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Final Report

Enhanced LAW Glass Property-Composition Models – Phase 2

prepared by

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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.

I.L. Pegg: _____ **Date:** 9/2/14
VSL Program Director/Principal Investigator

I. Joseph: Innocent Joseph **Date:** 9/2/14
Energy*Solutions* Sub-Contract Manager

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List of Abbreviations

AIC	Akaike Information Criterion
AICc	Corrected Akaike Information Criterion
ANL-LRM	Argonne National Laboratory – Low Activity Reference Material
ASTM	American Society for Testing and Materials
BIC	Bayesian Information Criterion
BNI	Bechtel National, Inc.
CCC	Canister Centerline Cooling
DCP-AES	Direct Current Plasma - Atomic Emission Spectroscopy
DF	Degrees of Freedom
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-activity waste (LAW) and high-level waste (HLW) 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 HLW.

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

The baseline WTP 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 to address 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.

The present report describes work to further the development of extended glass property-composition databases for WTP LAW glasses which 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 Conservations 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.

Under Phase 1 of this effort, the LAW glass property-composition data were reviewed to identify gaps in the composition space that need to be filled to develop new models to support waste processing at Hanford using the new higher waste loading ORP glass compositions [21]. The WTP baseline models were evaluated against the new data in terms of region of validity and prediction performance. The results were used to identify the composition spaces where gaps exist and need to be filled by new compositions to be tested. A statistically-designed glass composition matrix was developed to guide the selection of test glasses to fill those data gaps. A large composition matrix of 816 glass compositions was developed for this purpose. From this

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. The scope of Phase 1 of this effort supported the preparation and characterization of crucible melts of 20 glass compositions selected from this matrix; testing of these glasses was completed and the results were reported earlier [23].

During the present Phase 2 of this effort, an additional 20 glasses were selected and characterized to further fill the data gaps. A strategy similar to that employed during Phase 1 was used to select the twenty glasses for testing. Crucible melts of these 20 glass compositions were prepared and tested for the properties of interest. All of the available LAW glass property-composition data were used in the development of enhanced models that cover a larger composition space. The results of enhanced LAW property-composition model development are presented in this report.

1.2 Objectives

The objectives of this work are to develop 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 extended database and identify composition spaces in the database that need augmentation.
- Select an additional 20 glass compositions from the matrix developed in Phase 1 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.
- Develop new preliminary LAW glass property-composition 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 designed[1] 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 originally 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. Since the development of the baseline WTP LAW glass property-composition models, 12 additional glasses were prepared and subjected to VHT. Another five glasses, with vanadium oxide as a glass former additive for which viscosity and electrical conductivity data are available, were originally excluded from the WTP-LAW dataset because of the presence of vanadium. Data for these 17 glasses were added to the WTP-LAW dataset for the present modeling effort.

The ORP glass property-composition dataset that contains data from 209 glasses including two replicates (referred to as ORP-LAW glasses) nearly doubles the total number of LAW glass data available for modeling. Early 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. Recently, under the LAW property-composition model development effort, a total of 40 glasses (referred to as LORPM glasses) from a statistically designed composition matrix were prepared and characterized in order to fill data gaps in the LAW glass property-composition data. Table 2.1 provides a comparison of the number of glasses and composition regions for the WTP baseline datasets and the ORP-LAW datasets for each of the glass properties. Property data from the 40 LORPM glasses prepared and characterized during Phase 1 and Phase 2 of this work scope also are included in the 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, 23]. Compositions used in modeling were normalized to 100% with XRF measured SO_3 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,

[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.

especially at high sodium concentrations [24, 25], while vanadium oxide was added to improve sulfate incorporation [6-12, 26-33].

In the following sections, the various studies from which the two sets of glass data were generated are summarized. References to the corresponding glass development reports and/or melter test reports for the data have been provided earlier [1, 21, 23]. The property data that were collected from each set of glasses are also identified. Assessment of the LAW glass property-composition data for data gaps, development of statistically designed matrices to address the data gaps, and selection of glass compositions from this matrix for characterization are also provided in this section.

2.1 WTP- LAW Glasses

The following sections provide short descriptions of the 288 WTP-LAW 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 [1]. Target compositions and references to the corresponding test matrix development reports and/or data summary reports for all these glasses are provided in earlier reports [1, 2]. 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. Five glasses containing V_2O_5, which were earlier excluded from the dataset due to the presence of vanadium (which was not one of the baseline WTP additives), were added back to the dataset because the combined dataset (WTP-LAW and ORP-LAW) contains many glasses with vanadium as a component.

- 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 [1].

- To these were added a smaller third group of glasses derived from the LAW Correlation that employs waste composition information to determine the appropriate waste loading, glass composition, and amounts and types of glass former additives [34]. The design of these glass formulations introduced correlations in the additives because they are directly linked to Na_2O, K_2O, and SO_3 levels in any potential LAW Hanford waste; these glasses 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 276 WTP-LAW glasses in the modeling dataset [1], 161 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 [35] in terms of the molar ratios of various species to sodium. The primary source of tank waste compositional data were a BNI test specification [36], the Best Basis Inventory (2001) [37] , and subsequent revisions to the tank waste compositions (TFCOUP Rev. 2, Rev. 3 and Rev. 3A) [38-40]. 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 to perform all of the property measurements. Five glasses containing V_2O_5 (LAWB39, LAWB47, LAWB48, LAWB49, LAWC13), which were originally excluded from the dataset due to the presence of vanadium, were added back because they are within the composition region of the combined dataset (WTP-LAW and ORP-LAW).

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 ±15% variation in the blending of waste and glass former additives (A88Si+15, A88Si-15, C22Si+15 and C22Si-15) and formulations at ¼, ½, and ¾ 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 dataset available for modeling, particularly near the contractual limit of 50 g/m^2/day. For this second set, Na_2O and K_2O ranges were set beyond the upper bounds of the earlier set and increased from 22 to 23 wt% for Na_2O and 4 to 5.4 wt% for K_2O.

2.1.3 LAW Correlation and High Cr_2O_3, P_2O_5 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 (SO_4/Na). These relationships together define the LAW Correlation designed by VSL for WTP LAW [34], which uses a two-step algorithm to calculate glass compositions for a given waste stream composition. Na_2O, K_2O, and SO_3 concentrations define waste loading limits. The concentrations of the additives CaO, Li_2O, and MgO vary with this waste loading, while the other six additives are kept at fixed concentrations (Al_2O_3, B_2O_3, Fe_2O_3, TiO_2, ZnO, ZrO_2) and the SiO_2 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 LAW Correlation, but with increased Cr_2O_3 (from 0.35 to 1.4 wt%) and P_2O_5 (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 ^{90}Sr/TRU by precipitation, ultrafiltration to remove entrained solids, ion exchange to remove ^{137}Cs and ^{99}Tc, 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 [41] 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 [42] 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 [43].

- AP-101 Actual is a glass sample prepared at PNNL from an actual Tank 241-AP-101 waste sample [44] 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 [45] 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 [42] 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 [46], 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 [47] and in the small-scale crucible-type melter system, respectively [48], 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 dataset 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 high alkali LAW 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). To these were added a total of 40 statistically designed glasses (referred to as LORPM glasses) to fill composition gaps in the property-composition databases. Twenty of the LORPM glasses were prepared and characterized during Phase 1 of this modeling effort and the remaining 20 during Phase 2.

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 54 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, 26-33]. 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:

- WVW-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 preparation 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 ranges 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 regions 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 [36] and included a 2.5 % increase in sodium concentration to account for sodium additions in pretreatment [37]. The primary objective of this effort was to develop glass formulations that could accommodate higher concentrations of Na_2O. 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 the 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 therefore cover the region from 23 to 26 wt% Na_2O and 0.16 to 0.88 wt% SO_3. These formulations also include additions of chromium (up to 0.5 wt% Cr_2O_3) and tin (up to 5 wt% SnO_2) as new glass former additives, as well as higher concentrations of zirconium (up to 6 wt% ZrO_2). Moderate amounts of vanadium (less than 1 wt% V_2O_5) 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 SO_4/Na ratios may be as high as 2.11×10^{-2}. In these formulations, sodium varies from 21 to 25 wt%, while SO_3 ranges from 0.45 to 1.0 wt%. In view of the higher sulfate levels, additions of vanadium in the range of 1 to 2 wt% as V_2O_5 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% SO_3 if all of it were retained in the glass. Such glasses were prepared for 29 of 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 (i.e., similar in all constituents except SO_3) glasses, as discussed in Section 5. Only three of these samples were used in assessing %RSD on VHT since comparison is made with high sulfate content glasses produced in DM10 melter tests, as described below. The sodium content in these glasses measured by XRF was found to be within ±1.8% to ±7.1% of the original glass measurement, with no systematic trend.

Further increases in sulfate to the maximum levels expected in LAW streams (Regions E and F) were studied in the 26 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 SO_4/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 10.1 to 20.0 wt% and with the addition of lithium (up to 5 wt% Li_2O) to improve sulfate incorporation (up to 1.5 wt% SO_3). 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 SO_3), and Z10-G-153B (based on ORLF7-high SO_3).

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% Na_2O + 19.61 wt% K_2O on a waste oxide basis). Twenty nine glasses were formulated in which the waste loading was varied such that Na_2O loadings in the glasses increased from 18.5 wt% to 21.5 wt% (and K_2O from 5 to 5.75 wt%). Iron oxide was eliminated from the additives blend to make room for additional tin oxide and zirconia, with ZrO_2 + SnO_2 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 near-replicates crucible melts of the corresponding target formulations in Section 5.

2.2.3 Statistically Designed ORP-LAW Glasses (LORPM Glasses)

A total of 40 statistically designed ORP-LAW glasses (referred to as LORPM glasses) were prepared and characterized as part of the enhanced LAW glass property-composition modeling effort. Twenty of the glasses were characterized during Phase 1 of this effort and the other 20 during Phase 2. To select these glass compositions for testing, 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. The ORP glasses cover a wider composition range but tend to be less evenly distributed in composition space when compared to the WTP glasses. In addition, the ORP formulations employ glass components (vanadium and tin oxides) that were not present in the WTP-LAW glasses.

The approach used to design the new glasses was generally similar to that used in the statistical design of the WTP baseline glasses [1]. A 3-layer matrix was developed by using the Design of Experiments routines of the program JMP® (SAS Institute - Version 10.0) with the "Mixture Design" option and the "Optimal" type of mixture for each layer. 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 and MnO which was a batching impurity. 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 2.2, and "Others" listed in Table 2.3. The following additional constraints were also imposed:

$$13.92 \text{ wt\%} < (K_2O + Li_2O + Na_2O) < 27.39 \text{ wt\%}$$

and

$$42.13 \text{ wt\%} < (Al_2O_3 + SiO_2 + ZrO_2) < 58.87 \text{ wt\%},$$

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 yielded 272 compositions giving a total of 816 designed compositions. During Phase 1, 50 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 20 compositions by eliminating the compositions with total alkali (defined as ALK = wt% Na_2O + 0.66 wt% K_2O + 2 wt% Li_2O) 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 statistically designed Phase 1 glasses were designated LORPM1 to LORPM20. PCT, VHT, melt viscosity, and melt electrical conductivity data were collected on all of the 20 Phase 1 LORPM glasses.

Scatter plots of WTP-LAW glasses, ORP-LAW glasses and 20 Phase 1 LORPM glasses as functions of 15 glass components ("others" not shown) are given in Figure 2.2 where data gaps are clearly visible. The objective of the selection of second set of 20 LORPM glasses was to provide an additional step in efforts to fill those gaps and provide a combined dataset that was better suited to building extended glass property models. Using the 796 candidate compositions remaining after Phase 1 LORPM glass selection, Phase 2 glasses were selected to occupy under-populated compositions regions and aimed to support improvement of the poorest performing models, which are the PCT and VHT models based on the results from the Phase 1 work. Consequently, the preliminary ORP models from Phase 1 and the WTP baseline models were applied to the 796 remaining designed matrix compositions and their predicted properties were compared in an effort to identify compositions that might provide the greatest benefit for the extended models. Formulations yielding extremely low or excessively high PCT and VHT responses in any model were discarded, while those for which the response (PCT-B, PCT-Na or VHT) approached the contractual limit were scrutinized further. Among those, preference was given to formulations that showed the most significant differences between the responses predicted by the baseline WTP models and the corresponding Phase 1 ORP models. An iterative process was necessary because some glasses of interest for PCT models were predicted to clearly fail VHT and were therefore eliminated for the purpose of the Phase 2 LORPM glass selection. Finally, of the potential remaining glasses, those lying in under-populated compositions regions were selected based on reviews of the 2-D scatter-plots as well as selected 3-D regions. This exercise resulted in the selection of the 20 LORPM formulations listed in Table 2.4. The compositions of these 20 glasses are plotted as the red circles in Figure 2.2 and in selected 3-D plots in Figures 2.3 – 2.5. The predicted properties using the Phase 1 ORP models and the baseline WTP models are displayed in Figure 2.6 in comparison to the contractual limits for PCT and VHT.

PCT, VHT, melt viscosity, and melt electrical conductivity data were collected on all of the 20 Phase 2 LORPM glasses.

2.3 Summary of Combined LAW Glass Property-Composition Dataset

The 288 glasses in the WTP-LAW dataset include 271 glasses used in the development of the WTP LAW glass property-composition models, 5 newly added glasses containing V_2O_5 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, 266 glasses have data on PCT boron (PCT-B), PCT sodium (PCT-Na), and PCT silicon (PCT-Si) releases, 193 glasses have VHT data, many in replicates,

and 186 glasses have melt viscosity and melt electrical conductivity data, as summarized in Table 2.5. 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 249 ORP-LAW glasses, 211 have PCT data, 243 have VHT data, 159 have viscosity data, and 162 have electrical conductivity data, as summarized in Table 2.6.

In comparison to the WTP datasets on which the baseline models were developed, these additional data represent an increase of 79%, 126%, 85%, and 87% in the data available for the PCT, VHT, viscosity, and electrical conductivity models, respectively.

The statistically designed LORPM glasses complement the coverage provided by the actively designed ORP glasses. An example is provided in Figure 2.1 in terms of concentrations of Na_2O and SO_3 in the forty LORPM glasses as compared to the actively designed ORP-LAW glasses that are clustered in this composition space. As shown in Figure 2.7, the ORP-LAW data expand the compositional ranges for Al_2O_3, CaO, MgO, Na_2O, SiO_2, and ZrO_2, increase the measured SO_3 content, and introduce the new components V_2O_5 and SnO_2. Iron is generally much lower in the ORP-LAW dataset, with a median value of 0.9 wt% Fe_2O_3 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 LAW Glass Property-Composition Data from Other Sources

Property-composition data have been previously compiled for over 3400 glasses from a large number of studies of waste glasses by various organizations [49, 50]. Approximately half of those glasses, and more than half of the property data, are from previous studies performed at VSL. The data in those compilations were extracted from various publications, reports, and databases of glass properties irrespective of the quality assurance status of the data. The data were evaluated for possible use in the present work. Comparison of these data against the compositional window of the present LAW glasses resulted in excluding more than 75% of the glass compositions. This is primarily because most of the glasses are HLW glass compositions, which typically contain greater than 1 wt% of many components considered as minor components in the present LAW models (e.g., CeO_2 in CVS glasses, ThO_2 in West Valley glasses, etc.). Of the remaining 25%, more than 90% are VSL glasses that are already included in this study. The remaining additional glass compositions that were identified have PCT-Na, PCT-B, or VHT data and are listed in Table 2.7. The net result is that the only additional compositions of interest for the present LAW glass property-composition modeling effort for which data were available are those collected at PNNL [49 - 52].

The glasses listed in Table 2.7 for the most part belong to the Hanford LAW product acceptance (HLP) series with five from the in-container vitrification (ICV) series (AMP2-02, AMP2-03, AMP2-16, S22-16 and S22-26). Some of the HLP glasses were excluded from the list in Table 2.7 because their compositions were outside of the current LAW glass composition region, or their PCT releases were much higher than the WTP limit.

VHT alteration depth at 200°C and 24 days (the nominal values for the baseline WTP models) were either extracted from the literature or calculated from the published rate value and the reported glass density when available [52, 53]. If the density was not reported, an average LAW glass density of 2.65 g/cc was used. The VHT data were often extrapolated from tests with test periods other than 24 days; data from test periods that were too disparate from 24 days were excluded. Some of the VHT data relate to temperatures greater than 200°C, which were not used.

Since QA information was not available for the data extracted from the literature, these data were not used in model development or validation. Instead, an assessment of the applicability of the selected models to these datasets was made.

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 2.4.

A blender was used to mix and homogenize the starting materials before they were loaded into platinum-gold (Pt-Au) crucibles 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) [54] and Savannah River Laboratory – Environmental Assessment (SRL-EA) glass [55]. 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 20 new 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:HNO_3 was diluted to 50 ml and used for the dissolution. This procedure is similar to the ASTM Test Method C 1412-99, which also employs a mixture of concentrated HF and HNO_3 in microwave digestion of pulverized glass samples. However, supplemental use of HCl/H_3BO_3 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 SO_3, the batched (target) glass compositions are expected to be more accurate than the analyzed compositions because the batched compositions are derived from simple weighings of pure chemicals. Hence, the target compositions for all major constituents, except SO_3, 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 SO_3 is a constituent that limits waste loading in LAW glasses and has a tendency to volatilize during glass preparation, the SO_3 concentration to be used in modeling LAW glass properties was of particular interest. Analysis of crucible melts and melter discharge glass samples have shown SO_3 analyzed values to be consistently below target values due to volatilization [29]. For this reason, it was decided during WTP baseline model development that XRF analyzed SO_3 values would better represent the LAW glass composition. Accordingly, XRF measured SO_3 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 90ºC for 7 days according to ASTM C 1285 [56], in accordance with the current WTP contract requirement [35]. All tests were conducted in triplicate, in parallel with the LAW standard glass included in each test set (ANL-LRM [54]). The leachates were sampled after seven days. One milliliter of sampled leachate was mixed with 20 ml of 1 M HNO_3 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:

$$C_i = \frac{c_i}{f_i} \ , \tag{3.1}$$

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 [56]. 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

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

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 g/L = 1000 g/m^3). Specification 2.2.2.17.2 in the WTP contract [35] sets a limit of 2 g/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 g/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 the corresponding VSL procedure which conforms to ASTM C 1663. Glass specimens were cut to produce coupons about 1 x 1 x 0.18 cm using a 600 grit diamond saw blade, or polished to 600 grit finish after cutting. In either case, a 600 grit finish was achieved. Precise dimensional measurements were made of each coupon using optical scanning with image analysis for the broad, flat faces, and with digital micrometer at five locations for thickness to permit calculation of the total surface area of the coupon. Each coupon was weighed before and after the VHT on a balance having a resolution of 100 μg. Coupons were suspended with their broad, flat surfaces horizontal from inert wire supports in the pressure vessels, and enough de-ionized water was added to the vessel to saturate the volume at the test temperature of 200ºC and to allow for a non-dripping layer covering the coupon based on its measured total surface area. The pressure vessels were sealed, weighed on a high capacity balance having a resolution of 1 mg, and placed

in an oven held at 200ºC. The temperature was monitored continuously with an independent calibrated 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 and dry, the vessel was 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. If weighing indicated an acceptable test, the pressure vessel was then opened and if the coupon had not fallen from its hanger during the test, it was removed and weighed. Post-VHT coupons were placed on an optical scanner and the scanned images examined and stored for future reference. Coupons were usually mounted whole in epoxy in a standard 1-inch diameter SEM mounting cup with the broad surfaces supported vertically so that subsequent grinding and polishing would produce a representative cross-section of the reacted layer and the remaining glass for SEM examination and measurement. If it was necessary to have a portion of the coupon available for other examination (e.g., by XRD), the coupon was sectioned by dry cutting on a diamond saw and only one piece mounted for SEM examination. For consistency with existing data, the nominal test duration was 24 days.

