1.4 PCT Replicates

Table 5.9 lists 27 sets of replicate and near-replicate glasses and the corresponding PCT-B and PCT-Na normalized releases; twelve are from the WTP-LAW dataset and fifteen are from the ORP-LAW dataset. Table 5.9 also lists estimates of percent relative standard deviations

² Grubbs' test is a statistical test used to detect outliers in a data set assumed to come from a normally distributed population. Grubbs' test detects one outlier at a time. The outlier is removed from the dataset, and the test is repeated until no outliers are detected. The test quantifies how far an outlier is from the rest of the population by calculating the ratio $Z = (\bar{y} - y_i)/SD$ and comparing to tabulated critical values for various sample sizes.

(%RSDs) for each replicate set, as well as pooled estimates over all of the replicate sets. A pooled %RSD combines the separate %RSD estimates from each replicate set so that a more accurate combined estimate of the %RSD is obtained. These pooled %RSDs include uncertainties in fabricating glasses, performing the PCT, and chemically analyzing leachates to determine elemental releases. In the case of near-replicates, the uncertainties also reflect the difference in fabrication scale, thermal history (some are also heat treated according to canister centerline cooling profile), sulfate content, and minor components that may have been added as tracers for volatile radionuclides in melter testing (such as cesium and iodine). Nonetheless, the magnitudes of the pooled %RSDs in the two sections of Table 5.9 for WTP-LAW and ORP-LAW glasses are similar (24.89% and 19.07% for WTP-LAW glasses, versus 17.95% and 17.97% for ORP-LAW glasses). The overall %RSD therefore changes very little over the 27 replicates sets, for a final %RSD of 20.58 and 18.13% for boron and sodium normalized releases, respectively. These compare well to the corresponding %RSD obtained from round robin testing of the ANL-LRM glass, which are 27% (PCT-B) and 21% (PCT-Na), indicating that any differences arising from inclusions of glasses produced at various scales (crucible and melter glasses), radioactive and non-radioactive glasses, and quenched and canister-centerline-cooled glasses, are comparable to those arising from replicate measurements on the same glass made at different laboratories. These estimates of uncertainty in replicate measurements for PCT-B and PCT-Na releases are used subsequently to statistically assess lack-of-fit (LOF) of the various models considered in Section 5.1.5 below.

5.1.5 Preliminary PCT Models

The baseline WTP LAW models provided reasonable fits to the WTP-LAW dataset for PCT leaching of boron and sodium (R^2 of 0.87) but a marked decrease in R^2 was observed when the models were applied to the ORP-LAW dataset [21], most particularly for PCT-Na release (R^2 was calculated to be 0.43 for PCT-Na for the ORP-LAW glass dataset). This may be due in part to the extended sodium range stemming from designing higher waste loading glasses in the ORP-LAW dataset. Similarly poor results were observed for the 20 LORPM glasses added to the model dataset. The twenty LORPM glasses identified by red triangles in Figure 5.3 highlight the limitations of the WTP baseline models over the composition range covered by the ORP-LAW glasses.

The model forms considered for the new models remained in the general class of *mixture experiment models* and relied on the experience from the previous WTP baseline model development work [1]. Starting from the partial quadratic mixture (PQM) model selected as the WTP baseline model [1], regression models were successively developed with incremental improvement in the model statistics. Summaries of the status of these enhanced models for PCT-Na and PCT-B releases are given in Tables 5.10 and 5.11, respectively.

Initially, the strategy to progressively improve the model performance was identical for both PCT-Na and PCT-B models:

- Model 1 corresponds to the previous 17-Term Reduced Partial Quadratic Mixture Model (PQM), used as starting model coefficient set, and is presented here for comparison.

- Model 2 uses identical sets of model terms (17-term PQM) but these have been updated for the expanded dataset – the only compositional outliers in this model are those with MgO concentrations higher than 5.1 wt%, for which PCT-Na releases always exceeded 8 g/L (ORPLA28, ORPLA29, ORPLA31, ORPLA32 and LAWA65) and four high chromium glasses that crystallized after CCC heat treatment (LAW3Cr2CCC, LAW9HCr1CCC, LAW9HCr2CCC and LAW10HCr3CCC). As can be seen from Tables 5.10 and 5.11, the performance of the model is worse than that of the WTP baseline model.
- Model 3 (17-term PQM) was designed after successive iterations of Model 2 for possible outliers by Grubbs' test, which identified seven additional glasses with PCT-Na releases greater than 8 g/L (LAWM12, LAWM17, LAWM35, LAWM55, LAWM56, ORPLG13 and ORPLG15). In the new model, the most affected model coefficients were ZrO_2 , $CaO \times Li_2O$ and $B_2O_3 \times MgO$. As expected, since some of the uncertainty associated with the high leaching replicates LAWM12/LAWM55 and LAWM35/LAWM56 has been removed, this reduced the root mean square error (RMSE). These outliers remained excluded for the rest of the modeling stages described below.

The possible addition of model terms for SnO_2 and V_2O_5 were considered at this point. V_2O_5 did not contribute significantly to the model performance and was easily ruled out as a model term but the SnO_2 term was significant in both the PCT-Na and the PCT-B models.

For the PCT-Na model, the successive steps of model improvement summarized in Table 5.10 were as follows:

- Model 4 (18-term PQM) revises the model terms after removing LORPM13 as a Grubbs' test outlier from the previous model and adds a term for SnO_2 , which was found to be a significant component based on the p -values calculated in t -tests (limit of significance level used was $p\text{-value} < 0.0025$)³. Improvements are noticeable in most of the model and validation statistics, except for a small increase in the validation RMSE.

³ The t -test was used in a stepwise regression process to identify unnecessary terms in a model. The t -test computes a t -statistic equal to a model coefficient divided by its standard deviation. The t -statistic is then compared to the t probability distribution to determine the probability of getting a t -statistic at least as large as a pre-determined limit. The resulting probability is referred to as t -test p -value, and represents the probability of incorrectly deciding a coefficient is significantly different than zero. JMP outputs estimated model coefficients, coefficients standard errors, t -statistics, and p -values. The smaller the p -value the stronger is the evidence that the coefficient is significantly different from zero, and that the corresponding model term is needed. To avoid running models with too many potentially unnecessary terms in a model, the t statistics is run looking at p -values for the coefficients in a "full" model, and the model term whose coefficient is least statistically significant (here more than 0.0025) is not included.

- JMP® Response Surface methodology⁴ was used in Models 5 and 6 to identify any other significant compositional interaction effects, using the stepwise statistical method (same limits of significance as above p -value < 0.0025). Model 5 used the Mixture Response Surface (MRS), which permits optimization of quadratic terms but does not include square terms, while Model 6 used Response Surface (RS), which also identifies square terms.

Of the six PCT-Na models listed in Table 5.10, Model 5 (18-term PQM), which includes additional quadratic terms for $\text{Na}_2\text{O} \times \text{SiO}_2$, $\text{CaO} \times \text{SnO}_2$, $\text{CaO} \times \text{Fe}_2\text{O}_3$ and $\text{Al}_2\text{O}_3 \times \text{Fe}_2\text{O}_3$, shows the best regression statistics but Model 6 (17-term PQM) shows somewhat better validation statistics. Optimization that will follow in later phases of this work may yet consider the quadratic term for $\text{Al}_2\text{O}_3 \times \text{K}_2\text{O}$ that is present in Model 6, which does appear significant. Figure 5.4 displays the predicted versus measured plot for Model 5 and shows a tight distribution of points around the 45° line for the WTP model dataset and the additional ORP dataset alike.

Similar incremental improvements were obtained for the PCT-B model. Since ORPLM13 was identified as an outlier in the PCT-Na modeling work, it was also omitted in the PCT-B modeling work. The PCT-B models listed in Table 5.11 are described below.

- Model 4 (18-term PQM) adds a SnO_2 term. Model statistics improve slightly but remain generally lower than with the corresponding PCT-Na model.
- Model 5 is a 22-term PQM obtained by MRS, which includes new quadratic terms for $\text{Al}_2\text{O}_3 \times \text{K}_2\text{O}$, $\text{B}_2\text{O}_3 \times \text{K}_2\text{O}$, $\text{K}_2\text{O} \times \text{SiO}_2$, $\text{Li}_2\text{O} \times \text{SiO}_2$, $\text{CaO} \times \text{SnO}_2$, $\text{K}_2\text{O} \times \text{SnO}_2$ and $\text{CaO} \times \text{ZrO}_2$. A p -value smaller than 0.0025 was returned for all except $\text{CaO} \times \text{SnO}_2$ (at 0.076), which indicates that this term may not be significant. The regression and validation statistics are much improved for this model and the calculated RMSE of 0.276 is comparable to the 27% RSD for the PCT-B round robin [48] and 21% for the replicates evaluated above.
- Model 6 (23-term PQM) includes an additional square term for $\text{Al}_2\text{O}_3 \times \text{Al}_2\text{O}_3$ and provides somewhat better regression statistics but worse validation statistics.

Among the currently evaluated PCT-B models, the 22-term Model 5 shows the best combination of regression statistics and validation performance. Figure 5.5 shows a predicted versus measured plot resulting from this model. A tight distribution of points around the 45° line is seen for both the WTP dataset and the additional ORP dataset. A very slight under-prediction is observed for PBT-B releases near and above the limit of 4 g/L, although this tendency remains smaller than was observed in WTP models.

The variance/covariance matrices for the best performing PCT-Na model (Model 5) and PCT-B model (Model 5) are provided in the Appendix.

⁴ JMP offers two Response Surface Methodologies providing methods of augmenting a linear mixture model with quadratic terms or other nonlinear blending terms. The Mixture Response Surface (MRS) model suppresses the intercept, includes all the linear main-effect terms, excludes all the square terms (such as $X_1 \times X_1$), but includes all cross terms (such as $X_1 \times X_2$). The Response Surface (RS) is different from MRS only by including all square terms ($X_1 \times X_1$).

5.2 VHT Modeling

The VHT data used for model development are described in Section 5.2.1. The composition range covered by the model and identification of outliers are discussed in Section 5.2.2 and validation dataset selection is described in Section 5.2.3. Replicates and near-replicates used to evaluate the lack of fit of the models are presented and discussed in Section 5.2.4. The status of VHT model development for the combined dataset is discussed in Section 5.2.5.

5.2.1 VHT Dataset

Of the 512 LAW glasses collected and discussed in Sections 2 and 4 above, 416 have VHT results. Multiple replicates have been included in the dataset in an effort to estimate and possibly improve on the large variation observed in various replicate VHT measurements. In all, 430 VHT data have been collected for development of an enhanced model. The VHT alteration depths and alteration rates for these glasses vary from undetectable, and estimated to be less than $0.05\ \mu\text{m}$ ($0.006\ \text{g/m}^2/\text{day}$), to greater than $1200\ \mu\text{m}$ ($133\ \text{g/m}^2/\text{day}$). This range excludes the results for 40 VHT coupons, including two in duplicate, that were altered completely before the end of the 24-day test period. Because the ORP-LAW glasses are aimed at maximizing waste loadings, they are designed to determine the likely limits of LAW sodium and sulfur loadings in the glass. Multiple glasses were prepared at increased waste loading with the intent to approach or even slightly exceed the VHT limit so that the limit of waste loading can be determined. As a result, many more ORP-LAW glasses (32) than WTP-LAW glasses (6) had the VHT test coupons completely altered, and many ORP-LAW glass samples exceeded the contractual limit for VHT alteration. In total, 111 glasses have VHT alteration rates above the $50\ \text{g/m}^2/\text{d}$ limit [53], 138 from the ORP-LAW dataset, and 29 from the WTP-LAW dataset. The 111 glasses with VHT alteration rates above the $50\ \text{g/m}^2/\text{d}$ limit include the 40 VHT tests mentioned above for which the extent of alteration was so high that the entire glass coupon was altered and therefore a rate could not be calculated. The VHT alteration rates for these glasses, listed as “greater than” values in the dataset, can still be used as secondary validation for the models.

5.2.2 VHT Model Range and Outliers

In the WTP baseline model development [1], 16 WTP-LAW glasses were excluded from the ILAW VHT modeling dataset: 6 were excluded as compositional outliers, 4 were container-centerline-cooled glasses with high Cr_2O_3 content that were considered non-representative, and VHT alteration exceeded the sample thickness in 6 samples. Expansion of the compositional space now permitted inclusion of 6 of the 16 glasses previously excluded as compositional outliers. The other 10 samples remained excluded for the current modeling work. The samples for which alteration exceeded the sample thickness can however be used to validate model predictions with very high alteration rates as is discussed below, in Section 5.2.5.

The overall compositional range considered at the onset of the current model development was kept as broad as possible, encompassing both WTP-LAW and ORP-LAW

datasets (Table 5.6). As with the PCT dataset, MgO is the only component for which a limit (of 5.1 wt%) was applied. Table 5.12 lists the nine LAW glasses excluded from the current VHT modeling dataset and the reason each glass was excluded. Glasses formerly excluded due to high concentrations of CaO, Fe₂O₃, and ZnO were all kept in the dataset used for the present VHT model development and their possible status as outliers was reevaluated individually during model development. Similarly, the new glass LORPM8R1, which showed about 2 vol% crystallization, was kept in the model dataset and later individually evaluated as a possible outlier, as discussed in Section 5.2.4 below. However, LORPM13, which crystallized and was clearly identified as a PCT outlier, was not included in the model dataset. Table 5.13 lists the 38 glasses for which VHT alteration exceeded the sample thickness (32 ORP-LAW + 6 WTP-LAW). The final data set for modeling contains 385 VHT test results, including replicates.

5.2.3 VHT Validation Set Selection

Model validation was accomplished in the WTP baseline VHT model development by data-splitting, data-partitioning, and by applying the models to calculate the properties of outlying glass compositions. The data available was limited to 165 VHT test results and therefore reducing the modeling set by reserving data for independent validation was undesirable. The data-splitting method permitted use of all the available data in the VHT modeling dataset. The present VHT dataset of 385 results allowed reserving samples for independent validation of the new VHT models. To select the validation dataset, all actively designed glasses were sorted by increasing VHT alteration rate and one glass out of every ten samples was pulled from the set, resulting in a validation set of 27 glasses. None of the statistically designed glasses or replicates were pulled from the modeling dataset. The selected validation glasses are listed in Table 5.14.

5.2.4 VHT Replicates

Table 5.15 lists 30 sets of replicate and near-replicate LAW glasses, fifteen each from the WTP-LAW and the ORP-LAW VHT datasets. The table also lists estimates of percent relative standard deviations (%RSDs) for each replicate set, as well as pooled estimates over all the replicate sets. Note that the standard deviations in all of these sets also account for the uncertainties due to fabricating glasses at crucible scale or in melter tests, and difference in thermal history, and sulfate content of the glass. The %RSD in the first part of Table 5.15 (for WTP-LAW replicates) is much improved by the addition of ten replicates, all showing medium to large VHT alteration rates (28.45%, versus 41.87% in the previous dataset [1]). The %RSD calculated from ORP-LAW replicates, which includes twelve near replicates, mostly with variation in minor components (sulfate and halide components), shows larger variation (47.29% RSD) but this is lower (24.04% RSD) for the three true replicates.

As shown in Table 5.15, the overall RSD over the thirty replicates sets is 40% for near-replicates and 23% for true replicates. These estimates of replicate uncertainty for the VHT are used subsequently to statistically assess lack-of-fit (LOF) of the various models considered in Section 5.2.5 below.

5.2.5 Preliminary VHT Models

The recommended baseline WTP LAW VHT model, which contains four cubic terms, predicts VHT alteration depths reasonably well near and above the WTP contract limit (R^2 of 0.74) when applied to the WTP-LAW VHT data. However, a marked decrease in R^2 was observed when the model was applied to the ORP-LAW dataset [21], (R^2 of 0.35 for ORP-LAW VHT data). The extended sodium range, beyond the design range of the WTP baseline VHT model for high waste loading glasses in the ORP-LAW dataset, is a major reason for the poor performance. A similar result was observed for the VHT data on the twenty LORPM glasses. The twenty LORPM glasses identified by red triangles in Figure 5.6 cover a broad range of VHT alterations and the lack of agreement between measured VHT alterations and values predicted using the baseline model is comparable to what was seen with the rest of the ORP-LAW glasses.

Improvements to the VHT model followed the same strategy as was used for the PCT models described in Section 5.1. The model forms considered are still from the general class of *mixture experiment models* and started from the partial quadratic mixture (PQM) model with four cubic terms selected as the WTP baseline VHT model [1]. Regression models were successively developed with incremental improvement in the model statistics, as summarized in Table 5.16, where model parameters and statistics are provided in the upper part and validation statistics in the lower part. The strategy to progressively improve the model performance was as follows:

- Model 1 is the WTP baseline VHT model, which is a 15-Term Reduced Partial Cubic Mixture Model (PCM), and is included here for comparison.
- Model 2 uses identical sets of model terms (15-term PCM) but these have been updated for the expanded dataset. The model does not provide much improvement over the WTP baseline VHT model.
- In Model 3 (16-term PCM), addition of model terms for SnO_2 and V_2O_5 were both considered but only tin oxide was retained based on its significance (based on t -test results). From this point on, the mixture term for “Others” applies to the sum of the minor components (Ag_2O , BaO , Br , CdO , Cs_2O , I , La_2O_3 , MnO , MoO_3 , NiO , PbO , Re_2O_7 , SeO_2 , SrO , and “Unknown”), Cl , Cr_2O_3 , F , SO_3 , TiO_2 , ZnO and V_2O_3 . An improvement, although minor, is observed in the regression as well as validation statistics.
- Model 4 (16-term PCM) provides updated terms from Model 3 after the Grubbs’ test identified LORPM13 as an outlier, as was also the case for PCT-Na modeling; normal quantile plots of model residuals are presented in Figure 5.7 where LORPM13 is identified as an outlier. Exclusion of this additional outlier improves the model statistics.
- Model 5 is a 13-term PQM obtained by MRS: none of the square or cubic terms of alkalis are included in this case and the only quadratic term identified to be of significance is

$\text{CaO} \times \text{SiO}_2$. Performance statistics from fitting this much simplified model do not show any improvement from Model 4.

- Model 6 (20-term PQM) is a Response Surface (RS) model that includes the square terms $(\text{CaO})^2$, $(\text{K}_2\text{O})^2$ and $(\text{Na}_2\text{O})^2$ as well as the quadratic alkali terms $\text{K}_2\text{O} \times \text{Na}_2\text{O}$ and $\text{Li}_2\text{O} \times \text{Na}_2\text{O}$ along with $\text{CaO} \times \text{SiO}_2$, $\text{K}_2\text{O} \times \text{MgO}$ and $\text{Al}_2\text{O}_3 \times \text{Na}_2\text{O}$. The regression statistics and validation R^2 are improved with this model but the validation RSME is slightly worse than for Models 3, 4, and 5. These performance statistics for Model 6 are also better than those obtained for the WTP baseline VHT model and the dataset on which it was regressed, which showed an R^2 and R^2_{Adjusted} of 0.744 and 0.720, respectively, and an RMSE of 0.848.
- Model 7 (26-term PCM) was the last attempt at improving the VHT model by applying a factorial model of 3rd degree⁵. Although slightly better regression statistics were obtained than those for Model 6, the validation statistics were much worse.

Despite the significantly extended composition range in the dataset, several of the models explored here show as good or better predictive performance as does the WTP baseline VHT model over the smaller composition range on which it was built. Among the currently developed models, Model 6, the 20-term PQM VHT model performs the best. Figure 5.8 shows a predicted versus measured plot resulting from this model. The distribution of points around the 45° line shows a similarly large scatter for the WTP dataset and the ORP dataset. However, the distribution is even around the diagonal, indicating an unbiased prediction. The variance/covariance matrix for Model 6 is provided in the Appendix.

5.3 Electrical Conductivity Modeling

The electrical conductivity data used for model development are described in Section 5.3.1. The model range and any outliers are described in Section 5.3.2 and validation set selection is described in Section 5.3.3. Near-replicates used to evaluate the model lack of fit are discussed in Section 5.3.4. The status of development of enhanced electrical conductivity (EC) models for the combined WTP-LAW and ORP-LAW datasets is discussed in Section 5.3.5.

5.3.1 Dataset for Electrical Conductivity

Of the 512 LAW glasses collected and discussed in Sections 2 and 4 above, 323 glasses have electrical conductivity data, which were generally measured at four temperatures, resulting in a dataset of 1290 data points. Measurements are available at only three temperatures for glasses LAW145 and ORPLA6.

⁵ Factorial of third degree models include any possible interactions of three components ($X_1 \times X_2 \times X_3$) or any factorial of one (X_1^3) or two components ($X_1^2 \times X_2$).

The current WTP requirement [53] for glass melt electrical conductivity is that it be within the range of 0.1 to 0.7 S/cm in the temperature range of 1100 to 1200 °C. Among 323 ORP-LAW glasses, fifteen of the measurements were above this range, with values from 0.702 to 0.820 S/cm, mostly among glasses with the highest alkali contents, and particularly glasses in the ORPLA, ORPLB and ORPLC series formulated at 25 wt% Na₂O.

Electrical conductivity was measured at temperatures close to the four nominal values (950, 1050, 1150, and 1250°C) for most WTP-LAW and ORP-LAW glasses. C22AN107, C22Si-15, C22Si+15, and LAWE7H, have highest measurement temperatures of approximately 1200°C instead of 1250°C, while LAWB82, LAWM42, and LAWM48 have all four measurement temperatures noticeably below the nominal values. Two other glasses that have measurement temperatures significantly different from the nominal values are LAWC103 and ORPLE2. These have minimum measurement temperatures of 988°C instead of 950°C and a maximum measurement temperature of 1202°C instead of 1250°C, respectively. These observations are provided for information only, since they do not affect the suitability of the associated data for developing electrical conductivity models.

5.3.2 Electrical Conductivity Model Range and Outliers

The WTP baseline EC model excluded 10 WTP-LAW glasses from the ILAW EC and viscosity modeling datasets, in all cases because their compositions were outside a compositional range. The ORP-LAW dataset broadens the compositional range, as shown in Table 5.6, and all of the above outliers can now be included in the modeling dataset. In the WTP baseline modeling work [1], two WTP-LAW glasses were identified as significant outliers: LAWM30 tended to be grossly over-predicted with any of the models suggested, while LAWM40 was under predicted. No specific reason could be found to exclude these glasses and they were included in the dataset. Among the ORP-LAW glasses, the preliminary EC models developed herein also identified LORPM13 as an outlier, as also was the case based on observations from PCT and VHT modeling.

5.2.3 Electrical Conductivity Validation Set Selection

Model validation was accomplished during the WTP baseline model development by data-splitting, data-partitioning, and by applying the models to calculate the properties of outlying glass compositions. The data available was limited to 171 glasses (682 EC data) and it was undesirable to reduce the dataset by reserving data for validation. The data-splitting method permitted use of all the data available in the EC modeling dataset. The current set of 323 glasses (1290 EC data points) is large enough to allow for a set of glasses to be reserved for independent validation of the new predictive models. To select the validation set, all actively designed glasses were sorted by increasing electrical conductivity near 1150 °C (third measurement) and one glass out of every seven samples was pulled from the set, resulting in a validation set of 30 glasses with 120 EC measurements. None of the statistically designed glasses or replicates were pulled from the modeling set. The selected validation glasses are listed in Table 5.17.

5.3.4 Electrical Conductivity Replicates

Only four near-replicate pairs of electrical conductivity versus temperature values are available to use in model lack-of-fit evaluation. Table 5.18 summarizes the replicate measurements and Figure 5.9 shows the electrical conductivity values plotted against $1/T$ (with T in Kelvin) for the two near-replicate glasses LAWC100R1, a crucible melt, and WVY-G-95A from a DM100 melter run. The lines correspond to the fit of the Arrhenius equation:

$$\ln(EC) = A + B(1/T). \quad (5.1)$$

These data indicate a 5.8% RSD over the four measured temperatures and a 3.3% RSD over the four nominal temperatures.

5.3.4 Preliminary Electrical Conductivity Models

The recommended WTP model (25-Term Reduced Truncated Linear Mixture Models with three Quadratic Terms) provides a good fit to the EC data for the WTP glasses ($R^2 = 0.948$) on which it was developed. However, the prediction performance was significantly worse ($R^2 = 0.748$) for the ORP-LAW dataset, or the 20 LORPM glasses identified by red triangles in Figure 5.10. The error in prediction varied from 28% under-predicted (for a glass such as ORPLE12) to 100% over-predicted (in LAWC100R1 or LAWA194, for example), with greater deviation at higher conductivity.

Improvements in EC models were achieved through the same strategy as was used for the PCT and VHT models discussed above. This time, as was used in WTP modeling, the model form considered for EC was a slightly modified version of the Arrhenius equation with its two parameters expanded as functions of LAW glass composition. The partial quadratic mixture (PQM) model form to predict the natural logarithm of EC was as follows:

$$\ln(EC) = \sum_{i=1}^q a_i x_i + a_{CaOLi_2O} x_{CaO} x_{Li_2O} + a_{CaONa_2O} x_{CaO} x_{Na_2O} + a_{Li_2ONa_2O} x_{Li_2O} x_{Na_2O} + \sum_{i=1}^q b_i \frac{x_i}{T/1000}, \quad (5.2)$$

which is the same form as that used for the baseline WTP LAW EC model [1] and the same quadratic terms are retained. The x_i ($i = 1, 2, \dots, q$) are normalized mass fractions of the q glass oxide components such that

$$\sum_{i=1}^q x_i = 1. \quad (5.3)$$

The modification to the Arrhenius equation is that temperature (T in Kelvin) is divided by the scaling factor of 1000 so that the b_i coefficients are similar in magnitude to the a_i coefficients.

Regression models were successively developed with improvements in the model statistics, as summarized in Table 5.19 in which model parameters and statistics are given in the upper part and validation statistics in the lower part. The strategy to progressively improve the model performance is described below.

- Model 1 corresponds to the previous 25-term reduced Arrhenius-linear mixture model with three cross-product terms selected for the WTP baseline model. This, when applied to the same set of 171 glasses (excluding 10 outliers) returned very close yet slightly different coefficients than reported earlier [1], but identical other statistics. This is presented here for comparison to the other models. The validation model statistics when the model is applied to the 15 glasses not used in model development (the 15 ORP-LAW glasses from the 30-glass validation set) are worse than those obtained by data splitting during WTP baseline model development ($R^2 = 0.80$, RMSE 0.305 versus 0.947 and 0.175, respectively [1]).
- Model 2 uses identical sets of model terms (25 terms) but they have been updated for the expanded dataset (excluding the single compositional outlier, LORPM13). In all, 1166 composition and temperature data points are used in modeling and another 120 in validation. The quadratic coefficient $\text{Li}_2\text{O} \times \text{Na}_2\text{O}$ is most changed in comparison to Model 1, which may be a consequence of the increased alkali content in the ORP-LAW glasses. Model 2 shows much improved validation statistics with $R^2 = 0.967$ and RMSE = 0.121; in addition, the model statistics are as good or better than those for the WTP baseline model [1].
- In Model 3 (27-term) the addition of model terms for SnO_2 and $\text{SnO}_2/(T/1000)$ is explored while keeping all of the other terms from Model 2. The performance of Model 3 is identical to that of Model 2 in model and validation statistics. In addition, since the p -values calculated in t -tests on the two SnO_2 terms were very high (0.398 for the mixture term, 0.231 for the temperature term), it is likely that SnO_2 is not a significant factor in the EC model.
- In Model 4 (27-term) addition of model terms for V_2O_5 and $\text{V}_2\text{O}_5/(T/1000)$ is explored. Model and validation statistics for Model 4 are worse than those for Model 2. The p -values calculated in t -tests were 0.235 and 0.0227 for the V_2O_5 mixture term and $\text{V}_2\text{O}_5/(T/1000)$ term, respectively. Thus, vanadium does not appear to have any significant effect in the EC model. Note also that Grubbs test did identify the statistically designed WTP glass LAWM30 as an outlier, as was the case in WTP modeling.

Among the EC models considered during the present work, Model 2, the 25-term reduced Arrhenius-linear mixture model with three cross-product terms, provides the best model and validation statistics when applied to the extended dataset comprising of WTP-LAW and ORP-LAW glasses. Figure 5.11 displays the predicted versus measured plot for this EC model. The tight distribution of points around the 45° line shows that this model provides good and unbiased predictions over the full range of measured EC values. The scatter observed is mostly due to some previously identified WTP outlying data points. The variance/covariance matrix for this model is provided in the Appendix.

5.4 Viscosity Modeling

The viscosity data used for model development are presented in Section 5.4.1. The model range and any outliers are described in Section 5.4.2 and the validation set selection is described in Section 5.4.3. Near-replicates used to evaluate the model lack of fit are presented in Section 5.4.4. The status of viscosity model development for the combined dataset (WTP-LAW and ORP-LAW glasses) is discussed in Section 5.4.5.

5.4.1 Viscosity Dataset

Of the 512 LAW glasses collected and discussed in Sections 2 and 4 above, 321 glasses have viscosity results. Because of crystallization, viscosity measurements were not conducted on glasses LORPM8R1 and LORPM13. Melt viscosities were generally measured at four temperatures, with the exception of LAWM7 for which five measurements were taken, resulting in a dataset of 1285 records. Among WTP glasses, LAWA51, LAWA128R1, LAWA129R1, and LAWM5 had viscosities exceeding the recommended WTP upper limit of 150 poise at 1100°C [53]; among ORP glasses ORPLA5, ORPLA6, ORPLA11, ORPLA12, ORPLA13, ORPLA14, ORPLG1, ORPLG2, ORPLG4, ORPLG5, LORPM5, and LORPM9 had viscosities exceeding the recommended upper limit [53]. These are glass formulations with high waste loadings for which high concentrations of zirconia and addition of tin oxide were used to compensate for the detrimental effects of higher sodium on glass leaching.

Viscosity was measured at temperatures close to the four nominal values (950, 1050, 1150, and 1250°C) for all ORP-LAW glasses with very few exceptions (e.g., for ORPLA3 viscosity was measured at 1219°C instead of 1250°C; for ORPLE9 viscosity was measured at 992°C instead of 950°C). These observations are noted but they do not affect the suitability of the associated data for developing viscosity models since actual measurement temperatures are used in the models.

Overall, the measured viscosity values for the 321 LAW glasses vary from 5.99 to 2461 poise, with smaller viscosity values generally corresponding to higher temperatures and larger viscosity values corresponding to lower temperatures. The range of viscosity values is similar for the ORP-LAW and WTP-LAW glasses.

5.4.3 Viscosity Validation Set Selection

Selection of validation glasses was made following a similar strategy to that used for the electrical conductivity data. To select the validation set, all actively designed glasses were sorted by increasing viscosity near 1150 °C (third measurement) and one glass out of every eight samples was pulled from the set, resulting in a set of 28 glasses (112 viscosity-temperature data points) that were reserved for independent validation of the models. None of the statistically designed glasses or any replicates were pulled from the modeling dataset. The selected glasses are listed in Table 5.20.

5.4.4 Viscosity Replicates

One near-replicate pair of viscosity versus temperature values is compared in Table 5.21. Figure 5.12 shows the two sets of viscosity values plotted against $1/T$ (with T in Kelvin), with a line corresponding to the fit of the Arrhenius equation (similar to Equation 5.1 with viscosity replacing electrical conductivity) for the two LAW glasses. The data indicate a 2% RSD over the four measured temperatures and also over the four nominal temperatures.

5.4.5 Preliminary Viscosity Models

The WTP baseline viscosity model provided the best fit to the WTL-LAW dataset ($R^2 = 0.988$). As expected, the performance of the model is worse for the OPR-LAW glasses and for the new LORPM glasses, as can be seen in Figure 5.13. ($R^2 = 0.961$ and 0.884 for OPR-LAW and LORPM, respectively).

Attempts to expand and improve viscosity models followed the same steps as for the electrical conductivity models described above. The model form considered for viscosity was the same as that used for the baseline WTP LAW viscosity model, as described below. Unlike the case of the electrical conductivity, significant curvature is evident in Arrhenius plots for the viscosity [1]. Consequently, the Vogel-Fulcher equation generally provides a better representation of the temperature dependence of the viscosity than does the Arrhenius equation. A simplification of the Vogel-Fulcher equation in terms of a truncated second-order Taylor series expansion, referred to as the “truncated T2 model” [55], was used as the basis for the baseline WTP LAW viscosity model [1]. Expansion of the two parameters in that model as functions of LAW glass composition leads to the partial quadratic mixture (PQM) model that was used as the WTP LAW baseline viscosity model form to predict the natural logarithm of viscosity [1]:

$$\ln(\eta) = \sum_{i=1}^q a_i x_i + \text{Selected} \left\{ \sum_{i=1}^q a_{ii} x_i^2 + \sum_{i < j}^{q-1} \sum_j^q a_{ij} x_i x_j \right\} + \sum_{i=1}^q b_i \frac{x_i}{(T/1000)^2}, \quad (5.4)$$

where the x_i ($i = 1, 2, \dots, q$) are normalized mass fractions of the q glass oxide components such that

$$\sum_{i=1}^q x_i = 1. \quad (5.5)$$

Note that the temperature (T in Kelvin) is divided by the scaling factor of 1000 so that the b_i coefficients are similar in magnitude to the a_i coefficients. The WTP baseline model used 26 terms.

Table 5.22 provides a summary of the successive regression models developed for predicting the melt viscosity, with model parameters and statistics in the upper part and

validation statistics in the lower part. The strategy to progressively improve the model performance was as follows:

- Model 1 corresponds to the WTP baseline model [1], which is a 26-term reduced truncated T2 mixture model with four quadratic terms $((\text{B}_2\text{O}_3)^2, (\text{Li}_2\text{O})^2, (\text{MgO})^2$ and $\text{Al}_2\text{O}_3 \times \text{Li}_2\text{O})$. This, model when applied to the same set of data from 171 glasses (excluding 10 outliers) returned very close yet slightly different coefficients than the previous model [1], but identical other statistics. Note that the temperature terms $\text{B}_2\text{O}_3/(T/1000)^2$ and $\text{K}_2\text{O}/(T/1000)^2$ are not included (the p -values calculated in t -tests were 0.792 and 0.615, respectively, indicating little significance for these terms). This starting model is presented here for comparison. The validation model statistics obtained using the 14 glasses not used in the model (ORP-LAW glasses) are poorer than the validation statistics obtained by data splitting during the WTP baseline model development but are still indicative of good prediction performance ($R^2 = 0.961$, RMSE 0.354 versus 0.988 and 0.145, respectively [1]).
- Model 2 uses the same set of model terms (26 terms) as Model 1 but the coefficients are regressed on the expanded dataset. In all, 1173 combined composition and temperature data points were used to develop Model 2 and another 112 data points were reserved for validation. The model shows improved validation statistics and only slightly worse regression statistics. One of the largest changes noted is in both the magnitude and the uncertainty in the $(\text{MgO})^2$ term, with the large uncertainty suggesting that this term may not be significant. (The $\text{B}_2\text{O}_3/(T/1000)^2$ and $\text{K}_2\text{O}/(T/1000)^2$ terms continued to show little significance with the expanded data set.)
- Model 3 (28-term) considered the addition of model terms for SnO_2 and $\text{SnO}_2/(T/1000)^2$ while keeping all other terms the same as in Model 2. Both the regression and validation statistics are improved in this case. Both SnO_2 terms had p -values of less than 0.0025, indicating that they are significant. The $(\text{MgO})^2$ term, for which the t -test p -value has increased to 0.466, remains of questionable significance.
- Model 4 (28-term) considered the addition of model terms for V_2O_5 and $\text{V}_2\text{O}_5/(T/1000)^2$, while keeping all other terms the same as in Model 2. However, this resulted in small decreases in the regression and validation statistics. The p -values calculated in t -tests were 0.015 and 0.011 for the V_2O_5 mixture term and $\text{V}_2\text{O}_5/(T/1000)^2$ term, respectively. The t -test p -value for the $(\text{MgO})^2$ term increased to 0.760 for this model.
- Model 5 (27-term) is the same as Model 3 but deletes the $(\text{MgO})^2$ term, which appeared to be insignificant in all of the new models investigated. This is confirmed by the regression and validation statistics for this model, which are essentially identical to those obtained for Model 3.

Among the models considered for LAW glass melt viscosity, Model 5, the 27-term truncated T2 mixture model with three cross-product terms gives the best model and validation statistics. This model is the same as Model 3 except for the deletion of the $(\text{MgO})^2$ term and

provides essentially identical performance with one less parameter. In contrast to the WTP baseline dataset, the $(\text{MgO})^2$ term appears to be of low significance for the extended data set. Figure 5.14 displays the predicted versus measured plot for this viscosity model. The tight distribution of points around the 45° line shows that this model provides an excellent and unbiased prediction over the full range of measured viscosity values. The variance/covariance matrix for this model is provided in the Appendix.

SECTION 6.0

SUMMARY AND CONCLUSIONS

The ORP dataset is comprised of data from a series of LAW glass development and melter testing studies for ORP in which incremental improvements of the WTP LAW facility was considered over several years. These improvements focused primarily on increasing the waste loading, particularly with respect to sulfate and sodium, but also investigated increasing the processing temperature, and increasing the fraction of the sulfur in the feed that is partitioned to the off-gas stream to further increase the waste loading. The applicability of these improvements over the expected range of sodium, potassium, and sulfur concentrations was demonstrated for a wide range of Hanford LAW compositions. The resulting ORP-LAW glass compositions are significantly different from the WTP-LAW glass compositions in both the concentration ranges of glass components as well as in the use of SnO_2 and V_2O_5 as new glass former additives, primarily in place of Fe_2O_3 and TiO_2 . With the increases in waste loadings, the concentrations of glass formers such as Al_2O_3 , CaO , and ZrO_2 have also been significantly increased. All of the original ORP glasses were actively designed formulations. While the ORP data significantly expand both the number of glasses available for modeling and the composition ranges, not surprisingly, gaps were identified in the combined WTP and ORP datasets, in both the compositions and in the glass property responses.

As an initial step towards addressing these gaps, 20 new ORP glasses were statistically designed, focusing in particular on the composition gaps. Data collected from these new glasses have been compiled to support the revision of the baseline WTP LAW glass property models. The new data, compiled together with previous ORP and WTP data, include glass compositions, PCT releases, VHT response, melt electrical conductivity, and melt viscosity. The overall LAW datasets now consists of 512 glasses after adding 229 ORP glasses to the original 271 WTP-LAW glasses collected to develop models in 2006, plus the 12 WTP glasses added to augment the VHT dataset in 2008 but not considered in the earlier WTP models. In addition, many of the 20 glasses excluded as compositional outliers in the baseline WTP modeling work could be retained in the modeling dataset for the expanded composition region.

The new datasets were used to develop revised LAW models for the extended glass composition range that includes the higher waste loading ORP formulations. Models were developed for five glass properties: PCT-Na response, PCT-B response, VHT response, melt viscosity, and melt electrical conductivity. In general, the regression and validation statistics for these models are comparable to those for the original WTP baseline models but the new models are valid over much wider composition ranges. R^2 and R^2_{Adjusted} model statistics vary from 0.987 and 0.987, respectively, for melt viscosity to 0.776 and 0.763, respectively, for VHT. As found previously, the VHT response is the most challenging property for model development, in part due to the inherent variability in the test and the complex nature of the underlying phenomena. Interestingly, although many of the ORP glasses include SnO_2 and V_2O_5 , which is not the case for the WTP glasses, model terms involving V_2O_5 were not found to be significant for any of the

five properties. Model terms involving SnO_2 were not found to be significant for electrical conductivity but were found to be significant for the other four properties.

As noted above, this is the first step in a multi-stage process to improve and to extend the range of validity of the current baseline WTP LAW glass property-composition models to encompass the higher waste loading glass formulations that have been developed for ORP. Work is ongoing to continue to address gaps in the data in order to improve the support for model development and to further refine the model forms to improve their performance over the extended composition range. During this preliminary phase of the work, the focus was on determining whether model forms similar to the WTP baseline models perform as well with the expanded composition range. In the next phase of the work, other model forms will be explored in an attempt to further improve the performance of the models.

SECTION 7.0 QUALITY ASSURANCE

This work was conducted under a quality assurance program compliant with the applicable criteria of 10 CFR 830.120; the American Society of Mechanical Engineers (ASME) NQA-1, 2004; and DOE Order 414.1 C, Quality Assurance. These QA requirements are implemented through a Quality Assurance Project Plan for ORP/RPP-WTP work [56] that is conducted at VSL. Test and procedure requirements by which the testing activities are planned and controlled are also defined in this plan. The program is supported by VSL standard operating procedures that were used for this work [57].

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Table 2.1. Minimums and Maximums of LAW Glass Components (Mass Fractions) in Datasets Used for the WTP-LAW Glass Property Models [1] and the ORP-LAW Datasets.

LAW Glass Property	PCT		VHT		Viscosity & Electrical Conductivity ^(b)		Glasses in Any Property Modeling Dataset	
Number of Glasses in Baseline Modeling Set	244 (+20 excluded)		165 (+16 excluded) +12 augmentation ^(a)		171 (+10 excluded)		271+12 augmentation ^(a)	
Number of ORP-LAW Glasses	171 + 20 augmentation		203 + 20 augmentation		122 + 20 augmentation		209+ 20 augmentation	
Total	455		416		323		512	
WTP-LAW Glass Component	Min	Max	Min	Max	Min	Max	Min	Max
Al ₂ O ₃	0.03499	0.09044	0.03503	0.09044	0.03499	0.09043	0.03499	0.09044
B ₂ O ₃	0.05999	0.13263	0.06008	0.13262	0.05999	0.13057	0.05999	0.13263
CaO	0	0.10463	0	0.10463	0	0.10462	0	0.10463
Cl	0	0.01171	0	0.00914	0	0.01171	0	0.01171
Cr ₂ O ₃	0	0.00631	0	0.00631	0.00008	0.00592	0	0.00631
F	0	0.00471	0	0.00470	0	0.00351	0	0.00471
Fe ₂ O ₃	0	0.08412	0	0.08039	0	0.08412	0	0.08412
K ₂ O	0	0.05559	0	0.05413	0	0.05412	0	0.05559
Li ₂ O	0	0.05825	0	0.05825	0	0.05825	0	0.05825
MgO	0	0.05019	0	0.05019	0	0.05019	0	0.05019
Na ₂ O	0.02457	0.24007	0.02457	0.24007	0.02457	0.23002	0.02457	0.24007
P ₂ O ₅	0	0.04752	0	0.03020	0	0.04023	0	0.04752
SiO ₂	0.38007	0.52148	0.38362	0.52148	0.38007	0.52147	0.38007	0.52148
SO ₃	0.00070	0.01060	0.00070	0.01021	0.00070	0.01060	0.00070	0.01060
TiO ₂	0	0.03015	0	0.03015	0	0.03014	0	0.03015
ZnO	0.00100	0.05366	0.00999	0.05366	0.00998	0.05365	0.00998	0.05366
ZrO ₂	0	0.05003	0	0.05003	0	0.05001	0	0.05003
Others	0	0.00451	0	0.00280	0	0.00280	0	0.00451
ORP-LAW Glass Component	Min	Max	Min	Max	Min	Max	Min	Max
Al ₂ O ₃	0.05514	0.13854	0.05514	0.13854	0.05818	0.13854	0.05514	0.13854
B ₂ O ₃	0.06061	0.13740	0.06061	0.13740	0.06061	0.13740	0.06056	0.13740
CaO	0	0.12241	0	0.12241	0	0.12241	0	0.12241
Fe ₂ O ₃	0	0.03019	0	0.03019	0	0.06984	0	0.06984
K ₂ O	0.00110	0.05881	0.00110	0.05881	0.00110	0.05881	0.00110	0.05881
Li ₂ O	0	0.05023	0	0.05023	0	0.05023	0	0.05023
MgO	0	0.09939	0	0.09939	0	0.03369	0	0.09939
Na ₂ O	0.09989	0.26005	0.09989	0.26005	0.09993	0.25040	0.09989	0.26005
P ₂ O ₅	0	0.02500	0	0.02500	0	0.02010	0	0.02500
SiO ₂	0.29824	0.46178	0.29824	0.46178	0.34364	0.46178	0.29824	0.46178
SO ₃	0.00160	0.02170	0.00160	0.02170	0.00120	0.02100	0.00120	0.02170
TiO ₂	0	0.01549	0	0.01549	0	0.01549	0	0.01549
ZnO	0.01000	0.03652	0.01000	0.03652	0.01000	0.03652	0.00998	0.03652
ZrO ₂	0.02559	0.06753	0.02559	0.06753	0.02951	0.06753	0.02559	0.06753
SnO ₂ (new)	0	0.05001	0	0.05001	0	0.04830	0	0.05001
V ₂ O ₅ (new)	0	0.03001	0	0.03001	0	0.04001	0	0.04001
Others	0.00220	0.03780	0.00220	0.03780	0.00220	0.02931	0.00220	0.03780

(a) 12 VHT augmentation glasses were added after the baseline model work was completed.

(b) Viscosity and electrical conductivity data were collected on exactly the same glasses, so their information is combined.

Table 2.1. Minimums and Maximums of LAW Glass Components (in Mass Fractions) in the Datasets Used for the WTP Baseline LAW Glass Property Models [1] and ORP-LAW Datasets (continued).

LAW Glass Property	PCT		VHT		Viscosity & Electrical Conductivity ^(a)		Glasses in Any Property Modeling Dataset	
	Min	Max	Min	Max	Min	Max	Min	Max
WTP-LAW Glass Components in “Others”								
BaO	0	0.00020	0	0.00010	0	0.01000	0	0.00020
Br	0	0.00079	0	0.00079	0	0	0	0.00079
CdO	0	0.00100	0	0.00010	0	0.00010	0	0.00100
Cs ₂ O	0	0.00180	0	0.00180	0	0.00180	0	0.00180
I	0	0.00101	0	0	0	0	0	0.00101
MnO	0	0.00005	0	0	0	0	0	0.00005
MoO ₃	0	0.00012	0	0.00012	0	0.00010	0	0.00012
NiO	0	0.00036	0	0.00036	0	0.00031	0	0.00036
PbO	0	0.00031	0	0.00031	0	0.00031	0	0.00031
Re ₂ O ₇	0	0.00111	0	0.00111	0	0.00111	0	0.00111
SeO ₂	0	0.00100	0	0	0	0	0	0.00100
SrO	0	0.00002	0	0	0	0	0	0.00002
Unknown	0	0.00264	0	0	0	0	0	0.00264
ORP-LAW Glass Components in “Others”	Min	Max	Min	Max	Min	Max	Min	Max
Cl	0.0001	0.01170	0.0001	0.01170	0.0001	0.01161	0.0001	0.01170
Cr ₂ O ₃	0.0002	0.00600	0.0002	0.00600	0.00018	0.00600	0.0002	0.00600
Cs ₂ O	0	0.00190	0	0.00190	0	0.00190	0	0.00190
F	0	0.00490	0	0.00491	0	0.00490	0	0.00491
I	0	0.00100	0	0.00100	0	0.00100	0	0.00100
MnO	0	0.00060	0	0.00060	0	0.00060	0	0.00060
NiO	0	0.00040	0	0.00043	0	0.00040	0	0.00043
P ₂ O ₅	0	0.02500	0	0.02500	0	0.02010	0	0.02500
PbO	0	0.00020	0	0.00020	0	0.00020	0	0.00020

(a) Viscosity and electrical conductivity data were collected on exactly the same glasses, so their information is combined.

Table 2.2. WTP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity.

Glass ID	PCT ^(a)	VHT ^(a)	Viscosity ^(a)	Electrical ^(a) Conductivity
LAWA44R10	1	1	1	1
LAWA53	1	1	1	1
LAWA56	1	1	1	1
LAWA88	1	0	1	1
LAWA88R1	1	1	0	0
LAWA102R1	1	1	1	1
LAWA126	1	1	1	1
LAWA128	1	1	0	0
LAWA128R1	0	0	1	1
LAWA130	1	1	1	1
LAWB65	1	1	1	1
LAWB66	1	1	1	1
LAWB68	1	1	1	1
LAWB78	1	1	1	1
LAWB79	1	1	1	1
LAWB80	1	1	1	1
LAWB83	1	1	1	1
LAWB84	1	1	1	1
LAWB85	1	1	1	1
LAWB86	1	1	1	1
C100-G-136B	1	1	1	1
LAWC27	1	1	1	1
LAWC32	1	1	1	1
LAWM1	1	1	1	1
LAWM2	1	1	1	1
LAWM3	1	1	1	1
LAWM4	1	1	1	1
LAWM5	1	1	1	1
LAWM6	1	1	1	1
LAWM7	1	1	1	1
LAWM8	1	1	1	1
LAWM9	1	1	1	1
LAWM10	1	1	1	1
LAWM11	1	1	1	1
LAWM12	1	1	1	1
LAWM13	1	1	1	1
LAWM14	1	1	1	1
LAWM15	1	1	1	1

Glass ID	PCT	VHT	Viscosity	Electrical Conductivity
LAWM16	1	1	1	1
LAWM17	1	1	1	1
LAWM18	1	1	1	1
LAWM19	1	1	1	1
LAWM20	1	1	1	1
LAWM21	1	1	1	1
LAWM22	1	1	1	1
LAWM23	1	1	1	1
LAWM24	1	1	1	1
LAWM25R1	1	1	1	1
LAWM26	1	1	1	1
LAWM27	1	1	1	1
LAWM28	1	1	1	1
LAWM29	1	1	1	1
LAWM30	1	1	1	1
LAWM31	1	1	1	1
LAWM32	1	1	1	1
LAWM33R1	1	1	1	1
LAWM34	1	1	1	1
LAWM35	1	1	1	1
LAWM36	1	1	1	1
LAWM37	1	1	1	1
LAWM38	1	1	1	1
LAWM39	1	1	1	1
LAWM40	1	1	1	1
LAWM41	1	1	1	1
LAWM42	1	1	1	1
LAWM43	1	1	1	1
LAWM44	1	1	1	1
LAWM45	1	1	1	1
LAWM46	1	1	1	1
LAWM47	1	1	1	1
LAWM48	1	1	1	1
LAWM49	1	1	1	1
LAWM50	1	1	1	1
LAWM51	1	1	1	1
LAWM52	1	1	1	1
LAWM53	1	1	1	1

(a) An entry of 1 indicates data is available for that property on that glass, while an entry of 0 indicates no data is available for that property on that glass.

Table 2.2. WTP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity (continued).

Glass ID	PCT ^(a)	VHT ^(a)	Viscosity ^(a)	Electrical Conductivity ^(a)
LAWM54R1	1	1	1	1
LAWM55	1	1	1	1
LAWM56	1	1	1	1
LAWM57	1	1	1	1
LAWM58	1	1	0	0
LAWM59	1	1	1	1
LAWM60	1	1	1	1
LAWM61	1	1	0	0
LAWM62	1	1	0	0
LAWM63	1	1	1	1
LAWM64	1	1	0	0
LAWM65	1	1	0	0
LAWM66	1	1	1	1
LAWM67	1	1	0	0
LAWM68	1	1	1	1
LAWM69	1	1	0	0
LAWM70	1	1	0	0
LAWM71	1	1	1	1
LAWM72	1	1	0	0
LAWM73	1	1	1	1
LAWM74	1	1	0	0
LAWM75	1	1	1	1
LAWM76	1	1	0	0
LAWE2H	1	1	1	1
LAWE3	1	1	1	1
LAWE3H	1	1	1	1
LAWE4	0	0	1	1
LAWE4H	1	1	1	1
LAWE5	0	0	1	1
LAWE5H	1	1	1	1
LAWE7	0	1	1	1
LAWE7H	1	1	1	1
LAWE9H	1	1	1	1
LAWE10H	1	1	1	1
LAWE11	1	1	1	1
LAWE12	1	1	1	1
LAWE13	1	1	1	1
LAWE14	1	1	0	0

Glass ID	PCT	VHT	Viscosity	Electrical Conductivity
LAWE15	1	1	0	0
LAWE16	1	1	1	1
LAWE3Cr2CCC	1	1	0	0
LAWE9HCr1CCC	1	1	0	0
LAWE9HCr2CCC	1	1	0	0
LAWE10HCr3CCC	1	1	0	0
LAWCrP1R	1	1	1	1
LAWCrP2R	1	1	1	1
LAWCrP3R	1	1	1	1
LAWCrP4R	1	1	1	1
LAWCrP5	1	1	1	1
LAWCrP6	1	1	0	0
LAWCrP7	1	1	0	0
LAWA41	1	0	1	1
LAWA42	1	0	1	1
LAWA43-1	1	0	1	1
LAWA44	1	0	0	0
LAWA45	1	0	1	1
LAWA49	1	1	1	1
LAWA50	1	0	1	1
LAWA51	1	1	1	1
LAWA52	1	1	1	1
LAWA60	1	1	1	1
LAWA65	1	0	0	0
LAWA76	1	0	0	0
LAWA81	1	0	1	1
LAWA82	1	0	1	1
LAWA83	1	0	1	1
LAWA84	1	0	0	0
LAWA87	1	0	0	0
LAWA89	1	0	1	1
LAWA90	1	0	1	1
LAWA93	1	0	1	1
LAWA96	1	0	1	1
LAWA102R2	1	0	0	0
LAWA104	1	1	0	0
LAWA105	1	1	0	0
LAWA112B14	1	0	0	0

(a) An entry of 1 indicates data is available for that property on that glass, while an entry of 0 indicates no data is available for that property on that glass.

Table 2.2. WTP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity (continued).

Glass ID	PCT ^(a)	VHT ^(a)	Viscosity ^(a)	Electrical Conductivity ^(a)
LAWA112B15	1	0	0	0
LAWA125	1	1	1	1
LAWA127R1	1	0	1	1
LAWA127R2	1	0	0	0
LAWA129	1	0	0	0
LAWA129R1	0	0	1	1
LAWA133	1	1	0	0
LAWA134	1	1	1	1
LAWA135	1	1	1	1
LAWA136	1	1	1	1
LAWA170	1	0	0	0
LAWB30	1	0	1	1
LAWB31	1	0	0	0
LAWB32	1	0	0	0
LAWB33	1	0	0	0
LAWB34	1	0	1	1
LAWB35	1	0	0	0
LAWB37	1	0	1	1
LAWB38	1	0	1	1
LAWB40	1	0	0	0
LAWB41	1	0	0	0
LAWB60	1	1	1	1
LAWB61	1	0	1	1
LAWB62	1	1	1	1
LAWB63	1	1	1	1
LAWB64	1	1	1	1
LAWB67	1	1	1	1
LAWB69	1	1	1	1
LAWB70	1	1	1	1
LAWB71	1	1	1	1
LAWB72	1	1	1	1
LAWB73	1	1	1	1
LAWB74	1	1	1	1
LAWB75	1	1	1	1
LAWB76	1	1	1	1
LAWB77	1	1	1	1
LAWB81	1	1	1	1
LAWB82	1	1	1	1

Glass ID	PCT	VHT	Viscosity	Electrical Conductivity
LAWB87	1	0	1	1
LAWB88	1	0	1	1
LAWB89	1	1	1	1
LAWB90	1	1	1	1
LAWB91	1	1	0	0
LAWB92	1	1	1	1
LAWB93	1	1	0	0
LAWB93R1	0	0	1	1
LAWB94	1	1	1	1
LAWB95	1	1	1	1
LAWB96	1	0	0	0
LAWC12	1	0	1	1
LAWC15	1	1	0	0
LAWC21	1	0	0	0
LAWC21rev2	1	0	1	1
LAWC22	1	0	0	0
LAWC23	1	0	0	0
LAWC24	1	0	0	0
LAWC25	1	0	0	0
LAWC26	1	1	0	0
LAWC28	1	1	0	0
LAWC29	1	1	1	1
LAWC30	1	1	1	1
LAWC31	1	1	0	0
LAWC31R1	0	0	1	1
LAWC33	1	1	0	0
TFA-BASE	1	1	0	0
C22AN107	1	1	1	1
A88AP101R1	1	1	0	0
A88Si+15	1	1	1	1
A88Si-15	1	1	1	1
C22Si+15	1	1	1	1
C22Si-15	1	1	1	1
A1C1-1	1	1	1	1
A1C1-2	1	1	1	1
A1C1-3	1	1	0	0
C1-AN107	1	1	1	1
A2-AP101	1	1	1	1

(a) An entry of 1 indicates data is available for that property on that glass, while an entry of 0 indicates no data is available for that property on that glass.