For an average reacted layer thickness greater than 100 microns, the layer thickness (which can be uneven) was determined by measuring the remaining glass thickness at ten points throughout the cross-section of the coupon and subtracting the average remaining thickness from the original thickness of the coupon and dividing that value by 2. For average layer thicknesses less than or about equal to 100 microns, the thickness of the altered layer was measured directly at 3 points in each of 6 evenly spaced regions of the coupon using the digital caliper in the SEM software package and the resulting set of 18 measurements was averaged. For VHT coupons exhibiting sever attack, excessive cracking, or separation of the layer, measurement were made in regions in which linear advance of the modified layer could be judged to have occurred without interference of adjoining regions, thus sometimes limiting the number of measurements to less than the 18 normally made. The altered layer thickness, which given certain assumptions relates directly to the mean glass alteration rate over the test interval, was the variable used in modeling.

WTP Contract Specification 2 [35] requires that the VHT alteration rate determined from tests of seven days or longer duration be less than 50 g/m^2/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/m^2/d) is related to the measured altered layer thickness D in microns by

$$r = \rho D/t, \tag{3.3}$$

where ρ is the glass density in g/cm^3 and t is the test duration. Under this assumption, for a typical glass density of 2.65 g/cm^3, a layer thickness of 453 microns in a 24-day VHT would correspond to a mean glass alteration rate of 50 g/m^2/day.

Although in some previous VHT modeling work the test duration was included as a modeling variable [57], the VHT modeling work in this report is similar to that in the preceding reports [1, 58] 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. Note that this is not the case for many of the VHT data collected from other sources described in Section 2.4.

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 1250ºC 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 ºC [59].

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 1250ºC. 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 ºC, with the preferred range being 40-80 poise at 1150^{o}C [59].

SECTION 4.0
PREPARATION AND TESTING OF NEW LORPM GLASSES

This section describes the preparation of 20 LORPM glasses (LORPM21 thru LORPM40) 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, electrical conductivity, 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 dataset.

4.1 Preparation and Analysis of Twenty New LORPM Glasses

The target and analyzed compositions of the 20 LORPM glasses (LORPM21-40) 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 LORPM24, LORPM30, and LORPM31 SnO_2 is low (-13 %, -19% and -13% relative deviations, respectively). In three others (LORPM23, LORPM26, and LORPM29), the deviation is below but close to 10 relative percent and the deviation appears to be consistent in XRF and DCP analyses. However, in LORPM24, DCP analysis showed the measured value to be much closer to target for SnO_2.

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 less than 1 vol% in LORPM24 and LORPM29 glasses. The amount of tin oxide crystals varies from 0.1 vol% (LORPM24) to 1.5 vol% (LORPM29), and could account for the SnO_2 deficiency in the glass analysis. Optical and SEM evaluations were conducted on all LORPM glass samples to assess homogeneity. Similar tin oxide subhedral clusters were observed in LORPM23 (0.2 vol%), LORPM26 (1.3 vol%) and LORPM31 (0.6 vol%). Two of these samples, which also have the highest ZrO_2 glass concentration of 6.0 wt%, LORPM23 and LORPM31, were found to contain 1.2 and 1.4 vol%, respectively, of zirconium oxide crystals in clusters. The zirconia contents measured in these two glasses from both XRF and DCP analyses were below target but within 10 relative percent. Trace amounts of a Cr-Zn-Fe spinel (0.1 – 0.2 vol%) were observed in LORPM29 and LORPM31.

4.2 Properties of the Twenty 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 LORPM21-40 glasses. The PCT releases vary from 0.284 g/L (0.142 g/m^2) to 7.690 g/L (3.845 g/m^2) for

PCT-B, 0.336 g/L (0.168 g/m^2) to 4.248 g/L (2.174 g/m^2) for PCT-Na, and 0.125 g/L (0.063 g/m^2) to 0.997 g/L (0.499 g/m^2) for PCT-Si. The normalized PCT mass loss for Si remains well below the PCT contract limit of 2 g/m^2 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 for PCT release was exceeded only for glass LORPM28R1, which was tested in duplicate. This glass was designed at the highest B_2O_3 (13.73 wt%) and Li_2O (5 wt%) concentrations combined with lowest concentrations of Al_2O_3 (3.5 wt%), CaO, and MgO (both zero). As a result, lithium and boron showed similarly high PCT releases (3.0 g/m^2 lithium and 3.8 g/m^2 boron for the average of two replicates, which were in close agreement), and much higher PCT releases than sodium (2.2 g/m^2 on average). Calcium and magnesium are constituents of particular importance as they can play important roles in the development of alteration layers formed during PCT or VHT testing of nuclear waste glass. Formulations such as LORPM28R1 provide the opportunity to identify leaching model coefficients of importance involving alkalis, alkaline earths, and B_2O_3. Similar behavior is observed for LORPM39 in which B_2O_3 and Li_2O concentrations are 12.18 wt% and 4 wt%, respectively, along with concentrations of Al_2O_3, CaO, and MgO of 5.57 wt%, 2.45 wt%, and 1.00 wt%, respectively. All other LORPM glasses show relatively low leach rates with the observed sodium and boron releases generally congruent, as can be seen in Figure 4.3. The data are well distributed between values of 0.1 and 1.0 g/m^2. A high PCT-Na value that remains well within the WTP contract limit [35], but for which sodium leaching greatly exceeds that of boron (0.70 versus 0.18 g/m^2), is evident for glass sample LORPM22. This is not unusual for glasses of high sodium content with associated low alumina and silica levels; this is the highest sodium glass in the current set (21.7 wt% Na_2O) while Al_2O_3 (3.5 wt%) and SiO_2 (35 wt%) are at their respective lower limits.

The PCT leachate pH values for the 20 new LORPM glasses range from 9.9 (LORPM31) to 11.8 (LORPM39). This compares well with the range of pH values from previous sets ranging from 9 to 12.5. 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 actively designed ORP-LAW glasses, the first 20 LORPM glasses (LORPM1-20), and the new 20 LORPM glasses (LORPM21-40). 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, which was specifically investigated in one 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 behavior of the LORPM21-40 glasses. Nonetheless, LORPM28R1 with high concentrations of B_2O_3 and Li_2O and no MgO or CaO, has a pH value that is

noticeably above the trend for the LORPM glasses, indicating a possible model outlier (discussed in Section 5). It is possible that, in this case, PCT leachate concentrations are driven by the growth of aluminosilicate secondary phases in which lithium is the primary component involved in charge compensation.

PCT boron and sodium releases for the LORPM glasses are compared to the corresponding results for the WTP-LAW and ORP-LAW 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 Na_2O + $0.6K_2O$+ $2Li_2O$, 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 primary contributors in the inter-diffusion during the first stage of leaching. In this stage (Stage I)[2], 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. All new glasses follow the expected trend of PCT releases on the basis of alkali content (Figure 4.5). Glasses LORPM28R1 (in duplicate) and LORPM39, noted in the figure, have the highest alkali concentrations for glasses in the LORPM21-40 set.

4.2.2 Vapor Hydration Test

The VHT alteration depths (in μm) and alteration rates (in $g/m^2/d$) are given in Table 4.3 for the 20 new LORPM glasses (LORPM21-40). The VHT alteration depths and rates for the LORPM21-40 glasses vary from 1.4 to 550 μm (0.2 to 60.8 g/m^2/day). None of the data from the tests in this series had to be excluded since the alteration depth at the end of the 24-day test period, even when large, never exceeded the thickness of the coupon itself. While measuring alteration layers under SEM, frequent observations were noted of large re-deposited crystals of Na-aluminosilicates (likely analcime) or Na-K-aluminosilicate (possibly zeolite) on top of sodium-depleted alteration layers. This layer is also enriched in tin oxide. Behind the outer layer, multiple occurrences of another inner layer containing Zn-silicate (in LORPM25, LORPM29), Zn-Fe-Ca silicate (LORPM26), or enriched in Zn and Fe (LORPM39) were also observed.

[2] We are using here the stages as described by Frugier *et. al.* (*J. Nucl. Materials*, 380, 8-21, 2008), and multiple others, because this more recent nomenclature does not ignore the important ion exchange / interdiffusion stage. However, we note that there is some inconsistency in the published record as some others combine Stages I and II under "forward rate Stage I".

Spherical Zn-silicate re-deposited crystals were also observed in LORPM25, LORPM34, LORPM37, and LORPM40.

As was previously demonstrated for WTP-LAW and ORP-LAW glasses, finding general trends for VHT alteration rate as a function of glass composition is more challenging than with PCT data. This is in part due to the fact that VHT is designed to assess a late-stage feature of the complex alteration process, which also involves a period of incubation.

Figure 4.6 shows the VHT alteration rates as a function of the alkali oxide concentration for the 20 new LORPM glasses (LORPM21-40), along with data for the previous 203 ORP-LAW glasses [21], the 171 WTP-LAW glasses [1], and the 20 LORPM glasses (LORPM1-20) from Phase 1 of this work [23]. The WTP baseline model for VHT was based on the data from the 171 WTP-LAW glasses. As was discussed in past model analyses [2, 21, 23], 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; LORPM26 is a good example of this type of glass, which shows a low VHT alteration even in the absence of zirconia. There are, however, a few glasses falling out of the general trend among the latest LORPM set: glasses LORPM31 and LORPM32. No particular component combinations can be readily identified as a reason for this behavior.

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 LORPM21-40 glass. The electrical conductivity versus temperature values are given in Table 4.4 for the 20 new LORPM21-40 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 between 0.1 to 0.7 S/cm in the temperature range of 1100 to 1200ºC [59]. Among the measurements taken in this temperature range, electrical conductivity values were acceptable for all glasses, ranging from 0.139 at 1160°C for LORPM26 to 0.697 S/cm at 1164°C for LORPM39.

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 nineteen of the twenty LORPM21-40 glasses. Measurements on glass sample LORPM31 revealed non-Newtonian behavior at all four measurement temperatures and high torque values indicative of crystallization (probably ZrO_2 crystals, as described above in Section 4.1). This

glass was, therefore, excluded from the dataset for viscosity modeling. Each row of Table 4.5 provides the viscosity data for a given glass at up to four temperatures. There are four columns of data for each glass corresponding to the four temperatures at which viscosity data were measured. Measurements on glasses LORPM23, LORPM24, LORPM26, LORPM29, and LORPM30 could not be performed at all four temperatures as non-Newtonian behavior was observed at the lower temperatures. These are all glasses with high concentrations of tin and zirconium oxides and the small amounts of crystallization observed in the as-melted samples (Section 4.1) are likely to increase as temperature is decreased during viscosity measurement. Only stable measurements at the highest temperature were used in model development. Apart from these exceptions, all glasses in the LORPM21-40 series had viscosities within the recommended WTP limits of 10 to 150 poise at 1100ºC [59].

Figures 4.7 and 4.8 show the distribution of temperature values at which electrical conductivity and viscosity were measured for each LORPM21-40 glass melt, respectively. The figures show that the measurements were taken at temperatures close to the four nominal values of 950, 1050, 1150, and 1250ºC.

SECTION 5.0
LAW GLASS DATASET 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. 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 presented in Phase 1 of this work [23], with the combined dataset described in the following sections.

In total, there are now 537 LAW glasses with data for at least one of the five properties (PCT-Na, PCT-B, VHT, melt viscosity and melt electrical conductivity), as well as many replicates, as discussed below. More than half of these glasses (300) 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.

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).

From these can be calculated the Residual Sum of Squares (RSS) = $\sum_{i=1}^{n}(\hat{y}_i - y_i)^2$, which would equal zero if the model was perfect, i.e, for all n data points, the predicted property value coincides perfectly with the measured value.

This can be compared to the total variability in the regression model, or Total Sum of Squares (TSS) expressed as the sum of the squared difference between each measured property value y_i and the average $\bar{y}$.

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:

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

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:

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

Generally, the R^2 statistics take values between 0 and 1. Negative values of R^2 estimated on the validation set or $R^2_{Adjusted}$ 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 standard deviation associated with melting glasses and measuring the property values

which are being modeled. *RMSE* is therefore expected to be comparable to the measured glass preparation and property measurement standard deviation assessed from replicates testing. The statistic *RMSE* is included as a standard output in the JMP software used in modeling, and is given by:

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

where p is omitted when estimating $RMSE_{Validation}$ on a validation dataset of n_v data points (i.e., no adjustment for the degrees of freedom).

A simple measure of the ability of the model to predict the property is based on the Predictive Error Sum of Squares (*PRESS*), which is the sum of squared differences between the measured and the predicted property values; $\hat{y}_{(i)}$, the predicted property value, is estimated when y_i is left out of the modeling dataset. It is defined as:

$$PRESS = \sum_{i=1}^{n}(\hat{y}_{(i)p} - y_i)^2 \tag{5.4}$$

The residual value of each predicted/measured row is computed by a matrix-vector formula in the modeling software JMP®, which is equivalent to dropping that row from the computations. *Press RMSE* helps in comparing the performance of multiple models and is given by:

$$PressRMSE = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_{(i)p} - y_i)^2}{n-1}} \tag{5.5}$$

Models with lower *Press RMSE* are favored.

An equivalent parameter to R^2 in terms of model performance is defined using the *PRESS* quantity instead of *RSS;* this cross-validated R^2 will be termed $R^2_{Predict}$ in our discussions and summary tables and is given by:

$$R^2_{\mathrm{Pr}edict} = 1 - \frac{PRESS}{TSS} = 1 - \frac{\sum_{i=1}^{n}(\hat{y}_{(i)p} - y_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \tag{5.6}$$

Optimal prediction yields $R^2_{Predict}$ closest to 1 but a poor predictive model can also yield negative values of $R^2_{Predict}$ when *PRESS* is greater than *TSS*, which occurs when the one-at-a-time (PRESS) validation dataset performs worse than the mean response of the modeling dataset.

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:

$$F = \frac{(\text{SSE} - \text{SSPE})/(n - p - f)}{\text{SSPE}/f} = \frac{\left[\left(\sum_{i=1}^{n}(\hat{y}_i - y_i)^2 - \sum_{k=1}^{K}\sum_{j=1}^{m_k}(y_{kj} - \bar{y}_k)^2\right)\Big/(n-p-f)\right]}{\left.\sum_{k=1}^{K}\sum_{j=1}^{m_k}(y_{kj} - \bar{y}_k)^2\right/f} \tag{5.7}$$

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 squares 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, $k = 1, 2, \ldots, K$.

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 537 LAW glasses collected and discussed in Sections 2 and 4 above, 477 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), and a replicate of LORPM28R1, the full PCT model dataset has 481 sets of PCT data. For *every one* of these 477 glasses, the normalized PCT mass loss for Si is below the PCT contract limit of 2 g/m^2. In fact, the Si mass loss only exceeds 1 g/m^2 (half the limit) in the PCT leachates of the statistically designed WTP-LAW glasses LAWM12 and LAWM55 [60], reported as 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 477 LAW glasses are less than the contract limit of 2 g/m^2 (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 477 LAW glasses with PCT results, 28 glasses have PCT-B releases greater than 2 g/m^2 and 21 have PCT-Na releases greater than 2 g/m^2. 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 Cr_2O_3 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 Phase 1 glasses LORPM8R1 and LORPM13, which showed about 2 vol% crystallization were individually evaluated as possible outliers [23]. The outlier diagnostics (using Grubbs' test[3]), also identified as outliers five statistically designed WTP-LAW glasses, two high sodium and potassium ORP-LAW glasses for which the PCT-Na release is greater than 8 g/L, and LORPM13, all of which are listed in Table 5.7. No outliers were identified in the current set of statistically designed glasses, LORPM21 to LORPM40.

5.1.3 PCT Validation Set Selection

Model validation was accomplished during the WTP baseline model development by data-splitting[4], data-partitioning[5], 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 now doubled in size, a validation set of 27 samples was reserved during Phase 1 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 27 validation glasses was considered to be a reasonable compromise between sufficiency for validation and not unduly reducing the size of the modeling dataset. A list of the validation glasses is provided in Table 5.8. The glasses with their normalized releases for boron and sodium are listed in Table 5.8 in the order of increasing PCT-Na release. As was done in Phase 1, the same validation dataset was used for both PCT models.

5.1.4 PCT Replicates

Table 5.9 lists 28 sets of replicate and near-replicate glasses and the corresponding PCT-B and PCT-Na normalized releases; 12 are from the WTP-LAW dataset and 16 are from the ORP-LAW dataset. Table 5.9 also lists estimates of percent relative standard deviations (%RSDs) for each replicate set, as well as pooled estimates over all of the replicate sets. Note that the replicate dataset now includes one more duplicate testing of statistically designed glass LORPM28R1. 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

[3] Grubbs' test is a statistical test used to detect outliers in a data set assuming residuals after fitting are normally distributed. 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.

[4] In the data-splitting approach, the modeling dataset was split into five sets of modeling and validation subsets, using roughly 80% of the data for modeling and 20% for validation.

[5] In the data partition approach, the modeling datasets were partitioned into a modeling dataset (comprised of the WTP statistically designed glasses) and a validation subset (comprised of all remaining glasses, most or all of which were actively designed).

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 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 17.54% and 17.56% for ORP-LAW glasses). The overall %RSD therefore changes very little over the 28 replicates sets, for a final %RSD of 20.29 and 17.88% for boron and sodium normalized releases, respectively. These uncertainties for measurements conducted over a period of about 15 years 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 consistency over time and 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 PCT Model Development

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], 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 with the two sets of LORPM glasses added to the model dataset. The LORPM glasses identified in Figure 5.2 highlight the limitations of the WTP baseline models over the composition range covered by the ORP-LAW glasses, particularly for the statistically designed LORPM 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]. During Phase 1 of this work [23], the modeling effort made use of the partial quadratic mixture (PQM) model selected as the WTP baseline model [1, 61] as the starting point for further development of regression models with incremental improvement in the model statistics. During the present Phase 2 of model development, however, the model terms were entirely reevaluated. First, a subset of 111 PCT data from statistically designed WTP-LAW and ORP-LAW glasses were considered separately in an effort to identify essential compositional contributions without any potential bias inherent in the actively designed formulations in which component correlations are necessarily present [1]. Then, the full modeling dataset was fit to a first-order model (no cross nor square terms) in order to identify which components are significant, followed by stepwise optimization of the model quadratic

components using different stopping rules, including maximum R^2 using k-fold[6] validation or *p*-value threshold to identify any significant compositional interaction effects. These were defined using JMP® Response Surface methodology[7] with the full dataset of 436 PCT values in the modeling dataset (both RS and MRS were tested).

Results of model development for PCT-Na and PCT-B releases are given in Tables 5.10 and 5.12, respectively. Highlights of the cross-terms optimization process using the regression coefficient *p*-values are provided in Tables 5.11 and 5.13 for PCT-Na and PCT-B models, respectively.

In Phase 1 of this work, preliminary models were explored using parallel strategies for PCT-Na and PCT-B releases; these were based on progressive improvement of the model performance, using the JMP® Response Surface methodology to identify any significant compositional interaction effects not detected in the WTP dataset. The stepwise statistical method permitted selection of the significant terms based on the *p*-values calculated in *t*-tests (limit of significance level used was *p*-value < 0.0025)[8].