Table 2.2. WTP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity (continued).

Glass ID	PCT ^(a)	VHT ^(a)	Viscosity ^(a)	Electrical Conductivity ^(a)
A2B1-1	1	1	1	1
A2B1-2	1	1	1	1
B1-AZ101	1	1	1	1
C2-AN102C35	1	1	1	1
A3-AN104	1	1	1	1
A2B1-3	1	0	1	1
A3C2-1	1	0	1	1
A3C2-2	1	0	1	1
A3C2-3	1	0	1	1
A1-AN105R2	1	0	1	1
12U-G-86A	1	0	0	0
LA44PNCC	1	0	0	0
LA44CCCR2	1	0	0	0
WVF-G-21B	1	0	0	0
PNLA126CC	1	0	0	0
LA126CCC	1	0	0	0
WVM-G-142C	1	0	0	0
A100G115A	1	0	0	0
A100CC	1	0	0	0
WVB-G-124B	1	0	0	0
LA137SRCCC	1	0	0	0
WVR-G-127A	1	0	0	0

Glass ID	PCT	VHT	Viscosity	Electrical Conductivity
LB83PNCC	1	0	0	0
LB83CCC-1	1	0	0	0
WVJ-G-109D	1	0	0	0
GTSD-1126	1	0	0	0
LB88CCC	1	0	0	0
AZ-102 Surr SRNL	1	0	0	0
12S-G-85C	1	0	0	0
C100GCC	1	0	0	0
AN-102 Surr LC Melter	1	0	0	0
WVH-G-57B	1	0	0	0
GTSD-1437	1	0	0	0
PLTC35CCC	1	0	0	0
AN-103 Actual	1	0	0	0
AW-101 Actual	1	0	0	0
AP-101 Actual	1	0	0	0
AZ-101 Actual	1	0	0	0
AZ-102 Actual	1	0	0	0
AZ-102 Actual CCC	1	0	0	0
AN-107 Actual (LAWC15)	1	0	0	0
AN-102 Actual LC Melter	1	0	0	0
AN-102 Actual	1	0	0	0
Totals	264	181	181	181

(a) An entry of 1 indicates data is available for that property on that glass, while an entry of 0 indicates no data is available for that property on that glass.

Table 2.3. ORP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity.

Glass ID	VHT ^(a)	PCT ^(a)	Viscosity ^(a)	Electrical Conductivity ^(a)
LAWA143	0	0	1	1
LAWA144	0	0	1	1
LAWA145	0	0	1	1
LAWA161	1	1	0	0
LAWA161-duplicate	1	0	0	0
LAWA161S2	0	0	1	1
LAWA171	1 ^{*(b)}	1	1	1
LAWA172	1 [*]	1	1	1
LAWA173	1	1	1	1
LAWA174	1	1	1	1
LAWA175	1	1	1	1
LAWA176	1	1	1	1
LAWA177	1 [*]	1	1	1
LAWA178	1 [*]	1	1	1
LAWA179	1 [*]	1	1	1
LAWA180	1	1	1	1
LAWA181	1 [*]	1	1	1
LAWA182	1 [*]	1	1	1
LAWA183	1	1	1	1
LAWA184	1	1	1	1
LAWA185	1	1	1	1
LAWA186	1	1	1	1
LAWA187	1	1	1	1
LAWA187-duplicate	1	0	0	0
LAWA187CCC	0	1	0	0
LAWA188	1	1	1	1
LAWA189	1	1	1	1
LAWA190	1	1	1	1
LAWA191	1	1	1	1
LAWA192	1	1	1	1
LAWA193	1	1	1	1
LAWA194	1	1	1	1
LAWA195	1	1	1	1
LAWA196	1	1	1	1
LAWA197	1	1	1	1
LAWB97	1	1	1	1
LAWB98	1	1	1	1
LAWB99	1	1	1	1
LAWB100	1	1	1	1
LAWB101	1	1	1	1
LAWB102	1	1	1	1
LAWB103	1	1	1	1
LAWB104	1	1	1	1
LAWB105	1	1	1	1

(b) An entry of 1 indicates data is available for that property on that glass, while an entry of 0 indicates no data is available for that property on that glass.

(c) An entry of 1^{*} for VHT denotes a test for which the glass test coupon was fully reacted and only a “greater than” value is available.

Table 2.3. ORP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity (continued).

Glass ID	VHT	PCT	Viscosity	Electrical Conductivity
LAWC100R1	1	1	1	1
LAWC101	1	1	1	1
LAWC102	1	1	1	1
LAWC103	1	1	1	1
ORPLA1	1 ^{*(b)}	1	1	1
ORPLA1S4	1*	0	0	0
ORPLA2	1	1	1	1
ORPLA2S4	1	0	0	0
ORPLA3	1	1	1	1
ORPLA3S4	1	0	0	0
ORPLA4	1	1	1	1
ORPLA4S4	1	0	0	0
ORPLA5	1	1	1	1
ORPLA5S4	1*	0	0	0
ORPLA6	1	1	1	1
ORPLA6S4	1	0	0	0
ORPLA7	1	1	1	1
ORPLA7S4	1	0	0	0
ORPLA8	1	1	1	1
ORPLA8S4	1*	0	0	0
ORPLA9	1	1	1	1
ORPLA9S4	1	0	0	0
ORPLA10	1	1	1	1
ORPLA10S4	1	0	0	0
ORPLA11	1*	1	1	1
ORPLA11S4	1*	0	0	0
ORPLA12	1	1	1	1
ORPLA12S4	1	0	0	0
ORPLA13	1	1	1	1
ORPLA13S4	1	0	0	0
ORPLA14	1	1	1	1
ORPLA14S4	1	0	0	0
ORPLA15	1	1	1	1
ORPLA15S4	1	0	0	0
ORPLA16	1	1	1	1
ORPLA16S4	1	0	0	0
ORPLA17	1	1	1	1
ORPLA17S4	1	0	0	0
ORPLA18	1	1	1	1
ORPLA19	1	1	1	1
ORPLA20	1	1	1	1
ORPLA21	1	1	0	0
ORPLA22	1	1	0	0
ORPLA23	1	1	0	0
ORPLA24	1	1	0	0

(a) An entry of 1 indicates data is available for that property on that glass, while an entry of 0 indicates no data is available for that property on that glass.

(b) An entry of 1* for VHT denotes tests for which the glass test coupon was fully reacted and only a “greater than” value is available.

Table 2.3. ORP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity (continued).

Glass ID	VHT ^(a)	PCT ^(a)	Viscosity ^(a)	Electrical Conductivity ^(a)
ORPLA25	1	1	0	0
ORPLA26	1	1	0	0
ORPLA27	1 ^{*(b)}	1	0	0
ORPLA28	1	1	0	0
ORPLA29	1	1	0	0
ORPLA30	1*	1	0	0
ORPLA31	1*	1	0	0
ORPLA32	1	1	0	0
ORPLA33	1	1	0	0
ORPLA33-1	1	1	1	1
ORPLA34	1	1	0	0
ORPLA35	1	1	0	0
ORPLA36	1	1	0	0
ORPLA37	1	1	0	0
ORPLA38	1	1	0	0
ORPLA38-1	1	1	1	1
ORPLB1	1*	1	1	1
ORPLB1S4	1*	0	0	0
ORPLB2	1	1	1	1
ORPLB2S4	1	0	0	0
ORPLB3	1	1	1	1
ORPLB3S4	1	0	0	0
ORPLB4	1	1	1	1
ORPLB4S4	1	0	0	0
ORPLC1	1	1	1	1
ORPLC1S4	1	0	0	0
ORPLC2	1*	1	1	1
ORPLC2S4	1	0	0	0
ORPLC3	1*	1	0	0
ORPLC3S4	1*	0	0	0
ORPLC4	1*	1	0	0
ORPLC4S4	1*	0	0	0
ORPLC5	1	1	1	1
ORPLC5S4	1	0	0	0
ORPLD1	1	1	1	1
ORPLD1S4	1	0	0	0
ORPLD2	1	1	0	0
ORPLD2S4	1	0	0	0
ORPLD3	1	1	0	0
ORPLD3S4	1	0	0	0
ORPLD4	1	1	1	1
ORPLD5	1	1	1	1
ORPLD6	1	1	1	1
ORPLD7	1	1	1	1
ORPLD8	1	1	1	1
ORPLD9	1	1	1	1

(a) An entry of 1 indicates data is available for that property on that glass, while an entry of 0 indicates no data is available for that property on that glass.

(b) An entry of 1* for VHT denotes tests for which the glass test coupon was fully reacted and only a “greater than” value is available.

Table 2.3. ORP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity (continued).

Glass ID	VHT^(a)	PCT^(a)	Viscosity^(a)	Electrical Conductivity^(a)
ORPLE1	1	1	1	1
ORPLE2	1	1	1	1
ORPLE3	1	1	1	1
ORPLE4	1	1	1	1
ORPLE5	1	1	1	1
ORPLE6	1	1	1	1
ORPLE7	1	1	1	1
ORPLE8	1	1	1	1
ORPLE9	1	1	1	1
ORPLE10	1	1	1	1
ORPLE11	1	1	1	1
ORPLE12	1	1	1	1
ORPLF1	1	1	1	1
ORPLF2	1	1	1	1
ORPLF3	1	1	1	1
ORPLF4	1	1	1	1
ORPLF5	1	1	0	0
ORPLF6	1	1	0	0
ORPLF7	1	1	1	1
ORPLF8	1	1	1	1
ORPLF9	1	1	1	1
ORPLF10	1	1	1	1
ORPLF11	1	1	0	0
ORPLF12	1	1	1	1
ORPLF13	1	1	1	1
ORPLF14	1	1	1	1
ORPLG1	1	1	1	1
ORPLG2	1	1	1	1
ORPLG3	1	1	0	0
ORPLG4	1	1	1	1
ORPLG5	1	1	1	1
ORPLG6	1	1	1	1
ORPLG7	1	1	1	1
ORPLG8	1	1	1	1
ORPLG9	1	1	1	1
ORPLG10	1	1	1	1
ORPLG11	1	1	1	1
ORPLG12	1	1	1	1
ORPLG13	1	1	0	0
ORPLG14	1 ^{*(b)}	1	0	0
ORPLG15	1	1	0	0
ORPLG16	1*	1	0	0
ORPLG17	1*	1	0	0
ORPLG18	1*	1	0	0
ORPLG19	1*	1	0	0

(a) An entry of 1 indicates data is available for that property on that glass, while an entry of 0 indicates no data is available for that property on that glass.

(b) An entry of 1* for VHT denotes tests for which the glass test coupon was fully reacted and only a “greater than” value is available.

Table 2.3. ORP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity (continued).

Glass ID	VHT^(a)	PCT^(a)	Viscosity^(a)	Electrical Conductivity^(a)
ORPLG20	1	1	0	0
ORPLG21	1	1	1	1
ORPLG22	1	1	1	1
ORPLG23	1	1	1	1
ORPLG24	1	1	1	1
ORPLG25	1	1	1	1
ORPLG26	1	1	1	1
ORPLG27	1	1	1	1
Q10-G-134A (ORPLE12)	1	1	0	0
R10-G-155A (ORPLA15)	1	1	0	0
S10-G-101B (ORPLC5)	1	1	0	0
S10-G-45A (ORPLB4)	1	1	0	0
T10-G-16A (ORPLD1)	1	1	0	0
WVW-G-11A (LAWA161)	1	1	0	0
Y10-G-146C (ORPLA20)	1	1	0	0
Z10-G-122B (ORLF7-low SO ₃)	1	1	0	0
Z10-G-153B (ORLF7-high SO ₃)	1	1	0	0
Z10-G-60C (ORPLD6)	0	1	0	0
10A-G-53C (ORPLD6)	1	1	0	0
10A-G-43B (ORPLG9)	1 ^{*(b)}	1	0	0
DWV-G-123C (LAWB99)	1	1	0	0
EWV-G-89B (LAWA187)	1	1	0	0
EWV89BCCC (LAWA187)	1	1	0	0
EWV-G-93B (LAWA187)	1	0	0	0
EWV93BCCC (LAWA187)	1	0	0	0
EWV-G-108B (LAWA187)	1	0	0	0
WVY-G-95A (LAWC100)	1	1	1	1
J10-G-24B (ORPLA38-1)	1	1	0	0
I10-G-135A (ORPLG27)	1	1	0	0
Totals (# Glasses = 207)	203	171	122	122

(a) An entry of 1 indicates data is available for that property on that glass, while an entry of 0 indicates no data is available for that property on that glass.

(b) An entry of 1* for VHT denotes tests for which the glass test coupon was fully reacted and only a “greater than” value is available.

Table 2.4. Three-Layer Component Constraints for the ORP Test Matrix (wt%).

Oxides	Outer Layer		Middle Layer		Inner Layer	
	Lower limit	Upper limit	Lower limit	Upper limit	Lower limit	Upper limit
Al ₂ O ₃	3.500	13.850	5.570	11.780	6.605	10.745
B ₂ O ₃	6.000	13.730	7.546	12.184	8.319	11.411
CaO	0.000	12.240	2.448	9.792	3.672	8.568
Fe ₂ O ₃	0.300	8.000	1.840	6.460	2.610	5.690
K ₂ O	0.110	5.880	1.264	4.726	1.841	4.149
Li ₂ O	0.000	5.000	1.000	4.000	1.500	3.500
MgO	0.000	5.000	1.000	3.500	1.500	2.500
Na ₂ O	5.000	25.000	10.000	22.000	14.000	20.000
SO ₃	0.100	1.000	0.240	0.600	0.350	0.500
SiO ₂	35.000	52.000	38.400	48.600	40.100	46.900
SnO ₂	0.000	5.000	1.000	4.000	1.500	3.500
TiO ₂	0.000	3.000	0.600	2.400	0.900	2.100
V ₂ O ₅	0.000	4.000	0.800	3.200	1.200	2.800
ZnO	1.000	5.000	1.800	4.200	2.200	3.800
ZrO ₂	0.000	6.000	2.000	5.000	3.000	5.000
Others	0.050	2.000	0.050	2.000	0.050	2.000

Table 2.5. Composition of the Grouped Component “Others” for the ORP Test Matrix.

Components	Relative Amount (wt%)	Maximum Amount in Glass (wt%)
BaO	0.50	0.01
CdO	0.50	0.01
Cl	40.01	0.80
Cr ₂ O ₃	16.07	0.32
F	14.97	0.30
NiO	1.50	0.03
PbO	1.50	0.03
P ₂ O ₅	24.95	0.50
Subtotal	100.00	2.00

Table 2.6. Compositions of the Twenty LORPM Glasses.

LORPM Glass #	Al ₂ O ₃	B ₂ O ₃	CaO	Fe ₂ O ₃	K ₂ O	Li ₂ O	MgO	Na ₂ O	SO ₃	SiO ₂	SnO ₂	TiO ₂	V ₂ O ₅	ZnO	ZrO ₂	Others	Sum
1	6.870	8.267	1.274	1.363	0.110	5.000	0.000	10.641	1.000	52.000	2.559	0.474	3.442	5.000	0.000	2.000	100
2	12.876	6.520	10.588	0.300	5.253	2.663	4.609	6.823	0.190	35.000	2.159	0.284	3.733	1.000	6.000	2.000	100
3	4.201	7.296	1.762	7.208	1.014	0.000	2.476	22.803	0.548	37.088	5.000	3.000	2.500	1.706	1.619	1.778	100
4	9.443	12.378	5.054	0.300	5.880	0.000	4.922	13.957	0.740	35.971	0.000	1.080	4.000	4.415	0.000	1.861	100
5	10.833	6.000	4.300	8.000	0.637	5.000	0.000	8.283	0.910	48.037	5.000	0.000	0.000	1.000	0.000	2.000	100
6	3.500	13.730	12.240	0.300	0.774	0.000	4.105	13.146	0.100	35.000	5.000	0.000	0.000	5.000	5.105	2.000	100
7	13.850	7.793	2.295	4.092	2.017	3.029	1.258	14.054	0.180	37.785	0.404	0.523	1.458	5.000	5.491	0.771	100
8	13.850	6.891	0.000	0.756	3.202	2.376	5.000	8.342	1.000	40.345	4.616	2.622	4.000	5.000	0.000	2.000	100
9	8.582	6.935	0.000	0.300	0.847	0.000	0.000	23.898	0.100	49.298	0.000	0.000	4.000	5.000	0.989	0.050	100
10	3.500	6.000	12.240	8.000	5.880	5.000	4.502	5.000	0.887	38.991	0.000	3.000	4.000	1.000	0.000	2.000	100
11	3.500	6.000	0.000	0.300	0.110	0.000	5.000	19.620	0.100	49.370	0.000	3.000	0.000	5.000	6.000	2.000	100
12	3.500	12.425	0.765	1.183	5.267	4.424	4.204	5.000	0.910	52.000	4.341	2.700	0.000	1.499	0.000	1.782	100
13	13.850	13.730	0.000	8.000	0.110	0.500	0.000	13.310	1.000	37.060	1.390	0.000	4.000	1.000	6.000	0.050	100
14	5.570	7.546	9.792	2.395	4.726	3.611	3.500	13.273	0.240	38.400	3.622	0.600	2.875	1.800	2.000	0.050	100
15	5.570	7.546	5.897	6.460	1.264	4.000	3.500	10.000	0.600	40.343	3.610	0.884	3.200	1.800	5.000	0.326	100
16	11.780	12.184	2.448	2.626	2.509	4.000	1.963	10.638	0.564	38.400	2.933	0.925	0.800	3.935	2.295	2.000	100
17	10.759	7.546	2.670	5.747	4.217	1.000	3.500	18.667	0.539	38.607	1.000	0.762	0.800	2.137	2.000	0.050	100
18	5.570	7.546	2.448	1.840	1.264	3.345	3.173	10.583	0.276	47.889	4.000	2.400	3.200	1.800	4.615	0.050	100
19	8.593	9.253	4.300	2.918	2.802	1.733	2.263	14.747	0.350	40.100	1.715	1.955	2.265	3.391	3.152	0.464	100
20	9.785	8.563	3.672	2.962	3.499	2.991	1.500	15.546	0.500	40.100	2.783	0.924	1.651	2.200	3.274	0.050	100

Table 4.1. XRF and DCP Analyses of the Twenty LORPM Glasses.

Glass	LORPM1			LORPM2R1			LORPM3			LORPM4R1			LORPM5		
	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis
Al ₂ O ₃	6.87	6.79	6.56	12.88	12.83	13.08	4.20	4.19	4.07	9.44	9.32	9.45	10.83	10.76	10.34
B ₂ O ₃	8.27	NA	8.01	6.52	NA	6.49	7.30	NA	7.42	12.38	NA	11.89	6.00	NA	6.12
BaO	0.01	0.00	0.02	0.01	0.00	0.01	0.01	0.00	0.01	0.01	0.00	0.01	0.01	0.03	0.01
CaO	1.27	1.42	1.44	10.59	10.94	10.94	1.76	1.87	1.79	5.05	5.10	5.06	4.30	4.70	4.41
CdO	0.01	0.04	NA	0.01	0.00	NA	0.01	0.04	NA	0.01	0.00	NA	0.01	0.05	NA
Cr ₂ O ₃	0.32	0.34	0.33	0.32	0.47	0.33	0.29	0.40	0.31	0.30	0.47	0.23	0.32	0.38	0.32
Fe ₂ O ₃	1.36	1.52	1.36	0.30	0.32	0.31	7.21	7.28	6.79	0.30	0.34	0.30	8.00	8.55	7.69
K ₂ O	0.11	0.11	0.09	5.25	5.12	4.81	1.01	0.70	0.95	5.88	5.77	5.59	0.64	0.42	0.54
Li ₂ O	5.00	NA	4.99	2.66	NA	2.60	0.00	NA	0.02	0.00	NA	0.03	5.00	NA	5.03
MgO	0.00	0.00	0.01	4.61	4.45	4.60	2.48	2.41	2.38	4.92	4.78	4.63	0.00	0.00	0.01
Na ₂ O	10.64	10.04	10.13	6.82	6.97	6.73	22.80	23.13	21.54	13.96	14.19	13.49	8.28	8.19	7.82
NiO	0.03	0.04	0.04	0.03	0.04	0.07	0.03	0.04	0.03	0.03	0.04	0.07	0.03	0.04	0.01
PbO	0.03	0.03	NA	0.03	0.03	NA	0.03	0.03	NA	0.03	0.03	NA	0.03	0.03	NA
SiO ₂	52.00	52.48	52.37	35.00	35.19	35.09	37.09	37.06	36.89	35.97	36.32	36.35	48.04	48.51	46.93
SnO ₂	2.56	2.56	2.58	2.16	1.92	2.19	5.00	4.73	4.97	0.00	0.00	0.01	5.00	4.40	5.00
TiO ₂	0.47	0.53	0.52	0.28	0.31	0.32	3.00	3.15	3.12	1.08	1.08	1.13	0.00	0.02	0.01
V ₂ O ₅	3.44	3.63	3.58	3.73	3.78	3.89	2.50	2.51	2.61	4.00	3.99	4.00	0.00	0.00	0.01
ZnO	5.00	5.35	5.09	1.00	0.97	1.01	1.71	1.71	1.78	4.42	4.37	4.42	1.00	1.08	1.05
ZrO ₂	0.00	0.01	0.00	6.00	5.98	5.77	1.62	1.67	1.63	0.00	0.01	0.02	0.00	0.00	0
Cl	0.80	0.56	NA	0.80	0.47	NA	0.71	0.55	NA	0.74	0.52	NA	0.80	0.45	NA
F	0.30	NA	NA	0.30	NA	NA	0.27	NA	NA	0.28	NA	NA	0.30	NA	NA
P ₂ O ₅	0.50	0.57	0.50	0.50	0.59	0.42	0.44	0.51	0.50	0.46	0.55	0.27	0.50	0.60	0.47
SO ₃	1.00	0.72	NA	0.19	0.17	NA	0.55	0.60	NA	0.74	0.70	NA	0.91	0.76	NA
Sum	100.0	100.0	97.6	100.0	99.7	98.7	100.0	99.9	96.8	100.0	100.0	97.0	100.0	100.0	95.8

NA = Not analyzed

Table 4.1. XRF and DCP Analyses of the Twenty LORPM Glasses (continued).

Glass	LORPM6			LORPM7R1			LORPM8R1			LORPM9			LORPM10R1		
	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis
Al ₂ O ₃	3.50	3.51	3.59	13.85	13.55	13.95	13.85	13.94	13.95	8.58	8.35	7.96	3.50	3.66	3.54
B ₂ O ₃	13.73	NA	13.54	7.79	NA	7.56	6.89	NA	6.9	6.94	NA	6.90	6.00	NA	6.05
BaO	0.01	0.00	0.01	0.00	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.01
CaO	12.24	13.35	12.43	2.30	2.42	2.34	0.00	0.00	0.03	0.00	0.02	0.03	12.24	12.28	12.66
CdO	0.01	0.04	NA	0.00	0.00	NA	0.01	0.00	NA	0.00	0.00	NA	0.01	0.02	NA
Cr ₂ O ₃	0.32	0.34	0.37	0.12	0.08	0.13	0.32	0.37	0.17	0.01	0.00	0.02	0.32	0.47	0.34
Fe ₂ O ₃	0.30	0.32	0.35	4.09	4.36	3.93	0.76	0.89	0.75	0.30	0.33	0.31	8.00	8.06	7.90
K ₂ O	0.77	0.63	0.69	2.02	2.15	2.07	3.20	3.22	3.02	0.85	0.71	0.75	5.88	5.40	5.41
Li ₂ O	0.00	NA	0.05	3.03	NA	3.02	2.38	NA	2.33	0.00	NA	0.01	5.00	NA	5.10
MgO	4.11	3.96	3.97	1.26	1.22	1.34	5.00	4.75	4.66	0.00	0.00	0.01	4.50	4.39	4.60
Na ₂ O	13.15	12.98	12.66	14.05	13.66	13.74	8.34	7.60	8.29	23.90	24.47	22.56	5.00	5.43	5.01
NiO	0.03	0.04	0.03	0.01	0.01	0.03	0.03	0.04	0.07	0.00	0.00	0.00	0.03	0.03	0.07
PbO	0.03	0.04	NA	0.01	0.01	NA	0.03	0.04	NA	0.00	0.00	NA	0.03	0.03	NA
SiO ₂	35.00	34.54	35.24	37.79	37.57	37.58	40.35	41.87	40.73	49.30	49.05	49.22	38.99	39.57	39.04
SnO ₂	5.00	4.67	5.03	0.40	0.38	0.41	4.62	3.76	4.08	0.00	0.00	0.01	0.00	0.00	0.01
TiO ₂	0.00	0.00	0.02	0.52	0.53	0.59	2.62	2.88	2.72	0.00	0.01	0.01	3.00	3.02	3.10
V ₂ O ₅	0.00	0.00	0.01	1.46	1.44	1.51	4.00	4.35	4.14	4.00	3.92	4.07	4.00	3.84	4.14
ZnO	5.00	5.18	5.03	5.00	5.20	4.99	5.00	5.29	4.98	5.00	4.96	5.00	1.00	1.01	1.01
ZrO ₂	5.11	5.32	5.17	5.49	5.66	5.24	0.00	0.01	0.01	0.99	1.04	0.98	0.00	0.00	0.00
Cl	0.80	0.55	NA	0.31	0.26	NA	0.80	0.52	NA	0.02	0.04	NA	0.80	0.27	NA
F	0.30	0.00	NA	0.12	0.00	NA	0.30	0.00	NA	0.01	0.00	NA	0.30	0.00	NA
P ₂ O ₅	0.50	0.56	0.60	0.19	0.24	0.00	0.50	0.63	0.59	0.01	0.02	0.08	0.50	0.60	0.39
SO ₃	0.10	0.09	NA	0.18	0.23	NA	1.00	0.56	NA	0.10	0.11	NA	0.89	0.81	NA
Sum	100.0	99.9	98.8	100.0	99.8	98.4	100.0	100.0	97.4	100.0	100.0	97.9	100.0	99.9	98.4

NA = Not analyzed

Table 4.1. XRF and DCP Analyses of the Twenty LORPM Glasses (continued).