In the present Phase 2 work, the modeling parameters were identified anew, fitting successively the 111 statistically designed, and the full set of 436 PCT values to a first-order model (no quadratic terms) in order to identify which components are most significant among the following 18 components for which the maximum value in the compositional range exceeded 1.2 wt%: Al_2O_3, B_2O_3, CaO, Cr_2O_3, Fe_2O_3, K_2O, Li_2O, MgO, Na_2O, P_2O_5, SiO_2, SnO_2, SO_3, TiO_2, V_2O_5, ZnO, ZrO_2, and Others. Components that we determined to be of least significance (using the evaluation process described in Appendix A) were then included in "Others." Other iterations were explored comparing both RS and MRS methods to identify the significant second-order terms, which were selected by stepwise regression and "stopping rules" based on a *p*-value threshold or "Max R^2 *k*-fold" using a 5-fold cross-validation model. Not all iterations of the PCT-Na models that were explored are included in the summary Table 5.10, which provides

[6] In k-fold validation, JMP divides the original data into k subsets. In turn, each of the subsets is used to validate the model fit on the rest of the data, fitting a total of k models. The model giving the best validation statistic is chosen as the final model. In the following five models, k=5.

[7] 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*X_1), but includes all cross terms (such as X_1*X_2). The Response Surface (RS) is different from MRS only by including all square terms (X_1*X_1).

[8] The *t-test* was used in a stepwise regression process to identify necessary cross-terms in a model while linear terms were selected on the basis of their confidence interval (see Appendix A). The mixed direction (alternating forward and backward steps) approach was selected. 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 cross-term coefficient is significantly different from zero, and that the corresponding model cross-term is needed. To avoid running models with too many potentially unnecessary terms, JMP evaluates *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.

the major improvements identified as the dataset increased. Some of the intermediate model parameters and their associated *p*-values are listed in Table 5.11 to support the discussion.

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

- Model 1 is the WTP baseline model (a 17-term Reduced PQM model) that is presented here for comparison.

- Model 2 is the preliminary model recommended at the end of Phase 1 (18-term PQM) [23]. During the development of this model a number of data points were identified as outliers and were dropped from the dataset. First, five glasses with MgO concentrations higher than 5.1 wt% were dropped as compositional outliers. PCT-Na releases of these glasses (ORPLA28, ORPLA29, ORPLA31, ORPLA32, and LAWA65) always exceeded 8 g/L. The four high chromium glasses that crystallized after CCC heat treatment (LAWE3Cr2CCC, LAWE9HCr1CCC, LAWE9HCr2CCC, and LAWE10HCr3CCC), also were identified as outliers during the WTP baseline model [1] and the Phase 1 model [23] development work. Grubbs' test further identified seven glasses as outliers, all with PCT-Na releases greater than 8 g/L (LAWM12, LAWM17, LAWM35, LAWM55, LAWM56, ORPLG13, and ORPLG15). The possible addition of SnO_2 and V_2O_5 as main model terms were considered during Phase 1 model development work. 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. With SnO_2 as a significant model coefficient, LORPM13 (a Phase 1 glass in which some SnO_2 was partially undissolved or recrystallized) was also flagged as an outlier in Grubbs'test; it was therefore eliminated from the dataset. The coefficients of this model are given in Table 5.10.

- Model 3 was developed in two steps. First, the data were fitted to a full linear model to determine the components that are significant (Model 3A in Table 5.11). Various reduced models were then compared against the full model to evaluate the significance of model terms using the process described in Appendix A. Second, a stepwise model optimization with "Max R^2 *k*-fold" stopping rule was performed to identify the cross-terms of significance. Refining the model using the RS and MRS methods with 5-fold cross-validation technique presents a choice between a two PQM models, a 32-term (Model 3) and a 36-term (Model 3B). The 32-term PQM model yields slightly better model statistics and lack-of-fit; it is also favored as it is less prone to overfitting. This model has 13 main component coefficients, 17 cross terms, and 2 square terms (for Al_2O_3 and TiO_2). These bring the most improvement in the model statistics with R^2, $R^2_{Adjusted}$, and $R^2_{Predict}$ of 0.878, 0.868, and 0.857, respectively, as well as some improvement in validation statistics. The RMSE is almost identical to the value for the Phase 1 model (Model 2 in Table 5.11).

- Model 4 results from refinement of Model 3 using the mixture response surface method (MRS) cross-term construct followed by mixed direction stepwise regression in which all

cross-term combinations are tested against a *p*-value of 0.01. This resulted in dropping the terms Al_2O_3*B_2O_3, Al_2O_3*SiO_2, B_2O_3*CaO, B_2O_3*Li_2O, MgO*P_2O_5, Na_2O*TiO_2, P_2O_5*TiO_2, and $(TiO_2)^2$. The resulting 24-term PQM model has 11 cross terms and the square term $(Al_2O_3)^2$ in addition to the 13 main component coefficients. It offers a slightly decreased but still very good set of model statistics of R^2, $R^2_{Adjusted}$, and $R^2_{Predict}$ of 0.866, 0.858, and 0.849, respectively. Lack of fit dropped from 0.027 to 0.015, indicating a slightly inferior model but validation statistics for the 27 glasses improved.

Of the two PCT-Na models developed during the present Phase 2 work (Models 3 and 4 in Table 5.10), Model 3 (32-term PQM) shows the best regression statistics. However, Model 4 (24-term PQM) has eight fewer terms and shows somewhat better validation statistics, and is the recommended model for PCT-Na. Figure 5.3 displays the predicted versus measured plot for Model 4 and shows a tight distribution of points around the 45º line for the 231 WTP-LAW, 205 ORP-LAW, and 27 validation data points.

Strategies similar to those used in the development of the PCT-Na models were used in the development of the PCT-B models. A summary of the PCT-B models is provided in Table 5.12 and described below.

- Model 1 is the WTP baseline model [1](17-term PQM) that is presented here for comparison.

- Model 2 is the 22-term PQM preliminary model recommended at the end of Phase 1 work, which includes SnO_2 as a component and nine quadratic terms (Al_2O_3×K_2O, B_2O_3×Li_2O, B_2O_3×K_2O, CaO×Fe_2O_3, CaO×SnO_2, CaO×ZrO_2, K_2O×SiO_2, Li_2O×SiO_2, and K_2O×SnO_2). This model returned similar or better model statistics than the WTP baseline model (R^2, $R^2_{Adjusted}$, and $R^2_{Predict}$ of 0.865, 0.858, and 0.844, respectively), which are also comparable to the PCT-Na model statistics.

- Model 3 was developed from a larger dataset of 436 PCT-B data using a two-step process as was done for the PCT-Na model. First, a linear model fit (Model 3A in Table 5.13) was used to identify components of significance starting with the 18 components for which the maximum value exceeds 1.2 wt%: Al_2O_3, B_2O_3, CaO, Cr_2O_3, Fe_2O_3, K_2O, Li_2O, MgO, Na_2O, P_2O_5, SiO_2, SnO_2, SO_3, TiO_2, V_2O_5, ZnO, ZrO_2, and Others. Using the approach described in Appendix A, Cr_2O_3, SO_3, V_2O_5, and ZnO were eliminated as not significant. Second, a 5-fold cross-term stepwise optimization with "Max R^2 *k*-fold" as the stopping rule was performed to identify the cross-terms of significance among the 14 remaining components. Successive application of the RS and MRS cross-term construct methods with subsequent 5-fold cross-validation stepwise analysis narrowed the choices to a 56-term (Model 3B in Table 5.13) or a 37-term PQM model (Model 3 in Table 5.13). Model 3 has 14 main component coefficients along with 23 cross terms, and the model statistics (R^2, $R^2_{Adjusted}$, and $R^2_{Predict}$ of 0.885, 0.875, and 0.853, respectively), as well as the validation statistics ($R^2_{validation}$ = 0.825) are very good. The lack of fit value (0.022) would indicate additional terms for improvement. Model 3B, shown in Table 5.13, with

56 terms gives 0.113 lack-of-fit, but some of the *p*-values for the model terms show very low significance (e.g., $MgO \times ZrO_2$ with *p*-value of 0.919).

- Models 4, 5, and 6 result from a down-selection of quadratic terms from Model 3 by the MRS construct approach using mixed direction stepwise regression in which all cross-term combinations are tested against set *p*-values of 0.025, 0.01, and 0.005, respectively. This was done after attempting manual selection based on expectations from knowledge of glass leaching mechanisms, which did not provide much improvement in the model statistics and sometimes even led to much higher number of terms with no improvement in model statistics. Screening at the *p*-value of 0.025 removed the terms $Al_2O_3 \times Fe_2O_3$, $Al_2O_3 \times SnO_2$, $CaO \times TiO_2$, $CaO \times ZrO_2$, $Fe_2O_3 \times TiO_2$, and $Na_2O \times SiO_2$, eliminating both TiO_2 cross-terms. In terms of modeling statistics (R^2, $R^2_{Adjusted}$, and $R^2_{Predict}$ of 0.874, 0.865, and 0.848, respectively, and lack of fit of 0.012), the 31-term PCT-B model (Model 4 in Table 5.12) performs similarly to the recommended 24-term PCT-Na model (Model 4 in Table 5.10). Further reducing the *p*-value to 0.01 as was done with the PCT-Na model reduces the model terms to 30, removing only the term, $CaO \times P_2O_5$. The model statistics were not affected greatly except for the validation R^2, which decreased from 0.813 to 0.748. Further reduction to a 26-term PQM model is achieved when the *p*-value is set to 0.005. Eliminating $Al_2O_3 \times$Others, $Li_2O \times SnO_2$, $SiO_2 \times$Others, and $SiO_2 \times P_2O_5$ in this model yields statistics that are as high as those for the recommended WTP model and the Phase 1 model (R^2, $R^2_{Adjusted}$, and $R^2_{Predict}$ of 0.862, 0.853, and 0.838, respectively). Note that in this case, R^2 on the validation dataset improves to 0.797 and RMSE (0.18) compares well with the replicates standard deviation (18% RSD).

Among the PCT-B models evaluated during Phase 2, the 37-term (Model 3) or 31-term (Model 4) models show the best combination of regression statistics, but does not permit calculation of RMSE because the validation data set contains fewer data points than the model terms. Down-selection to the 26-term Model 6 offers a practical combination of number of cross terms and good regression and validation statistics. Figure 5.4 shows a predicted versus measured plot resulting from this model. A tight distribution of points around the 45º line is seen for both the WTP-LAW and the ORP-LAW datasets. A very slight under-prediction is observed for PCT-B releases near and above the limit of 4 g/L, although this bias remains smaller than was observed for the WTP models.

The variance/covariance matrices for the recommended PCT-Na model (Model 4) and PCT-B model (Model 6) are provided in Appendix B.

5.1.6 Evaluation of PCT Data from Other Sources

As described in Section 2.4, even though more than 3400 glass property data from other sources were considered, only forty three HLP glasses [49 - 52] with PCT measurements and compositions within the current compositional domain were identified for evaluation with the presently selected LAW models for PCT-B and PCT-Na. Applying the PCT-Na model to this

dataset returned an R^2 value of 0.164 and an RMSE of 0.527. Similarly, the PCT-B model returned an R^2 of 0.207 and an RMSE of 0.628. The PCT release values predicted by the model are on average ~75% of the measured value, with the bias increasing with increasing measured PCT release values (Figure 5.5).

Since the HLP glass PCT data from PNNL exhibited a significant bias in the predicted versus measured values, further evaluation was performed to see whether any bias is present in other PCT data from sources other than VSL. As part of the glass development effort for WTP under the BNI contract, seven glass formulations were prepared and subjected to PCT at VSL and at PNNL or Savannah River National Laboratory (SRNL). In these tests, simulant melts were prepared and subjected to PCT at the VSL, whereas samples with the same composition, but with actual waste from the Hanford tanks were prepared and subjected to PCT at PNNL or SRNL. The data presented in Table 5.14 and plotted in Figure 5.6 do not show any bias in the PCT data collected at VSL as compared to the data collected at PNNL and SRNL. A previous review of these data [43] also did not identify any significant differences in the PCT results from VSL, PNNL, and SRNL. The PCT round-robin tests with an LAW glass [54], which included VSL among multiple other laboratories, also did not show any bias in the VSL PCT data as compared to other laboratories. In another study with HLW glasses, 46 replicate pairs of PCT data were collected at VSL and SRNL [62]. Analysis of the data showed very good agreement between the data collected at VSL and SRNL with no bias or any other systematic differences in the measured PCT values. The data analysis showed %RSD values of 7.6% and 5.2% for PCT-B and PCT-Na respectively, pooled over 46 pairs. This is well within the %RSD values of 27% and 21% for PCT-B and PCT-Na, respectively obtained from PCT round-robin with the ANL-LRM glass [54]. Based on the above analysis, and given that only HLP glasses that are within the composition region were used in the present evaluation, it is clear that the bias observed with the HLP glass PCT data is an issue that is specific to the HLP glass dataset, and is not related to any systematic differences in the glass preparation or PCT procedures employed at VSL, PNNL, and SRNL.

A thorough examination of the source data and a review of the glass preparation and PCT measurement procedures employed in the collection of the HLP glass PCT data would be necessary to identify the cause(s) of the bias in the PNNL HLP data. Until such an analysis is performed, it is recommended that those data should not be used for modeling purposes.

5.2 VHT Modeling

The VHT data used in model development are described in Section 5.2.1. The composition region covered by the model and identification of outliers are discussed in Section 5.2.2; 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 results from VHT model development are presented and discussed in Section 5.2.5.

5.2.1 VHT Dataset

Of the 537 LAW glasses discussed in Sections 2 and 4 above, 436 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, 436 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 μm (0.006 g/m^2/day), to greater than 1200 μm (133 g/m^2/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 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, 114 glasses have VHT alteration rates above the 50 g/m^2/d limit [35], 94 from the ORP-LAW dataset, and 20 from the WTP-LAW dataset. The 114 glasses with VHT alteration rates above the 50 g/m^2/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. However, 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 discussed below, in Section 5.2.5.

The overall compositional region considered at the onset of the current model development work was kept as broad as possible, encompassing both the 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 5.15 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, Fe_2O_3, 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. None were later flagged as outliers and all were kept in the model dataset. Conversely, Phase-1 glass LORPM13, which crystallized and was identified as an outlier, was not included in the model dataset. Table 5.16 lists the 38 glasses for which VHT alteration exceeded the sample thickness (32 ORP-LAW + 6 WTP-LAW).

With the exclusion of all outliers, including LORPM13, the final dataset for modeling contains 404 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 were then limited to 165 VHT test results and therefore reducing the modeling dataset 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 404 results within measurable range allowed reserving samples for independent validation of the new VHT models. To select the validation dataset during Phase 1 of the work, 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. Neither statistically designed glasses nor any of the replicates were pulled from the modeling dataset. The recent addition of data for the new LORPM glasses does not change the selection because the LORPM glass compositions were statistically designed. The selected validation glasses are listed in Table 5.17.

5.2.4 VHT Replicates

Table 5.18 lists 30 sets of replicate and near-replicate LAW glasses, 15 each from the WTP-LAW and the ORP-LAW VHT datasets. The table also lists estimates of %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 5.18 (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), shows larger variation (47.29% RSD) but the %RSD is lower for the three true replicates (24.04% RSD).

As shown in Table 5.18, 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 VHT Model Development

The Phase 2 VHT model development was performed using 377 VHT data in the modeling dataset and 27 in the validation dataset. The recommended baseline WTP LAW VHT model [1] predicts VHT alteration depths reasonably well (R^2 of 0.74) near and above the WTP contract limit when applied to the WTP-LAW VHT data. However, a marked decrease in R^2 was observed (R^2 of 0.35 for ORP-LAW VHT data) when the model was applied to the ORP-LAW dataset [21]. 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. The addition of new glass formers such as SnO_2 is another important reason. A similar result was observed for the VHT data on the two sets of LORPM glasses. The Phase 1 and Phase 2 sets of LORPM glasses, shown in Figure 5.7, 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.

Development of the Phase 2 VHT models 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*. In Phase 1, model development 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.

The present Phase 2 VHT model development started with assessment of significant components from the linear mixture model followed by identification of relevant quadratic and square terms. The results of VHT model development are summarized in Table 5.19, 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 (20-term PQM) is the recommended Phase 1 model. In comparison to the WTP model, the regression and validation statistics were all better with this model.

- Model 3 (22-term PQM) was developed during Phase 2 of the work as described below. First, a linear model of the eighteen main components with a maximum concentration (in at least one glass) of 1.2 wt% or greater (Al_2O_3, B_2O_3, CaO, Cr_2O_3, Fe_2O_3, K_2O, Li_2O, MgO, Na_2O, P_2O_5, SiO_2, SnO_2, SO_3, TiO_2, V_2O_5, ZnO, ZrO_2, and Others) was fitted. This model returned poor statistics but its primary purpose was to identify the components of little significance. The resulting evaluation (see Appendix A) eliminated the model terms for V_2O_5, SO_3, MgO, Cr_2O_3, and ZnO. The model developed from the 11 main constituents plus "Others" and cross terms identified using the RS cross-term construct method to fit the 377 VHT data is presented as Model 3 in Table 5.19. An improvement is observed in the regression statistics (R^2, $R^2_{Adjusted}$, and $R^2_{Predict}$ of 0.770, 0.757, and 0.739, respectively) in comparison to the Phase 1 recommended model for which the

statistics became worse when applied to the current modeling dataset; the validation statistics remain good.

- Model 4 (23-term PQM) re-introduces ZnO as a linear coefficient because zinc was observed in many SEM evaluations of the hydration layers after alteration of the LORPM glasses (see discussion in Section 4.2.2). No change was made to the cross-terms. The resulting model statistics show a minor increase in R^2 but a noticeable decrease in validation R^2.

- Model 5, also with ZnO, is the result of using the RS cross-term construct methods with subsequent 5-fold cross-validation stepwise analysis with "Max R^2 *k*-fold" as the stopping rule for cross-term selection. The modest improvement in prediction statistics does not seem to justify adding the 6 quadratic terms $(Al_2O_3)^2$, $B_2O_3 \times CaO$, $CaO \times SnO_2$, $Fe_2O_3 \times K_2O$,$K_2O \times ZrO_2$,$Li_2O \times SiO_2$. The 23% RSD among true replicates and 40% RSD among near replicates in VHT hardly justify the addition of so many model terms for the observed improvement in model predictions.

Despite the significantly extended composition region in the dataset, several of the models explored in Phase 2 show as good or better predictive performance than does the WTP baseline VHT model over the smaller composition region on which it was built. Among the currently developed models, Model 3, the 22-term PQM VHT model is recommended. Figure 5.8 shows a predicted versus measured plot resulting from this model. The distribution of points around the 45º line shows a similarly large scatter for the WTP-LAW and the ORP-LAW datasets, in line with the large %RSD observed on replicate VHT testing. However, the distribution is even around the diagonal, indicating unbiased prediction. The predicted alterations for all fully altered glasses are shown in Figure 5.8 (black squares), all placed at a measured alteration corresponding to half the thickness of the coupon (800 μm for LAWE14 and 1200 μm for the thirty-seven others listed in Table 5.16). As expected, these points are also evenly distributed around the diagonal and provide additional (although not quantifiable) validation of the current model.

The variance/covariance matrix for Model 3 is provided in Appendix B.

5.2.6 Evaluation of VHT Data from Other Sources

Forty-four HLP and ICV glasses from PNNL [49 - 52] with VHT data and with compositions within the compositional domain of the Phase 2 VHT model were assessed against the selected LAW model. All of the VHT data from VSL used in model development and validation were from 24-day tests, whereas the PNNL data were from tests at various time durations from which 24-day alteration depths were calculated. The resulting statistics (R^2 of -2.753 and RMSE of 2.927) indicate that the model does not fit this data well, which is also illustrated in Figure 5.9. The model under predicts most of the PNNL VHT data. Two near-replicate samples are highlighted in Figure 5.9. One set is the LAWA44 glass sample tested at VSL and a sample of the same composition tested at PNNL termed HLP-56. Another set is TFA-Base glass samples tested at VSL and multiple times at PNNL. As is evident from Figure

5.9, the replicate measurements from VSL and PNNL show good agreement. The standard deviation in the VHT results for these replicates were found to be 0.238 and 0.266 for the pairs of LAWA44 and TFA-Base, respectively, which are well within the range of 0.239 for true replicates and 0.463 for near replicates from VHT data collected at the VSL. The reason(s) for the under prediction of the remaining VHT data from PNNL has not been identified. However, as stated above, there is a clear difference in the way the data were collected in that the VSL data used in model development were all collected at 24-day duration, whereas the PNNL data were collected at various test durations.

5.3 Electrical Conductivity Modeling

The electrical conductivity data used for model development are described in Section 5.3.1. The model region 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 537 LAW glasses collected and discussed in Sections 2 and 4 above, 348 glasses have electrical conductivity data, which were generally measured at four temperatures, resulting in a dataset of 1386 data points. Measurements are available at only three temperatures for glasses LAWA145 and ORPLA6.

The current WTP requirement [59] 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 1200ºC. Among 162 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% Na_2O.

Electrical conductivity was measured at temperatures close to the four nominal values (950, 1050, 1150, and 1250ºC) for most WTP-LAW and ORP-LAW glasses. C22AN107, C22Si-15, C22Si+15, and LAWE7H, have the highest measurement temperatures of approximately 1200ºC instead of 1250ºC, while LAWB82, LAWM42, and LAWM48 have all four measurement temperatures noticeably below the nominal values. Two other glasses have measurement temperatures significantly different from the nominal values. ORPLE2 has a minimum measurement temperatures of 988ºC instead of 950ºC and LAWC103 has a maximum measurement temperature of 1202ºC instead of 1250ºC. These observations are provided for information only, since they do not affect the suitability of the associated data for developing electrical conductivity models. As described in Section 4.2.3 above, data for all statistically designed LORPM glasses provided in this report have been measured close to the nominal temperature values (1 to 2% deviation from nominal).

5.3.2 Electrical Conductivity Model Range and Outliers

The WTP baseline EC model excluded 10 WTP-LAW glasses from the ILAW EC modeling dataset, in all cases because their compositions were outside the compositional region of the model. The ORP-LAW dataset broadens the compositional region, 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, for no apparent reason. Archive samples of these glasses were retested in the present work and use of the new measurements resolved that situation. Among the ORP-LAW glasses, the EC models developed during Phase 1 identified LORPM13 as an outlier (due to 2 vol% undissolved or recrystallized zirconium oxide), as also was the case based on observations from PCT and VHT modeling. Data for this glass were not used in the EC modeling dataset.

The electrical conductivity data for the combined dataset (WTP-LAW and ORP-LAW glasses) span the electrical conductivity range of 0.01 to 1.10 S/cm and temperature range of 891°C to 1279°C, as compared to the WTP requirement of 0.10 to 0.70 S/cm in the temperature range of 1100°C to 1200°C.

5.3.3 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 at that time 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 348 glasses (1386 EC data points) is large enough to allow for a set of glasses to be reserved for independent validation of the new models. To select the validation set, all actively designed glasses were sorted by increasing electrical conductivity near 1150ºC (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. The statistically designed glasses or replicates were not pulled from the modeling set. The selected validation glasses are listed in Table 5.20.

5.3.4 Electrical Conductivity Replicates

Six WTP-LAW and one ORP-LAW near-replicate pairs of electrical conductivity versus temperature values are available for use in model lack-of-fit evaluation. Table 5.21 summarizes the replicate measurements and Figure 5.10 shows the electrical conductivity values plotted against $1/T$ (with T in Kelvin) for the two ORP 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:

$$\ln(\mathrm{EC}) = A + B/T\,. \tag{5.1}$$

The data for this replicate set indicate a 5.8% RSD over the four measured temperatures and a 3.3% RSD over the four nominal temperatures. This set, added to the WTP near-replicate set [1], yields a 14% RSD pooled over 7 replicate sets at four temperature measurements and is used in the evaluation of model lack-of-fit.

5.3.5 Electrical Conductivity Model Development

The recommended WTP model (25-term Reduced Truncated Linear Mixture Model with three Quadratic Terms) provides a good fit to the EC data for the WTP glasses (R^2 = 0.951) on which it was developed. However, the prediction performance was significantly worse (R^2 = 0.748) for the ORP-LAW dataset or the LORPM glasses shown in Figure 5.11. The error in prediction varied from 28% under-predicted (for a glass such as ORPLE12) to 100% over-predicted (for LAWC100R1 or LAWA194, for example), with greater deviation at higher conductivity values.

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:

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

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

$$\sum_{i=1}^{q} x_i = 1\,. \tag{5.3}$$

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 5.22 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 was as follows:

- 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 those 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 validation = 0.80, RMSE = 0.305 versus 0.947 and 0.175, respectively [1]).

- Model 2 (25-term) is the recommended EC model from Phase 1 of this work (excluding the single compositional outlier, LORPM13). The model statistics are as good or better than those for the WTP baseline model [1]. Evaluation of possible terms for SnO_2 or V_2O_5 showed that neither appeared to have any significant effect in the EC model.

- Model 3 (27-term), as well as other model evaluations not shown in Table 5.22, explores the addition of model terms for V_2O_5 and $V_2O_5/(T/1000)$ for the expanded dataset (see Appendix A). Multiple other possible cross terms were also investigated, but $CaO \times Li_2O$, $CaO \times Na_2O$ and $Li_2O \times Na_2O$ were the terms that were most significant (low p-value). Vanadium does not appear to contribute significantly, even with the expanded dataset, including the new statistically designed glasses LORPM21-40.

- Model 4 (25-term) is one of several further optimizations of linear and quadratic mixture terms using the JMP® stepwise regression procedure with a p-value threshold stopping rule and MRS initial cross terms construct. This particular optimization yielded improvements in the model statistics with R^2, $R^2_{Adjusted}$, and $R^2_{Predict}$ of 0.961, 0.960, and 0.959, respectively, and a validation R^2 of 0.967. Similar improvements were obtained for other optimizations. For example, a model that made use of the additional cross terms $CaO \times SiO_2$, $K_2O \times Na_2O$, and $Al_2O_3 \times Fe_2O_3$, which have low p-values and removed B_2O_3 and its temperature-dependent terms from the model increased R^2 and $R^2_{Adjusted}$ very slightly (0.962 and 0.961 respectively) but decreased the validation R^2 to 0.966.

Among the EC models considered during the present work, Model 4, the 25-term reduced Arrhenius-linear mixture model with three cross-product terms $CaO \times Li_2O$, $CaO \times Na_2O$, and $Li_2O \times Na_2O$, provides the best model and validation statistics when applied to the extended dataset of 1386 electrical conductivity/temperature data from the WTP-LAW and ORP-LAW modeling and validation datasets. Figure 5.12 displays the predicted versus measured plot for this EC model. The tight distribution of points around the 45º line shows that this model provides good and unbiased predictions over the full range of measured EC values. The variance/covariance matrix for this model is provided in Appendix B.

5.4 Viscosity Modeling

The viscosity data used for model development are presented in Section 5.4.1. The model region 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 548 LAW glasses collected and discussed in Sections 2 and 4 above, 340 glasses have viscosity data. Because of crystallization, viscosity measurements were not conducted on glass LORPM31 (due to non-Newtonian behavior induced by zirconia crystals). Melt viscosities were generally measured at four temperatures, with the exception of LAWM7 for which five measurements were taken, resulting in a dataset of 1379 records. Among WTP glasses, LAWA51, LAWA128R1, LAWA129R1, and LAWM5 had viscosities exceeding the recommended WTP upper limit of 150 poise at 1100ºC [59]; among ORP glasses, ORPLA5, ORPLA6, ORPLA11, ORPLA12, ORPLA13, ORPLA14, ORPLG1, ORPLG2, ORPLG4, ORPLG5, LORPM5, and LORPM9 had viscosities exceeding the recommended upper limit [59]. 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. All glasses in the present LORPM21-40 series had viscosities within the recommended WTP limits.

Viscosity was measured at temperatures close to the four nominal values (950, 1050, 1150, and 1250ºC) for all ORP-LAW glasses with very few exceptions (e.g., for ORPLA3 viscosity was measured at 1219ºC instead of 1250ºC; for ORPLE9 viscosity was measured at 992ºC instead of 950ºC). 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. Measurements for the 19 statistically designed LORPM glasses collected in the present work were measured close to the nominal temperature values (less than 1% deviation from nominal).

Overall, the measured viscosity values for the 340 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.

5.4.2 Viscosity Model Range and Outliers

During the WTP baseline viscosity model development, the same 10 WTP-LAW glasses excluded from the EC model dataset were excluded from the viscosity model dataset also because their compositions were outside the compositional range of the model. The ORP-LAW

dataset broadens the compositional region, as shown in Table 5.6, and all of the above glasses can now be included in the modeling dataset. Among the ORP-LAW glasses, models developed during Phase 1 identified LORPM13 as an outlier (due to 2 vol% undissolved or recrystallized zirconium oxide). Data for this glass were not used in the present viscosity modeling dataset. Finally, as discussed in Section 4.2.3, non-Newtonian behavior was suspected at the lower measurement temperatures for a few of the glasses in LORPM21-40 set. Viscosity measurements for LORPM23 at 1155°C, LORPM24 at 1251°C, LORPM26 at 1251°C, LORPM29 at 1250°C and LORPM30 at 1057°C are the lowest measurement temperatures used in the dataset for these glasses because crystallization was suspected at lower temperatures.

The viscosity data for the combined dataset (WTP-LAW and ORP-LAW glasses) span the viscosity range from 4 to 2534 poise and temperature range of 888°C to 1280°C, as compared to the WTP requirement of 10 to 150 poise at 1100°C.

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 1150ºC (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 5.23.

5.4.4 Viscosity Replicates

Six WTP-LAW and one ORP-LAW near-replicate pairs of viscosity versus temperature values are listed in Table 5.24. Figure 5.13 shows the viscosity values plotted against $1/T$ (with T in Kelvin), with lines connecting the data points for the two ORP-LAW glasses. An Arrhenius fit was not used because some curvature is evident in Figure 5.13. The data for this replicate set indicate a 2% RSD over the four measured and four nominal temperatures. The seven replicate pairs provide a pooled RSD over four measurement temperatures of 13%, which can be used in the evaluation of model lack-of-fit.

5.4.5 Viscosity Model Development

The WTP baseline viscosity model provided the best fit to the WTP-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 5.14. (R^2 = 0.961 and 0.884 for OPR-LAW and LORPM glasses, respectively).

Attempts to expand and improve viscosity models followed similar steps as for the electrical conductivity models described above. However, dependence of viscosity on temperature generally shows more evident departure from Arrhenius behavior than do electrical conductivity data (see the curvature in Figure 5.13, for example).

The dependence of melt viscosity on temperature can generally be represented quite well by the Vogel-Fulcher equation:

$$\ln \eta = A_f/(T-T_o) + B \,, \tag{5.4}$$

where η is viscosity (herein, in poise), T is the absolute temperature (in Kelvin), and A_f, B, and T_o are adjustable parameters, all of which depend on glass composition. If the temperature is sufficiently far above glass transition temperature and does not span too wide a range, an Arrhenius equation,

$$\ln \eta = A/T + B \,, \tag{5.5}$$

may describe viscosity data quite well; the parameter A is proportional to the activation energy for viscous flow, and B is usually referred to as the pre-exponential factor. However, even though the viscosity data of interest here relate to temperatures several hundred degrees above the glass transition temperature, we have found previously that the Vogel-Fulcher equation fits such data significantly better than does the Arrhenius equation, which is confirmed once again in the present work. However, a disadvantage with the Vogel-Fulcher equation is that it is not linear in all of its parameters (it is non-linear in T_0), which means that non-linear regression must be used. To address this issue, VSL proposed in past model development [57, 63, 64] an approximate form of the Vogel-Fulcher equation that allows linear regression. Since, for the data of interest here, T_0/T is always smaller than unity, the Vogel-Fulcher equation can be expanded in a Taylor series:

$$\ln \eta = B + \frac{A_f}{T}(1 - T_0/T)^{-1} = B + \frac{A_f}{T}(1 + \frac{T_0}{T} + (\frac{T_0}{T})^2 + ...) \,. \tag{5.6}$$

We see that the zeroth-order approximation is the Arrhenius equation, whereas the first-order approximation yields:

$$\ln \eta = B + \frac{A_f}{T} + \frac{A_f T_0}{T^2} \quad . \tag{5.7}$$

Equation (5.7) was found to provide a significantly better representation of the temperature dependence of the melt viscosity data than does the Arrhenius equation [57, 63, 64]. Furthermore, we have found that a reduced form of Equation (5.7),

$$\ln \eta = B + \frac{A_f T_0}{T^2} \,, \tag{5.8}$$

frequently outperforms the Arrhenius equation and compares very favorably with Equation (5.7).

The curvature evident in Arrhenius plots for the viscosity [1] inevitably leads also to skewed prediction when modeling the viscosity/temperature data using $1/T$ temperature dependence terms (as demonstrated below). The simplification of the Vogel-Fulcher equation (5.8) above referred to as the "truncated T2 model" [63], 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 PQM model that was used as the WTP LAW baseline viscosity model form to predict the natural logarithm of viscosity [1]:

$$\ln(\eta) = \sum_{i=1}^{q} a_i x_i + \text{Selected}\left\{\sum_{i=1}^{q} a_{ii} x_i^2 + \sum_{i<}^{q-1}\sum_{j}^{q} a_{ij} x_i x_j\right\} + \sum_{i=1}^{q} b_i \frac{x_i}{(T/1000)^2}, \quad (5.9)$$

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

$$\sum_{i=1}^{q} x_i = 1. \quad (5.10)$$

as for all previous model forms.

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 and the Phase 1 model used 27 terms with a new compositional term for SnO_2.

Table 5.25 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 (26-term) corresponds to the WTP baseline model [1], which is a 26-term reduced truncated T2 mixture model with four quadratic terms ($(B_2O_3)^2$, $(Li_2O)^2$, $(MgO)^2$ and $Al_2O_3 \times Li_2O$). This, model when applied to the same set of data from 171 WTP-LAW 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 $B_2O_3/(T/1000)^2$ and $K_2O/(T/1000)^2$ are not included as the p-values calculated in t-tests were high (0.792 and 0.615, respectively), indicating little significance for these terms. This model is presented here for comparison. The validation 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 versus 0.988 [1]).

- Model 2 (27-term) is the recommended Phase 1 model in which the $(MgO)^2$ term, also of low significance, was removed but two terms for SnO_2 (SnO_2 mixture and $SnO_2/(T/1000)^2$) were added to better fit all the ORP-LAW glass data now in the

modeling dataset. The model returned excellent statistics for the combined WTP-LAW and ORP-LAW dataset of 1238 viscosity/temperature data and 112 validation data points.

- Model 3 results from first fitting the dataset of 1265 viscosity/temperature data using an Arrhenius mixture model form to verify whether the current expanded dataset, which spans viscosity values from 3.6 to 2190 poise, could be fit acceptably using such a model (i.e., with $1/T$ terms replacing the $1/T^2$ terms). In this case, $R^2_{Predict}$ decreased (0.984) with minor changes in other model statistics. However, the model residual (lower part of Table 5.25) shows unacceptable skewness (0.157), which is also evident in Figure 5.15. Given the large size of the viscosity dataset, this cannot be simply attributed to a skewed sample distribution but is instead due to an incorrect model form. This could be corrected by adding back the $1/T^2$ coefficients, which then required as many as 37 terms and did not yield any improvement to the model statistics.

- Model 4 (27-term reduced truncated T2-linear mixture model) resulted from three successive optimizations using the linear mixture and $1/T^2$ terms. Again, V_2O_5 is not found to be a significant contributor, but SnO_2 remains significant (see Appendix A). The resulting model includes 13 linear terms and 11 $1/T^2$ terms. Among the quadratic terms, $Al_2O_3 \times Li_2O$, $Al_2O_3 \times Na_2O$, $(B_2O_3)^2$, $B_2O_3 \times Li_2O$, and $(Li_2O)^2$ are most significant. In this model, the terms $Al_2O_3 \times Li_2O$, $(B_2O_3)^2$, and $(Li_2O)^2$, which were previously used in Model 2, were also tested. The model statistics are similar to the results obtained in previous viscosity models: R^2, $R^2_{Adjusted}$, and $R^2_{Predict}$ all equal to 0.986, and a validation R^2 of 0.974.

- Model 5 (28-term) is obtained by replacing $Al_2O_3 \times Li_2O$ with $Al_2O_3 \times Na_2O$ from the list of cross terms tested in Model 4, and adding a $B_2O_3 \times Li_2O$ term, which is the next most significant term with lowest *p*-value (see Table 5.26). Minor improvement is evident in R^2 (to 0.987) but with increased skewness in the residuals as compared to Model 4, but less than that in Model 3.

Among the models considered for LAW glass melt viscosity, Model 4, the 27-term truncated T2 mixture model with three cross-product terms, gives the best fit of the modeling and validation data. This model provides a good empirical relationship to predict melt viscosity of LAW glasses in the composition region and temperature range covered by the data. Figure 5.16 displays the predicted versus measured plot for this viscosity model. The tight distribution of points around the 45º 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 Appendix B.

5.5 Alternate Neural Network Modeling

5.5.1 PCT Neural Network Modeling

Neural Network (NN) modeling provides a potential alternative approach to PQM models and such modeling capability is now included in many statistical software packages, including

JMP. This section describes the application of such models to the PCT and VHT datasets in order to provide an initial evaluation of this approach. The NN approach has been previously applied to modeling various material property-composition relationships including data relating to glass liquidus temperature [65] and, more recently, to waste glass VHT data [50].

The NN selected for modeling PCT-Na and PCT-B glass properties employed one hidden layer network with 5 nodes. The input parameters were the 18 major glass components for which the maximum value exceeds 1.2 wt%: Al_2O_3, B_2O_3, CaO, Cr_2O_3, Fe_2O_3, K_2O, Li_2O, MgO, Na_2O, P_2O_5, SiO_2, SnO_2, SO_3, TiO_2, V_2O_5, ZnO, ZrO_2 and Others. The network outputs are the two glass properties selected – Ln(PCT-Na) and Ln(PCT-B) – as illustrated in Figure 5.17. The 'Random Holdback' validation method was chosen with ratio of training to validation dataset equal to 33.33%. Thus, from the initial dataset of 436 glasses, 290 glasses were used for network training and 146 glasses were used for validation. The hyperbolic tangent function was selected as the node transfer function. To maintain repeatability of model creation steps, the random seed that defines all initial model estimates was set to '12345' and the order of the glasses in the dataset was held constant.

Table 5.27 provides the R^2 values obtained for PCT-Na and PCT-B. The NN model R^2 values for Ln(PCT-Na) and Ln(PCT-B) of 0.898 and 0.886, respectively, are slightly higher than the corresponding statistics for the PQM models of 0.866 and 0.862, respectively. Predictive R^2 values obtained when applying the models to the reserved validation dataset of 27 glasses for Ln(PCT-Na) and Ln(PCT-B) were 0.892 and 0.880, respectively, as compared to 0.890 and 0.797, respectively, for the corresponding selected PQM models described in Section 5.1.5.

The generalized NN model R^2 value of 0.99 reflects high correlation between the outputs for Ln(PCT-Na) and Ln(PCT-B). Analysis of the NN residuals identified glass LORPM28 as an outlier. LORPM28 has an atypical ratio of PCT-Na to PCT-B values and the non-congruence and high pH of this particular glass sample was discussed in Section 4.2.1.

The Final Layer Formulas used to calculate the NN predicted PCT-B and PCT-Na values are provided in the top section of Table 5.28 using the hyperbolic tangent functions for the five nodes described in the lower section. This representation also serves to illustrate the relatively large number of effective parameters in the NN model. Visual comparison of the two predictions from the NN model are provided in Figure 5.18 (PCT-Na) and Figure 5.19 (PCT-B), which also highlights the inconsistency for LORPM22.