Glass	LORPM11			LORPM12R1			LORPM13			LORPM14R1			LORPM15		
	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis
Al ₂ O ₃	3.50	3.53	3.60	3.50	3.59	3.52	13.85	13.63	13.37	5.57	5.39	5.63	5.57	5.30	5.45
B ₂ O ₃	6.00	NA	5.98	12.43	NA	12.09	13.73	NA	13.83	7.55	NA	7.32	7.55	NA	7.76
BaO	0.01	0.00	0.02	0.01	0.00	0.01	0.00	0.00	0	0.00	0.00	0.00	0.00	0.00	0
CaO	0.00	0.02	0.02	0.77	0.83	0.86	0.00	0.00	0.02	9.79	10.07	10.09	5.90	6.53	5.77
CdO	0.01	0.00	NA	0.01	0.05	NA	0.00	0.00	NA	0.00	0.00	NA	0.00	0.00	NA
Cr ₂ O ₃	0.32	0.32	0.28	0.29	0.30	0.30	0.01	0.00	0.01	0.01	0.00	0.01	0.05	0.00	0.06
Fe ₂ O ₃	0.30	0.36	0.33	1.18	1.25	1.18	8.00	8.33	7.92	2.40	2.45	2.32	6.46	6.98	6.41
K ₂ O	0.11	0.11	0.12	5.27	5.39	5.13	0.11	0.11	0.10	4.73	4.82	4.46	1.26	1.05	1.12
Li ₂ O	0.00	NA	0.03	4.42	NA	4.37	0.50	NA	0.51	3.61	NA	3.75	4.00	NA	4.04
MgO	5.00	4.81	4.49	4.20	3.87	3.98	0.00	0.00	0.00	3.50	3.17	3.49	3.50	3.17	3.39
Na ₂ O	19.62	19.45	19.14	5.00	4.80	5.00	13.31	13.36	12.9	13.27	13.88	12.92	10.00	9.94	9.92
NiO	0.03	0.05	0.04	0.03	0.04	0.03	0.00	0.00	0.04	0.00	0.00	0.03	0.00	0.00	0.04
PbO	0.03	0.04	NA	0.03	0.05	NA	0.00	0.00	NA	0.00	0.00	NA	0.00	0.01	NA
SiO ₂	49.37	48.72	49.12	52.00	53.35	53.15	37.06	37.19	37.00	38.40	37.75	38.31	40.34	39.37	40.03
SnO ₂	0.00	0.00	0.08	4.34	4.09	4.54	1.39	1.25	1.34	3.62	3.46	3.77	3.61	3.44	3.60
TiO ₂	3.00	3.24	3.17	2.70	2.80	2.82	0.00	0.02	0.02	0.60	0.66	0.66	0.88	0.99	0.85
V ₂ O ₅	0.00	0.00	0.03	0.00	0.00	0.01	4.00	4.23	4.04	2.88	2.93	2.96	3.20	3.35	3.20
ZnO	5.00	5.27	4.98	1.50	1.43	1.48	1.00	1.07	1.01	1.80	1.75	1.76	1.80	1.99	1.83
ZrO ₂	6.00	6.58	5.92	0.00	0.00	0.00	6.00	5.93	6.02	2.00	2.03	1.97	5.00	5.44	5.04
Cl	0.80	0.71	NA	0.71	0.35	NA	0.02	0.03	NA	0.02	0.03	NA	0.13	0.09	NA
F	0.30	0.00	NA	0.27	0.00	NA	0.01	0.00	NA	0.01	0.00	NA	0.05	0.00	NA
P ₂ O ₅	0.50	0.55	0.68	0.44	0.52	0.34	0.01	0.04	0.14	0.01	0.02	0.00	0.08	0.10	0.20
SO ₃	0.10	0.10	NA	0.91	0.41	NA	1.00	0.44	NA	0.24	0.26	NA	0.60	0.54	NA
Sum	100.0	99.9	98.0	100.0	100.0	98.8	100.0	99.9	98.3	100.0	99.8	99.5	100.0	99.8	98.7

NA = Not analyzed

Table 4.1. XRF and DCP Analyses of the Twenty LORPM Glasses (continued).

Glass	LORPM16R1			LORPM17R1			LORPM18			LORPM19R1			LORPM20R1		
	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis	Target	XRF Analysis	DCP Analysis
Al ₂ O ₃	11.78	11.62	12.01	10.76	10.34	10.95	5.57	5.30	5.51	8.59	8.29	8.61	9.79	9.52	9.86
B ₂ O ₃	12.18	NA	11.91	7.55	NA	7.51	7.55	NA	7.52	9.25	NA	9.11	8.56	NA	8.39
BaO	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0	0.00	0.00	0	0.00	0.00	0.00
CaO	2.45	2.58	2.51	2.67	2.72	2.75	2.45	2.71	2.57	4.30	4.41	4.26	3.67	3.71	3.63
CdO	0.01	0.00	NA	0.00	0.00	NA	0.00	0.00	NA	0.00	0.00	NA	0.00	0.00	NA
Cr ₂ O ₃	0.32	0.35	0.24	0.01	0.00	0.01	0.01	0.00	0.01	0.07	0.08	0.08	0.01	0.00	0.01
Fe ₂ O ₃	2.63	2.78	2.53	5.75	5.72	5.77	1.84	2.19	1.81	2.92	2.99	2.89	2.96	2.97	2.90
K ₂ O	2.51	2.62	2.43	4.22	4.40	4.21	1.26	1.12	1.13	2.80	2.87	2.75	3.50	3.60	3.44
Li ₂ O	4.00	NA	4.02	1.00	NA	1.19	3.35	NA	3.25	1.73	NA	1.98	2.99	NA	3.05
MgO	1.96	1.72	1.84	3.50	3.26	3.64	3.17	2.82	3.01	2.26	2.06	2.19	1.50	1.31	1.63
Na ₂ O	10.64	10.89	10.38	18.67	20.09	18.27	10.58	9.56	10.00	14.75	15.91	14.27	15.55	16.52	15.15
NiO	0.03	0.04	0.04	0.00	0.00	0.01	0.00	0.00	0.03	0.01	0.02	0.04	0.00	0.00	0.02
PbO	0.03	0.05	NA	0.00	0.01	NA	0.00	0.00	NA	0.01	0.01	NA	0.00	0.00	NA
SiO ₂	38.40	38.65	38.56	38.61	37.78	40.19	47.89	47.60	47.41	40.10	39.58	40.48	40.10	39.66	40.27
SnO ₂	2.93	2.89	3.08	1.00	0.93	1.07	4.00	3.72	3.96	1.72	1.56	1.83	2.78	2.56	2.85
TiO ₂	0.93	0.94	1.01	0.76	0.75	0.89	2.40	2.70	2.47	1.96	2.04	2.07	0.92	0.98	1.04
V ₂ O ₅	0.80	0.81	0.84	0.80	0.81	0.85	3.20	3.47	3.31	2.27	2.28	2.4	1.65	1.68	1.95
ZnO	3.94	3.87	3.93	2.14	2.01	2.24	1.80	1.99	1.84	3.39	3.17	3.38	2.20	2.02	2.17
ZrO ₂	2.30	2.35	2.28	2.00	1.98	2.15	4.62	5.41	4.61	3.15	3.06	3.12	3.27	3.24	3.19
Cl	0.80	0.54	NA	0.02	0.03	NA	0.02	0.03	NA	0.19	0.13	NA	0.02	0.02	NA
F	0.30	0.00	NA	0.01	0.00	NA	0.01	0.00	NA	0.07	0.00	NA	0.01	0.00	NA
P ₂ O ₅	0.50	0.55	0.35	0.01	0.02	0.00	0.01	0.03	0.18	0.12	0.12	0.07	0.01	0.03	0.00
SO ₃	0.56	0.51	NA	0.54	0.53	NA	0.28	0.28	NA	0.35	0.35	NA	0.50	0.49	NA
Sum	100.0	99.9	98.0	100.0	99.9	101.7	100.0	99.8	98.6	100.0	99.9	99.5	100.0	99.9	99.6

NA = Not Analyzed

Table 4.2. PCT Results^(a) for the Twenty LORPM Glasses.

Glass ID	pH	Concentration (ppm)			Normalized Concentration (g/L)			Normalized Mass Loss (g/m ²)		
		B	Na	Si	B	Na	Si	B	Na	Si
LORPM1	10.02	12.1	29.27	90.68	0.470	0.370	0.372	0.235	0.185	0.186
LORPM2R1	10.54	5.6	19.36	17.21	0.277	0.383	0.105	0.138	0.191	0.053
LORPM3	11.46	35.49	268.97	115.44	1.568	1.592	0.667	0.784	0.796	0.333
LORPM4R1	10.34	72.45	171.94	47.64	1.885	1.660	0.283	0.942	0.830	0.142
LORPM5	10.26	4.92	12.34	46.24	0.264	0.200	0.206	0.132	0.100	0.103
LORPM6	10.81	71.53	171.88	33.58	1.678	1.763	0.205	0.839	0.882	0.103
LORPM7R1	10.71	10.93	55.49	40.74	0.452	0.532	0.231	0.226	0.266	0.115
LORPM8R1	9.63	7.57	18.81	42.68	0.352	0.303	0.225	0.176	0.151	0.113
LORPM9	11.61	36.3	298.3	135.77	1.687	1.683	0.589	0.843	0.842	0.295
LORPM10R1	11.81	66.56	151.86	131.29	3.573	4.094	0.721	1.786	2.047	0.360
LORPM11	10.62	27.36	193.04	134.77	1.469	1.326	0.584	0.734	0.663	0.292
LORPM12R1	9.71	34.51	27.5	101.81	0.890	0.737	0.417	0.445	0.368	0.208
LORPM13	9.02	28.09	49.96	44.59	0.655	0.503	0.256	0.328	0.251	0.128
LORPM14R1	11.7	32.8	172.14	82.46	1.401	1.748	0.460	0.701	0.874	0.230
LORPM15	11.01	31.91	103.87	71.06	1.361	1.399	0.377	0.681	0.699	0.188
LORPM16R1	10.12	21.23	39.09	43.6	0.561	0.495	0.243	0.280	0.248	0.121
LORPM17R1	11.35	25.2	151.98	66.24	1.076	1.098	0.367	0.538	0.549	0.184
LORPM18	10.21	9.59	39.67	57.75	0.409	0.505	0.258	0.205	0.253	0.129
LORPM19R1	10.71	18.67	68.32	49.76	0.650	0.625	0.266	0.325	0.312	0.133
LORPM20R1	11.15	20.72	92.37	57.84	0.780	0.801	0.309	0.390	0.400	0.154

(a) 7-Day PCT, stainless steel vessel with S/V = 2000 m⁻¹. The PCT release concentrations (ppm) are as measured. Normalized concentrations (g/L) and normalized mass losses (g/m²) are normalized based on the target compositions discussed in Section 2.

Table 4.3. VHT Results for the Twenty LORPM Glasses.

Glass ID	Alteration Depth (μm)	Ln (μm)	Days	Rate (g/m ² /d) Calculated for Estimated Average Density of 2.65 g/cc	Comparison to Limit of 50 g/m ² /d
LORPM1 (triplicate test results and average)	528	6.2691	24	58.3	117%
	620	6.4297	24	68.5	137%
	342	5.8348	24	37.8	76%
	Average = 497 μm	6.178	-	Average = 54.8	110%
	%RSD^(a) = 28.5%	SD=0.3078			
LORPM2R1	34.1	3.5290	24	3.8	8%
LORPM3	602	6.3999	24	66.4	133%
LORPM4R1	688	6.5339	24	76.0	152%
LORPM5	97.0	4.5742	24	10.7	21%
LORPM6	Non-detectable ^(b)	-2.9957	24	0.0	0%
LORPM7R1	99.5	4.6004	24	11.0	22%
LORPM8R1	323	5.7761	24	35.6	71%
LORPM9	390	5.9649	24	43.0	86%
LORPM10R1	120	4.7875	24	13.3	27%
LORPM11	1.12	0.1133	24	0.1	0%
LORPM12R1	7.39	2.0001	24	0.8	2%
LORPM13	466	6.1449	24	51.5	103%
LORPM14R1	85.5	4.4485	24	9.4	19%
LORPM15	4.55	1.5151	24	0.5	1%
LORPM16R1	107	4.6681	24	11.8	24%
LORPM17R1	Fully altered	>7	24	>100	>200%
LORPM18	3.46	1.2413	24	0.4	1%
LORPM19R1	3.32	1.2000	24	0.4	1%
LORPM20R1	777	6.6559	24	85.8	172%

(a) %RSD = 100×(Standard Deviation / Mean).

(b) Based on SEM magnification, the alteration is less than 50 nm.

Table 4.4. Melt Electrical Conductivity Data for the Twenty LORPM Glasses.

Glass ID	Temp1 (°C)	EC1 (S/cm)	Temp2 (°C)	EC2 (S/cm)	Temp3 (°C)	EC3 (S/cm)	Temp4 (°C)	EC4 (S/cm)
LORPM1	940	0.218	1048	0.332	1147	0.486	1245	0.602
LORPM2R1	951	0.048	1052	0.096	1151	0.166	1248	0.273
LORPM3	957	0.333	1056	0.485	1151	0.675	1247	0.811
LORPM4R1	958	0.105	1060	0.173	1157	0.265	1253	0.364
LORPM5	960	0.142	1060	0.225	1154	0.335	1248	0.470
LORPM6	963	0.051	1060	0.106	1155	0.190	1250	0.301
LORPM7R1	965	0.181	1063	0.292	1159	0.406	1254	0.528
LORPM8R1	948	0.092	1052	0.138	1151	0.211	1248	0.286
LORPM9	963	0.383	1062	0.509	1158	0.655	1253	0.873
LORPM10R1	956	0.128	1057	0.231	1154	0.367	1251	0.524
LORPM11	967	0.189	1064	0.290	1159	0.406	1254	0.567
LORPM12R1	965	0.080	1061	0.138	1157	0.218	1251	0.301
LORPM13	963	0.155	1060	0.244	1155	0.317	1253	0.397
LORPM14R1	962	0.197	1059	0.319	1154	0.495	1250	0.669
LORPM15	965	0.143	1061	0.244	1157	0.383	1252	0.532
LORPM16R1	962	0.160	1059	0.254	1152	0.368	1249	0.523
LORPM17R1	961	0.203	1058	0.309	1153	0.455	1248	0.601
LORPM18	961	0.130	1060	0.223	1156	0.323	1252	0.452
LORPM19R1	964	0.167	1059	0.268	1155	0.387	1250	0.554
LORPM20R1	966	0.218	1062	0.335	1157	0.474	1252	0.654

Table 4.5. Melt Viscosity Data for the Twenty LORPM Glasses.

Glass ID	Temp1 (°C)	Vis1 (P)	Temp2 (°C)	Vis2 (P)	Temp3 (°C)	Vis3 (P)	Temp4 (°C)	Vis4 (P)
LORPM1	956	608.01	1056	178.43	1158	67.22	1258	31.13
LORPM2R1	959	2617.43	1058	217.41	1158	45.66	1257	17.43
LORPM3	952	210.04	1054	53.1	1157	18.71	1259	8.21
LORPM4R1	952	276.32	1053	77.14	1155	28.71	1256	12.93
LORPM5	957	2516.93	1057	574.63	1157	129.71	1257	48.00
LORPM6	950	503.27	1052	83.96	1154	19.40	1256	8.34
LORPM7R1	957	734.07	1058	172.89	1159	59.02	1260	23.86
LORPM9	953	818.04	1055	239.27	1158	91.49	1260	41.58
LORPM10R1	948	59.54	1050	17.76	1152	7.20	1255	3.58
LORPM11	954	2416.50	1054	463.27	1156	126.90	1256	45.61
LORPM12R1	949	885.72	1049	212.52	1150	71.78	1251	32.38
LORPM14R1	947	100.51	1048	29.00	1150	11.30	1251	5.16
LORPM15	958	255.39	1058	61.27	1159	19.47	1259	8.65
LORPM16R1	945	343.74	1045	94.22	1146	34.02	1247	15.28
LORPM17R1	945	562.51	1045	148.03	1145	52.30	1246	23.49
LORPM18	956	1115.91	1054	249.48	1154	77.90	1252	31.07
LORPM19R1	947	447.78	1045	113.11	1145	39.14	1244	17.17
LORPM20R1	950	327.12	1049	90.55	1149	33.32	1249	15.27

Table 5.1. Model Summary for the WTP Baseline 17-Term Reduced Partial Quadratic Mixture Model on the Natural Logarithm of ILAW PCT-B [1].

<p>Model form to predict the natural logarithm of the normalized PCT-B release (in g/L):</p> $\ln(PCT - B) = \sum_{i=1}^q b_i x_i + \text{Selected} \left\{ \sum_{i < j}^{q-1} \sum_j^q b_{ij} x_i x_j \right\}$ <p>The x_i ($i = 1, 2, \dots, q$) are normalized mass fractions of q glass oxide components such that $\sum_{i=1}^q x_i = 1$.</p> <p>The b_i ($i = 1, 2, \dots, q$) and selected b_{ij} are coefficients listed below.</p>		
ln(PCT-B) Reduced PQM Model Term	Coefficient Estimate	Coefficient Stand. Dev.
Al ₂ O ₃	-31.3612	2.1310
B ₂ O ₃	11.8101	2.5505
CaO	-13.8404	3.0142
Fe ₂ O ₃	-16.5948	3.2161
K ₂ O	7.9687	1.7452
Li ₂ O	83.3036	8.4889
MgO	-21.2343	8.2492
Na ₂ O	46.1599	5.2140
P ₂ O ₅	-19.2540	2.8180
SiO ₂	-1.6161	1.1133
ZrO ₂	-6.6289	2.7866
Others ^(a)	-5.1690	1.8573
CaO×Li ₂ O	-251.2654	53.4354
B ₂ O ₃ ×MgO	488.8612	89.5443
B ₂ O ₃ ×Li ₂ O	-374.9533	72.1448
Na ₂ O×SiO ₂	-74.3462	13.1157
CaO×Fe ₂ O ₃	212.0947	46.0965
Modeling Data Statistic (applied to 244 WTP Glasses):		R² = 0.866

(a) “Others” components include Ag₂O, BaO, Br, CdO, Cs₂O, I, La₂O₃, MnO, MoO₃, NiO, PbO, Re₂O₇, SeO₂, SrO, and “Unknown” plus Cl, Cr₂O₃, F, SO₃, TiO₂, and ZnO.

Table 5.2. Model Summary for the WTP Baseline 17-Term Reduced Partial Quadratic Mixture Model on the Natural Logarithm of ILAW PCT-Na [1].

<p>Model form to predict the natural logarithm of the normalized PCT-Na release (in g/L):</p> $\ln(PCT - Na) = \sum_{i=1}^q b_i x_i + \text{Selected} \left\{ \sum_{i=1}^q b_{ii} x_i^2 + \sum_{i < j}^{q-1} \sum_{j=1}^q b_{ij} x_i x_j \right\}$ <p>The x_i ($i = 1, 2, \dots, q$) are normalized mass fractions of q glass oxide components such that $\sum_{i=1}^q x_i = 1$.</p> <p>The b_i ($i = 1, 2, \dots, q$) and selected b_{ii} and b_{ij} are coefficients listed below.</p>		
ln(PCT-Na) Reduced PQM Model Term	Coefficient Estimate	Coefficient Stand. Dev.
Al ₂ O ₃	-20.7142	1.6238
B ₂ O ₃	-6.5489	2.7610
CaO	0.0151	2.5591
Fe ₂ O ₃	-8.4617	2.6039
K ₂ O	-0.8724	3.9729
Li ₂ O	44.7604	3.5466
MgO	-13.8667	7.2503
Na ₂ O	9.9942	1.6770
P ₂ O ₅	-14.5324	2.4027
SiO ₂	-4.8834	0.5143
ZrO ₂	-0.6200	2.2096
Others ^(a)	3.3450	1.4341
CaO×Li ₂ O	-232.1695	46.7097
CaO×Fe ₂ O ₃	182.6191	40.4128
B ₂ O ₃ ×MgO	437.4267	77.8463
B ₂ O ₃ ×Na ₂ O	87.6716	19.0092
K ₂ O×K ₂ O	315.6867	83.2397
Modeling Data Statistic (applied to 244 WTP Glasses):		R² = 0.870

(a) “Others” components include Ag₂O, BaO, Br, CdO, Cs₂O, I, La₂O₃, MnO, MoO₃, NiO, PbO, Re₂O₇, SeO₂, SrO, and “Unknown” plus Cl, Cr₂O₃, F, SO₃, TiO₂, and ZnO.

Table 5.3. Model Summary for the WTP Baseline 15-Term Reduced Partial Cubic Mixture Model on the Natural Logarithm of ILAW VHT Alteration Depth [1].

<p>Model form to predict the natural logarithm of the VHT alteration depth, D, in microns:</p> $\ln(D) = \sum_{i=1}^q b_i x_i + \text{Selected} \left\{ \sum_{i=1}^q b_{iii} x_i^3 + \sum_{i < j}^{q-1} \sum_{j=1}^q b_{ijj} x_i^2 x_j + \sum_{i < j < k}^{q-2} \sum_{j=1}^{q-1} \sum_{k=1}^q b_{ijk} x_i x_j x_k \right\}$ <p>The x_i ($i = 1, 2, \dots, q$) are normalized mass fractions of q glass oxide components such that $\sum_{i=1}^q x_i = 1$.</p> <p>The b_i ($i = 1, 2, \dots, q$) and selected b_{iii}, b_{ijj} and b_{ijk} are coefficients listed below.</p>		
ln(D) Reduced Partial Cubic Mixture Model Term	Coefficient Estimate	Coefficient Stand. Dev.
Al ₂ O ₃	19.5685	6.0850
B ₂ O ₃	18.5336	5.9232
CaO	38.2412	9.4479
Fe ₂ O ₃	-8.4126	4.7225
K ₂ O	-39.3124	10.7075
Li ₂ O	-17.8250	20.0670
MgO	-8.3068	8.0413
Na ₂ O	-20.6518	10.4755
SiO ₂	-0.5137	2.2871
ZrO ₂	-62.8457	7.5911
Others ^(a)	-0.4293	5.3481
(K ₂ O) ² ×Na ₂ O	10138.2817	1198.5167
(Na ₂ O) ³	872.6563	130.6419
Li ₂ O×Na ₂ O×SiO ₂	2139.8048	387.6038
B ₂ O ₃ ×CaO×Na ₂ O	-1943.0687	773.3618
Modeling Data Statistic (applied to 165 WTP Glasses)		R² = 0.744

(a) “Others” components include Ag₂O, BaO, Br, CdO, Cs₂O, I, La₂O₃, MnO, MoO₃, NiO, PbO, Re₂O₇, SeO₂, SrO, and “Unknown” plus Cl, Cr₂O₃, F, SO₃, TiO₂, and ZnO.

Table 5.4. Model Summary for the WTP Baseline 25-Term Reduced Arrhenius-Linear Mixture Model with Three Crossproduct Terms on the Natural Logarithm of ILAW Electrical Conductivity [1].

<p>Model form to predict the natural logarithm of EC, in ln(S/cm):</p> $\ln(EC) = \sum_{i=1}^q a_i x_i + a_{CaOLi_2O} x_{CaO} x_{Li_2O} + a_{CaONa_2O} x_{CaO} x_{Na_2O} + a_{Li_2ONa_2O} x_{Li_2O} x_{Na_2O} + \sum_{i=1}^q b_i \frac{x_i}{T/1000}$ <p>The x_i ($i = 1, 2, \dots, q$) are normalized mass fractions of q glass oxide components such that $\sum_{i=1}^q x_i = 1$.</p> <p>The b_i ($i = 1, 2, \dots, q$) and selected a_{ij} are coefficients listed below.</p>					
Mixture Terms (a_i)	Coefficient Estimate	Coefficient Stand. Dev.	Mixture-Temp. Terms [$x_i/(T/1000)$]	Coefficient Estimate	Coefficient Stand. Dev.
Al ₂ O ₃	2.3854	2.5456	Al ₂ O ₃ /(T/1000)	-9.0593	3.1966
B ₂ O ₃	7.9750	1.7536	B ₂ O ₃ /(T/1000)	-11.0983	2.1885
CaO	5.2093	3.0161	CaO/(T/1000)	-30.6535	1.8797
Fe ₂ O ₃	4.3935	1.6656	Fe ₂ O ₃ /(T/1000)	-9.2407	2.0700
K ₂ O	7.6774	2.1834	K ₂ O/(T/1000)	-11.5299	2.7137
Li ₂ O	4.2464	5.0291	Li ₂ O/(T/1000)	30.4827	4.2400
MgO	15.1675	3.2610	MgO/(T/1000)	-25.0634	4.0719
Na ₂ O	-2.0291	1.2653	Na ₂ O/(T/1000)	12.3822	1.2516
SiO ₂	3.6811	0.7384	SiO ₂ /(T/1000)	-10.1563	0.9047
ZrO ₂	7.8740	3.3302	ZrO ₂ /(T/1000)	-16.5390	4.1850
Others ^(a)	11.2069	2.1288	Others/(T/1000)	-17.7117	2.6254
CaO×Li ₂ O	144.9519	44.2208			
CaO×Na ₂ O	79.0190	14.6533			
Li ₂ O×Na ₂ O	-130.1441	17.2032			
Modeling Data Statistic (applied to 171 WTP Glasses)				R² = 0.951	

(a) The “Others” components include Ag₂O, BaO, Br, CdO, Cs₂O, I, La₂O₃, MnO, MoO₃, NiO, PbO, Re₂O₇, SeO₂, SrO, and “Unknown” plus Cl, Cr₂O₃, F, P₂O₅, SO₃, TiO₂, and ZnO.

Table 5.5. Model Summary for the WTP Baseline 26-Term Reduced Truncated T2-Linear Mixture Model with Four Quadratic Terms on the Natural Logarithm of ILAW Viscosity [1].

<p>Model form to predict the natural logarithm of viscosity, in $\ln(P)$</p> $\ln(\eta) = \sum_{i=1}^q a_i x_i + \text{Selected} \left\{ \sum_{i=1}^q a_{ii} x_i^2 + \sum_{i < j}^{q-1} \sum_{j=1}^q a_{ij} x_i x_j \right\} + \sum_{i=1}^q b_i \frac{x_i}{(T/1000)^2}$ <p>The x_i ($i = 1, 2, \dots, q$) are normalized mass fractions of q glass oxide components such that $\sum_{i=1}^q x_i = 1$.</p> <p>The b_i ($i = 1, 2, \dots, q$) and selected a_{ii} or a_{ij} are coefficients listed below.</p> <p>The temperature (T in Kelvin) is divided by the scaling factor of 1000 so that the b_i coefficients are similar in magnitude to the a_i coefficients.</p>					
Mixture Terms (x_i)	Coefficient Estimate	Coefficient Stand. Dev.	Mixture-Temp. Terms $[x_i/(T/1000)^2]$	Coefficient Estimate	Coefficient Stand. Dev.
Al_2O_3	5.5124	2.0960	$\text{Al}_2\text{O}_3/(T/1000)^2$	24.6423	2.2683
B_2O_3	-42.3772	6.8657	$\text{B}_2\text{O}_3/(T/1000)^2$	(b)	(b)
CaO	-10.6445	0.9836	$\text{CaO}/(T/1000)^2$	13.7793	1.3498
Fe_2O_3	-4.6220	1.0390	$\text{Fe}_2\text{O}_3/(T/1000)^2$	15.2036	1.4269
K_2O	-0.8689	0.9358	$\text{K}_2\text{O}/(T/1000)^2$	(b)	(b)
Li_2O	10.9390	4.5502	$\text{Li}_2\text{O}/(T/1000)^2$	-82.4815	2.9954
MgO	-5.6188	5.5224	$\text{MgO}/(T/1000)^2$	22.7608	2.8130
Na_2O	0.9073	0.6740	$\text{Na}_2\text{O}/(T/1000)^2$	-14.5621	0.8958
P_2O_5	-0.8081	2.8760	$\text{P}_2\text{O}_5/(T/1000)^2$	24.0339	4.2324
SiO_2	1.5575	0.5247	$\text{SiO}_2/(T/1000)^2$	24.4077	0.5709
ZrO_2	-12.0741	2.0755	$\text{ZrO}_2/(T/1000)^2$	48.2286	2.9522
Others ^(a)	-9.3903	1.4313	Others $/(T/1000)^2$	17.3800	2.0519
$(\text{B}_2\text{O}_3)^2$	198.7360	36.5259			
$(\text{Li}_2\text{O})^2$	133.6906	43.1873			
$\text{Al}_2\text{O}_3 \times \text{Li}_2\text{O}$	-136.5095	56.0571			
$(\text{MgO})^2$	-179.8249	103.5284			
Modeling Data Statistic (applied to 171 WTP Glasses)				$R^2 = 0.988$	

(a) The “Others” components include Ag_2O , BaO , Br , CdO , Cs_2O , I , La_2O_3 , MnO , MoO_3 , NiO , PbO , Re_2O_7 , SeO_2 , SrO , and “Unknown” plus Cl , Cr_2O_3 , F , P_2O_5 , SO_3 , TiO_2 , and ZnO .

(b) This term was not statistically significant and hence was omitted from the model.

Table 5.6. Composition Range and Component Limits Applied in Modeling (Mass Fraction).

	Minimum Round Down	Maximum Round Up	Adjusted
Al ₂ O ₃	0.034	0.14	-
B ₂ O ₃	0.059	0.152	-
CaO	0	0.129	-
Fe ₂ O ₃	0	0.120	-
K ₂ O	0	0.081	-
Li ₂ O	0	0.063	-
MgO	0	0.100	0.051
Na ₂ O	0.024	0.261	-
SiO ₂	0.298	0.528	-
ZrO ₂	0	0.068	-
SnO ₂	0	0.051	-
V ₂ O ₅	0	0.041	-
P ₂ O ₅	0	0.048	-
Others 2006 Model	0.016	0.185	-
Others 2012 Model	0.014	0.103	-
Others 2012 Model with V ₂ O ₅	0.016	0.138	-
SO ₃ XRF Measured or Interpolated	0	0.022	-
TiO ₂	0	0.04	-
ZnO	0.009	0.059	-
BaO	0	0.001	-
Br	0	0.001	-
CdO	0	0.002	-
Cl	0	0.012	-
Cr ₂ O ₃	0	0.015	-
Cs ₂ O	0	0.002	-
F	0	0.005	-
I	0	0.002	-
MnO	0	0.001	-
MoO ₃	0	0.001	-
NiO	0	0.003	-
PbO	0	0.001	-
Re ₂ O ₇	0	0.002	-
SeO ₂	0	0.002	-
SrO	0	0.001	-
Unknown	0	0.003	-

- Empty data field

Table 5.7. Eight LAW Glasses Excluded from the PCT Modeling Dataset.

Glass ID	Comments
ORPLA28	Outlying composition (MgO = 7.02 wt%)
ORPLA29	Outlying composition (MgO = 10.04 wt%)
ORPLA31	Outlying composition (MgO = 7.02 wt%)
ORPLA32	Outlying composition (MgO = 10.04 wt%)
LAWA65	Outlying composition (MgO = 6.03 wt%)
LAW3Cr2CCC	Non-representative composition & heat treatment
LAW9HCr1CCC	Non-representative composition & heat treatment
LAW9HCr2CCC	Non-representative composition & heat treatment
LAW10HCr3CCC	Non-representative composition & heat treatment
LAWM12	PCT-Na Grubbs' test outlier with PCT release greater than 8 g/L
LAWM17	PCT-Na Grubbs' test outlier with PCT release greater than 8 g/L
LAWM35	PCT-B Grubbs' test outlier with PCT release greater than 8 g/L
LAWM55	PCT-Na Grubbs' test outlier with PCT release greater than 8 g/L
LAWM56	PCT-Na Grubbs' test outlier with PCT release greater than 8 g/L
ORPLG13	PCT-Na Grubbs' test outlier with PCT release greater than 8 g/L
ORPLG15	PCT-Na Grubbs' test outlier with PCT release greater than 8 g/L
LORPM13 ^(a)	PCT-Na Grubbs' test outlier

(a) Only identified as outlier in later models.

Table 5.8. Twenty-Eight Glasses Reserved from the PCT Dataset for Validation and their Normalized PCT Releases.

Glass ID	Normalized PCT-B Release (g/L):	Normalized PCT-Na Release (g/L):
LAWB98	0.2420	0.3533
LAWB104	0.2166	0.4079
LAWB102	0.2724	0.4490
B1-AZ101	0.7804	0.5295
LAWB96	0.5504	0.5648
ORPLG1	0.4724	0.6409
LAWB105	0.5136	0.6568
LAWA127R1	0.6667	0.6836
ORPLF9	0.6168	0.7330
WVR-G-127A	0.8066	0.7905
LAWA43-1	0.7664	0.8612
LAWA11	1.0947	0.9060
LAWC22	1.0349	0.9374
ORPLA12	0.7516	1.0128
LAWA53	0.8043	1.0588
A3C2-2	1.0924	1.1058
A88AP101R1	1.3720	1.1687
ORPLD5	1.0059	1.2556
ORPLB1	1.2102	1.3058
ORPLD7	1.1520	1.3993
ORPLA5	1.2661	1.4895
ORPLD8	1.3797	1.5779
ORPLD9	1.5115	1.6816
LAWA197	1.5580	1.9497
LAWA12	2.4012	2.1190
LAWA189	2.3285	2.3643
ORPLA37	4.5818	3.1776
ORPLG14	10.3069	7.0219

Table 5.9. Variation in PCT-Boron and PCT-Sodium Responses for Replicate and Near-Replicate Pairs.

Glass IDs of Replicate and Near-Replicate Pairs ^(a)	PCT-Boron		PCT-Sodium	
	g/L	ln(g/L)	g/L	ln(g/L)
LAWM01	0.152	-1.88387	0.290	-1.23787
LAWM53	0.178	-1.72597	0.267	-1.32051
	%RSD^(b) = 11.14	SD = 0.1117	%RSD = 5.84	SD = 0.0584
LAWM09	0.210	-1.56065	0.513	-0.66748
LAWM54R1	0.372	-0.98886	0.367	-1.00239
	%RSD = 39.36	SD = 0.4043	%RSD = 23.46	SD = 0.2368
LAWM12	29.686	3.39068	16.081	2.77764
LAWM55	35.657	3.57395	22.937	3.13275
	%RSD = 12.92	SD = 0.1296	%RSD = 24.85	SD = 0.2511
LAWM35	10.526	2.35385	6.625	1.89085
LAWM56	14.603	2.68123	9.797	2.28208
	%RSD = 22.94	SD = 0.2315	%RSD = 27.32	SD = 0.2766
LAWM50	0.647	-0.43541	0.630	-0.46204
LAWM51	0.692	-0.36817	0.717	-0.33268
	%RSD = 4.75	SD = 0.0475	%RSD = 9.13	SD = 0.0915
LAWM52	1.444	0.36742	1.161	0.14928
LAWA88R1	1.633	0.49042	1.295	0.25851
LAWA88	0.867	-0.14272	0.852	-0.16017
	%RSD = 43.33	SD = 0.3357	%RSD = 29.18	SD = 0.2172
C100-G-136B	0.734	-0.30925	0.697	-0.36097
C100GCC ^(c)	0.463	-0.77003	0.484	-0.72567
	%RSD = 32.02	SD = 0.3258	%RSD = 25.51	SD = 0.2579
LA44PNCC ^(d)	0.666	-0.40647	0.672	-0.39750
LA44CCCR2 ^(d)	0.660	-0.51552	0.723	-0.32435
	%RSD = 0.64	SD = 0.0064	%RSD = 5.17	SD = 0.0517
PNLA126CC ^(e)	0.895	-0.11093	0.785	-0.24207
LA126CCC ^(e)	0.945	-0.05657	0.853	-0.15900
	%RSD = 3.84	SD = 0.0384	%RSD = 5.87	SD = 0.0587
LB83PNCC ^(f)	0.466	-0.76357	0.463	-0.77003
LB83CCC-1 ^(f)	0.522	-0.65009	0.443	-0.81419
	%RSD = 8.02	SD = 0.0802	%RSD = 3.12	SD = 0.0312
AZ-102 Actual ^(g)	0.399	-0.91879	0.318	-1.14570
AZ-102 Actual CCC ^(g)	0.317	-1.14885	0.272	-1.30195
	%RSD = 16.20	SD = 0.1627	%RSD = 11.03	SD = 0.1105
GTSD-1437	0.705	-0.34956	0.732	-0.31197
PLTC35CCC ^(h)	0.506	-0.68122	0.616	-0.48451
	%RSD = 23.24	SD = 0.2345	%RSD = 12.17	SD = 0.1220
Pooled Over 12 WTP Replicates Pairs	%RSD = 24.89	SD = 0.2259	%RSD = 19.07	SD = 0.1789

^(a) Because glass compositions were renormalized based on analyzed (or estimates of analyzed) SO₃ values, the compositions of replicate pairs may not match exactly. However, they were still treated as replicate pairs for statistical data analyses.

^(b) %RSD = 100 × (Standard Deviation / Mean)

^(c) Container centerline cooled (CCC) sample of C100-G-136B (which was a DM100 melter glass).

^(d) Crucible glasses with the same target glass composition but independently batched and melted. A CCC curve was used for LA44PNCC, while a slightly different cooling curve was used for LA44CCCR2.

^(e) Crucible glasses with the same target glass composition but independently batched and melted. A CCC curve was used for PNLA126CC, while a slightly different cooling curve was used for LA126CCC.

^(f) Crucible glasses with the same target glass composition but independently batched and melted. A CCC curve was used for LB83PNCC, while a slightly different cooling curve was used for LB83CCC-1.

^(g) Crucible glass made from AZ-102 waste, and sample subjected to a CCC curve.

^(h) A CCC sample of GTSD-1437, which was a LAW pilot melter glass.

Table 5.9. Variation in PCT-Boron and PCT-Sodium Responses for Replicate and Near-Replicate Pairs (continued).

Glass IDs of Near-Replicates	PCT-Boron		PCT-Sodium	
	g/L	ln(g/L)	g/L	ln(g/L)
LAWA161	1.343	0.29517	1.333	0.28741
WWV-G-11A	1.272	0.24021	1.151	0.14039
	%RSD^(a) = 3.88	SD = 0.0389	%RSD = 10.38	SD = 0.1040
LAWA187	3.420	1.22958	2.921	1.07193
LAWA187CCC ^(b)	2.055	0.72024	1.678	0.51731
EWV-G-89B	2.120	0.75128	1.900	0.64188
EWV89BCCC ^(b)	2.248	0.81015	1.705	0.53331
	%RSD = 26.19	SD = 0.2375	%RSD = 28.70	SD = 0.2598
LAWB99	0.236	-1.44259	0.413	-0.88351
DWV-G-123C	0.180	-1.71263	0.330	-1.10723
	%RSD = 18.98	SD = 0.1909	%RSD = 15.75	SD = 0.1582
LAWC100R1	1.678	0.51779	1.508	0.41065
WVY-G-95A-1	1.832	0.60558	1.574	0.45372
WVY-G-95A-2	1.845	0.61222	1.566	0.44866
WVY-G-95A-3	1.753	0.56143	1.568	0.44960
WVY-G-95A-4	1.817	0.59709	1.619	0.48181
	%RSD = 3.88	SD = 0.0393	%RSD = 2.53	SD = 0.0253
ORPLA15	1.318	0.27576	1.362	0.30866
R10-G-155A	1.866	0.62365	1.661	0.50731
	%RSD = 24.35	SD = 0.2460	%RSD = 14.00	SD = 0.1405
ORPLA20	1.449	0.37092	1.468	0.38382
Y10-G-146C	1.304	0.26514	1.322	0.27903
	%RSD = 7.47	SD = 0.0748	%RSD = 7.40	SD = 0.0741
ORPLA38-1	1.453	0.37361	1.350	0.29980
J10-G-24B	1.754	0.56178	1.649	0.50003
	%RSD = 13.27	SD = 0.1331	%RSD = 14.11	SD = 0.1416
ORPLB4	1.403	0.33894	1.326	0.28187
S10-G-45A	1.634	0.49085	1.408	0.34211
	%RSD = 10.72	SD = 0.1074	%RSD = 4.26	SD = 0.0426
ORPLC5	1.699	0.52997	1.489	0.39825
S10-G-101B	1.350	0.30030	1.209	0.19013
	%RSD = 16.17	SD = 0.1624	%RSD = 14.66	SD = 0.1472
ORPLD1	1.319	0.27697	1.437	0.36227
T10-G-16A	0.686	-0.37687	0.681	-0.38425
	%RSD = 44.65	SD = 0.4623	%RSD = 50.46	SD = 0.5279
ORPLD6	1.128	0.12049	1.343	0.29497
Z10-G-60C	1.246	0.21964	1.584	0.46017
	%RSD = 7.01	SD = 0.0701	%RSD = 11.65	SD = 0.1168
ORPLE12	0.503	-0.68704	0.793	-0.23190
Q10-G-134A	0.504	-0.68456	0.774	-0.25633
	%RSD = 0.18	SD = 0.0018	%RSD = 1.73	SD = 0.173
ORPLF7	0.329	-1.11036	0.709	-0.34436
Z10-G-122B	0.406	-0.90241	0.594	-0.52075
Z10-G-153B	0.434	-0.83573	0.629	-0.46409
	%RSD = 13.83	SD = 0.1432	%RSD = 9.13	SD = 0.0901
ORPLG9	1.485	0.39567	1.530	0.42547
10A-G-43B	1.299	0.26157	1.558	0.44354
	%RSD = 9.47	SD = 0.0948	%RSD = 1.28	SD = 0.0128
ORPLG27	1.327	0.28274	1.540	0.43164
I10-G-135A	1.857	0.61912	2.038	0.71214
	%RSD = 23.56	SD = 0.2379	%RSD = 19.71	SD = 0.1983
Pooled Over 15 ORP Replicates	%RSD = 17.95	SD = 0.1773	%RSD = 17.97	SD = 0.1770
Pooled Over 27 Sets of Replicates	%RSD = 20.58	SD = 0.1945	%RSD = 18.13	SD = 0.1752

^(a) %RSD = 100 × (Standard Deviation / Mean); ^(b) Container centerline cooled (CCC) sample of above samples.

Table 5.10. Coefficients and Performance Summary for Various Reduced Partial Quadratic Mixture Models on the Natural Logarithm of ILAW PCT-Na.

PCT Model	Model Number											
	1 [1]		2		3		4		5		6	
Glass Count	244 (+20 outliers)		421 (+8 outliers +28 validation)		414 (+15 outliers +28 validation)		413 (+16 outliers +28 validation)		413 (+16 outliers +28 validation)		413 (+16 outliers +28 validation)	
Model Terms	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.
Al ₂ O ₃	-20.714	1.624	-12.154	0.901	-9.922	0.799	-10.768	0.780	-10.587	1.215	-2.658	1.489
B ₂ O ₃	-6.549	2.761	-0.241	2.658	1.313	2.286	-0.885	2.237	2.682	0.919	8.090	1.625
CaO	0.015	2.559	-0.110	1.130	-0.523	0.967	-0.997	0.947	-5.122	1.111	2.946	1.610
Fe ₂ O ₃	-8.462	2.604	-5.517	1.242	-5.562	1.064	-7.659	1.079	-4.370	2.316	-1.145	1.914
K ₂ O	-0.872	3.973	6.493	3.472	4.168	3.004	4.815	2.887	9.042	0.841	25.526	3.074
Li ₂ O	44.760	3.547	37.229	2.980	28.097	2.856	31.994	2.815	29.000	2.819	28.950	2.313
MgO	-13.867	7.250	1.836	6.033	5.305	5.269	-1.222	5.161	13.734	1.475	5.892	5.021
Na ₂ O	9.994	1.677	12.432	1.319	12.440	1.130	13.193	1.091	22.979	2.124	20.317	1.498
P ₂ O ₅	-14.532	2.403	-14.685	2.622	-14.171	2.241	-13.895	2.150	-15.710	2.069	-6.327	2.582
SiO ₂	-4.883	0.514	-5.705	0.455	-5.215	0.394	-5.229	0.387	-3.422	0.586	-27.784	4.954
SnO ₂	-	-	-	-	-	-	-8.089	1.504	-18.225	2.499	-0.863	1.947
ZrO ₂	-0.620	2.210	0.165	1.469	-1.365	1.263	-0.689	1.264	-4.158	1.271	5.258	1.962
Others ^(a)	3.345	1.434	-1.684	1.015	-2.470	0.873	-0.484	0.992	-3.197	0.988	5.025	1.652
CaO×Li ₂ O	-232.176	46.710	-153.230	35.238	-1.365	1.263	-110.476	30.97838	-105.377	30.144	-	-
CaO×Fe ₂ O ₃	182.619	40.413	137.117	19.138	-2.470	0.873	154.8693	16.10487	-	-	153.297	15.517
B ₂ O ₃ ×MgO	437.426	77.846	201.813	65.661	-87.583	31.969	200.599	56.79774	-	-	180.655	52.889
B ₂ O ₃ ×Na ₂ O	87.672	19.009	36.653	14.778	133.894	16.382	23.15339	12.26838	-	-	-	-
K ₂ O×K ₂ O	315.687	83.240	71.464	62.377	121.472	57.579	101.4636	51.86806	-	-	-	-
Na ₂ O×SiO ₂	-	-	-	-	-	-	-	-	-24.057	5.552	-	-
CaO×SnO ₂	-	-	-	-	-	-	-	-	200.605	45.582	-	-
CaO*Fe ₂ O ₃	-	-	-	-	-	-	-	-	158.307	16.345	-	-
Al ₂ O ₃ *Fe ₂ O ₃	-	-	-	-	-	-	-	-	-95.941	29.875	-	-
Al ₂ O ₃ ×K ₂ O	-	-	-	-	-	-	-	-	-	-	-144.411	42.483
SiO ₂ ×SiO ₂	-	-	-	-	-	-	-	-	-	-	32.883	7.348
Modeling Data Statistics												
R ²	0.870		0.817		0.837		0.851		0.861		0.857	
R ² _{Adjusted}	0.861		0.810		0.831		0.845		0.855		0.851	
RMSE	0.255		0.304		0.259		0.248		0.240		0.244	
PRESS RMSE	0.274		0.319		0.270		0.257		0.247		0.252	
Model LOF p-value	0.055		0.00007		0.0025		0.0057		0.011		0.008	
Validation Statistics on 28 Glasses Selected Over Full Data Range – 18 ORP-LAW and 10 WTP-LAW Glasses												
R ²	0.473 ^(b)		0.873 ^(b) /0.861		0.842		0.855		0.846		0.850	
RMSE	2.271 ^(b)		1.114 ^(b) /0.383		0.409		0.411		0.424		0.398	

(a) “Others” components include the original “Others” component (which contains Ag₂O, BaO, Br, CdO, Cs₂O, I, La₂O₃, MnO, MoO₃, NiO, PbO, Re₂O₇, SeO₂, SrO, and “Unknown”) plus Cl, Cr₂O₃, F, SO₃, TiO₂, ZnO and V₂O₃. In models 1, 2 and 3, SnO₂ is also added to “Others”.

(b) Validation set was limited to 18 ORP-LAW glasses since 10 WTP-LAW glasses were already used in the model design [1] and none were set aside for independent validation.

Table 5.11. Coefficients and Performance Summary for Various Reduced Partial Quadratic Mixture Models on the Natural Logarithm of ILAW PCT-B.

PCT Model	Model Number											
	1 [1]		2		3		4		5		6	
PCT Data Count	244 (+20 outliers)		421 (+9 outliers +28 validation)		414 (+16 outliers +28 validation)		413 (+17 outliers +28 validation)		413 (+17 outliers +28 validation)		413 (+17 outliers +28 validation)	
Model Terms	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.
Al ₂ O ₃	-31.361	2.131	-19.553	1.339	-18.073	1.195	-19.238	1.167	-9.063	1.252	-29.031	5.347
B ₂ O ₃	11.810	2.550	13.409	1.805	11.943	1.605	9.655	1.590	18.482	1.268	17.210	1.511
CaO	-13.840	3.014	-12.644	1.464	-13.689	1.306	-14.534	1.274	-22.305	1.858	-20.987	1.846
Fe ₂ O ₃	-16.595	3.216	-10.708	1.461	-11.004	1.300	-13.700	1.324	-13.267	1.376	-12.482	1.364
K ₂ O	7.969	1.745	6.426	1.179	4.755	1.072	6.260	1.063	112.383	17.487	121.818	17.264
Li ₂ O	83.304	8.489	59.611	7.160	50.173	6.430	53.504	6.190	-49.706	11.101	-31.257	11.754
MgO	-21.234	8.249	8.208	6.957	11.232	6.310	4.339	6.153	24.264	1.723	5.283	6.089
Na ₂ O	46.160	5.214	31.225	2.982	33.233	2.652	35.204	2.568	15.164	0.661	16.125	0.682
P ₂ O ₅	-19.254	2.818	-16.989	0.798	-16.456	2.680	-16.284	2.569	-11.459	2.408	-11.671	2.361
SiO ₂	-1.616	1.113	-3.967	1.731	-2.313	0.730	-2.232	0.705	-7.674	0.440	-6.322	0.529
SnO ₂	-	-	-	-			-15.501	1.869	-9.135	3.426	-7.845	3.363
ZrO ₂	-6.629	2.787	-2.272	3.028	-3.998	1.540	-3.146	1.567	-10.105	2.293	-8.405	2.295
Others ^(a)	-5.169	1.857	-6.741	1.295	-7.968	1.161	-5.360	1.279	-3.175	1.205	-3.038	1.180
CaO×Li ₂ O	-251.265	53.435	-148.379	41.159	-76.299	38.999	-104.514	37.744	-	-	-	-
B ₂ O ₃ ×MgO	488.862	89.544	176.169	75.587	92.044	68.860	172.311	67.410	-	-	204.503	64.710
B ₂ O ₃ ×Li ₂ O	-374.954	72.145	-230.477	61.177	-232.653	54.802	-222.587	52.541	-161.944	49.820	-220.520	50.545
Na ₂ O×SiO ₂	-74.346	13.116	-42.446	7.980	-51.683	7.144	-54.067	6.861	-	-	-	-
CaO×Fe ₂ O ₃	212.095	46.097	186.611	22.466	176.746	19.945	202.078	19.602	278.781	20.570	268.322	20.401
Al ₂ O ₃ ×Al ₂ O ₃	-	-	-	-	-	-	-	-	-	-	120.544	31.454
Al ₂ O ₃ ×K ₂ O	-	-	-	-	-	-	-	-	-277.876	57.221	-255.344	56.488
B ₂ O ₃ ×K ₂ O	-	-	-	-	-	-	-	-	-270.939	58.868	-269.679	57.565
K ₂ O ×SiO ₂									-131.361	34.008	-157.955	33.828
Li ₂ O ×SiO ₂									209.400	22.592	183.993	23.039
CaO×SnO ₂									99.796	56.039	54.383	55.892
K ₂ O×SnO ₂									-284.835	67.949	-280.581	66.595
CaO×ZrO ₂									230.541	40.879	217.937	40.142
Modeling Data Statistics												
R ²	0.866		0.819		0.826		0.841		0.865		0.872	
R ² _{Adjusted}	0.857		0.812		0.819		0.834		0.858		0.864	
RMSE	0.291		0.352		0.312		0.299		0.276		0.270	
PRESS RMSE	0.312		0.374		0.329		0.316		0.290		0.289	
Model LOF p-value	0.122		0.00003		0.00055		0.0014		0.0067		0.0102	
Validation Statistics on 28 Glasses Selected Over Full Data Range – 18 ORP-LAW and 10 WTP-LAW Glasses												
R ²	0.743 ^(b)		0.819		0.803		0.815		0.844		0.819	
RMSE	2.060 ^(b)		0.545		0.569		0.578		0.684		0.904	

(a) “Others” components include the original “Others” component (which contains Ag₂O, BaO, Br, CdO, Cs₂O, I, La₂O₃, MnO, MoO₃, NiO, PbO, Re₂O₇, SeO₂, SrO, and “Unknown”) plus Cl, Cr₂O₃, F, SO₃, TiO₂, ZnO and V₂O₅. In models 1, 2 and 3, SnO₂ is also added to “Others”.

(b) Validation set was limited to 18 ORP-LAW glasses since 10 WTP-LAW glasses were already used in the model design [1] and none were set aside for independent validation.

Table 5.12. Nine LAW Glasses Excluded from VHT Modeling Data Set.

Glass ID	Comments
ORPLA28	Outlying composition (MgO = 7.02 wt%)
ORPLA29	Outlying composition (MgO = 10.04 wt%)
ORPLA31	Outlying composition (MgO = 7.02 wt%) and alteration depth > 1100 μ m
ORPLA32	Outlying composition (MgO = 10.04 wt%)
LAW3Cr2CCC	Non-representative composition & heat treatment
LAW9HCr1CCC	Non-representative composition & heat treatment
LAW9HCr2CCC	Non-representative composition & heat treatment
LAW10HCr3CCC	Non-representative composition & heat treatment
LORPM13 ^(a)	Non-representative composition - SnO ₂ crystallization

^(a) Composition deviation from batching due to crystallization and identified as outlier in PCT-Na models.

Table 5.13. Thirty-Eight LAW Glasses with Alteration Depth Exceeding Coupon Thickness and Excluded from VHT Modeling Data Set.

LAWM12	ORPLA8S4
LAWM13	ORPLA11
LAWM14	ORPLA11S4
LAWM32	ORPLA27
LAWM55	ORPLA30
LAW14	ORPLA31
10A-G-43B	ORPLB1
LAWA171	ORPLB1S4
LAWA172	ORPLC2
LAWA177	ORPLC3
LAWA178	ORPLC3S4
LAWA179	ORPLC4
LAWA181	ORPLC4S4
LAWA182	ORPLG13
LAW17(T1)	ORPLG16
LAW17(T2)	ORPLG17
ORPLA1	ORPLG18
ORPLA1S4	ORPLG19
ORPLA5S4	LORPM17R1

Table 5.14. Twenty-Seven Glasses Reserved from the VHT Dataset as Validation Set and Their VHT Alteration Depth.

Glass ID	VHT Alteration Depth (μm)	$\ln(\mu\text{m})$
A88Si-15	4	1.3863
A2B1-2	6	1.7918
LAWB65	10	2.3026
LAWA88R1	13	2.5649
LAWB93	15	2.7081
LAWA126	22	3.0910
LAWA49	30	3.4012
LAWB11	33	3.4965
ORPLA36	57	4.0431
ORPLA38-1	71	4.2627
LAWC28	92	4.5218
WVY-G-95A	102	4.6250
ORPLA10S4	114	4.7362
LAWA185	129	4.8598
LAWC102	141	4.9488
LAWB102	156	5.0499
LAWB97	172	5.1475
ORPLF5	200	5.2983
LAWCrP2R	216	5.3753
LAWA183	230	5.4381
LAWB104	273	5.6095
ORPLC5	362	5.8916
ORPLG21	415	6.0283
LAWB13	615	6.4216
LAWA196	712	6.5681
ORPLA2S4	858	6.7546
ORPLA4	1031	6.9383

Table 5.15. Variation in VHT Alterations for Replicate and Near-Replicate Pairs.

Glass ID	VHT Alteration Depth		%RSD ^(a) on Alteration Depth (μm)	Standard Deviation ln (μm)
	μm	ln(μm)		
LAWM01	82	4.4067	%RSD ^(a) = 6.58	SD = 0.0658
LAWM53	90	4.4998		
LAWM09	1	0.0000	%RSD = 70.71	SD = 0.7768
LAWM54R1	3	1.0986		
LAWM12	>1100	>7.0030	NA	NA
LAWM55	>1100	>7.0030		
LAWM35	4	1.3863	%RSD = 28.28	SD = 0.2867
LAWM56	6	1.7916		
LAWM50	4	1.3863	%RSD = 15.71	SD = 0.1578
LAWM51	5	1.6094		
LAWM52	28	3.3322	%RSD = 51.74	SD = 0.5425
LAWA88R1	13	2.5649		
LAWA137 (T1)	118	4.7707	%RSD = 22.22	SD = 0.2241
LAWA137 (T2)	162	5.0876		
LAWE17(T1) and (T2)	>1200	>7.090	NA	NA
LAWE18(T1)	556	6.3208	%RSD = 4.19	SD = 0.0419
LAWE18(T2)	524	6.2615		
LAWE19(T1)	212	5.3566	%RSD = 31.56	SD = 0.3348
LAWE19(T2)	175	5.1648		
LAWE19 (T3)	109	4.6913		
LAWE20(T1)	972	6.8794	%RSD = 27.14	SD = 0.2748
LAWE20(T2)	659	6.4907		
LAWE21(T1)	310	5.7366	%RSD = 8.17	SD = 0.0818
LAWE21(T2)	348	5.8522		
LAWE22(T1)	167	5.1180	%RSD = 21.84	SD = 0.2202
LAWE22(T2)	228	5.4293		
LAWE23(T1)	382	5.9454	%RSD = 7.37	SD = 0.0074
LAWE23(T2)	386	5.9558		
LAWE24(T1)	585	6.3716	%RSD = 25.21	SD = 0.2548
LAWE24(T2)	408	6.0113		
LAWE25(T1)	408	6.0113	%RSD = 36.70	SD = 0.3756
LAWE25(T2)	694	6.5425		
LAWE26(T1)	401	5.9940	%RSD = 17.47	SD = 0.1755
LAWE26(T2)	514	6.2422		
Pooled Over All 15 WTP-LAW Replicates and Near-Replicates			%RSD = 28.45	SD = 0.2980
Pooled Over All 10 WTP-LAW True Replicates (T1 and T2) (Identical Glass Samples Tested Separately)			%RSD = 21.61	SD = 0.2243

(a) %RSD = 100×(Standard Deviation / Mean).