It is worth emphasizing that both PCT-B and PCT-Na predictions are obtained from the same NN model since the network is set up to produce two outputs. Additional outputs could be added for additional glass properties and, in principle, all of the desired properties could be obtained from a single network with multiple outputs.

5.5.2 VHT Neural Network Modeling

The NN modeling approach was also applied to the VHT data, where an NN with one hidden layer of 5 hidden nodes was used. The decision to use a separate neural network to model the VHT data was based on the fact that VHT response has a very different scaling from the PCT-B and PCT-Na responses. This can be a problem for successful creation of a NN with several outputs and requires additional input data preparation [66].

All major glass components for which the maximum value exceeded 1.2 wt% were used as input parameters: Al_2O_3, B_2O_3, CaO, Cr_2O_3, Fe_2O_3, K_2O, Li_2O, MgO, Na_2O, P_2O_5, SiO_2, SnO_2, SO_3, TiO_2, V_2O_5, ZnO, ZrO_2 and Others were selected.

As for the PCT data, the hyperbolic tangent function was selected as the transfer function and the 'random holdback' validation approach was applied. To maintain repeatability of process of network creation, the random seed that controls the initial nodes weights was set to "12345". The resulting fitting statistics are given in Table 5.29 and the NN model formulas are presented in Table 5.30.

Comparison of the NN model statistics with those for the previously selected VHT PQM-model shows that the NN R^2 value is much higher than that obtained from VHT PQM Model-3 (0.917 vs. 0.770), while the R^2 validation on the selected 27 validation glasses is also somewhat better (0.779 vs. 0.724). However, visual comparison of the performance of the two types of models, provided in Figure 5.20, does not show any obvious improvement with the NN model, particularly with respect to under-predicting near the limit (red line). Nevertheless, further investigation of the NN approach for VHT modeling for LAW glasses may be useful.

SECTION 6.0
SUMMARY AND CONCLUSIONS

The ORP dataset is comprised of data from a series of LAW glass development and melter testing studies performed 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 limits. The applicability of these improvements over the expected ranges of sodium, potassium, and sulfur concentrations was demonstrated for a wide region of Hanford LAW compositions. The resulting ORP-LAW glass compositions are significantly different from the WTP-LAW glass compositions in both the concentration regions 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 regions, not surprisingly, gaps were identified in the combined WTP-LAW and ORP-LAW datasets, in both the compositions and in the glass property responses.

Steps towards addressing these gaps included the statistical design, preparation, and testing of forty additional glasses, focusing in particular on the composition gaps. Data collected from these new glasses have been compiled to support the revision of the LAW glass property-composition models. The new data, together with previous ORP and WTP data, include glass composition, PCT release, VHT response, melt electrical conductivity, and melt viscosity. The overall LAW dataset now consists of 537 glasses after adding 249 ORP-LAW glasses to the original 271 WTP-LAW glasses collected to develop the WTP baseline models in 2006, plus the 12 WTP-LAW glasses added to augment the VHT dataset in 2008 but not considered in the earlier WTP models, and five earlier formulations containing vanadium which is now one of the glass constituents of interest. In addition, many of the 20 glasses excluded as compositional outliers in the baseline WTP modeling work could now be retained in the modeling dataset for the expanded composition region.

The new datasets were used to develop LAW glass property-composition models for the extended glass composition region 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 regions. R^2 and $R^2_{Adjusted}$ model statistics vary from 0.986 and 0.986, respectively, for melt viscosity to 0.770 and 0.757, 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 contain 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. Addition of the forty statistically designed LORPM glasses led to identification of TiO_2 as a significant term in all three leaching models (PCT-Na, PCT-B, and VHT). Conversely, MgO was found not to be significant in the VHT model. Although ZnO is generally enriched in the VHT layer, it is not found to contribute significantly to the VHT model; however, the variability in VHT response is large (23 to 40% RSD among true or near-replicates), which makes it very challenging to fit the data with acceptable lack-of-fit.

The new models extend the region of validity of the baseline WTP LAW glass property-composition models to encompass the higher waste loading glass formulations that have been developed for ORP. Forty statistically designed glasses added to address gaps in the data have already proven invaluable in supporting model development and have improved their performance over the extended composition region. Model forms similar to the WTP baseline models can still perform quite well with the expanded composition region even if significant changes to the coefficients are necessary.

An initial evaluation of neural network models was made for the PCT and VHT as an alternative to the mixture models obtained by least squares regression. Although these models improved the performance of the models in terms of the R^2 statistics, the improvement was much less evident when applied to an independent set of validation glasses.

The five LAW glass property-composition models developed during Phase 2 of this work and recommended here are summarized below and in Table 6.1. The component response-trace plots, which show the effects of individual component concentration changes on each of the properties for the five selected models, are presented in Figures 6.1 to 6.5. In the figures, each curve spans the range of the corresponding component concentration in each model database and is centered on the centroid of composition region. The five centroid compositions are provided in Table 6.2.

- **PCT-Na:** A 24-term partial quadratic mixture model was developed to relate the natural logarithm of PCT-Na to LAW glass composition using data from WTP-LAW, ORP-LAW and LORPM glasses. The data span the PCT-Na release rates from 0.2 g/L to 4.9 g/L, as compared to the WTP required release rate of 4 g/L or less. The recommended Phase 2 model provides good fit of the data with model R^2 of 0.866 and independent validation R^2 of 0.890. Further refinement of this type of model with the present dataset is unlikely to provide much improvement when considering the %RSD of 17.88 for replicate measurements of PCT-Na releases.

- **PCT-B:** A 26-term partial quadratic mixture model was developed to relate the natural logarithm of PCT-B to LAW glass composition using data from WTP-LAW, ORP-LAW and LORPM glasses. The data span the PCT-B release rates from 0.15 g/L to 7.7 g/L, as compared to the WTP required release rate of 4 g/L or less. The recommended Phase 2 model provides good fit of the data with model R^2 of

0.862 and independent validation R^2 of 0.797. Further refinement of this type of model with the present dataset is unlikely to provide much improvement when considering the %RSD of 20.29 for replicate measurements of PCT-B releases.

- **VHT:** A 22-term partial quadratic mixture model was developed to relate the natural logarithm of the VHT alteration depth to LAW glass composition using data from WTP-LAW, ORP-LAW, and LORPM glasses. The data span VHT alteration depths from 0.05 μm to 1212 μm, as compared to the WTP required alteration depth of 453 μm or less on a 24-day VHT test at 200°C. VHT alteration depth measurements on replicate and near-replicate LAW glasses showed %RSD of 22.89 for true replicates and 39.78 for near-replicates. Considering this variation inherent in VHT alteration depth measurements, the recommended Phase 2 model provides a good fit of the data with model R^2 of 0.770 and independent validation R^2 of 0.724. While other modeling approaches such as neural network modeling could provide better model statistics, it is doubtful that such approaches would provide better prediction of VHT alteration depths.

- **Electric Conductivity:** A 25-term Arrhenius linear mixture model was developed to relate the natural logarithm of electrical conductivity to LAW glass composition using data from WTP-LAW, ORP-LAW, and LORPM glasses. The data span the electrical conductivity range of 0.01 to 1.10 S/cm and temperature range of 891°C to 1279°C, as compared to the WTP requirement of 0.10 to 0.70 S/cm in the temperature range of 1100°C to 1200°C. Replicate electrical conductivity measurements on LAW glasses showed a %RSD of 13.74. The recommended Phase 2 model provides a good fit of the data with model R^2 of 0.961 and independent validation R^2 of 0.967.

- **Viscosity:** A 27-term reduced truncated T2 linear mixture model was developed to relate the natural logarithm of viscosity to LAW glass composition using data from WTP-LAW, ORP-LAW, and LORPM glasses. The data span the viscosity range from 4 to 2534 poise and temperature range of 888°C to 1280°C, as compared to the WTP requirement of 10 to 150 poise at 1100°C. Replicate viscosity measurements on LAW glasses showed a %RSD of 12.98. The recommended Phase 2 model provides a good fit of the data with model R^2 of 0.986 and independent validation R^2 of 0.974.

The five LAW glass property-composition models developed during Phase 2 of this work and described in this report show good model statistics and property prediction capability. Further refinements of the models with the current datasets are unlikely to provide much improvement in model predictions. However, further refinement of the models is recommended as more data are added to the current datasets, especially if the new data expand the LAW glass composition region.

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 [67] 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 [68].

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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 Dataset	**244+2 (+20 excluded)**		**165 (+16 excluded) +12 augmentation[(a)]**		**171+5 (+10 excluded)**		**271+17 augmentation[(a)]**	
Number of ORP-LAW Glasses	**171 + 40 LORPM**		**203 + 40 LORPM**		**122 + 40 LORPM**		**209+ 40 LORPM**	
Total	**477**		**436**		**348**		**537**	
WTP-LAW Glass Component	**Min**	**Max**	**Min**	**Max**	**Min**	**Max**	**Min**	**Max**
Al_2O_3	0.03499	0.09044	0.03503	0.09044	0.03499	0.09043	0.03499	0.09044
B_2O_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_2O_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_2O_3	0	0.08412	0	0.08039	0	0.08412	0	0.08412
K_2O	0	0.05559	0	0.05413	0	0.05412	0	0.05559
Li_2O	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_2O	0.02457	0.24007	0.02457	0.24007	0.02457	0.23002	0.02457	0.24007
P_2O_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_2O_3	0.05514	0.13854	0.05514	0.13854	0.05818	0.13854	0.05514	0.13854
B_2O_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_2O_3	0	0.03019	0	0.03019	0	0.06984	0	0.06984
K_2O	0.00110	0.05881	0.00110	0.05881	0.00110	0.05881	0.00110	0.05881
Li_2O	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_2O	0.09989	0.26005	0.09989	0.26005	0.09993	0.25040	0.09989	0.26005
P_2O_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
SnO2 (new)	0	0.05001	0	0.05001	0	0.04830	0	0.05001
V_2O_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) Addition of V_2O_5 to the model components allows addition of 2 PCT from earlier WTP data [25], 5 viscosity and electrical conductivity data and 12 VHT augmentation glasses which 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 – some viscosity measurements not performed on every glass or at every temperature.

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**	
WTP-LAW Glass Components in "Others"	**Min**	**Max**	**Min**	**Max**	**Min**	**Max**	**Min**	**Max**
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_2O	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_2O_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**
BaO	0	0.00010	0	0.00010	0	0.00010	0	0.00010
CdO	0	0.00010	0	0.00010	0	0.00010	0	0.00010
Cl	0.0001	0.01170	0.0001	0.01170	0.0001	0.01161	0.0001	0.01170
Cr_2O_3	0.0002	0.00600	0.0002	0.00600	0.00018	0.00600	0.0002	0.00600
Cs_2O	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_2O_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. 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_2O_3	3.500	13.850	5.570	11.780	6.605	10.745
B_2O_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_2O_3	0.300	8.000	1.840	6.460	2.610	5.690
K_2O	0.110	5.880	1.264	4.726	1.841	4.149
Li_2O	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_2O	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_2O_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 2.3. 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_2O_3	16.07	0.32
F	14.97	0.30
NiO	1.50	0.03
PbO	1.50	0.03
P_2O_5	24.95	0.50
Subtotal	100.00	2.00

Table 2.4. Compositions of the LORPM21-40 Glasses.

LORPM Glass #	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SO_3	SiO_2	SnO_2	TiO_2	V_2O_5	ZnO	ZrO_2	Others	Sum
21	4.846	12.865	11.450	7.122	1.037	0.000	0.000	16.047	0.100	44.882	0.000	0.600	0.000	1.000	0.000	0.051	100
22	3.500	6.000	10.607	7.242	1.075	0.000	0.000	21.722	0.100	35.000	5.000	0.000	0.562	3.142	6.000	0.050	100
23	12.614	7.070	1.811	6.858	0.110	5.000	4.329	8.810	0.100	36.686	2.884	2.679	4.000	1.000	6.000	0.049	100
24	11.379	6.000	0.000	7.097	5.880	0.000	3.854	13.477	0.280	35.980	2.176	0.000	4.000	4.574	5.253	0.050	100
25	13.850	12.757	0.000	0.997	2.626	2.367	4.333	18.274	0.100	37.146	0.305	0.000	0.000	1.000	6.000	0.245	100
26	10.049	6.000	10.038	7.196	5.306	0.000	0.000	10.919	0.910	35.000	5.000	2.582	0.000	5.000	0.000	2.000	100
27	12.868	6.000	1.184	8.000	5.375	5.000	4.611	8.695	1.000	38.752	0.000	1.464	0.000	1.000	6.000	0.051	100
28	3.500	13.730	0.000	0.300	0.110	5.000	0.000	14.311	0.100	45.144	5.000	0.000	4.000	1.000	6.000	1.805	100
29	9.388	9.918	0.000	0.300	5.880	5.000	4.642	8.855	1.000	35.000	5.000	3.000	0.000	4.600	5.416	2.001	100
30	3.500	6.000	12.240	8.000	5.880	4.359	3.000	5.000	0.100	35.000	5.000	0.502	4.000	1.000	6.000	0.419	100
31	10.938	10.133	0.000	6.377	0.110	4.354	0.632	9.456	1.000	35.000	5.000	0.000	4.000	5.000	6.000	2.000	100
32	5.570	11.589	2.448	4.333	4.726	3.570	3.500	10.000	0.600	43.045	1.000	2.400	1.083	3.890	2.000	0.246	100
33	11.780	11.572	2.448	2.301	1.264	4.000	3.170	10.000	0.240	40.532	1.000	0.600	2.093	2.000	5.000	2.000	100
34	7.173	12.184	2.448	1.840	4.726	4.000	3.500	10.078	0.420	38.400	1.898	2.400	2.186	2.063	4.684	2.000	100
35	10.373	7.546	4.925	1.840	3.239	2.889	3.128	17.300	0.284	38.400	1.000	1.334	0.893	1.800	5.000	0.049	100
36	6.654	12.184	2.448	1.840	2.508	4.000	3.500	12.817	0.276	39.741	2.485	2.204	0.800	1.800	5.000	1.743	100
37	5.570	11.624	2.448	2.161	4.726	3.659	3.500	12.197	0.240	39.471	4.000	2.400	0.800	4.200	2.468	0.536	100
38	5.570	7.546	2.448	6.460	4.726	1.000	3.500	13.391	0.600	39.659	1.000	2.400	0.800	4.200	4.700	2.000	100
39	5.570	12.184	2.448	6.460	1.264	4.000	1.000	17.384	0.240	38.400	1.000	0.600	3.200	1.800	4.400	0.050	100
40	11.780	7.546	2.448	5.710	4.726	4.000	3.500	10.000	0.240	38.400	1.000	0.600	0.800	4.200	5.000	0.050	100

Table 2.5. WTP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity.

Glass ID	PCT[a]	VHT[a]	Viscosity[a]	Electrical[a] Conductivity	Glass ID	PCT	VHT	Viscosity	Electrical Conductivity
LAWA44R10	1	1	1	1	LAWM16	1	1	1	1
LAWA53	1	1	1	1	LAWM17	1	1	1	1
LAWA56	1	1	1	1	LAWM18	1	1	1	1
LAWA88	1	0	1	1	LAWM19	1	1	1	1
LAWA88R1	1	1	0	0	LAWM20	1	1	1	1
LAWA102R1	1	1	1	1	LAWM21	1	1	1	1
LAWA126	1	1	1	1	LAWM22	1	1	1	1
LAWA128	1	1	0	0	LAWM23	1	1	1	1
LAWA128R1	0	0	1	1	LAWM24	1	1	1	1
LAWA130	1	1	1	1	LAWM25R1	1	1	1	1
LAWB65	1	1	1	1	LAWM26	1	1	1	1
LAWB66	1	1	1	1	LAWM27	1	1	1	1
LAWB68	1	1	1	1	LAWM28	1	1	1	1
LAWB78	1	1	1	1	LAWM29	1	1	1	1
LAWB79	1	1	1	1	LAWM30	1	1	1	1
LAWB80	1	1	1	1	LAWM31	1	1	1	1
LAWB83	1	1	1	1	LAWM32	1	1	1	1
LAWB84	1	1	1	1	LAWM33R1	1	1	1	1
LAWB85	1	1	1	1	LAWM34	1	1	1	1
LAWB86	1	1	1	1	LAWM35	1	1	1	1
C100-G-136B	1	1	1	1	LAWM36	1	1	1	1
LAWC27	1	1	1	1	LAWM37	1	1	1	1
LAWC32	1	1	1	1	LAWM38	1	1	1	1
LAWM1	1	1	1	1	LAWM39	1	1	1	1
LAWM2	1	1	1	1	LAWM40	1	1	1	1
LAWM3	1	1	1	1	LAWM41	1	1	1	1
LAWM4	1	1	1	1	LAWM42	1	1	1	1
LAWM5	1	1	1	1	LAWM43	1	1	1	1
LAWM6	1	1	1	1	LAWM44	1	1	1	1
LAWM7	1	1	1	1	LAWM45	1	1	1	1
LAWM8	1	1	1	1	LAWM46	1	1	1	1
LAWM9	1	1	1	1	LAWM47	1	1	1	1
LAWM10	1	1	1	1	LAWM48	1	1	1	1
LAWM11	1	1	1	1	LAWM49	1	1	1	1
LAWM12	1	1	1	1	LAWM50	1	1	1	1
LAWM13	1	1	1	1	LAWM51	1	1	1	1
LAWM14	1	1	1	1	LAWM52	1	1	1	1
LAWM15	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 2.5. WTP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity (continued).

Glass ID	PCT[(a)]	VHT[(a)]	Viscosity[(a)]	Electrical[(a)] Conductivity
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 2.5. WTP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity (continued).

Glass ID	PCT[(a)]	VHT[(a)]	Viscosity[(a)]	Electrical[(a)] Conductivity
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
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	1	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 2.5. WTP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity (continued).

Glass ID	PCT[a]	VHT[a]	Viscosity[a]	Electrical[a] Conductivity
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
-				
LAWB39[b]	1	0	1	1
LAWB47[b]	0	0	1	1
LAWB48[b]	0	0	1	1
LAWB49[b]	0	0	1	1
LAWC13[b]	1	0	1	1
LAWA137[c]	0	1	0	0
LAWE17[c]	0	1	0	0
LAWE18[c]	0	1	0	0
LAWE19[c]	0	1	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
-				
LAWE20[c]	0	1	0	0
LAWE21[c]	0	1	0	0
LAWE22[c]	0	1	0	0
LAWE23[c]	0	1	0	0
LAWE24[c]	0	1	0	0
LAWE25[c]	0	1	0	0
LAWE26[c]	0	1	0	0
Totals	**266**	**193**	**186**	**186**

(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) WTP glass containing vanadium [25] added to the model dataset in this report since V_2O_5 is now a component in modeling.
(c) WTP new high alkali glasses measured in 2008 to augment the VHT data set.
- Empty data field.

Table 2.6. ORP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity.