**Table 5.15. Variation in VHT Alterations for Replicate and Near-Replicate Pairs
(continued).**

Glass ID	VHT Alteration Depth		%RSD ^(a) on Alteration Depth (μm)	Standard Deviation ln(μm)
	μm	ln(μm)		
LAWA161(T1)	223	5.4072	%RSD ^(a) = 34.78%	SD = 0.4017
LAWA161(T2)	230	5.4381		
WVW-G-11A (LAWA161)	113	4.7274		
LAWA187(T1)	230	5.4381	for the crucible pair %RSD = 26.08% for all Seven Glasses %RSD = 58.49%	SD = 0.2638 SD = 0.5264
LAWA187(T2)	334	5.8111		
EWV89BCCC (LAWA187)	230	5.4381		
EWV-G-89B (LAWA187)	736	6.6012		
EWV-G-93B (LAWA187)	719	6.5779		
EWV93BCCC (LAWA187) [§]	223	5.4072		
EWV-G-108B (LAWA187)	291	5.6733		
LAWB99	135	4.9053	%RSD = 26.76%	SD = 0.2708
DWV-G-123C (LAWB99)	198	5.2883		
LAWC100R1	144	4.9698	%RSD = 24.15%	SD = 0.2438
WVY-G-95A (LAWC100)	102	4.6250		
ORPLA15	230	5.4381	%RSD = 68.50%	SD = 0.6348
ORPLA15S4	279	5.6312		
R10-G-155A (ORPLA15)	751	6.6214		
ORPLA20	65	4.1744	%RSD = 51.74%	SD = 0.5425
Y10-G-146C (ORPLA20)	140	4.9416		
ORPLA38-1	71	4.2627	%RSD = 25.34%	SD = 0.2562
J10-G-24B (ORPLA38-1)	102	4.6250		
ORPLB4	369	5.9108	%RSD = 21.16%	SD = 0.2068
ORPLB4S4	320	5.7683		
S10-G-45A (ORPLB4)	481	6.1759		
ORPLC5	362	5.8916	%RSD = 15.14%	SD = 0.1520
S10-G-101B (ORPLC5)	292	5.6768		
ORPLD1	99	4.5951	%RSD = 21.46%	SD = 0.2042
ORPLD1S4	141	4.9488		
T10-G-16A (ORPLD1)	99	4.5951		
ORPLD6	164	5.0999	%RSD = 28.28%	SD = 0.2867
10A-G-53C (ORPLD6)	246	5.5053		
ORPLE12	277	5.6240	%RSD = 5.87%	SD = 0.0588
Q10-G-134A (ORPLE12)	301	5.7071		
ORPLF7	164	5.0999	%RSD = 14.51%	SD = 0.1400
Z10-G-122B (ORLF7-low SO ₃)	164	5.0999		
Z10-G-153B (ORLF7-high SO ₃)	209	5.3423		

(a) RSD = 100×(Standard Deviation / Mean). [§]Composition replicate of EWV-G-93B, CCC heat-treated different

**Table 5.15. Variation in VHT Alterations for Replicate and Near-Replicate Pairs
(continued).**

Glass ID	VHT Alteration Depth		%RSD ^(a) on Alteration Depth (μm)	Standard Deviation ln(μm)
	μm	ln(μm)		
ORPLG9	450	24	NA	NA
10A-G-43B (ORPLG9)	>1200	NA		
ORPLG27	34	3.5264	%RSD = 127.52%	SD = 2.0950
I10-G-135A (ORPLG27)	658	6.4892		
LORPM1(T1)	528	6.2691	%RSD = 28.51%	SD = 0.3078
LORPM1(T2)	620	6.4297		
LORPM1 (T3)	342	5.8348		
Pooled Over All 15 ORP-LAW Replicates			%RSD = 47.29	SD = 0.5665
Pooled Over All 3 ORP-LAW True Replicates (Identical Glass Samples Tested Separately)			%RSD = 24.04	SD = 0.2547
Pooled Over All 30 WTP-LAW and ORP-LAW Replicates and Near-Replicates			%RSD = 39.78	SD = 0.4632
Pooled Over 13 True WTP-LAW and ORP-LAW Replicates (Identical Glass Samples Tested Separately)			%RSD = 22.89	SD = 0.2389

(a) %RSD = 100×(Standard Deviation / Mean).

Table 5.16. Coefficients and Performance Summary for Various Reduced Partial Quadratic Mixture Models on the Natural Logarithm of VHT Alteration Depth.

PCT Model	Model Number													
	1 [1]		2		3		4		5		6		7	
Glass Count	165 (+16 outliers)		358 (+46 outliers + 27 validation)		358 (+46 outliers + 27 validation)		357 (+47 outliers + 27 validation)		357 (+47 outliers + 27 validation)		357 (+47 outliers + 27 validation)		357 (+47 outliers + 27 validation)	
Model Terms	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.
Al ₂ O ₃	19.569	6.085	24.176	3.060	24.294	2.957	20.415	2.943	23.252	3.355	52.822	7.146	12.682	17.450
B ₂ O ₃	18.534	5.923	24.913	4.394	23.648	4.253	18.789	4.202	1.557	3.433	15.480	3.413	5.917	18.260
CaO	38.241	9.448	34.885	5.306	31.167	5.180	29.423	5.002	-163.096	19.840	-127.339	19.772	353.037	54.883
Fe ₂ O ₃	-8.413	4.722	-0.985	3.206	-3.392	3.135	-6.588	3.082	-11.723	3.077	5.015	3.137	-168.059	29.573
K ₂ O	-39.312	10.707	-31.033	8.355	-27.37	8.11	-22.657	7.862	44.691	3.583	-109.334	16.281	135.656	18.423
Li ₂ O	-17.825	20.067	4.368	16.998	-4.716	16.523	2.961	15.987	116.722	7.819	-5.494	17.695	168.309	19.454
MgO	-8.307	8.041	0.142	5.866	0.545	5.669	5.007	5.528	17.451	6.130	-8.420	7.653	211.976	54.744
Na ₂ O	-20.652	10.476	1.445	6.645	-4.754	6.538	-4.255	6.300	51.088	2.577	-57.013	12.545	210.459	19.978
SiO ₂	-0.514	2.287	-6.562	1.504	-6.361	1.454	-5.014	1.424	-16.868	2.055	-4.874	2.262	9.382	6.593
SnO ₂	-	-	-	-	-22.998	5.175	-26.531	5.032	-20.444	5.802	-14.520	5.109	-79.788	9.146
ZrO ₂	-62.846	7.591	-59.559	4.977	-53.572	4.953	-57.845	4.842	-44.480	4.940	-44.557	4.428	-95.713	6.707
Others ^(a)	-0.429	5.348	-1.845	3.129	7.7754	3.5767	6.700	3.452	6.049	3.976	14.012	3.576	-37.105	6.074
(K ₂ O) ² × Na ₂ O	10138.3	1198.52	7743.43	836.53	7981.26	809.69	7759.06	781.28	-	-	-	-	-	-
(Na ₂ O) ³	872.656	130.64	516.55	73.07	588.72	72.05	610.515	69.539	-	-	-	-	-	-
Li ₂ O × Na ₂ O × SiO ₂	2139.80	387.60	1758.73	308.25	1985.00	301.23	1932.04	290.40	-	-	-	-	-	-
B ₂ O ₃ × CaO × Na ₂ O	-1943.1	773.36	-2197.84	348.90	-2061.53	338.21	-1812.31	329.32	-	-	-	-	-	-
CaO × SiO ₂	-	-	-	-	-	-	-	-	392.633	49.153	271.908	45.046	-561.563	129.247
CaO × CaO	-	-	-	-	-	-	-	-	-	-	219.306	57.309	-	-
K ₂ O × K ₂ O	-	-	-	-	-	-	-	-	-	-	1374.019	234.831	-	-
K ₂ O × MgO	-	-	-	-	-	-	-	-	-	-	911.815	262.425	-	-
Al ₂ O ₃ × Na ₂ O	-	-	-	-	-	-	-	-	-	-	-149.973	43.427	-	-
K ₂ O × Na ₂ O	-	-	-	-	-	-	-	-	-	-	444.083	70.439	-	-
Li ₂ O × Na ₂ O	-	-	-	-	-	-	-	-	-	-	953.798	140.547	-	-
(Na ₂ O) ²	-	-	-	-	-	-	-	-	-	-	353.518	38.237	-	-
Al ₂ O ₃ × B ₂ O ₃	-	-	-	-	-	-	-	-	-	-	-	-	-644.901	207.932
Al ₂ O ₃ × MgO	-	-	-	-	-	-	-	-	-	-	-	-	-3458.738	767.416
B ₂ O ₃ × Fe ₂ O ₃	-	-	-	-	-	-	-	-	-	-	-	-	370.747	119.852
B ₂ O ₃ × K ₂ O	-	-	-	-	-	-	-	-	-	-	-	-	-938.131	195.775
B ₂ O ₃ × MgO	-	-	-	-	-	-	-	-	-	-	-	-	-3970.122	686.340
CaO × K ₂ O	-	-	-	-	-	-	-	-	-	-	-	-	-1184.125	127.863
CaO × Li ₂ O	-	-	-	-	-	-	-	-	-	-	-	-	-1273.580	222.919
CaO × Na ₂ O	-	-	-	-	-	-	-	-	-	-	-	-	-2493.596	329.160
Fe ₂ O ₃ × SiO ₂	-	-	-	-	-	-	-	-	-	-	-	-	197.149	64.128
MgO × SnO ₂	-	-	-	-	-	-	-	-	-	-	-	-	1133.079	342.603
Na ₂ O × SiO ₂	-	-	-	-	-	-	-	-	-	-	-	-	-361.418	55.915
Al ₂ O ₃ × B ₂ O ₃ × MgO	-	-	-	-	-	-	-	-	-	-	-	-	57000.695	9316.930
CaO × Na ₂ O × SiO ₂	-	-	-	-	-	-	-	-	-	-	-	-	4307.447	759.237

- Empty data field

Table 5.16. Coefficients and Performance Summary for Various Reduced Partial Quadratic Mixture Models on the Natural Logarithm of VHT Alteration Depth (continued).

PCT Model	Model Number						
	1 [1]	2	3	4	5	6	7
Modeling Data Statistic							
R ²	0.744	0.706	0.727	0.746	0.671	0.776	0.787
R ² _{Adjusted}	0.720	0.694	0.715	0.735	0.660	0.763	0.771
RMSE	0.848	0.943	0.911	0.878	0.995	0.831	0.817
PRESS RMSE	0.884	0.980	0.949	0.903	1.019	0.852	0.865
Model LOF p-value	0.032 ^(b)	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
Validation Statistic , 27 Selected Glasses over Full Expanded Range – 16 from ORP Set and 11 from WTP set							
R ²	-2.407 ^(c)	-0.611 ^(c) /0.633	0.668	0.645	0.594	0.724	0.682
RMSE	6.153 ^(c)	4.231 ^(c) /1.366	1.358	1.404	1.330	1.551	4.409

(a) “Others” components include the original “Others” component (which contains Ag₂O, BaO, Br, CdO, Cs₂O, I, La₂O₃, MnO, MoO₃, NiO, PbO, Re₂O₇, SeO₂, SrO, and “Unknown”) plus Cl, Cr₂O₃, F, SO₃, TiO₂, ZnO and V₂O₃. In Models 1 and 2, SnO₂ is also added to “Others”.

(b) Value was taken from [1] as JMP® only calculates LOF when glass compositions of replicates are exactly the same.

(c) Validation set was limited to 16 ORP-LAW glasses since 11 WTP-LAW glasses were already used in the model design [1] and none were set aside for independent validation.

Table 5.17. Thirty Glasses Reserved from the Electrical Conductivity Dataset as Validation Set and their Temperatures and EC Measurements.

Glass ID	Temp1 (°C)	EC1 (S/cm)	Temp2 (°C)	EC2 (S/cm)	Temp3 (°C)	EC3 (S/cm)	Temp4 (°C)	EC4 (S/cm)
LAWB80	943	0.054	1040	0.105	1138	0.172	1239	0.264
LAWB79	949	0.079	1045	0.142	1142	0.217	1239	0.338
LAWB37	947	0.083	1042	0.144	1139	0.229	1247	0.297
LAWB89	945	0.090	1038	0.157	1131	0.252	1223	0.359
LAWB105	949	0.095	1040	0.164	1132	0.257	1224	0.368
LAWC31R1	947	0.100	1043	0.167	1140	0.271	1238	0.401
A3C2-2	963	0.114	1058	0.188	1154	0.278	1248	0.392
LAWB103	947	0.114	1039	0.193	1131	0.290	1222	0.426
A3C2-1	955	0.130	1051	0.211	1147	0.315	1240	0.418
C22Si-15	948	0.121	1046	0.206	1144	0.302	1193	0.346
ORPLF12	953	0.125	1050	0.212	1147	0.326	1243	0.506
LAWA102R1	945	0.156	1043	0.238	1142	0.368	1240	0.523
LAWE5	934	0.163	1026	0.250	1116	0.349	1208	0.489
ORPLG7	950	0.178	1049	0.261	1146	0.375	1243	0.547
A1C1-2	963	0.178	1058	0.272	1153	0.402	1247	0.555
LAWA60	950	0.197	1050	0.293	1148	0.415	1257	0.543
LAWA53	946	0.163	1045	0.262	1142	0.426	1240	0.568
LAWA52	945	0.186	1043	0.305	1141	0.439	1247	0.657
ORPLG21	949	0.245	1047	0.354	1143	0.460	1239	0.666
LAWA193	948	0.230	1040	0.350	1132	0.481	1224	0.619
LAWA190	945	0.234	1035	0.354	1125	0.498	1214	0.647
LAWA172	941	0.258	1032	0.371	1125	0.515	1214	0.689
ORPLE9	985	0.230	1082	0.354	1180	0.521	1276	0.676
ORPLA20	979	0.287	1075	0.419	1170	0.530	1266	0.737
LAWA176	942	0.265	1031	0.384	1124	0.538	1216	0.689
LAWA42	956	0.248	1054	0.393	1152	0.561	1240	0.710
ORPLA12	961	0.281	1055	0.400	1149	0.584	1243	0.779
LAWA181	949	0.344	1041	0.503	1132	0.640	1224	0.864
ORPLA2	977	0.390	1072	0.545	1169	0.681	1266	0.942
ORPLA10	981	0.359	1078	0.573	1177	0.737	1275	1.013

Table 5.18. Variation in Electrical Conductivity Values for Near-Replicate Pairs.

Glass ID	Electrical Conductivity Values at Measurement Temperatures								Pooled Over Temperature	
	Near 950°C		Near 1050°C		Near 1150°C		Near 1250°C		%RSD	SD
	T (°C)	S/cm	T (°C)	S/cm	T (°C)	S/cm	T (°C)	S/cm	S/cm	ln(S/cm)
LAWC100R1	956	0.186	1049	0.245	1145	0.407	1238	0.529		
WVY-G-95A	959	0.177	1050	0.286	1144	0.412	1236	0.544		
%RSD^(a)	0.2%	3.5%	0.1%	10.9%	0.1%	0.9%	0.1%	2.0%	5.83%	0.0585
Glass ID	Electrical Conductivity Values at Nominal Temperatures								Pooled Over Temperature	
	950°C		1050°C		1150°C		1250°C		%RSD	SD
	S/cm	ln(S/cm)	S/cm	ln(S/cm)	S/cm	ln(S/cm)	S/cm	ln(S/cm)	S/cm	ln(S/cm)
LAWC100R1	0.173	-1.753	0.270	-1.311	0.395	-0.930	0.549	-0.600		
WVY-G-95A	0.168	-1.784	0.285	-1.255	0.420	-0.868	0.566	-0.569		
%RSD^(b), SD^(b)	2.1%	0.0215	3.9%	0.0391	4.4%	0.0442	2.1%	0.0215	3.32%	0.0332

(a) %RSD = $100 \times (\text{Standard Deviation} / \text{Mean})$, calculated using the S/cm values.

(b) Calculated using ln(S/cm) values.

Table 5.19. Coefficients and Performance Summary of Various Reduced Arrhenius-Linear Mixture Models with Three Cross product Terms on the Natural Logarithm of ILAW Electrical Conductivity.

EC Model	1 [1]		2		3		4	
Data Count	171 (+10 outliers)		292 (+ LORPM13 outlier +30 validation)		292 (+ LORPM13 outlier +30 validation)		292 (+ LORPM13 outlier +30 validation)	
Model Terms	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.
Al ₂ O ₃	4.229	6.207	2.213	2.897	2.275	2.901	3.791	2.976
B ₂ O ₃	7.566	4.253	4.489	2.920	4.407	2.949	3.813	2.929
CaO	2.188	3.917	1.877	2.362	1.952	2.402	3.141	2.404
Fe ₂ O ₃	3.983	4.020	6.882	2.620	6.819	2.667	6.198	2.627
K ₂ O	4.773	5.252	3.038	3.392	3.165	3.545	3.031	3.377
Li ₂ O	5.778	8.418	-2.520	6.727	-2.397	6.734	0.675	6.798
MgO	12.874	7.907	13.619	5.734	13.587	5.734	13.903	5.712
Na ₂ O	-1.653	2.458	-2.395	1.879	-2.420	1.878	-1.463	1.915
SiO ₂	3.511	1.757	5.646	1.138	5.623	1.146	4.806	1.199
SnO ₂	-	-	-	-	5.025	5.943	-	-
V ₂ O ₃	-	-	-	-	-	-	-8.796	7.400
ZrO ₂	10.237	8.121	13.955	4.593	14.183	4.723	12.431	4.626
Others ^(a)	12.840	5.089	5.528	3.069	5.774	3.490	8.725	3.477
CaO×Li ₂ O	145.252	22.879	177.415	14.196	174.679	14.285	171.012	14.301
CaO×Na ₂ O	79.122	7.579	39.402	4.549	38.921	4.557	38.451	4.539
Li ₂ O×Na ₂ O	-130.284	8.892	-55.557	5.496	-56.112	5.504	-57.371	5.505
Al ₂ O ₃ /(T/1000)	-11.571	8.400	-9.250	3.935	-9.321	3.940	-11.695	4.045
B ₂ O ₃ /(T/1000)	-10.551	5.749	-7.380	3.958	-7.367	3.998	-6.397	3.969
CaO/(T/1000)	-26.585	4.940	-21.062	2.956	-21.081	3.012	-22.603	3.020
Fe ₂ O ₃ /(T/1000)	-8.675	5.448	-11.759	3.556	-11.779	3.622	-10.753	3.567
K ₂ O/(T/1000)	-7.588	7.097	-5.878	4.608	-5.865	4.816	-5.842	4.586
Li ₂ O/(T/1000)	28.375	11.125	26.753	8.998	26.958	9.009	22.856	9.097
MgO/(T/1000)	-21.944	10.690	-23.195	7.784	-23.198	7.784	-23.703	7.753
Na ₂ O/(T/1000)	11.855	3.288	13.525	2.532	13.598	2.532	12.226	2.583
SiO ₂ /(T/1000)	-9.920	2.377	-12.734	1.544	-12.736	1.555	-11.481	1.627
ZrO ₂ /(T/1000)	-19.731	10.988	-24.479	6.229	-24.611	6.404	-22.230	6.276
SnO ₂ /(T/1000)	-	-	-	-	-9.711	8.102	-	-
V ₂ O ₃ /(T/1000)	-	-	-	-	-	-	12.223	10.114
Others/(T/1000)	-19.917	6.885	-9.456	4.169	-9.509	4.739	-14.396	4.719
Modeling Data Statistics								
R ²	0.951		0.952		0.952		0.952	
R ² _{Adjusted}	0.949		0.950		0.951		0.951	
RMSE	0.151		0.146		0.146		0.146	
PRESS RMSE	0.156		0.149		0.149		0.148	
Model LOF p-value	No replicate		0.0412		0.0412		0.0419	
Validation Statistics on 30 Glasses Selected Over Full Range – 15 each from ORP-LAW and WTP-LAW Glasses								
R ²	0.800 ^(b)		0.967		0.967		0.966	
RMSE	0.305 ^(b)		0.121		0.122		0.124	

(a) “Others” components include the original “Others” component (which contains Ag₂O, BaO, Br, CdO, Cs₂O, I, La₂O₃, MnO, MoO₃, NiO, PbO, Re₂O₇, SeO₂, SrO, and “Unknown”) plus Cl, Cr₂O₃, F, SO₃, TiO₂, and ZnO. In Models 1 and 2, SnO₂ and V₂O₃ are also added to “Others” if they are not included in the model terms. Model 3 includes V₂O₃ and Model 4 includes SnO₂.

(b) Validation set was limited to 15 ORP-LAW glasses since 15 WTP-LAW glasses were already used in the model design [1] and none were set aside for independent validation.

Table 5.20. Twenty-Eight Glasses Reserved from the Viscosity Dataset as a Validation Set and their Temperatures and Viscosity Measurements (112 data sorted near 1150 °C).

Glass ID	Temp1 (°C)	Vis1 (P)	Temp2 (°C)	Vis2 (P)	Temp3 (°C)	Vis3 (P)	Temp4 (°C)	Vis4 (P)
ORPLE8	969	93.10	1062	35.58	1157	16.52	1251	8.63
ORPLE11	986	106.21	1077	39.70	1169	19.27	1260	10.54
LAW7H	944	154.24	1045	51.83	1145	22.20	1245	11.32
ORPLD4	960	242.79	1060	66.51	1160	25.74	1260	12.13
ORPLF3	956	308.91	1057	83.22	1157	30.46	1257	13.95
LAW2H	939	271.78	1040	84.78	1142	34.08	1242	16.32
A3-AN104	950	309.47	1048	92.50	1146	35.69	1244	16.61
LAWA176	952	340.68	1050	97.93	1147	35.94	1246	16.22
LAWB101	947	363.8	1047	100.47	1146	36.68	1245	17.33
LAWA192	948	375.17	1047	106.03	1145	39.34	1245	17.95
LAWB78	971	374.92	1056	109.81	1156	40.12	1256	18.28
LAWB70	946	421.57	1043	114.17	1141	41.28	1239	17.57
LAWC21rev2	953	478.86	1052	133.96	1151	47.41	1251	21.85
LAWB86	968	478.21	1049	135.84	1149	50.37	1250	21.52
ORPLG12	953	639.80	1055	154.15	1157	48.10	1260	20.22
LAWA184	950	700.63	1047	169.15	1143	54.00	1241	23.28
ORPLA33-1	951	932.11	1053	184.85	1157	54.08	1259	21.04
ORPLG27	950	907.71	1052	187.18	1156	54.35	1258	20.66
LAWCrP3R	954	608.55	1052	156.94	1151	55.49	1248	24.93
C1-AN107	938	558.46	1032	151.51	1126	56.90	1220	25.84
LAWB95	942	739.97	1043	172.31	1144	58.67	1244	24.77
LAWA144	950	629.27	1045	165.45	1139	61.60	1234	26.58
ORPLA15	952	877.79	1052	201.81	1152	63.78	1252	25.37
LAWB38	943	722.92	1043	195.22	1143	70.03	1254	27.6
ORPLB1	957	1029.58	1060	231.27	1163	72.57	1266	28.65
LAWA60	945	911.46	1029	227.03	1130	77.64	1248	30.28
LAWA127R1	957	1031.48	1056	245.11	1156	78.49	1256	32.81
LAWA44R10	935	1001.77	1034	247.19	1134	83.13	1233	34.89

Table 5.21. Variation in Melt Viscosity Values for Near-Replicate Pair.

Glass ID	Viscosity Values at Measurement Temperatures								Pooled Over Temperature	
	Near 950°C		Near 1050°C		Near 1150°C		Near 1250°C		%RSD	SD
	T (°C)	Viscosity (P)	T (°C)	Viscosity (P)	T (°C)	Viscosity (P)	T (°C)	Viscosity (P)	S/cm	ln(Visc)
LAWC100R1	956	0.186	1049	0.245	1145	0.407	1238	0.529		
WVY-G-95A	959	0.177	1050	0.286	1144	0.412	1236	0.544		
%RSD^(a)	0.0%	0.7%	0.0%	1.1%	0.0%	0.9%	0.0%	3.5%	1.91%	0.0191
Glass ID	Viscosity Values at Nominal Temperatures								Pooled Over Temperature	
	950°C		1050°C		1150°C		1250°C		%RSD	SD
	Viscosity (P)	ln(Visc)	Viscosity (P)	ln(Visc)	Viscosity (P)	ln(Visc)	Viscosity (P)	ln(Visc)	Viscosity (P)	ln(Visc)
LAWC100R1	233.21	5.452	64.64	4.169	25.22	3.228	12.28	2.508		
WVY-G-95A	235.77	5.463	65.59	4.183	24.88	3.214	11.64	2.454		
%RSD^(a), SD^(b)	0.8%	0.0077	1.0%	0.0103	1.0%	0.0096	3.8%	0.0378	2.06%	0.0206

(a) %RSD = $100 \times (\text{Standard Deviation} / \text{Mean})$, calculated using the Viscosity values.

(b) Calculated using ln(S/cm) values.

Table 5.22. Coefficients and Performance Summary for Various Reduced Truncated T2 Mixture Models with Quadratic Terms on the Natural Logarithm of ILAW Viscosity.

Viscosity Model	1 [1]		2		3		4		5	
Data Count	171 (+10 outliers)		293 glasses (no outlier +28 validation)		293 glasses (no outlier +28 validation)		293 glasses (no outlier +28 validation)		293 glasses (no outlier +28 validation)	
Model Terms	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.
Al ₂ O ₃	5.699	3.073	1.124	1.816	0.799	1.540	1.629	1.691	0.779	1.538
B ₂ O ₃	-42.105	3.585	-27.371	2.808	-24.524	2.386	-24.856	2.599	-24.167	2.074
CaO	-10.823	1.781	-8.353	1.290	-10.135	1.124	-6.410	1.194	-10.162	1.120
Fe ₂ O ₃	-4.755	1.887	-4.846	1.552	-5.982	1.331	-2.703	1.429	-5.984	1.330
K ₂ O	-0.904	0.489	0.002	0.380	-1.420	0.331	-1.293	0.358	-1.457	0.308
Li ₂ O	11.231	4.481	9.468	4.355	10.485	3.696	7.637	4.030	10.506	3.693
MgO	-6.463	4.535	-15.140	4.050	-15.827	3.441	-20.422	3.683	-16.364	2.948
Na ₂ O	0.919	1.186	1.361	1.143	0.775	0.971	0.311	1.065	0.763	0.970
P ₂ O ₅	-1.246	5.530	0.546	7.102	-1.920	6.029	-3.936	6.508	-1.929	6.027
SiO ₂	1.520	0.772	1.682	0.610	0.959	0.524	-1.354	0.547	0.944	0.521
SnO ₂	-	-	-	-	-26.697	2.801	-	-	-26.722	2.798
V ₂ O ₃	-	-	-	-	-	-	-9.712	3.975	-	-
ZrO ₂	-11.599	3.886	-23.296	2.773	-19.362	2.447	-25.251	2.571	-19.358	2.446
Others ^(a)	-9.246	2.699	-13.040	2.003	-6.382	1.994	9.507	0.539	-6.404	1.992
B ₂ O ₃ × B ₂ O ₃	197.193	19.071	109.547	14.687	97.639	12.473	99.351	13.601	95.880	11.031
Li ₂ O ×Li ₂ O	132.727	22.574	123.887	23.942	109.094	20.319	110.487	22.006	108.753	20.279
Al ₂ O ₃ Li ₂ O	-137.475	29.287	-65.815	14.882	-84.520	12.659	-83.477	13.755	-84.640	12.648
MgO×MgO	-169.558	53.834	14.203	45.526	-11.689	38.628	-12.829	41.961	-	-
Al ₂ O ₃ /(T/1000) ²	24.234	5.421	31.746	3.290	32.333	2.790	30.731	3.067	32.327	2.789
CaO/(T/1000) ²	14.078	3.225	7.687	2.342	12.004	2.043	4.986	2.166	12.002	2.042
Fe ₂ O ₃ /(T/1000) ²	15.457	3.408	12.450	2.830	15.782	2.426	9.675	2.601	15.783	2.425
Li ₂ O/(T/1000) ²	-82.940	7.153	-83.236	7.308	-82.282	6.200	-77.377	6.776	-82.262	6.197
MgO/(T/1000) ²	23.561	6.720	25.039	6.326	28.666	5.378	37.307	5.731	28.633	5.374
Na ₂ O/(T/1000) ²	-14.632	2.140	-15.436	2.067	-14.566	1.757	-13.752	1.927	-14.561	1.756
P ₂ O ₅ /(T/1000) ²	24.785	10.107	22.082	13.011	27.095	11.045	30.902	11.922	27.110	11.041
SiO ₂ /(T/1000) ²	24.496	1.363	21.908	1.076	23.328	0.925	27.674	0.959	23.327	0.924
ZrO ₂ /(T/1000) ²	47.267	7.055	71.061	5.060	60.162	4.462	71.430	4.691	60.167	4.460
SnO ₂ /(T/1000) ²	-	-	-	-	68.349	5.122	-	-	68.348	5.120
V ₂ O ₃ /(T/1000) ²	-	-	-	-	-	-	18.560	7.288	-	-
Others/(T/1000) ²	17.008	4.900	28.711	3.653	11.047	3.637	-18.278	1.096	11.052	3.636
Modeling Data Statistics										
R ²	0.988		0.982		0.987		0.985		0.987	
R ² _{Adjusted}	0.987		0.982		0.987		0.985		0.987	
RMSE	0.147		0.180		0.152		0.165		0.152	
PRESS RMSE	0.151		0.185		0.156		0.169		0.156	
Model LOF p-value	No replicate		0.0002		0.0005		0.0003		0.0005	
Validation Statistics on 28 Glasses Selected over Full Range – 14 each ORP-LAW and WTP-LAW Glasses										
R ²	0.961		0.975		0.975		0.974		0.974	
RMSE	0.354 ^(b)		0.254		0.259		0.263		0.257	

- (a) “Others” components include the original “Others” component (which contains Ag₂O, BaO, Br, CdO, Cs₂O, I, La₂O₃, MnO, MoO₃, NiO, PbO, Re₂O₇, SeO₂, SrO, and “Unknown”) plus Cl, Cr₂O₃, F, SO₃, TiO₂, and ZnO. In Models 1 and 2, SnO₂ and V₂O₃ are also added to “Others” if they are not included in the model terms.
- (b) Validation set was limited to 14 ORP-LAW glasses since 14 WTP-LAW glasses were already used in the model design [1] and none were set aside for independent validation.

Figure 2.1. Na_2O and SO_3 concentrations for 153 high waste loading ORP-LAW glasses.

Figure 2.2. Range of concentrations for major components in the combined LAW glass dataset (478 glass samples).

Figure 2.4. Na₂O-K₂O-CaO scatter plot showing the WTP-LAW glasses (green triangles), the ORP-LAW glasses (black squares) and the LORPM glasses (red circles).

Figure 2.5. SnO_2 - V_2O_5 - Fe_2O_3 scatter plot showing the WTP-LAW glasses (green triangles), the ORP-LAW glasses (black squares) and the LORPM glasses (red circles).

Figure 2.6. K₂O-Li₂O-SnO₂ scatter plot showing the WTP-LAW glasses (green triangles), the ORP-LAW glasses (black squares) and the LORPM glasses (red circles).

Figure 2.7. K_2O - Li_2O - V_2O_5 scatter plot showing the WTP-LAW glasses (green triangles), the ORP-LAW glasses (black squares) and the LORPM glasses (red circles).

Figure 4.1. SEM images and EDS spectra of two types of crystals observed in LORPM8R1: 2 vol% of 0.5 to 2 micron size tin oxide crystals in clusters (top) and 1 vol% of Zn-chromite 0.5-1 μm in size homogeneously dispersed in the glass (bottom).

Figure 4.2. SEM images and EDS spectra of crystals observed in LORPM13: 2.1 vol% of 0.2-2 μm by 1-10 μm, partially clustered zirconium oxide crystals. The clusters show an exsolution pattern alignment.

Figure 4.3. PCT sodium and silicon releases (g/m^2) as a function of PCT boron release for 20 LORPM Glasses.

Figure 4.4. PCT boron release as a function of the pH measured at 20°C in the 7-day PCT leachate for 20 LORPM glasses and 171 ORP-LAW glasses with PCT data.

Figure 4.5. PCT sodium and silicon releases (g/m²) as a function of glass alkali concentration.

Figure 4.6. VHT alteration rate (g/m²/day) as a function of glass alkali concentration.

Figure 4.7. Distribution of temperature values at which melt electrical conductivity was measured for the 20 LORPM glasses.

Figure 4.8. Distribution of temperature values at which melt electrical conductivity was measured for the 20 LORPM glasses.

Figure 5.1. PCT sodium release as a function of PCT boron release (g/m²) for 455 LAW glasses considered in new models.

Figure 5.2. Distribution of the PCT sodium (top) and boron (bottom) releases for 455 LAW glasses considered in new models; the selection of the 28 validation glasses (red markers) was made after sorting by increasing $\ln(\text{Na})$.

Figure 5.3. Comparison of predicted versus measured PCT-Na for the WTP-LAW (including outliers), ORP-LAW and twenty LORPM glasses using the WTP baseline 17-Term Reduced Partial Quadratic Mixture PCT model [1]. The red lines represent the WTP contract limit (4 g/L) for PCT-Na release.

Figure 5.4. Predicted versus measured plot for 18-term mixture model #5 on PCT-Na. The red lines represent the WTP contract limit (4 g/L) for PCT-Na release.

Figure 5.5. Predicted versus measured plot for 22-term mixture model #5 on PCT-B. The red lines represent the WTP contract limit (4 g/L) for PCT-B release.

Figure 5.6. Comparison of predicted versus measured VHT for the WTP-LAW, outliers, ORP-LAW, and twenty LORPM glasses using the WTP baseline 17-Term Reduced Partial Quadratic Mixture model [1] on the natural logarithm of VHT alteration depth. The red lines represent the WTP contract limit (50 g/m²/day alteration rate).

Figure 5.7. Normal quantile plot applied to model residuals of PCT-Na Model 4 (top) and VHT Model 3 (bottom) in which sample LORPM13 is identified as one remaining outlier.

Figure 5.8. Predicted versus measured plot for 20-term mixture model #6 on VHT Alteration Depth (D). The red lines represent the WTP contract limit corresponding to $50 \text{ g/m}^2/\text{day}$ ($D = 453 \mu\text{m}$).

Figure 5.9. Melt electrical conductivity data measured on near-replicate glasses LAW100R1 (crucible) and WVY-G-95A (DM100 melter glass).

Figure 5.10. Comparison of predicted versus measured electrical conductivity for the WTP-LAW, ORP-LAW, and twenty LORPM glasses using the WTP baseline 25-Term Reduced Arrhenius-Linear Mixture Model with three crossproduct terms on the natural logarithm of electrical conductivity.

Figure 5.11. Predicted versus measured plot for 22-term Arrhenius-linear mixture model with three crossproduct terms on ILAW electrical conductivity.

Figure 5.12. Melt viscosity data measured on near-replicate glasses LAW100R1 (crucible) and WVY-G-95A (DM100 melter glass).

Figure 5.13. Comparison of predicted versus measured melt viscosity for the WTP-LAW, ORP-LAW, and eighteen LORPM glasses using the WTP baseline 26-term reduced truncated T2-linear mixture model with four quadratic terms on the natural logarithm of viscosity.

Figure 5.14. Predicted versus measured plot for 28-term reduced truncated T2-linear mixture model with three quadratic terms on ILAW viscosity.

APPENDIX

Variance-Covariance Matrices for Selected Models

Table A.1. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 18-Term Model (Model 5) for ln(PCT-Na, g/L) of Combined WTP/ORP/LORPM LAW Glasses.

Term	Al ₂ O ₃	B ₂ O ₃	CaO	Fe ₂ O ₃	K ₂ O	Li ₂ O	MgO	Na ₂ O	SiO ₂
Al ₂ O ₃	1.4751	0.1123	-0.0642	1.7473	0.1588	0.0509	0.2941	-1.5015	-0.2731
B ₂ O ₃	0.1123	0.8444	-0.0428	-0.0786	0.0886	0.0554	0.1788	-1.0486	-0.3541
CaO	-0.0642	-0.0428	1.2346	0.6924	0.1522	0.9633	0.3058	-0.8792	-0.2387
Fe ₂ O ₃	1.7473	-0.0786	0.6924	5.3624	0.0735	1.0161	0.4192	-1.4527	-0.4035
K ₂ O	0.1588	0.0886	0.1522	0.0735	0.7067	0.9266	0.1880	-0.3917	-0.1643
Li ₂ O	0.0509	0.0554	0.9633	1.0161	0.9266	7.9482	0.4025	-0.9538	-0.6833
MgO	0.2941	0.1788	0.3058	0.4192	0.1880	0.4025	2.1760	-0.8240	-0.3191
Na ₂ O	-1.5015	-1.0486	-0.8792	-1.4527	-0.3917	-0.9538	-0.8240	4.5128	1.0114
SiO ₂	-0.2731	-0.3541	-0.2387	-0.4035	-0.1643	-0.6833	-0.3191	1.0114	0.3438
SnO ₂	-0.0413	0.5325	1.3896	1.2284	-0.3979	-0.8449	0.4752	-1.4261	-0.4347
ZrO ₂	0.1076	0.3119	0.3246	0.2442	0.0629	0.4711	0.3003	-1.1720	-0.3561
P ₂ O ₅	0.0368	-0.0198	0.1645	-0.1313	0.1460	-0.1308	-0.1273	-0.3029	-0.1358
Others	-0.1518	0.2237	0.0439	-0.2913	-0.0030	0.0638	-0.2085	-0.5118	-0.2135
Al ₂ O ₃ *Fe ₂ O ₃	-24.2889	1.2166	2.4075	-60.4472	-0.7952	-10.0376	-4.2493	12.6572	2.6390
CaO*Fe ₂ O ₃	1.2824	4.7161	-10.8115	-15.6024	-0.2315	-3.8890	-0.5590	-2.8131	-0.8542
CaO*Li ₂ O	-0.3613	2.9579	-17.8969	-11.7783	-6.0755	-67.2512	-1.1368	11.4276	3.6584
Na ₂ O*SiO ₂	3.4374	2.8198	2.3274	3.2771	1.2484	4.4277	2.5049	-11.5069	-2.8611
CaO*SnO ₂	5.3253	-4.6583	-23.6440	-10.7189	1.4631	2.3747	-11.7497	13.2865	5.7304

Term	SnO ₂	ZrO ₂	P ₂ O ₅	Others	Al ₂ O ₃ *Fe ₂ O ₃	CaO*Fe ₂ O ₃	CaO*Li ₂ O	Na ₂ O*SiO ₂	CaO*SnO ₂
Al ₂ O ₃	-0.0413	0.1076	0.0368	-0.1518	-24.2889	1.2824	-0.3613	3.4374	5.3253
B ₂ O ₃	0.5325	0.3119	-0.0198	0.2237	1.2166	4.7161	2.9579	2.8198	-4.6583
CaO	1.3896	0.3246	0.1645	0.0439	2.4075	-10.8115	-17.8969	2.3274	-23.6440
Fe ₂ O ₃	1.2284	0.2442	-0.1313	-0.2913	-60.4472	-15.6024	-11.7783	3.2771	-10.7189
K ₂ O	-0.3979	0.0629	0.1460	-0.0030	-0.7952	-0.2315	-6.0755	1.2484	1.4631
Li ₂ O	-0.8449	0.4711	-0.1308	0.0638	-10.0376	-3.8890	-67.2512	4.4277	2.3747
MgO	0.4752	0.3003	-0.1273	-0.2085	-4.2493	-0.5590	-1.1368	2.5049	-11.7497
Na ₂ O	-1.4261	-1.1720	-0.3029	-0.5118	12.6572	-2.8131	11.4276	-11.5069	13.2865
SiO ₂	-0.4347	-0.3561	-0.1358	-0.2135	2.6390	-0.8542	3.6584	-2.8611	5.7304
SnO ₂	6.2465	0.1997	0.2739	0.2372	3.8548	-12.6513	2.8444	3.4605	-91.5720
ZrO ₂	0.1997	1.6159	0.0724	0.4018	1.9253	0.5681	-7.5014	2.7993	-9.0495
P ₂ O ₅	0.2739	0.0724	4.2813	0.0962	3.6097	-0.1742	5.8118	1.0467	-4.0140
Others	0.2372	0.4018	0.0962	0.9764	5.2390	2.0060	-1.3723	1.3102	-2.5057
Al ₂ O ₃ *Fe ₂ O ₃	3.8548	1.9253	3.6097	5.2390	892.5340	25.6705	86.2309	-27.2837	-136.8554
CaO*Fe ₂ O ₃	-12.6513	0.5681	-0.1742	2.0060	25.6705	267.1492	104.4268	10.6708	213.8887
CaO*Li ₂ O	2.8444	-7.5014	5.8118	-1.3723	86.2309	104.4268	908.6406	-33.6964	68.7134
Na ₂ O*SiO ₂	3.4605	2.7993	1.0467	1.3102	-27.2837	10.6708	-33.6964	30.8211	-34.7615
CaO*SnO ₂	-91.5720	-9.0495	-4.0140	-2.5057	-136.8554	213.8887	68.7134	-34.7615	2077.7329

Table A.2. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 22-Term Model (Model 5) for $\ln(\text{PCT-B, g/L})$ of Combined WTP/ORP/LORPM LAW Glasses.

Term	Al ₂ O ₃	B ₂ O ₃	CaO	Fe ₂ O ₃	K ₂ O	Li ₂ O	MgO	Na ₂ O	SiO ₂	SnO ₂	ZrO ₂	P ₂ O ₅
Al ₂ O ₃	1.5678	-0.5941	-0.3217	0.0568	6.6899	-0.9352	-0.0415	-0.4253	0.1421	-0.6041	-0.2706	-0.0573
B ₂ O ₃	-0.5941	1.6067	-0.5977	-0.3876	1.2306	4.6627	0.0196	-0.0130	-0.1571	0.6841	-0.1173	-0.4462
CaO	-0.3217	-0.5977	3.4524	1.6090	-11.8239	-4.7328	0.2719	0.0044	-0.2837	0.7600	2.8424	0.6220
Fe ₂ O ₃	0.0568	-0.3876	1.6090	1.8941	-4.0535	-4.5991	0.0633	-0.0102	-0.2453	1.2285	1.0448	0.3182
K ₂ O	6.6899	1.2306	-11.8239	-4.0535	305.8026	3.9184	-5.0570	-4.2242	3.4922	11.4049	-15.5438	-4.3355
Li ₂ O	-0.9352	4.6627	-4.7328	-4.5991	3.9184	123.2365	0.2492	-1.6945	1.3973	1.1916	-1.1733	-3.4559
MgO	-0.0415	0.0196	0.2719	0.0633	-5.0570	0.2492	2.9679	0.2226	-0.2096	0.5929	0.2005	-0.2430
Na ₂ O	-0.4253	-0.0130	0.0044	-0.0102	-4.2242	-1.6945	0.2226	0.4371	-0.1567	-0.3428	-0.2070	0.2185
SiO ₂	0.1421	-0.1571	-0.2837	-0.2453	3.4922	1.3973	-0.2096	-0.1567	0.1939	0.0036	-0.4173	-0.1507
SnO ₂	-0.6041	0.6841	0.7600	1.2285	11.4049	1.1916	0.5929	-0.3428	0.0036	11.7343	-1.1524	0.1309
ZrO ₂	-0.2706	-0.1173	2.8424	1.0448	-15.5438	-1.1733	0.2005	-0.2070	-0.4173	-1.1524	5.2562	0.3997
P ₂ O ₅	-0.0573	-0.4462	0.6220	0.3182	-4.3355	-3.4559	-0.2430	0.2185	-0.1507	0.1309	0.3997	5.8001
Others	-0.2048	-0.2038	0.2412	0.2304	-5.8127	-4.0291	-0.3449	0.0995	-0.2242	-0.6217	0.6178	0.1836
CaO*Fe ₂ O ₃	-0.5790	3.9106	-26.4665	-22.2394	15.5030	22.1971	-2.1258	2.4707	1.4184	-16.9844	-16.3508	-3.5999
Al ₂ O ₃ *K ₂ O	-49.1691	9.6420	23.3475	4.1817	-626.3513	-66.7506	2.7007	17.9051	-7.6811	-5.0784	22.7025	8.5671
B ₂ O ₃ *K ₂ O	9.4854	-31.0804	16.7624	6.3181	-293.4181	11.3336	-13.6478	-2.3498	2.5521	-32.8125	29.4567	16.7411
B ₂ O ₃ *Li ₂ O	6.5359	-32.3896	12.4027	9.4510	-96.0727	-241.1768	7.6949	6.7877	-1.1293	-5.6423	-5.9839	2.3578
K ₂ O*SiO ₂	-10.3571	2.3670	20.1872	7.2247	-554.5663	-7.6070	15.1565	8.0765	-7.7872	-17.2015	25.7897	6.1512
Li ₂ O*SiO ₂	-1.0158	-2.6518	7.1875	8.0245	-5.7111	-220.2251	-1.4408	4.6617	-3.9546	-4.4023	3.9839	8.2932
CaO*SnO ₂	10.0662	-12.6439	-6.6364	-13.9227	-198.3112	-69.5529	-12.1402	3.9863	0.1018	-153.4179	13.4961	-0.0019
K ₂ O*SnO ₂	10.4400	-14.9281	13.0560	13.8531	-349.6738	-22.2417	-12.3518	3.4074	-3.2881	-135.9849	19.0312	-2.8106
CaO*ZrO ₂	1.3827	5.4157	-61.9806	-16.3885	243.1571	13.8982	-0.7848	1.6515	5.3776	22.9836	-74.6935	-5.5791

Table A.2. Variance-Covariance Matrix Associated with the Estimated Coefficients of Terms in the 22-Term Model (Model 5) for $\ln(\text{PCT-B, g/L})$ of Combined WTP/ORP/LORPM LAW Glasses (continued).

Term	Others	CaO *Fe ₂ O ₃	Al ₂ O ₃ *K ₂ O	B ₂ O ₃ *K ₂ O	B ₂ O ₃ *Li ₂ O	K ₂ O *SiO ₂	Li ₂ O *SiO ₂	CaO *SnO ₂	K ₂ O *SnO ₂	CaO *ZrO ₂
Al ₂ O ₃	-0.2048	-0.5790	-49.1691	9.4854	6.5359	-10.3571	-1.0158	10.0662	10.4400	1.3827
B ₂ O ₃	-0.2038	3.9106	9.6420	-31.0804	-32.3896	2.3670	-2.6518	-12.6439	-14.9281	5.4157
CaO	0.2412	-26.4665	23.3475	16.7624	12.4027	20.1872	7.1875	-6.6364	13.0560	-61.9806
Fe ₂ O ₃	0.2304	-22.2394	4.1817	6.3181	9.4510	7.2247	8.0245	-13.9227	13.8531	-16.3885
K ₂ O	-5.8127	15.5030	-626.3513	-293.4181	-96.0727	-554.5663	-5.7111	-198.3112	-349.6738	243.1571
Li ₂ O	-4.0291	22.1971	-66.7506	11.3336	-241.1768	-7.6070	-220.2251	-69.5529	-22.2417	13.8982
MgO	-0.3449	-2.1258	2.7007	-13.6478	7.6949	15.1565	-1.4408	-12.1402	-12.3518	-0.7848
Na ₂ O	0.0995	2.4707	17.9051	-2.3498	6.7877	8.0765	4.6617	3.9863	3.4074	1.6515
SiO ₂	-0.2242	1.4184	-7.6811	2.5521	-1.1293	-7.7872	-3.9546	0.1018	-3.2881	5.3776
SnO ₂	-0.6217	-16.9844	-5.0784	-32.8125	-5.6423	-17.2015	-4.4023	-153.4179	-135.9849	22.9836
ZrO ₂	0.6178	-16.3508	22.7025	29.4567	-5.9839	25.7897	3.9839	13.4961	19.0312	-74.6935
P ₂ O ₅	0.1836	-3.5999	8.5671	16.7411	2.3578	6.1512	8.2932	-0.0019	-2.8106	-5.5791
Others	1.4517	1.2271	11.4166	7.1645	16.3614	10.0181	5.5236	10.6297	19.7172	-5.7277
CaO*Fe ₂ O ₃	1.2271	423.1205	47.0606	-13.2274	58.5708	-38.9765	-54.9696	230.4609	-15.7597	368.4695
Al ₂ O ₃ *K ₂ O	11.4166	47.0606	3274.2656	-172.8689	362.2599	1022.7092	135.1627	140.2939	-116.9894	-329.0351
B ₂ O ₃ *K ₂ O	7.1645	-13.2274	-172.8689	3465.4201	-449.3315	-51.4209	63.2418	368.8409	1307.8057	-330.7012
B ₂ O ₃ *Li ₂ O	16.3614	58.5708	362.2599	-449.3315	2482.0005	284.1965	-8.1683	455.2956	-78.7660	-81.2721
K ₂ O*SiO ₂	10.0181	-38.9765	1022.7092	-51.4209	284.1965	1156.5168	-7.4583	350.1853	444.0148	-430.6423
Li ₂ O*SiO ₂	5.5236	-54.9696	135.1627	63.2418	-8.1683	-7.4583	510.4186	90.8583	75.6521	-22.0030
CaO*SnO ₂	10.6297	230.4609	140.2939	368.8409	455.2956	350.1853	90.8583	3140.3251	1198.3503	-447.7191
K ₂ O*SnO ₂	19.7172	-15.7597	-116.9894	1307.8057	-78.7660	444.0148	75.6521	1198.3503	4617.0301	-420.5091
CaO*ZrO ₂	-5.7277	368.4695	-329.0351	-330.7012	-81.2721	-430.6423	-22.0030	-447.7191	-420.5091	1671.1325

Table A.3. Variance-Covariance Matrix Associated with the Estimated Coefficients of Terms in the 20-Term Model (Model 6) for ln(VHT Alteration Depth, μm) of Combined WTP/ORP/LORPM LAW Glasses.

Term	Al ₂ O ₃	B ₂ O ₃	CaO	Fe ₂ O ₃	K ₂ O	Li ₂ O	MgO	Na ₂ O	SiO ₂	SnO ₂
Al ₂ O ₃	51.0662	0.3361	-6.6199	-0.9431	-9.5255	-21.8652	-1.8932	-7.6095	-2.2594	-4.7481
B ₂ O ₃	0.3361	11.6466	-21.3151	3.9053	-3.4790	-24.3354	-0.2047	-17.7066	-0.9775	4.9498
CaO	-6.6199	-21.3151	390.9168	-10.1855	-31.0992	-73.3222	-15.5834	-88.2765	31.4936	-21.2648
Fe ₂ O ₃	-0.9431	3.9053	-10.1855	9.8390	-21.8715	-17.0642	-5.0763	-13.3927	-0.2757	7.8295
K ₂ O	-9.5255	-3.4790	-31.0992	-21.8715	265.0819	54.8379	50.3386	52.6107	-9.0719	-13.0483
Li ₂ O	-21.8652	-24.3354	-73.3222	-17.0642	54.8379	313.1044	1.3998	197.7507	-23.9649	-13.3418
MgO	-1.8932	-0.2047	-15.5834	-5.0763	50.3386	1.3998	58.5690	8.0462	-3.7978	-2.6784
Na ₂ O	-7.6095	-17.7066	-88.2765	-13.3927	52.6107	197.7507	8.0462	157.3811	-19.6904	-6.2835
SiO ₂	-2.2594	-0.9775	31.4936	-0.2757	-9.0719	-23.9649	-3.7978	-19.6904	5.1146	-0.9999
SnO ₂	-4.7481	4.9498	-21.2648	7.8295	-13.0483	-13.3418	-2.6784	-6.2835	-0.9999	26.1049
ZrO ₂	-4.3993	2.8022	-4.8266	4.7877	-5.2086	-10.4393	-7.0130	-5.8651	-0.4230	-0.0260
Others	-3.8279	3.6371	-17.4285	3.4427	-7.0839	-18.0678	-1.7978	-12.1699	-1.1799	3.7796
CaO*CaO	-39.1225	43.8573	-377.6797	53.7635	-203.5695	-96.2561	-18.9903	-61.4263	12.0315	67.6959
K ₂ O*K ₂ O	288.2633	101.4280	-521.1393	133.1959	-2044.9130	-223.4171	77.0403	18.6409	-53.3655	-28.3393
K ₂ O*MgO	-96.5095	8.8222	-216.4648	191.5216	-2030.2308	-45.8960	-1451.7469	-258.7869	73.6732	71.3797
Al ₂ O ₃ *Na ₂ O	-281.6619	3.8259	-72.6634	24.8328	12.7767	54.0357	24.9018	6.2690	11.9622	39.9980
K ₂ O*Na ₂ O	-37.1381	11.3772	324.3135	75.9927	-676.3377	-383.2032	-164.0251	-410.4064	66.1469	67.1635
Li ₂ O*Na ₂ O	138.2768	224.8711	448.5268	144.5115	-320.1617	-2297.6017	109.0939	-1560.3372	152.5532	75.3249
Na ₂ O*Na ₂ O	84.2479	55.2263	217.6587	33.7426	-136.4899	-564.4944	-13.2329	-454.0894	47.7788	7.5471
CaO*SiO ₂	24.6146	39.9867	-841.2984	16.4891	108.2285	169.2343	36.8328	205.6350	-77.2166	42.4238

Table A.3. Variance-Covariance Matrix Associated with the Estimated Coefficients of Terms in the 20-Term Model (Model 6) for $\ln(\text{VHT Alteration Depth, } \mu\text{m})$ of Combined WTP/ORP/LORPM LAW Glasses (continued).

Term	ZrO ₂	Others	CaO *CaO	K ₂ O *K ₂ O	K ₂ O *MgO	Al ₂ O ₃ *Na ₂ O	K ₂ O *Na ₂ O	Li ₂ O *Na ₂ O	Na ₂ O *Na ₂ O	CaO *SiO ₂
Al ₂ O ₃	-4.3993	-3.8279	-39.1225	288.2633	-96.5095	-281.6619	-37.1381	138.2768	84.2479	24.6146
B ₂ O ₃	2.8022	3.6371	43.8573	101.4280	8.8222	3.8259	11.3772	224.8711	55.2263	39.9867
CaO	-4.8266	-17.4285	-377.6797	-521.1393	-216.4648	-72.6634	324.3135	448.5268	217.6587	-841.2984
Fe ₂ O ₃	4.7877	3.4427	53.7635	133.1959	191.5216	24.8328	75.9927	144.5115	33.7426	16.4891
K ₂ O	-5.2086	-7.0839	-203.5695	-2044.9130	-2030.2308	12.7767	-676.3377	-320.1617	-136.4899	108.2285
Li ₂ O	-10.4393	-18.0678	-96.2561	-223.4171	-45.8960	54.0357	-383.2032	-2297.6017	-564.4944	169.2343
MgO	-7.0130	-1.7978	-18.9903	77.0403	-1451.7469	24.9018	-164.0251	109.0939	-13.2329	36.8328
Na ₂ O	-5.8651	-12.1699	-61.4263	18.6409	-258.7869	6.2690	-410.4064	-1560.3372	-454.0894	205.6350
SiO ₂	-0.4230	-1.1799	12.0315	-53.3655	73.6732	11.9622	66.1469	152.5532	47.7788	-77.2166
SnO ₂	-0.0260	3.7796	67.6959	-28.3393	71.3797	39.9980	67.1635	75.3249	7.5471	42.4238
ZrO ₂	19.6116	4.0804	28.6896	-95.3021	295.6795	26.6928	27.0078	53.6890	0.6768	3.2068
Others	4.0804	12.7896	12.6384	15.6474	30.7595	30.1483	52.2316	142.9084	30.7223	42.1817
CaO*CaO	28.6896	12.6384	3284.3416	721.9633	493.9537	449.2555	798.6641	373.6025	46.8344	72.4036
K ₂ O*K ₂ O	-95.3021	15.6474	721.9633	55145.8311	-6012.9616	-1359.8981	-4793.6389	3139.6006	565.4488	947.8778
K ₂ O*MgO	295.6795	30.7595	493.9537	-6012.9616	68866.8177	461.5346	7485.3331	-1983.9432	388.8277	690.4582
Al ₂ O ₃ *Na ₂ O	26.6928	30.1483	449.2555	-1359.8981	461.5346	1885.8677	467.5005	-313.4038	-460.9668	66.4066
K ₂ O*Na ₂ O	27.0078	52.2316	798.6641	-4793.6389	7485.3331	467.5005	4961.6906	2560.8002	952.1964	-835.7726
Li ₂ O*Na ₂ O	53.6890	142.9084	373.6025	3139.6006	-1983.9432	-313.4038	2560.8002	19753.4260	4692.3415	-994.4424
Na ₂ O*Na ₂ O	0.6768	30.7223	46.8344	565.4488	388.8277	-460.9668	952.1964	4692.3415	1462.0869	-467.4079
CaO*SiO ₂	3.2068	42.1817	72.4036	947.8778	690.4582	66.4066	-835.7726	-994.4424	-467.4079	2029.1449

Table A.4. Variance-Covariance Matrix Associated with the Estimated Coefficients of Terms in the 25-Term Model (Model 2) for ln(Electrical Conductivity, S/cm) of Combined WTP/ORP/LORPM LAW Glasses.