Glass ID	PCT[a]	VHT[a]	Viscosity[a]	Electrical[a] Conductivity		Glass ID	PCT	VHT	Viscosity	Electrical Conductivity
LAWA143	0	0	1	1		LAWB104	1	1	1	1
LAWA144	0	0	1	1		LAWB105	1	1	1	1
LAWA145	0	0	1	1		LAWC100R1	1	1	1	1
LAWA161	1	1	0	0		LAWC101	1	1	1	1
LAWA161-duplicate	0	1	0	0		LAWC102	1	1	1	1
LAWA161S2	0	0	1	1		LAWC103	1	1	1	1
LAWA171	1	1*[b]	1	1		ORPLA1	1	1*[b]	1	1
LAWA172	1	1*	1	1		ORPLA1S4	0	1*	0	0
LAWA173	1	1	1	1		ORPLA2	1	1	1	1
LAWA174	1	1	1	1		ORPLA2S4	0	1	0	0
LAWA175	1	1	1	1		ORPLA3	1	1	1	1
LAWA176	1	1	1	1		ORPLA3S4	0	1	0	0
LAWA177	1	1*	1	1		ORPLA4	1	1	1	1
LAWA178	1	1*	1	1		ORPLA4S4	0	1	0	0
LAWA179	1	1*	1	1		ORPLA5	1	1	1	1
LAWA180	1	1	1	1		ORPLA5S4	0	1*	0	0
LAWA181	1	1*	1	1		ORPLA6	1	1	1	1
LAWA182	1	1*	1	1		ORPLA6S4	0	1	0	0
LAWA183	1	1	1	1		ORPLA7	1	1	1	1
LAWA184	1	1	1	1		ORPLA7S4	0	1	0	0
LAWA185	1	1	1	1		ORPLA8	1	1	1	1
LAWA186	1	1	1	1		ORPLA8S4	0	1*	0	0
LAWA187	1	1	1	1		ORPLA9	1	1	1	1
LAWA187-duplicate	0	1	0	0		ORPLA9S4	0	1	0	0
LAWA187CCC	1	0	0	0		ORPLA10	1	1	1	1
LAWA188	1	1	1	1		ORPLA10S4	0	1	0	0
LAWA189	1	1	1	1		ORPLA11	1	1*	1	1
LAWA190	1	1	1	1		ORPLA11S4	0	1*	0	0
LAWA191	1	1	1	1		ORPLA12	1	1	1	1
LAWA192	1	1	1	1		ORPLA12S4	0	1	0	0
LAWA193	1	1	1	1		ORPLA13	1	1	1	1
LAWA194	1	1	1	1		ORPLA13S4	0	1	0	0
LAWA195	1	1	1	1		ORPLA14	1	1	1	1
LAWA196	1	1	1	1		ORPLA14S4	0	1	0	0
LAWA197	1	1	1	1		ORPLA15	1	1	1	1
LAWB97	1	1	1	1		ORPLA15S4	0	1	0	0
LAWB98	1	1	1	1		ORPLA16	1	1	1	1
LAWB99	1	1	1	1		ORPLA16S4	0	1	0	0
LAWB100	1	1	1	1		ORPLA17	1	1	1	1
LAWB101	1	1	1	1		ORPLA17S4	0	1	0	0
LAWB102	1	1	1	1		ORPLA18	1	1	1	1
LAWB103	1	1	1	1		ORPLA19	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 a test for which the glass test coupon was fully reacted and only a "greater than" value is available.

Table 2.6. ORP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity (continued).

Glass ID	PCT[(a)]	VHT[(a)]	Viscosity[(a)]	Electrical[(a)] Conductivity
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
ORPLA25	1	1	0	0
ORPLA26	1	1	0	0
ORPLA27	1	1*[(b)]	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	0	1*	0	0
ORPLB2	1	1	1	1
ORPLB2S4	0	1	0	0
ORPLB3	1	1	1	1
ORPLB3S4	0	1	0	0
ORPLB4	1	1	1	1
ORPLB4S4	0	1	0	0
ORPLC1	1	1	1	1
ORPLC1S4	0	1	0	0
ORPLC2	1	1*	1	1
ORPLC2S4	0	1	0	0
ORPLC3	1	1*	0	0
ORPLC3S4	0	1*	0	0
ORPLC4	1	1*	0	0
ORPLC4S4	0	1*	0	0
ORPLC5	1	1	1	1
ORPLC5S4	0	1	0	0
ORPLD1	1	1	1	1
ORPLD1S4	0	1	0	0
ORPLD2	1	1	0	0
ORPLD2S4	0	1	0	0
ORPLD3	1	1	0	0
ORPLD3S4	0	1	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
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

(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 a test for which the glass test coupon was fully reacted and only a "greater than" value is available.

Table 2.6. ORP-LAW Glasses Having Data for PCT, VHT, Viscosity, and Electrical Conductivity (continued).

Glass ID	PCT[a]	VHT[a]	Viscosity[a]	Electrical[a] Conductivity	Glass ID	PCT	VHT	Viscosity	Electrical Conductivity
ORPLG8	1	1	1	1	LORPM1	1	1[c]	1	1
ORPLG9	1	1	1	1	LORPM2R1	1	1	1	1
ORPLG10	1	1	1	1	LORPM3	1	1	1	1
ORPLG11	1	1	1	1	LORPM4R1	1	1	1	1
ORPLG12	1	1	1	1	LORPM5	1	1	1	1
ORPLG13	1	1	0	0	LORPM6	1	1	1	1
ORPLG14	1	1*[b]	0	0	LORPM7R1	1	1	1	1
ORPLG15	1	1	0	0	LORPM8R1	1	1	0	1
ORPLG16	1	1*	0	0	LORPM9	1	1	1	1
ORPLG17	1	1*	0	0	LORPM10R1	1	1	1	1
ORPLG18	1	1*	0	0	LORPM11	1	1	1	1
ORPLG19	1	1*	0	0	LORPM12R1	1	1	1	1
ORPLG20	1	1	0	0	LORPM13	1	1	0	1
ORPLG21	1	1	1	1	LORPM14R1	1	1	1	1
ORPLG22	1	1	1	1	LORPM15	1	1	1	1
ORPLG23	1	1	1	1	LORPM16R1	1	1	1	1
ORPLG24	1	1	1	1	LORPM17R1	1	1*[b]	1	1
ORPLG25	1	1	1	1	LORPM18	1	1	1	1
ORPLG26	1	1	1	1	LORPM19R1	1	1	1	1
ORPLG27	1	1	1	1	LORPM20R1	1	1	1	1
Q10-G-134A (ORPLE12)	1	1	0	0	LORPM21	1	1	1	1
R10-G-155A (ORPLA15)	1	1	0	0	LORPM22	1	1	1	1
S10-G-101B (ORPLC5)	1	1	0	0	LORPM23	1	1	1	1
S10-G-45A (ORPLB4)	1	1	0	0	LORPM24	1	1	1	1
T10-G-16A (ORPLD1)	1	1	0	0	LORPM25	1	1	1	1
WVW-G-11A (LAWA161)	1	1	0	0	LORPM26	1	1	1	1
Y10-G-146C (ORPLA20)	1	1	0	0	LORPM27	1	1	1	1
Z10-G-122B (ORLF7low SO_3)	1	1	0	0	LORPM28R1	1[d]	1	1	1
Z10-G-153B (ORLF7 high SO_3)	1	1	0	0	LORPM29	1	1	1	1
Z10-G-60C (ORPLD6)	1	0	0	0	LORPM30	1	1	1	1
10A-G-53C (ORPLD6)	1	1	0	0	LORPM31	1	1	0	1
10A-G-43B (ORPLG9)	1	1*[b]	0	0	LORPM32	1	1	1	1
DWV-G-123C (LAWB99)	1	1	0	0	LORPM33	1	1	1	1
EWV-G-89B (LAWA187)	1	1	0	0	LORPM34	1	1	1	1
EWV89BCCC (LAWA187)	1	1	0	0	LORPM35	1	1	1	1
EWV-G-93B (LAWA187)	0	1	0	0	LORPM36	1	1	1	1
EWV93BCCC (LAWA187)	0	1	0	0	LORPM37	1	1*[b]	1	1
EWV-G-108B (LAWA187)	0	1	0	0	LORPM38	1	1	1	1
WVY-G-95A (LAWC100)	1	1	1	1	LORPM39	1	1	1	1
J10-G-24B (ORPLA38-1)	1	1	0	0	LORPM40	1	1	1	1
I10-G-135A (ORPLG27)	1	1	0	0	**Totals (249 glasses)**	**211**	**243**	**159**	**162**

(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 a test for which the glass test coupon was fully reacted and only a "greater than" value is available.
(c) Triplicate VHT testing for assessment of replicate variability.
(d) Duplicate PCT testing for assessment of replicate variability.

Table 2.7. PCT and VHT Results for Forty Nine Glasses from Other Sources.

Glass ID	PCT B (g/L)	PCT Na (g/L)	VHT (μm)	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	P_2O_5	SiO_2	TiO_2	ZnO	ZrO_2	SO_3	Others	Sum
HLP-01	0.54	0.70	106	7.00	10.00	0.01	5.50	0.41	0.00	1.50	20.00	0.06	49.06	3.00	1.50	1.50	0.07	0.40	100.0
HLP-02	5.80	4.62	-	8.79	12.57	0.02	6.92	0.52	0.00	1.88	25.14	0.07	36.00	3.77	1.88	1.88	0.09	0.46	100.0
HLP-03	0.56	0.64	108	6.60	9.43	0.01	5.19	0.39	0.00	1.41	18.85	0.05	52.01	2.82	1.41	1.41	0.07	0.35	100.0
HLP-04	3.88	2.34	547	8.24	11.78	0.01	6.48	0.49	0.00	1.77	23.57	0.07	40.00	3.53	1.77	1.77	0.09	0.44	100.0
HLP-05	2.56	1.68	69	4.00	10.32	0.01	5.68	0.43	0.00	1.55	20.65	0.06	50.64	3.09	1.55	1.55	0.08	0.39	100.0
HLP-06	0.60	0.56	169	11.94	9.47	0.01	5.21	0.39	0.00	1.42	18.94	0.05	46.46	2.84	1.42	1.42	0.07	0.35	100.0
HLP-07	0.60	0.62	254	9.00	9.79	0.01	5.38	0.40	0.00	1.47	19.57	0.05	48.02	2.93	1.47	1.47	0.07	0.36	100.0
HLP-08	0.66	0.88	153	7.31	6.00	0.01	5.75	0.43	0.00	1.57	20.89	0.06	51.24	3.13	1.57	1.57	0.08	0.39	100.0
HLP-09	1.00	0.90	167	6.84	12.00	0.01	5.38	0.40	0.00	1.47	19.56	0.05	47.98	2.93	1.47	1.47	0.07	0.36	100.0
HLP-10	0.68	0.74	113	7.15	8.00	0.01	5.63	0.42	0.00	1.53	20.45	0.06	50.17	3.06	1.53	1.53	0.07	0.39	100.0
HLP-11	0.88	0.82	333	7.37	10.52	0.01	0.55	0.44	0.00	1.58	21.05	0.06	51.64	3.15	1.58	1.58	0.08	0.39	100.0
HLP-12	0.82	0.68	223	6.74	9.63	0.01	9.00	0.40	0.00	1.44	19.26	0.05	47.26	2.89	1.44	1.44	0.07	0.36	100.0
HLP-13	0.90	0.86	192	7.18	10.27	0.01	3.00	0.42	0.00	1.54	20.53	0.06	50.37	3.08	1.54	1.54	0.08	0.38	100.0
HLP-14	1.38	1.08	311	7.21	10.31	0.01	5.67	0.43	0.00	1.55	20.62	0.06	50.58	0.00	1.55	1.55	0.08	0.39	100.0
HLP-16	0.72	0.72	-	7.10	10.15	0.01	5.59	0.42	0.00	1.52	20.31	0.06	49.82	3.04	0.00	1.52	0.07	0.38	100.0
HLP-17	0.88	0.84	52	6.82	9.75	0.01	5.36	0.40	0.00	1.46	19.49	0.05	47.81	2.92	4.00	1.46	0.07	0.41	100.0
HLP-18	1.02	0.90	282	7.10	10.15	0.01	5.59	0.42	0.00	1.52	20.31	0.06	49.82	3.04	1.52	0.00	0.07	0.38	100.0
HLP-19	0.54	0.60	-	6.68	9.55	0.01	5.25	0.39	0.00	1.43	19.09	0.05	46.83	2.86	1.43	6.00	0.07	0.35	100.0
HLP-20	0.74	0.66	172	7.10	10.15	0.01	5.59	0.42	0.00	0.00	20.31	0.06	49.82	3.04	1.52	1.52	0.07	0.38	100.0
HLP-21	1.16	0.92	79	6.82	9.75	0.01	5.36	0.40	0.00	4.00	19.50	0.05	47.83	2.92	1.46	1.46	0.07	0.36	100.0
HLP-22	0.48	0.46	34	7.37	10.53	0.01	5.79	0.33	0.00	1.58	16.00	0.04	51.67	3.16	1.58	1.58	0.06	0.30	100.0
HLP-23	1.92	1.52	459	6.72	9.61	0.01	5.29	0.47	0.00	1.44	23.00	0.06	47.13	2.88	1.44	1.44	0.08	0.43	100.0
HLP-24	0.66	0.70	94	7.18	10.27	0.01	5.65	0.37	0.00	1.54	18.00	0.05	50.36	3.08	1.54	1.54	0.07	0.34	100.0
HLP-25	0.86	0.84	135	7.00	10.00	0.01	5.50	0.41	0.00	1.50	20.00	0.06	49.06	3.00	1.50	1.50	0.07	0.40	100.0
HLP-26	1.04	0.76	186	7.00	10.00	0.01	5.50	0.41	0.00	1.50	20.00	0.06	49.07	3.00	1.50	1.50	0.07	0.38	100.0

Table 2.7. PCT and VHT Results for Forty Nine Glasses from Other Sources (continued).

Glass ID	PCT B (g/L)	PCT Na (g/L)	VHT (μm)	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	P_2O_5	SiO_2	TiO_2	ZnO	ZrO_2	SO_3	Others	Sum
HLP-27	4.34	3.04	-	11.87	11.93	0.01	0.60	0.47	0.00	0.00	22.87	0.06	51.69	0.00	0.00	0.00	0.08	0.43	100.0
HLP-28	0.50	0.38	-	11.94	12.00	0.01	3.10	0.33	0.00	0.84	16.00	0.04	52.01	1.69	0.84	0.84	0.06	0.30	100.0
HLP-29	0.76	1.06	-	11.94	6.00	0.01	2.54	0.47	0.00	0.69	23.00	0.06	52.01	1.38	0.69	0.69	0.08	0.43	100.0
HLP-30	0.30	0.48	408	11.94	6.00	0.01	5.64	0.33	0.00	1.54	16.00	0.04	51.99	3.07	1.54	1.54	0.06	0.30	100.0
HLP-32	0.92	0.68	22	4.00	12.00	0.01	6.46	0.33	0.00	1.76	16.00	0.04	52.00	3.52	1.76	1.76	0.06	0.30	100.0
HLP-33	3.84	3.22	584	4.00	6.00	0.01	5.90	0.47	0.00	1.61	23.00	0.06	52.01	3.21	1.61	1.61	0.08	0.43	100.0
HLP-35	2.64	2.00	463	11.94	12.00	0.01	6.77	0.47	0.00	1.85	23.00	0.06	36.00	3.69	1.85	1.85	0.08	0.43	100.0
HLP-43	0.80	0.66	105	7.00	10.00	0.01	5.50	0.41	0.00	1.50	20.00	0.06	49.07	3.00	1.50	1.50	0.07	0.38	100.0
HLP-44	0.90	0.80	128	7.00	10.00	0.01	5.50	0.41	0.00	1.50	20.00	0.06	49.07	3.00	1.50	1.50	0.07	0.38	100.0
HLP-45	0.84	0.76	164	7.00	10.00	0.01	5.50	0.41	0.00	1.50	20.00	0.06	49.07	3.00	1.50	1.50	0.07	0.38	100.0
HLP-48	1.22	1.04	669	11.97	8.85	0.00	5.77	3.10	0.00	1.99	20.00	0.08	38.25	2.49	4.27	2.49	0.10	0.64	100.0
HLP-49	0.62	0.58	-	8.03	8.07	7.03	8.03	0.36	4.08	3.00	10.00	0.01	43.94	0.00	3.99	3.04	0.02	0.39	100.0
HLP-56	-	-	6	6.20	8.90	1.99	6.98	0.50	0.00	1.99	20.00	0.03	44.55	1.99	2.96	2.99	0.10	0.82	100.0
HLP-58	0.52	0.62	24	6.85	9.78	2.00	5.38	0.40	0.13	1.47	19.57	0.06	48.01	2.94	1.47	1.47	0.09	0.40	100.0
HLP-59	0.58	0.74	28	6.64	9.48	4.99	5.22	0.39	0.13	1.43	18.96	0.06	46.52	2.84	1.43	1.43	0.09	0.40	100.0
HLP-64	6.40	4.80	64	3.99	5.99	0.01	0.16	4.99	0.11	4.29	15.96	2.00	51.87	0.00	4.13	5.99	0.04	0.49	100.0
HLP-65	0.92	0.98	-	3.99	5.99	4.99	9.80	0.33	0.11	4.29	15.97	2.00	51.90	0.00	0.00	0.04	0.11	0.49	100.0
HLP-74	0.50	0.58	-	11.92	12.55	4.99	11.29	0.33	0.14	0.00	15.97	2.00	35.94	0.00	4.29	0.00	0.10	0.49	100.0
HLP-75	0.66	0.86	159	7.41	8.90	2.30	5.52	2.48	0.28	1.99	19.77	0.99	41.41	3.67	1.99	2.69	0.10	0.49	100.0
AMP2-03	-	-	363	8.00	6.00	2.50	11.00	2.50	0.00	0.90	18.00	1.60	43.85	2.00	0.00	2.00	0.95	0.70	100.0
AMP2-02	-	-	110	8.00	6.00	2.50	11.00	2.50	0.00	3.00	18.00	0.20	44.00	2.00	0.00	2.00	0.10	0.70	100.0
AMP2-16	-	-	127	8.00	6.00	5.50	4.00	0.90	0.00	3.00	20.52	1.60	44.83	2.00	0.00	2.85	0.10	0.70	100.0
S22-16	-	-	1241	12.56	6.00	2.50	3.95	2.50	0.00	3.00	23.00	2.50	40.01	0.00	0.00	2.75	0.00	1.23	100.0
S22-26	-	-	1133	8.00	6.00	5.50	3.95	0.00	0.00	0.00	23.00	2.50	45.65	2.00	0.00	2.75	0.00	0.65	100.0

Table 4.1. XRF and DCP Analyses of the Twenty LORPM21-40 Glasses.

Glass	LORPM21			LORPM22			LORPM23			LORPM24			LORPM25		
	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_2O_3	4.85	4.53	4.60	3.50	3.39	3.61	12.61	12.09	11.72	11.38	11.13	10.35	13.85	13.23	13.84
B_2O_3	12.87	NA	12.32	6.00	NA	6.03	7.07	NA	6.94	6.00	NA	5.98	12.76	NA	12.70
BaO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CaO	11.45	11.98	11.09	10.61	11.13	10.15	1.81	1.95	1.80	0.00	0.00	0.03	0.00	0.02	0.02
CdO	0.00	0.00	NA	0.00	0.00	NA	0.00	0.00	NA	0.00	0.00	NA	0.00	0.00	NA
Cr_2O_3	0.01	0.02	0.02	0.01	0.00	0.02	0.01	0.00	0.02	0.01	0.00	0.02	0.04	0.05	0.05
Fe_2O_3	7.12	7.20	7.18	7.24	7.11	7.08	6.86	7.15	7.16	7.10	7.15	7.15	1.00	1.04	1.09
K_2O	1.04	1.02	1.09	1.08	1.05	1.18	0.11	0.13	0.13	5.88	6.02	5.40	2.63	2.64	2.52
Li_2O	0.00	NA	0.05	0.00	NA	0.05	5.00	NA	4.63	0.00	NA	0.04	2.37	NA	2.35
MgO	0.00	0.00	0.01	0.00	0.00	0.01	4.33	3.92	3.92	3.85	3.50	3.32	4.33	3.89	4.30
Na_2O	16.05	16.13	14.98	21.72	21.89	19.87	8.81	9.30	8.52	13.48	13.54	12.78	18.27	18.48	17.42
NiO	0.00	0.00	0.04	0.00	0.00	0.05	0.00	0.00	0.08	0.00	0.00	0.07	0.00	0.01	0.01
PbO	0.00	0.00	NA	0.00	0.00	NA	0.00	0.00	NA	0.00	0.02	NA	0.00	0.01	NA
SiO_2	44.88	44.50	44.63	35.00	34.98	34.98	36.69	37.11	37.35	35.98	36.91	36.87	37.15	37.40	37.60
SnO_2	0.00	0.00	0.00	5.00	4.61	5.06	2.88	2.61	2.45	2.18	1.90	2.08	0.31	0.28	0.33
TiO_2	0.60	0.64	0.67	0.00	0.00	0.03	2.68	2.61	2.78	0.00	0.00	0.04	0.00	0.01	0.02
V_2O_5	0.00	0.00	0.02	0.56	0.53	0.61	4.00	4.18	4.03	4.00	4.17	4.06	0.00	0.00	0.02
ZnO	1.00	0.96	1.00	3.14	3.05	3.09	1.00	0.97	1.00	4.57	4.44	4.38	1.00	0.98	1.02
ZrO_2	0.00	0.00	0.01	6.00	5.88	6.04	6.00	5.40	5.74	5.25	4.79	5.08	6.00	6.34	6.04
Cl	0.02	0.03	NA	0.02	0.03	NA	0.02	0.03	NA	0.02	0.03	NA	0.10	0.09	NA
F	0.01	NA	NA	0.01	NA	NA	0.01	NA	NA	0.01	NA	NA	0.04	NA	NA
P_2O_5	0.01	0.02	0.04	0.01	0.03	0.04	0.01	0.03	0.06	0.01	0.02	0.03	0.06	0.08	0.02
SO_3	0.10	0.10	NA	0.10	0.18	NA	0.10	0.10	NA	0.28	0.28	NA	0.10	0.12	NA
Sum*	100.0	100.0	97.8	100.0	99.9	97.9	100.0	99.7	98.3	100.0	99.9	97.7	100.0	99.8	99.4

NA = Not analyzed.
* Sum includes target values for components that were not analyzed.