Term	Al ₂ O ₃	B ₂ O ₃	CaO	Fe ₂ O ₃	K ₂ O	Li ₂ O	MgO	Na ₂ O	SiO ₂	ZrO ₂	Others
Al ₂ O ₃	8.3933	-0.9138	-1.6482	0.6630	0.8446	-3.5288	-0.3631	-2.3577	0.2211	-1.3274	-1.4164
B ₂ O ₃	-0.9138	8.524	-1.4954	0.5308	0.6742	0.2338	-0.8322	-0.5538	-1.5642	0.6386	0.7537
CaO	-1.6482	-1.4954	5.5782	0.8316	0.5220	-3.5691	0.5997	0.3939	-0.1846	-0.0303	0.6519
Fe ₂ O ₃	0.6630	0.5308	0.8316	6.8627	-0.5503	1.2140	-1.4882	0.1087	-1.5602	4.1739	2.1400
K ₂ O	0.8446	0.6742	0.5220	-0.5503	11.5064	4.1379	2.6503	0.6601	-0.6040	-2.1047	-2.6249
Li ₂ O	-3.5288	0.2338	-3.5691	1.2140	4.1379	45.2525	4.7397	9.9587	-3.8932	-4.2333	-3.1280
MgO	-0.3631	-0.8322	0.5997	-1.4882	2.6503	4.7397	32.8739	2.4481	-1.5183	1.1437	-4.6532
Na ₂ O	-2.3577	-0.5538	0.3939	0.1087	0.6601	9.9587	2.4481	3.5305	-0.9577	-2.7261	-0.7522
SiO ₂	0.2211	-1.5642	-0.1846	-1.5602	-0.6040	-3.8932	-1.5183	-0.9577	1.2956	-0.9969	-1.1243
ZrO ₂	-1.3274	0.6386	-0.0303	4.1739	-2.1047	-4.2333	1.1437	-2.7261	-0.9969	21.0955	1.6307
Others	-1.4164	0.7537	0.6519	2.1400	-2.6249	-3.1280	-4.6532	-0.7522	-1.1243	1.6307	9.4214
CaO*Li ₂ O	0.3975	0.5849	-11.6164	0.5641	-0.3081	-11.2264	0.5189	-2.4152	0.6931	1.9028	1.3677
CaO*Na ₂ O	0.1604	-0.1748	-4.1324	0.3311	-0.1485	-1.9730	0.1568	-0.8746	0.2815	0.9649	0.3778
Li ₂ O*Na ₂ O	0.1288	0.0570	0.5500	0.1840	-0.2077	-4.4288	0.2956	-0.3273	0.0842	0.1703	0.1890
Al ₂ O ₃ /(T/1000)	-11.3610	1.2434	2.1904	-0.8929	-1.1541	4.6363	0.5403	3.1714	-0.2943	1.7968	1.9268
B ₂ O ₃ /(T/1000)	1.2429	-11.5150	1.9777	-0.7260	-0.9269	-0.4095	1.1380	0.7420	2.1190	-0.8682	-1.0195
CaO/(T/1000)	2.2047	2.0389	-6.4790	-1.2036	-0.6681	5.4971	-0.8520	-0.3050	0.1784	-0.1817	-0.9949
Fe ₂ O ₃ /(T/1000)	-0.8945	-0.7279	-1.2081	-9.2836	0.7427	-1.6946	2.0249	-0.1603	2.1190	-5.6309	-2.8995
K ₂ O/(T/1000)	-1.1473	-0.9316	-0.7365	0.7506	-15.5792	-5.5994	-3.5807	-0.8905	0.8241	2.8491	3.5389
Li ₂ O/(T/1000)	4.6892	-0.3864	5.6939	-1.7008	-5.5412	-59.5382	-6.5694	-13.2101	5.2018	5.5500	4.0678
MgO/(T/1000)	0.5398	1.1334	-0.8999	2.0293	-3.5889	-6.5882	-44.4824	-3.3584	2.0630	-1.5210	6.2989
Na ₂ O/(T/1000)	3.1750	0.761	-0.2574	-0.1668	-0.8693	-13.2397	-3.3500	-4.7072	1.2740	3.6199	0.9803
SiO ₂ /(T/1000)	-0.2960	2.1127	0.1782	2.1200	0.8180	5.2292	2.0591	1.2781	-1.7489	1.3668	1.5353
ZrO ₂ /(T/1000)	1.7917	-0.8789	-0.0788	-5.6340	2.8288	5.5957	-1.5335	3.6524	1.3595	-28.5098	-2.1694
Others/(T/1000)	1.9215	-1.022	-1.0027	-2.9027	3.5342	4.1102	6.2919	0.9863	1.5352	-2.1658	-12.7478

Table A.4. Variance-Covariance Matrix Associated with the Estimated Coefficients of Terms in the 25-Term Model (Model 2) for ln(Electrical Conductivity, S/cm) of Combined WTP/ORP/LORPM LAW Glasses (continued).

Term	CaO*Li ₂ O	CaO*Na ₂ O	Li ₂ O*Na ₂ O	Al ₂ O ₃ /(T/1000)	B ₂ O ₃ /(T/1000)	CaO/(T/1000)	Fe ₂ O ₃ /(T/1000)
Al ₂ O ₃	0.3975	0.1604	0.1288	-11.3610	1.2429	2.2047	-0.8945
B ₂ O ₃	0.5849	-0.1748	0.0570	1.2434	-11.5150	2.0389	-0.7279
CaO	-11.6164	-4.1324	0.5500	2.1904	1.9777	-6.4790	-1.2081
Fe ₂ O ₃	0.5641	0.3311	0.1840	-0.8929	-0.7260	-1.2036	-9.2836
K ₂ O	-0.3081	-0.1485	-0.2077	-1.1541	-0.9269	-0.6681	0.7427
Li ₂ O	-11.2264	-1.9730	-4.4288	4.6363	-0.4095	5.4971	-1.6946
MgO	0.5189	0.1568	0.2956	0.5403	1.1380	-0.8520	2.0249
Na ₂ O	-2.4152	-0.8746	-0.3273	3.1714	0.7420	-0.3050	-0.1603
SiO ₂	0.6931	0.2815	0.0842	-0.2943	2.1190	0.1784	2.1190
ZrO ₂	1.9028	0.9649	0.1703	1.7968	-0.8682	-0.1817	-5.6309
Others	1.3677	0.3778	0.1890	1.9268	-1.0195	-0.9949	-2.8995
CaO*Li ₂ O	201.5393	50.1129	1.1198	0.4634	0.3499	1.1718	0.3574
CaO*Na ₂ O	50.1129	20.6974	-4.5856	0.0082	0.3554	0.3773	-0.0481
Li ₂ O*Na ₂ O	1.1198	-4.5856	30.2087	0.1765	0.0588	0.0066	-0.1933
Al ₂ O ₃ /(T/1000)	0.4634	0.0082	0.1765	15.4849	-1.6952	-3.0181	1.2193
B ₂ O ₃ /(T/1000)	0.3499	0.3554	0.0588	-1.6952	15.6625	-2.7647	1.0056
CaO/(T/1000)	1.1718	0.3773	0.0066	-3.0181	-2.7647	8.7356	1.6463
Fe ₂ O ₃ /(T/1000)	0.3574	-0.0481	-0.1933	1.2193	1.0056	1.6463	12.6472
K ₂ O/(T/1000)	0.5894	0.3818	0.2320	1.5787	1.2863	0.9121	-1.0162
Li ₂ O/(T/1000)	-1.7249	-0.6838	1.0864	-6.3379	0.5343	-7.5815	2.2855
MgO/(T/1000)	0.5918	0.2186	-0.1364	-0.7893	-1.5522	1.1643	-2.7681
Na ₂ O/(T/1000)	-0.2689	-0.1685	0.2143	-4.3207	-1.0376	0.3915	0.2163
SiO ₂ /(T/1000)	-0.1292	-0.0145	-0.1106	0.4012	-2.8784	-0.2369	-2.8901
ZrO ₂ /(T/1000)	-1.0731	-0.6497	0.1608	-2.4273	1.2063	0.2440	7.6635
Others/(T/1000)	0.0733	-0.0050	-0.2950	-2.6205	1.4007	1.3737	3.9687

Table A.4. Variance-Covariance Matrix Associated with the Estimated Coefficients of Terms in the 25-Term Model (Model 2) for $\ln(\text{Electrical Conductivity, S/cm})$ of Combined WTP/ORP/LORPM LAW Glasses (continued).

Term	K ₂ O/(T/1000)	Li ₂ O/(T/1000)	MgO/(T/1000)	Na ₂ O/(T/1000)	SiO ₂ /(T/1000)	ZrO ₂ /(T/1000)	Others/(T/1000)
Al ₂ O ₃	-1.1473	4.6892	0.5398	3.1750	-0.2960	1.7917	1.9215
B ₂ O ₃	-0.9316	-0.3864	1.1334	0.7611	2.1127	-0.8789	-1.0221
CaO	-0.7365	5.6939	-0.8999	-0.2574	0.1782	-0.0788	-1.0027
Fe ₂ O ₃	0.7506	-1.7008	2.0293	-0.1668	2.1200	-5.6340	-2.9027
K ₂ O	-15.5792	-5.5412	-3.5889	-0.8693	0.8180	2.8288	3.5342
Li ₂ O	-5.5994	-59.5382	-6.5882	-13.2397	5.2292	5.5957	4.1102
MgO	-3.5807	-6.5694	-44.4824	-3.3500	2.0591	-1.5335	6.2919
Na ₂ O	-0.8905	-13.2101	-3.3584	-4.7072	1.2781	3.6524	0.9863
SiO ₂	0.8241	5.2018	2.0630	1.2740	-1.7489	1.3595	1.5352
ZrO ₂	2.8491	5.5500	-1.5210	3.6199	1.3668	-28.5098	-2.1658
Others	3.5389	4.0678	6.2989	0.9803	1.5353	-2.1694	-12.7478
CaO*Li ₂ O	0.5894	-1.7249	0.5918	-0.2689	-0.1292	-1.0731	0.0733
CaO*Na ₂ O	0.3818	-0.6838	0.2186	-0.1685	-0.0145	-0.6497	-0.0050
Li ₂ O*Na ₂ O	0.2320	1.0864	-0.1364	0.2143	-0.1106	0.1608	-0.2950
Al ₂ O ₃ /(T/1000)	1.5787	-6.3379	-0.7893	-4.3207	0.4012	-2.4273	-2.6205
B ₂ O ₃ /(T/1000)	1.2863	0.5343	-1.5522	-1.0376	-2.8784	1.2063	1.4007
CaO/(T/1000)	0.9121	-7.5815	1.1643	0.3915	-0.2369	0.2440	1.3737
Fe ₂ O ₃ /(T/1000)	-1.0162	2.2855	-2.7681	0.2163	-2.8901	7.6635	3.9687
K ₂ O/(T/1000)	21.2298	7.5409	4.8846	1.1685	-1.1196	-3.8473	-4.7937
Li ₂ O/(T/1000)	7.5409	80.9684	9.0294	17.9946	-7.0965	-7.5624	-5.5276
MgO/(T/1000)	4.8846	9.0294	60.5869	4.5872	-2.8071	2.0735	-8.5590
Na ₂ O/(T/1000)	1.1685	17.9946	4.5872	6.4131	-1.7361	-4.9323	-1.3272
SiO ₂ /(T/1000)	-1.1196	-7.0965	-2.8071	-1.7361	2.3825	-1.8618	-2.1011
ZrO ₂ /(T/1000)	-3.8473	-7.5624	2.0735	-4.9323	-1.8618	38.8057	2.9129
Others/(T/1000)	-4.7937	-5.5276	-8.5590	-1.3272	-2.1011	2.9129	17.3776

Table A.5. Variance-Covariance Matrix Associated with the Estimated Coefficients of Terms in the 27-Term Model (Model 5) for $\ln(\text{Viscosity, poise})$ of Combined WTP/ORP/LORPM LAW Glasses.

Term	Al ₂ O ₃	B ₂ O ₃	CaO	Fe ₂ O ₃	K ₂ O	Li ₂ O	MgO	Na ₂ O	P ₂ O ₅	SiO ₂	SnO ₂
Al ₂ O ₃	2.3649	-0.1624	-0.5492	0.2148	0.0144	-0.9730	-0.0489	-0.7389	0.4911	0.0238	-0.0587
B ₂ O ₃	-0.1624	4.3012	-0.1737	-0.1450	-0.1740	-0.2239	-0.1794	-0.2244	-0.1697	-0.2468	0.0234
CaO	-0.5492	-0.1737	1.2555	0.2777	0.0059	-1.0850	0.0839	0.0710	0.1854	-0.0485	0.7330
Fe ₂ O ₃	0.2148	-0.1450	0.2777	1.7702	0.0001	0.4250	-0.3371	0.0511	0.1776	-0.3398	0.8922
K ₂ O	0.0144	-0.1740	0.0059	0.0001	0.0947	0.0754	0.0254	0.0175	0.0263	0.0042	-0.0449
Li ₂ O	-0.9730	-0.2239	-1.0850	0.4250	0.0754	13.6410	0.8936	2.6013	1.0984	-0.9349	-0.6857
MgO	-0.0489	-0.1794	0.0839	-0.3371	0.0254	0.8936	8.6898	0.5494	-1.1225	-0.3777	-0.5358
Na ₂ O	-0.7389	-0.2244	0.0710	0.0511	0.0175	2.6013	0.5494	0.9413	0.2203	-0.2333	-0.1343
P ₂ O ₅	0.4911	-0.1697	0.1854	0.1776	0.0263	1.0984	-1.1225	0.2203	36.3223	-0.2603	-0.0020
SiO ₂	0.0238	-0.2468	-0.0485	-0.3398	0.0042	-0.9349	-0.3777	-0.2333	-0.2603	0.2718	-0.1096
SnO ₂	-0.0587	0.0234	0.7330	0.8922	-0.0449	-0.6857	-0.5358	-0.1343	-0.0020	-0.1096	7.8312
ZrO ₂	-0.3543	-0.2723	-0.0171	0.9461	-0.0033	-0.7901	0.2969	-0.6209	0.3229	-0.2988	-1.4852
Others	-0.1219	-0.1284	-0.1134	0.2495	-0.0086	-1.0768	-1.1979	-0.3320	-0.9056	-0.3699	0.5517
B ₂ O ₃ *B ₂ O ₃	0.8195	-22.7237	0.8776	0.8128	0.9324	1.0860	0.9261	1.1838	0.8657	1.2687	-0.0053
Li ₂ O*Li ₂ O	-1.0407	2.8446	0.9212	-0.1805	-0.7217	-24.1584	-0.2797	-0.2926	1.3355	0.0720	-0.3384
Al ₂ O ₃ *Li ₂ O	-2.0715	-2.0772	0.1940	-0.0218	0.1286	-13.0691	1.2490	0.5362	-0.0837	0.1680	-0.2660
Al ₂ O ₃ /(T/1000) ²	-4.1967	-0.0520	1.0065	-0.3790	-0.0001	2.1013	0.0835	1.3396	-0.8665	-0.0240	0.0955
CaO/(T/1000) ²	0.9978	0.0509	-2.2515	-0.4920	0.0019	1.8704	-0.1343	-0.1147	-0.3209	0.1046	-1.3306
Fe ₂ O ₃ /(T/1000) ²	-0.3788	-0.0461	-0.4881	-3.1768	-0.0010	-0.7386	0.6076	-0.0750	-0.3129	0.6283	-1.5992
Li ₂ O/(T/1000) ²	2.0957	-0.0261	1.8653	-0.7292	-0.0127	-20.8203	-1.7199	-4.6852	-2.0528	1.6772	1.2743
MgO/(T/1000) ²	0.0816	0.0301	-0.1379	0.6068	-0.0011	-1.7143	-15.6211	-0.9697	2.0255	0.6985	0.9537
Na ₂ O/(T/1000) ²	1.3346	0.0123	-0.1148	-0.0770	-0.0051	-4.6877	-0.9681	-1.6696	-0.3816	0.4421	0.2353
P ₂ O ₅ /(T/1000) ²	-0.8729	0.1273	-0.3195	-0.3205	-0.0011	-2.0759	2.0228	-0.3851	-65.6462	0.4790	-0.0238
SiO ₂ /(T/1000) ²	-0.0281	0.0045	0.1085	0.6252	0.0009	1.6670	0.7010	0.4426	0.4862	-0.4623	0.1941
ZrO ₂ /(T/1000) ²	0.6530	-0.0523	0.0532	-1.6820	0.0117	1.4277	-0.5368	1.1461	-0.5612	0.5677	2.6871
Others/(T/1000) ²	0.2275	0.0160	0.2110	-0.4428	0.0017	1.8800	2.1727	0.6014	1.6498	0.6820	-0.9853
SnO ₂ /(T/1000) ²	0.1011	-0.0605	-1.3267	-1.5975	-0.0118	1.2657	0.9480	0.2331	-0.0177	0.1996	-14.1033

Table A.5. Variance-Covariance Matrix Associated with the Estimated Coefficients of Terms in the 27-Term Model (Model 5) for $\ln(\text{Viscosity, poise})$ of Combined WTP/ORP/LORPM LAW Glasses (continued).

Term	ZrO ₂	Others	B ₂ O ₃ *B ₂ O ₃	Li ₂ O*Li ₂ O	Al ₂ O ₃ *Li ₂ O	Al ₂ O ₃ / (T/1000) ²
Al ₂ O ₃	-0.3543	-0.1219	0.8195	-1.0407	-2.0715	-4.1967
B ₂ O ₃	-0.2723	-0.1284	-22.7237	2.8446	-2.0772	-0.0520
CaO	-0.0171	-0.1134	0.8776	0.9212	0.1940	1.0065
Fe ₂ O ₃	0.9461	0.2495	0.8128	-0.1805	-0.0218	-0.3790
K ₂ O	-0.0033	-0.0086	0.9324	-0.7217	0.1286	-0.0001
Li ₂ O	-0.7901	-1.0768	1.0860	-24.1584	-13.0691	2.1013
MgO	0.2969	-1.1979	0.9261	-0.2797	1.2490	0.0835
Na ₂ O	-0.6209	-0.3320	1.1838	-0.2926	0.5362	1.3396
P ₂ O ₅	0.3229	-0.9056	0.8657	1.3355	-0.0837	-0.8665
SiO ₂	-0.2988	-0.3699	1.2687	0.0720	0.1680	-0.0240
SnO ₂	-1.4852	0.5517	-0.0053	-0.3384	-0.2660	0.0955
ZrO ₂	5.9825	0.7306	1.4918	-0.0187	0.5216	0.6473
Others	0.7306	3.9665	0.6905	0.3242	0.2959	0.2272
B ₂ O ₃ *B ₂ O ₃	1.4918	0.6905	121.6876	-16.0373	13.4223	0.2292
Li ₂ O*Li ₂ O	-0.0187	0.3242	-16.0373	411.2503	54.9661	0.1734
Al ₂ O ₃ *Li ₂ O	0.5216	0.2959	13.4223	54.9661	159.9600	-0.1215
Al ₂ O ₃ /(T/1000) ²	0.6473	0.2272	0.2292	0.1734	-0.1215	7.7803
CaO/ (T/1000) ²	0.0488	0.2099	-0.2503	-0.4658	0.2474	-1.8655
Fe ₂ O ₃ / (T/1000) ²	-1.6791	-0.4399	0.2402	0.0959	0.0643	0.7090
Li ₂ O/ (T/1000) ²	1.3786	1.8637	0.1475	-0.0319	0.3353	-3.8622
MgO/ (T/1000) ²	-0.5400	2.1725	-0.1051	-0.0387	-0.0874	-0.1639
Na ₂ O/ (T/1000) ²	1.1438	0.6027	-0.0489	-0.1950	0.1283	-2.4729
P ₂ O ₅ / (T/1000) ²	-0.5753	1.6457	-0.7207	0.6545	-0.1600	1.6155
SiO ₂ / (T/1000) ²	0.5644	0.6827	-0.0219	0.1911	-0.0170	0.0517
ZrO ₂ / (T/1000) ²	-10.7472	-1.2815	0.2414	-0.5533	-0.3095	-1.1953
Others/ (T/1000) ²	-1.2828	-7.1422	-0.1005	-0.1949	-0.1531	-0.4280
SnO ₂ / (T/1000) ²	2.6987	-0.9797	0.2941	0.1560	-0.1460	-0.1742

Table A.5. Variance-Covariance Matrix Associated with the Estimated Coefficients of Terms in the 27-Term Model (Model 5) for $\ln(\text{Viscosity, poise})$ of Combined WTP/ORP/LORPM LAW Glasses (continued).

Term	$\text{CaO}/(\text{T}/1000)^2$	$\text{Fe}_2\text{O}_3/(\text{T}/1000)^2$	$\text{Li}_2\text{O}/(\text{T}/1000)^2$	$\text{MgO}/(\text{T}/1000)^2$	$\text{Na}_2\text{O}/(\text{T}/1000)^2$
Al_2O_3	0.9978	-0.3788	2.0957	0.0816	1.3346
B_2O_3	0.0509	-0.0461	-0.0261	0.0301	0.0123
CaO	-2.2515	-0.4881	1.8653	-0.1379	-0.1148
Fe_2O_3	-0.4920	-3.1768	-0.7292	0.6068	-0.0770
K_2O	0.0019	-0.0010	-0.0127	-0.0011	-0.0051
Li_2O	1.8704	-0.7386	-20.8203	-1.7143	-4.6877
MgO	-0.1343	0.6076	-1.7199	-15.6211	-0.9681
Na_2O	-0.1147	-0.0750	-4.6852	-0.9697	-1.6696
P_2O_5	-0.3209	-0.3129	-2.0528	2.0255	-0.3816
SiO_2	0.1046	0.6283	1.6772	0.6985	0.4421
SnO_2	-1.3306	-1.5992	1.2743	0.9537	0.2353
ZrO_2	0.0488	-1.6791	1.3786	-0.5400	1.1438
Others	0.2099	-0.4399	1.8637	2.1725	0.6027
$\text{B}_2\text{O}_3 * \text{B}_2\text{O}_3$	-0.2503	0.2402	0.1475	-0.1051	-0.0489
$\text{Li}_2\text{O} * \text{Li}_2\text{O}$	-0.4658	0.0959	-0.0319	-0.0387	-0.1950
$\text{Al}_2\text{O}_3 * \text{Li}_2\text{O}$	0.2474	0.0643	0.3353	-0.0874	0.1283
$\text{Al}_2\text{O}_3/(\text{T}/1000)^2$	-1.8655	0.7090	-3.8622	-0.1639	-2.4729
$\text{CaO}/(\text{T}/1000)^2$	4.1685	0.9030	-3.4465	0.2480	0.2133
$\text{Fe}_2\text{O}_3/(\text{T}/1000)^2$	0.9030	5.8823	1.3415	-1.1073	0.1378
$\text{Li}_2\text{O}/(\text{T}/1000)^2$	-3.4465	1.3415	38.4037	3.2157	8.6474
$\text{MgO}/(\text{T}/1000)^2$	0.2480	-1.1073	3.2157	28.8839	1.7975
$\text{Na}_2\text{O}/(\text{T}/1000)^2$	0.2133	0.1378	8.6474	1.7975	3.0834
$\text{P}_2\text{O}_5/(\text{T}/1000)^2$	0.5928	0.5828	3.7757	-3.7292	0.6963
$\text{SiO}_2/(\text{T}/1000)^2$	-0.2013	-1.1560	-3.0962	-1.3024	-0.8190
$\text{ZrO}_2/(\text{T}/1000)^2$	-0.0990	3.1087	-2.5380	1.0392	-2.1145
Others/ $(\text{T}/1000)^2$	-0.3864	0.8200	-3.4088	-4.0324	-1.1017
$\text{SnO}_2/(\text{T}/1000)^2$	2.4605	2.9670	-2.3523	-1.7729	-0.4301

Table A.5. Variance-Covariance Matrix Associated with the Estimated Coefficients of Terms in the 27-Term Model (Model 5) for $\ln(\text{Viscosity, poise})$ of Combined WTP/ORP/LORPM LAW Glasses (continued).

Term	$\text{P}_2\text{O}_5/(\text{T}/1000)^2$	$\text{SiO}_2/(\text{T}/1000)^2$	$\text{ZrO}_2/(\text{T}/1000)^2$	$\text{Others}/(\text{T}/1000)^2$	$\text{SnO}_2/(\text{T}/1000)^2$
Al_2O_3	-0.8729	-0.0281	0.6530	0.2275	0.1011
B_2O_3	0.1273	0.0045	-0.0523	0.0160	-0.0605
CaO	-0.3195	0.1085	0.0532	0.2110	-1.3267
Fe_2O_3	-0.3205	0.6252	-1.6820	-0.4428	-1.5975
K_2O	-0.0011	0.0009	0.0117	0.0017	-0.0118
Li_2O	-2.0759	1.6670	1.4277	1.8800	1.2657
MgO	2.0228	0.7010	-0.5368	2.1727	0.9480
Na_2O	-0.3851	0.4426	1.1461	0.6014	0.2331
P_2O_5	-65.6462	0.4862	-0.5612	1.6498	-0.0177
SiO_2	0.4790	-0.4623	0.5677	0.6820	0.1996
SnO_2	-0.0238	0.1941	2.6871	-0.9853	-14.1033
ZrO_2	-0.5753	0.5644	-10.7472	-1.2828	2.6987
Others	1.6457	0.6827	-1.2815	-7.1422	-0.9797
$\text{B}_2\text{O}_3 * \text{B}_2\text{O}_3$	-0.7207	-0.0219	0.2414	-0.1005	0.2941
$\text{Li}_2\text{O} * \text{Li}_2\text{O}$	0.6545	0.1911	-0.5533	-0.1949	0.1560
$\text{Al}_2\text{O}_3 * \text{Li}_2\text{O}$	-0.1600	-0.0170	-0.3095	-0.1531	-0.1460
$\text{Al}_2\text{O}_3/(\text{T}/1000)^2$	1.6155	0.0517	-1.1953	-0.4280	-0.1742
$\text{CaO}/(\text{T}/1000)^2$	0.5928	-0.2013	-0.0990	-0.3864	2.4605
$\text{Fe}_2\text{O}_3/(\text{T}/1000)^2$	0.5828	-1.1560	3.1087	0.8200	2.9670
$\text{Li}_2\text{O}/(\text{T}/1000)^2$	3.7757	-3.0962	-2.5380	-3.4088	-2.3523
$\text{MgO}/(\text{T}/1000)^2$	-3.7292	-1.3024	1.0392	-4.0324	-1.7729
$\text{Na}_2\text{O}/(\text{T}/1000)^2$	0.6963	-0.8190	-2.1145	-1.1017	-0.4301
$\text{P}_2\text{O}_5/(\text{T}/1000)^2$	121.9011	-0.8949	1.0332	-3.0809	0.0231
$\text{SiO}_2/(\text{T}/1000)^2$	-0.8949	0.8547	-1.0416	-1.2659	-0.3606
$\text{ZrO}_2/(\text{T}/1000)^2$	1.0332	-1.0416	19.8946	2.3383	-4.9846
$\text{Others}/(\text{T}/1000)^2$	-3.0809	-1.2659	2.3383	13.2192	1.8201
$\text{SnO}_2/(\text{T}/1000)^2$	0.0231	-0.3606	-4.9846	1.8201	26.2184