Table 4.1. XRF and DCP Analyses of the Twenty LORPM21-40 Glasses (continued).

Glass	LORPM26			LORPM27			LORPM28R1			LORPM29			LORPM30		
	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_2O_3	10.05	9.94	9.64	12.87	12.47	12.34	3.50	3.44	3.51	9.39	9.36	8.57	3.50	3.28	3.54
B_2O_3	6.00	NA	5.97	6.00	NA	5.93	13.73	NA	13.25	9.92	NA	9.49	6.00	NA	***5.98***
BaO	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00
CaO	10.04	10.47	9.87	1.18	1.34	1.49	0.00	0.00	0.02	0.00	0.00	0.03	12.24	12.89	12.30
CdO	0.01	0.00	NA	0.00	0.00	NA	0.01	0.00	NA	0.01	0.00	NA	0.00	0.00	NA
Cr_2O_3	0.32	0.29	0.29	0.01	0.02	0.03	0.29	0.29	0.30	0.32	0.30	0.24	0.07	0.00	0.08
Fe_2O_3	7.20	7.37	7.43	8.00	8.37	8.35	0.30	0.34	0.33	0.30	0.35	0.43	8.00	7.95	7.90
K_2O	5.31	4.89	4.86	5.38	5.49	4.85	0.11	0.12	0.13	5.88	5.68	5.22	5.88	6.22	5.65
Li_2O	0.00	NA	0.04	5.00	NA	4.76	5.00	NA	4.83	5.00	NA	4.79	4.36	NA	4.34
MgO	0.00	0.00	0.02	4.61	4.19	4.23	0.00	0.00	0.01	4.64	4.41	4.15	3.00	2.65	3.01
Na_2O	10.92	11.29	10.27	8.70	8.81	8.38	14.31	14.15	13.83	8.86	8.79	8.56	5.00	5.45	4.87
NiO	0.03	0.04	0.08	0.00	0.00	0.06	0.03	0.03	0.05	0.03	0.04	0.09	0.01	0.01	0.04
PbO	0.03	0.07	NA	0.00	0.00	NA	0.03	0.05	NA	0.03	0.05	NA	0.01	0.04	NA
SiO_2	35.00	36.31	36.80	38.75	39.45	40.22	45.14	45.54	46.11	35.00	37.17	36.39	35.00	35.08	35.32
SnO_2	5.00	4.51	4.49	0.00	0.00	0.01	5.00	4.93	5.04	5.00	4.45	4.60	5.00	4.06	4.09
TiO_2	2.58	2.83	2.70	1.46	1.59	1.84	0.00	0.03	0.02	3.00	3.18	3.10	0.50	0.51	0.55
V_2O_5	0.00	0.00	0.03	0.00	0.00	0.01	4.00	3.98	4.02	0.00	0.00	0.02	4.00	4.02	4.03
ZnO	5.00	4.76	4.97	1.00	0.98	1.00	1.00	0.99	1.02	4.60	4.48	4.43	1.00	0.97	1.02
ZrO_2	0.00	0.00	0.03	6.00	5.65	5.84	6.00	6.15	6.00	5.42	5.23	5.42	6.00	5.83	5.82
Cl	0.80	0.33	NA	0.02	0.02	NA	0.72	0.48	NA	0.80	0.25	NA	0.17	0.12	NA
F	0.30	NA	NA	0.01	NA	NA	0.27	NA	NA	0.30	NA	NA	0.06	NA	NA
P_2O_5	0.50	0.43	0.51	0.01	0.03	0.05	0.45	0.44	0.39	0.50	0.55	0.50	0.10	0.12	0.08
SO_3	0.91	0.41	NA	1.00	0.46	NA	0.10	0.18	NA	1.00	0.52	NA	0.10	0.13	NA
Sum*	100.0	100.2	98.0	100.0	99.8	99.4	100.0	100.1	98.9	100.0	100.0	96.0	100.0	99.7	98.6

NA = Not analyzed.
* Sum includes target values for components that were not analyzed.

Table 4.1. XRF and DCP Analyses of the Twenty LORPM21-40 Glasses (continued).

Glass	LORPM31			LORPM32			LORPM33			LORPM34			LORPM35		
	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_2O_3	10.94	10.89	10.55	5.57	5.28	5.51	11.78	11.12	11.19	7.17	6.90	6.84	10.37	9.83	9.94
B_2O_3	10.13	NA	10.07	11.59	NA	11.29	11.57	NA	11.49	12.18	NA	12.10	7.55	NA	7.52
BaO	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.04	0.01	0.01	0.00	0.01	0.00	0.00	0.00
CaO	0.00	0.00	0.02	2.45	2.72	2.50	2.45	2.63	2.51	2.45	2.61	2.47	4.93	5.10	4.89
CdO	0.01	0.00	NA	0.00	0.00	NA	0.01	0.01	NA	0.01	0.01	NA	0.00	0.00	NA
Cr_2O_3	0.32	0.49	0.23	0.04	0.00	0.04	0.32	0.42	0.29	0.32	0.39	0.34	0.01	0.00	0.01
Fe_2O_3	6.38	6.67	6.31	4.33	4.53	4.28	2.30	2.55	2.30	1.84	1.93	1.88	1.84	1.93	1.89
K_2O	0.11	0.12	0.13	4.73	4.80	4.67	1.26	1.28	1.24	4.73	4.65	4.46	3.24	3.21	3.22
Li_2O	4.35	NA	4.34	3.57	NA	3.58	4.00	NA	3.99	4.00	NA	4.00	2.89	NA	2.91
MgO	0.63	0.60	0.60	3.50	3.04	3.20	3.17	2.76	3.18	3.50	3.04	3.47	3.13	2.74	3.12
Na_2O	9.46	9.90	9.17	10.00	9.74	9.85	10.00	10.11	9.45	10.08	10.34	9.56	17.30	17.57	16.31
NiO	0.03	0.04	0.06	0.00	0.00	0.02	0.03	0.03	0.05	0.03	0.04	0.05	0.00	0.00	0.01
PbO	0.03	0.05	NA	0.00	0.00	NA	0.03	0.03	NA	0.03	0.04	NA	0.00	0.00	NA
SiO_2	35.00	36.07	35.52	43.05	43.14	43.01	40.53	40.55	40.77	38.40	38.44	38.65	38.40	38.31	38.51
SnO_2	5.00	4.36	4.03	1.00	0.98	1.04	1.00	1.05	1.04	1.90	1.95	1.93	1.00	1.09	1.01
TiO_2	0.00	0.02	0.02	2.40	2.57	2.42	0.60	0.64	0.67	2.40	2.59	2.45	1.33	1.40	1.45
V_2O_5	4.00	4.33	4.04	1.08	1.13	1.09	2.09	2.23	2.16	2.19	2.25	2.24	0.89	0.93	0.90
ZnO	5.00	4.86	5.02	3.89	3.79	3.93	2.00	1.99	2.00	2.06	2.08	2.08	1.80	1.76	1.88
ZrO_2	6.00	5.60	5.65	2.00	2.04	1.96	5.00	5.34	5.14	4.68	4.82	4.65	5.00	5.19	5.06
Cl	0.80	0.28	NA	0.10	0.07	NA	0.80	0.46	NA	0.80	0.47	NA	0.02	0.03	NA
F	0.30	NA	NA	0.04	NA	NA	0.30	NA	NA	0.30	NA	NA	0.01	NA	NA
P_2O_5	0.50	0.50	0.54	0.06	0.07	0.06	0.50	0.51	0.48	0.50	0.51	0.49	0.01	0.03	0.03
SO_3	1.00	0.59	NA	0.60	0.48	NA	0.24	0.20	NA	0.42	0.35	NA	0.28	0.30	NA
Sum*	100.0	100.1	96.3	100.0	99.6	98.5	100.0	99.8	98.0	100.0	99.9	97.7	100.0	99.8	98.7

NA = Not analyzed.
* Sum includes target values for components that were not analyzed.

Table 4.1. XRF and DCP Analyses of the Twenty LORPM21-40 Glasses (continued).

Glass	LORPM36			LORPM37			LORPM38			LORPM39			LORPM40		
	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_2O_3	6.65	6.46	6.53	5.57	5.43	5.32	5.57	5.44	5.38	5.57	5.30	5.56	11.78	11.19	11.49
B_2O_3	12.18	NA	12.28	11.62	NA	11.61	7.55	NA	7.56	12.18	NA	12.04	7.55	NA	7.34
BaO	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
CaO	2.45	2.53	2.51	2.45	2.52	2.53	2.45	2.64	2.52	2.45	2.62	2.47	2.45	2.61	2.46
CdO	0.01	0.00	NA	0.00	0.00	NA	0.01	0.01	NA	0.00	0.00	NA	0.00	0.00	NA
Cr_2O_3	0.28	0.34	0.31	0.09	0.15	0.09	0.32	0.36	0.34	0.01	0.00	0.01	0.01	0.00	0.01
Fe_2O_3	1.84	1.87	1.89	2.16	2.22	2.21	6.46	6.76	6.59	6.46	6.53	6.45	5.71	5.88	5.68
K_2O	2.51	2.45	2.46	4.73	4.63	4.58	4.73	4.48	4.38	1.26	1.25	1.25	4.73	4.75	4.53
Li_2O	4.00	NA	3.99	3.66	NA	3.70	1.00	NA	1.11	4.00	NA	4.04	4.00	NA	4.03
MgO	3.50	3.20	3.37	3.50	3.08	3.36	3.50	3.06	3.33	1.00	0.97	1.08	3.50	3.41	3.32
Na_2O	12.82	13.35	12.29	12.20	12.16	11.64	13.39	13.48	12.53	17.38	17.32	16.05	10.00	9.85	9.32
NiO	0.03	0.03	0.04	0.01	0.01	0.02	0.03	0.03	0.05	0.00	0.00	0.02	0.00	0.00	0.01
PbO	0.03	0.03	NA	0.01	0.01	NA	0.03	0.03	NA	0.00	0.00	NA	0.00	0.00	NA
SiO_2	39.74	40.07	39.88	39.47	39.87	39.59	39.66	40.41	39.95	38.40	38.36	38.13	38.40	38.60	38.70
SnO_2	2.49	2.43	2.51	4.00	4.14	3.97	1.00	1.04	1.05	1.00	1.01	1.07	1.00	1.00	1.05
TiO_2	2.20	2.28	2.29	2.40	2.54	2.47	2.40	2.55	2.53	0.60	0.64	0.65	0.60	0.66	0.64
V_2O_5	0.80	0.84	0.83	0.80	0.83	0.83	0.80	0.83	0.83	3.20	3.27	3.23	0.80	0.83	0.85
ZnO	1.80	1.73	1.87	4.20	4.08	4.36	4.20	4.14	4.37	1.80	1.73	1.76	4.20	4.18	4.17
ZrO_2	5.00	4.95	5.08	2.47	2.46	2.47	4.70	4.77	4.79	4.40	4.38	4.32	5.00	5.03	5.04
Cl	0.70	0.45	NA	0.21	0.16	NA	0.80	0.39	NA	0.02	0.03	NA	0.02	0.03	NA
F	0.26	NA	NA	0.08	NA	NA	0.30	NA	NA	0.01	NA	NA	0.01	NA	NA
P_2O_5	0.43	0.47	0.46	0.13	0.15	0.17	0.50	0.53	0.50	0.01	0.02	0.01	0.01	0.03	0.01
SO_3	0.28	0.25	NA	0.24	0.23	NA	0.60	0.36	NA	0.24	0.25	NA	0.24	0.23	NA
Sum*	100.0	100.2	98.6	100.0	100.0	98.9	100.0	100.1	97.8	100.0	99.9	98.1	100.0	99.8	98.7

NA = Not analyzed.
* Sum includes target values for components that were not analyzed.

Table 4.2. PCT Results[(a)] for the Twenty LORPM21-40 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
LORPM21	10.66	15.48	80.83	44.88	0.388	0.679	0.214	0.194	0.339	0.107
LORPM22	11.71	6.85	224.24	41.18	0.368	1.393	0.252	0.184	0.696	0.126
LORPM23	10.51	12.92	35.76	53.68	0.589	0.547	0.313	0.294	0.274	0.157
LORPM24	10.51	9.64	70.6	44.83	0.517	0.706	0.267	0.259	0.353	0.133
LORPM25	11.05	58.57	159.24	46.74	1.479	1.175	0.269	0.739	0.587	0.135
LORPM26	10.45	5.31	34.27	20.62	0.284	0.421	0.125	0.142	0.210	0.063
LORPM27	10.81	10.94	40.34	50.55	0.584	0.622	0.278	0.292	0.311	0.139
LORPM28R1-1	10.42	327.59	444.32	195.66	7.690	4.188	0.928	3.845	2.094	0.464
LORPM28R1-2	10.48	315.99	461.22	191.40	7.418	4.248	0.908	3.709	2.174	0.454
LORPM29	10.66	25.86	48.78	48.16	0.836	0.739	0.293	0.418	0.369	0.146
LORPM30	11.2	17.64	48.88	36.67	0.947	1.318	0.224	0.474	0.659	0.112
LORPM31	9.91	18.73	23.65	54.6	0.593	0.336	0.332	0.296	0.168	0.166
LORPM32	10.42	41.5	77.4	73.61	1.152	1.042	0.365	0.576	0.521	0.183
LORPM33	10.06	18.75	30.85	42.35	0.522	0.416	0.223	0.261	0.208	0.112
LORPM34	10.41	37.95	65.21	48.9	1.002	0.872	0.272	0.501	0.436	0.136
LORPM35	11.51	29.52	172.75	66.45	1.260	1.346	0.370	0.630	0.673	0.185
LORPM36	10.61	29.93	71.27	52.13	0.791	0.749	0.281	0.395	0.375	0.140
LORPM37	10.8	37.53	86.72	70.39	1.040	0.958	0.382	0.520	0.479	0.191
LORPM38	10.6	17.42	77.44	54.14	0.742	0.778	0.291	0.371	0.389	0.146
LORPM39	11.77	202.11	513.17	178.97	5.343	3.979	0.997	2.672	1.990	0.499
LORPM40	10.87	14.14	45.89	45.9	0.603	0.618	0.256	0.302	0.309	0.128

(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/m^2) are normalized based on the target compositions presented in Section 2.

Table 4.3. VHT Results for the Twenty LORPM21-40 Glasses.

Glass ID	Alteration Depth (μm)	Ln (Depth, μm)	Days	Rate ($g/m^2/d$) Calculated for Estimated Average Glass Density of 2.65 g/cc	Comparison to Limit of 50 $g/m^2/d$
LORPM21	20.5	3.0204	24	2.3	5%
LORPM22	11.6	2.4484	24	1.3	3%
LORPM23	80.0	4.3822	24	8.8	18%
LORPM24	14.9	2.6987	24	1.6	3%
LORPM25	550	6.3103	24	60.8	122%
LORPM26	81.7	4.4031	24	9.0	18%
LORPM27	29.3	3.3759	24	3.2	6%
LORPM28R1	176.5	5.1733	24	19.5	39%
LORPM29	30.8	3.4285	24	3.4	7%
LORPM30	1.4	0.3075	24	0.2	0.3%
LORPM31	404	6.0014	24	44.6	89%
LORPM32	511	6.2365	24	56.4	113%
LORPM33	23.9	3.1718	24	2.6	5%
LORPM34	10.7	2.3702	24	1.2	2%
LORPM35	336	5.8171	24	37.1	74%
LORPM36	4.1	1.4207	24	0.5	1%
LORPM37	547	6.3050	24	60.4	121%
LORPM38	2.0	0.6931	24	0.2	0.4%
LORPM39	319	5.7636	24	35.2	70%
LORPM40	9.7	2.2701	24	1.1	2%

Table 4.4. Melt Electrical Conductivity Data for the Twenty LORPM21-40 Glasses.

Glass ID	Temp1 (ºC)	EC1 (S/cm)	Temp2 (ºC)	EC2 (S/cm)	Temp3 (ºC)	EC3 (S/cm)	Temp4 (ºC)	EC4 (S/cm)
LORPM21	971	0.101	1066	0.176	1161	0.267	1256	0.385
LORPM22	971	0.262	1066	0.393	1161	0.578	1256	0.783
LORPM23	969	0.173	1065	0.275	1162	0.387	1257	0.525
LORPM24	974	0.085	1068	0.160	1163	0.228	1258	0.309
LORPM25	972	0.222	1067	0.329	1163	0.455	1259	0.622
LORPM26	971	0.041	1066	0.083	1160	0.139	1256	0.212
LORPM27	971	0.138	1069	0.228	1163	0.337	1258	0.455
LORPM28R1	974	0.291	1070	0.431	1165	0.607	1260	0.76
LORPM29	973	0.172	1067	0.286	1162	0.418	1256	0.554
LORPM30	972	0.073	1068	0.157	1163	0.265	1258	0.471
LORPM31	974	0.211	1069	0.318	1164	0.432	1259	0.569
LORPM32	972	0.143	1068	0.235	1162	0.363	1258	0.513
LORPM33	974	0.132	1069	0.213	1164	0.309	1258	0.435
LORPM34	972	0.149	1068	0.244	1162	0.358	1257	0.558
LORPM35	974	0.232	1069	0.354	1165	0.498	1261	0.675
LORPM36	972	0.171	1067	0.280	1162	0.414	1257	0.568
LORPM37	972	0.172	1068	0.271	1163	0.405	1259	0.588
LORPM38	975	0.102	1070	0.173	1165	0.268	1260	0.382
LORPM39	973	0.354	1069	0.534	1164	0.697	1258	0.882
LORPM40	973	0.118	1067	0.202	1164	0.303	1258	0.443

Table 4.5. Melt Viscosity Data for the Twenty LORPM21-40 Glasses.

Glass ID	Temp1 (ºC)	Vis1 (P)	Temp2 (ºC)	Vis2 (P)	Temp3 (ºC)	Vis3 (P)	Temp4 (ºC)	Vis4 (P)
LORPM21	953	277.73	1053	70.77	1153	26.33	1253	12.29
LORPM22	951	288.93	1052	55.31	1152	16.76	1253	6.48
LORPM23	Non-Newtonian fluid (1.2 vol% $ZrO_{2)}$				1155	43.03	1255	14.74
LORPM24	Non-Newtonian fluid (1.0 vol% ZrO_2)						1251	77.49
LORPM25	946	454.16	1046	128.01	1146	46.77	1247	21.07
LORPM26	Non-Newtonian fluid (1.3 vol% SnO_2)						1251	35.36
LORPM27	950	590.17	1051	165.86	1151	55.32	1251	22.62
LORPM28R1	945	274.36	1046	72.21	1146	25.82	1246	11.44
LORPM29	Non-Newtonian fluid (1.5 vol% SnO_2)						1250	16.83
LORPM30	0.7 vol% SnO_2		1057	87.59	1158	12.45	1260	4.67
LORPM31	Non-Newtonian fluid (1.4 vol% ZrO_2 + spinels)							
LORPM32	949	206.19	1050	63.16	1150	25.15	1250	11.97
LORPM33	949	625.7	1050	160.61	1150	54.47	1250	23.38
LORPM34	946	198.61	1048	56.85	1149	21.24	1252	9.72
LORPM35	946	298.97	1047	83.82	1147	30.84	1247	14.38
LORPM36	948	195.65	1049	54.65	1150	20.82	1250	9.53
LORPM37	946	159.19	1047	46.22	1147	17.79	1247	8.23
LORPM38	951	795.77	1052	174.67	1152	55.04	1252	22.14
LORPM39	950	65.09	1051	23.11	1151	9.93	1251	5.11
LORPM40	948	532.12	1049	133.98	1150	45.74	1250	19.23

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].

Model form to predict the natural logarithm of the normalized PCT-B release (in g/L):

$$\ln(PCT-B) = \sum_{i=1}^{q} b_i x_i + \text{Selected}\left\{\sum_{i<}^{q-1}\sum_{j}^{q} b_{ij} x_i x_j\right\}$$

The x_i (i = 1, 2, …, q) are normalized mass fractions of q glass oxide components such that $\sum_{i=1}^{q} x_i = 1$.

The b_i (i = 1, 2, …, q) and selected b_{ij} are coefficients listed below.

ln(PCT-B) Reduced PQM Model Term	**Coefficient Estimate**	**Coefficient Stand. Dev.**
Al_2O_3	-31.3612	2.1310
B_2O_3	11.8101	2.5505
CaO	-13.8404	3.0142
Fe_2O_3	-16.5948	3.2161
K_2O	7.9687	1.7452
Li_2O	83.3036	8.4889
MgO	-21.2343	8.2492
Na_2O	46.1599	5.2140
P_2O_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_2O	-251.2654	53.4354
B_2O_3×MgO	488.8612	89.5443
B_2O_3×Li_2O	-374.9533	72.1448
Na_2O×SiO_2	-74.3462	13.1157
CaO×Fe_2O_3	212.0947	46.0965
Modeling Data Statistic (applied to 244 WTP Glasses):	R^2 = 0.866	

(a) "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, SO_3, TiO_2, 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].

Model form to predict the natural logarithm of the normalized PCT-Na release (in g/L):

$$\ln(PCT-Na) = \sum_{i=1}^{q} b_i x_i + \text{Selected}\left\{\sum_{i=1}^{q} b_{ii} x_i^2 + \sum_{i<}^{q-1}\sum_{j}^{q} b_{ij} x_i x_j\right\}$$

The x_i (i = 1, 2, …, q) are normalized mass fractions of q glass oxide components such that $\sum_{i=1}^{q} x_i = 1$.

The b_i (i = 1, 2, …, q) and selected b_{ii} and b_{ij} are coefficients listed below.

ln(PCT-Na) Reduced PQM Model Term	**Coefficient Estimate**	**Coefficient Stand. Dev.**
Al_2O_3	-20.7142	1.6238
B_2O_3	-6.5489	2.7610
CaO	0.0151	2.5591
Fe_2O_3	-8.4617	2.6039
K_2O	-0.8724	3.9729
Li_2O	44.7604	3.5466
MgO	-13.8667	7.2503
Na_2O	9.9942	1.6770
P_2O_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_2O	-232.1695	46.7097
CaO×Fe_2O_3	182.6191	40.4128
B_2O_3×MgO	437.4267	77.8463
B_2O_3×Na_2O	87.6716	19.0092
K_2O×K_2O	315.6867	83.2397
Modeling Data Statistic (applied to 244 WTP Glasses):	R^2 = 0.870	

(a) "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, SO_3, TiO_2, 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].

Model form to predict the natural logarithm of the VHT alteration depth, D, in microns:

$$\ln(D) = \sum_{i=1}^{q} b_i x_i + \text{Selected}\left\{\sum_{i=1}^{q} b_{iii} x_i^3 + \sum_{i<}^{q-1}\sum_{j}^{q} b_{iij} x_i^2 x_j + \sum_{i<}^{q-2}\sum_{j<}^{q-1}\sum_{k}^{q} b_{ijk} x_i x_j x_k\right\}$$

The x_i (i = 1, 2, …, q) are normalized mass fractions of q glass oxide components such that $\sum_{i=1}^{q} x_i = 1$.

The b_i (i = 1, 2, …, q) and selected b_{iii} , b_{iij} and b_{ijk} are coefficients listed below.

ln(D) Reduced Partial Cubic Mixture Model Term	**Coefficient Estimate**	**Coefficient Stand. Dev.**
Al_2O_3	19.5685	6.0850
B_2O_3	18.5336	5.9232
CaO	38.2412	9.4479
Fe_2O_3	-8.4126	4.7225
K_2O	-39.3124	10.7075
Li_2O	-17.8250	20.0670
MgO	-8.3068	8.0413
Na_2O	-20.6518	10.4755
SiO_2	-0.5137	2.2871
ZrO_2	-62.8457	7.5911
Others[(a)]	-0.4293	5.3481
$(K_2O)^2 \times Na_2O$	10138.2817	1198.5167
$(Na_2O)^3$	872.6563	130.6419
$Li_2O \times Na_2O \times SiO_2$	2139.8048	387.6038
$B_2O_3 \times CaO \times Na_2O$	-1943.0687	773.3618
Modeling Data Statistic (applied to 165 WTP Glasses)	R^2 = 0.744	

(a) "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, SO_3, TiO_2, and ZnO.

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

Model form to predict the natural logarithm of EC, in ln(S/cm):

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

The x_i (i = 1, 2, …, q) are normalized mass fractions of q glass oxide components such that $\sum_{i=1}^{q} x_i = 1$.

The b_i (i = 1, 2, …, q) and selected a_{ij} are coefficients listed below.

Mixture Terms (a_i)	**Coefficient Estimate**	**Coefficient Stand. Dev.**	**Mixture-Temp. Terms [x_i/(T/1000)]**	**Coefficient Estimate**	**Coefficient Stand. Dev.**
Al_2O_3	2.3854	2.5456	Al_2O_3/(T/1000)	-9.0593	3.1966
B_2O_3	7.9750	1.7536	B_2O_3/(T/1000)	-11.0983	2.1885
CaO	5.2093	3.0161	CaO/(T/1000)	-30.6535	1.8797
Fe_2O_3	4.3935	1.6656	Fe_2O_3/(T/1000)	-9.2407	2.0700
K_2O	7.6774	2.1834	K_2O/(T/1000)	-11.5299	2.7137
Li_2O	4.2464	5.0291	Li_2O/(T/1000)	30.4827	4.2400
MgO	15.1675	3.2610	MgO/(T/1000)	-25.0634	4.0719
Na_2O	-2.0291	1.2653	Na_2O/(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_2O	144.9519	44.2208			
CaO×Na_2O	79.0190	14.6533			
Li_2O×Na_2O	-130.1441	17.2032			
Modeling Data Statistic (applied to 171 WTP Glasses)				R^2 = 0.951	

(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.

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].

Model form to predict the natural logarithm of viscosity, in ln(P)

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

The x_i (i = 1, 2, …, q) are normalized mass fractions of q glass oxide components such that $\sum_{i=1}^{q} x_i = 1$.

The b_i (i = 1, 2, …, q) and selected a_{ii} or a_{ij} are coefficients listed below.

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.

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	$Al_2O_3/(T/1000)^2$	24.6423	2.2683
B_2O_3	-42.3772	6.8657	$B_2O_3/(T/1000)^2$	(b)	(b)
CaO	-10.6445	0.9836	$CaO/(T/1000)^2$	13.7793	1.3498
Fe_2O_3	-4.6220	1.0390	$Fe_2O_3/(T/1000^2$	15.2036	1.4269
K_2O	-0.8689	0.9358	$K_2O/(T/1000)^2$	(b)	(b)
Li_2O	10.9390	4.5502	$Li_2O/(T/1000)^2$	-82.4815	2.9954
MgO	-5.6188	5.5224	$MgO/(T/1000)^2$	22.7608	2.8130
Na_2O	0.9073	0.6740	$Na_2O/(T/1000)^2$	-14.5621	0.8958
P_2O_5	-0.8081	2.8760	$P_2O_5/(T/1000)^2$	24.0339	4.2324
SiO_2	1.5575	0.5247	$SiO_2/(T/1000)^2$	24.4077	0.5709
ZrO_2	-12.0741	2.0755	$ZrO_2/(T/1000)^2$	48.2286	2.9522
Others[(a)]	-9.3903	1.4313	Others/$(T/1000)^2$	17.3800	2.0519
$(B_2O_3)^2$	198.7360	36.5259			
$(Li_2O)^2$	133.6906	43.1873			
$Al_2O_3 \times Li_2O$	-136.5095	56.0571			
$(MgO)^2$	-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 Region and Component Limits Applied in Modeling (Mass Fraction).

Component	Minimum Rounded Down	Maximum Rounded Up	Adjusted
Al_2O_3	0.034	0.14	-
B_2O_3	0.059	0.152	-
CaO	0	0.129	-
Fe_2O_3	0	0.120	-
K_2O	0	0.081	-
Li_2O	0	0.063	-
MgO	0	0.100	0.051
Na_2O	0.024	0.261	-
SiO_2	0.332	0.522	-
ZrO_2	0	0.068	-
SnO_2	0	0.051	-
V_2O_5	0	0.041	-
P_2O_5	0	0.048	-
Others 2006 Model	0.016	0.185	-
Others 2012 Model	0.014	0.103	-
Others 2012 Model with V_2O_5	0.016	0.138	-
SO_3 XRF Measured or Interpolated	0	0.021	-
TiO_2	0	0.040	-
ZnO	0.009	0.059	-
BaO	0	0.001	-
Br	0	0.001	-
CdO	0	0.002	-
Cl	0	0.012	-
Cr_2O_3	0	0.015	-
Cs_2O	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_2O_7	0	0.002	-
SeO_2	0	0.002	-
SrO	0	0.001	-
Unknown	0	0.003	-

- Empty data field.

Table 5.7. Eighteen 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%)
LAWE3Cr2CCC	Non-representative composition & heat treatment
LAWE9HCr1CCC	Non-representative composition & heat treatment
LAWE9HCr2CCC	Non-representative composition & heat treatment
LAWE10HCr3CCC	Non-representative composition & heat treatment
LAWM12	PCT Grubbs' test outlier with one PCT release greater than 8 g/L
LAWM17	PCT Grubbs' test outlier with one PCT release greater than 8 g/L
LAWM35	PCT Grubbs' test outlier with one PCT release greater than 8 g/L
LAWM55	PCT Grubbs' test outlier with one PCT release greater than 8 g/L
LAWM56	PCT Grubbs' test outlier with one PCT release greater than 8 g/L
ORPLG13	PCT Grubbs' test outlier with one PCT release greater than 8 g/L
ORPLG14	PCT Grubbs' test outlier with one PCT release greater than 8 g/L
ORPLG15	PCT Grubbs' test outlier with one PCT release greater than 8 g/L
LORPM13[(a)]	PCT-Na Grubbs' test outlier

(a) Identified as outlier only in later models.

Table 5.8. Twenty-Seven 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
LAWE11	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
LAWE12	2.4012	2.1190
LAWA189	2.3285	2.3643
ORPLA37	4.5818	3.1776

Table 5.9. Variation in PCT-Boron and PCT-Sodium Releases 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)
LAWM1	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**
LAWM9	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[i]	29.686	3.39068	16.081	2.77764
LAWM55[i]	35.657	3.57395	22.937	3.13275
	%RSD = 12.92	**SD = 0.1296**	**%RSD = 24.85**	**SD = 0.2511**
LAWM35[i]	10.526	2.35385	6.625	1.89085
LAWM56[i]	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	-0.41552	0.723	-0.32435
	%RSD = 0.64	**SD = 0.0063**	**%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 = 0.2269**	**%RSD = 19.07**	**SD = 0.1760**

[a] Because glass compositions were renormalized based on analyzed (or estimates of analyzed) SO_3 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.
[i] These PCT data were not considered in later models where PCT releases greater than 8 g/L were excluded.

Table 5.9. Variation in PCT-Boron and PCT-Sodium Releases 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
WVW-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**
LORPM28R1-1	7.690	2.03989	4.188	1.43225
LORPM28R1-2	7.418	2.00384	4.347	1.46958
	%RSD = 2.55	**SD = 0.0255**	**%RSD = 2.64**	**SD = 0.0264**
Pooled Over 16 ORP Replicates	**%RSD = 17.54**	**SD = 0.1733**	**%RSD =17.56**	**SD = 0.1730**
Pooled Over 28 Sets of Replicates	**%RSD = 20.29**	**SD = 0.1918**	**%RSD =17.88**	**SD = 0.1728**

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

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

Model Number	**1 [1]**		**2 [23]**		**3**		**4**	
Glass Count	244 (+20 outliers)		413 (+16 outliers +28 validation)		436 (+17 outliers +27 validation)		436 (+17 outliers +27 validation)	
Model Terms	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.
Al_2O_3	-20.714	1.624	-10.587	1.215	1.845	11.805	-24.506	4.157
B_2O_3	-6.549	2.761	2.682	0.919	15.276	2.882	5.116	0.917
CaO	0.015	2.559	-5.122	1.111	-3.275	3.032	-5.155	1.409
Fe_2O_3	-8.462	2.604	-4.37	2.316	-	-	-	-
K_2O	-0.872	3.973	9.042	0.841	39.491	5.183	41.243	5.080
Li_2O	44.760	3.547	29	2.819	56.375	6.708	43.578	3.511
MgO	-13.867	7.250	13.734	1.475	12.483	1.759	15.980	1.335
Na_2O	9.994	1.677	22.979	2.124	10.070	1.018	13.148	0.519
P_2O_5	-14.532	2.403	-15.71	2.069	100.961	32.162	80.051	29.004
SiO_2	-4.883	0.514	-3.422	0.586	-4.528	0.845	-4.949	0.349
SnO_2	-	-	-18.225	2.499	-6.160	1.712	-2.325	1.595
TiO_2	-	-	-	-	-52.158	9.490	-16.527	2.977
ZrO_2	-0.620	2.210	-4.158	1.271	-5.407	1.391	-3.871	1.121
Others[(a)]	3.345	1.434	-3.197	0.988	7.835	3.375	7.314	3.099
$Al_2O_3 \times Al_2O_3$	-	-	-	-	77.509	29.375	108.571	24.734
$Al_2O_3 \times B_2O_3$	-	-	-	-	-99.784	29.968	-	-
$Al_2O_3 \times Fe_2O_3$	-	-	-95.941	29.875	-	-	-	-
$Al_2O_3 \times K_2O$	-	-	-		-165.260	37.237	-126.849	35.475
$Al_2O_3 \times Li_2O$	-	-	-		-179.499	40.501	-187.784	35.498
$Al_2O_3 \times SiO_2$	-	-	-		-36.324	20.554		
$B_2O_3 \times K_2O$	-	-		-	-205.257	45.321	-223.153	44.003
$B_2O_3 \times CaO$	-	-	-	-	-45.953	22.288	-	-
$B_2O_3 \times Li_2O$	-	-	-	-	-154.335	44.063	-	-
$B_2O_3 \times MgO$	437.426	77.846	-	-	-	-	-	-
$B_2O_3 \times Na_2O$	87.672	19.009	-		-	-	-	-
$CaO \times Fe_2O_3$	182.619	40.413	158.307	16.345	-	-	-	-
$CaO \times Li_2O$	-232.170	46.710	-105.377	30.144	-125.830	26.650	-116.819	25.514
CaO×Others	-	-			52.128	18.665	67.777	16.690
$CaO \times SnO_2$	-	-	200.605	45.582				
$CaO \times TiO_2$	-	-	-	-	276.653	56.951	159.881	43.720
$(K_2O)^2$	315.687	83.240	-	-	-			
$K_2O \times Li_2O$	-	-	-	-	-240.946	44.772	-207.756	43.082
$K_2O \times SnO_2$	-	-	-	-	-111.541	47.526	-158.678	47.769
$MgO \times P_2O_5$	-	-	-	-	708.515	321.075	-	-
$Na_2O \times SiO_2$	-	-	-24.057	5.552	-	-	-	-
$Na_2O \times TiO_2$	-	-	-	-	63.391	33.551	-	-
$(Others)^2$	-	-	-	-	-73.633	16.852	-61.290	16.141
$P_2O_5 \times TiO_2$	-	-	-	-	837.101	233.349	-	-
$SiO_2 \times P_2O_5$	-	-	-	-	-317.750	78.985	-212.005	64.466
$(TiO^2)^2$	-	-	-	-	557.798	155.643	-	-

(a) "Others" components include the original "Others" component (which contains 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, SO_3, ZnO, and V_2O_5, plus TiO_2 in Models 1 and 2, and SnO_2 in Model 1.

- Empty data field.

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

Model	**1 [1]**	**2 [23]**	**3**	**4**
Number of Terms	17	18	32	24
Modeling Data Statistics				
R^2	0.870	0.861/ 0.796[(c)]	0.878	0.866
$R^2_{Adjusted}$	0.861	0.855 0.787[(c)]	0.868	0.858
$R^2_{Predict}$	0.840	0.846	0.857	0.849
LOF	0.055	0.011	0.027	0.015
Validation Statistics on 27 Glasses Selected Over Full Data Range				
$R^2_{Validation}$	0.199[(b)]	0.864	0.862	0.890
$RMSE_{Validation}$	0.548	0.200	0.201	0.180

(a) "Others" components include the original "Others" component (which contains 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, SO_3, ZnO and V_2O_5, plus TiO_2 in Models 1 and 2, and SnO_2 in Model 1.

(b) Validation set was limited to 17 ORP-LAW glasses since 10 WTP-LAW glasses were already used in the model design [1] and none were set aside for independent validation.

(c) Statistics recalculated with the updated data set of 436 PCT-B including the LORPM glasses.

Table 5.11. Regression Coefficients' *p*-Values for PCT-Na Model Quadratic Terms.

Model Number	**Model 3**	**3B**	**Model 4**
Model Terms	RS 5 Fold Optimization	MRS 5 Fold Optimization	RS at *p*-value thresholds of 0.01
$(Al_2O_3)^2$	0.0086	-	<.0001
$Al_2O_3 \times B_2O_3$	0.0009	<.0001	-
$Al_2O_3 \times K_2O$	<.0001	<.0001	0.0004
$Al_2O_3 \times Li_2O$	<.0001	0.011	<.0001
$Al_2O_3 \times MgO$	-	0.0038	-
$Al_2O_3 \times Na_2O$	-	0.0224	-
$Al_2O_3 \times SiO_2$	0.0779	<.0001	-
$B_2O_3 \times CaO$	0.0399	-	-
$B_2O_3 \times K_2O$	<.0001	<.0001	<.0001
$B_2O_3 \times Li_2O$	0.0005	-	-
$B_2O_3 \times TiO_2$	-	0.0105	-
$CaO \times Li_2O$	<.0001	<.0001	<.0001
$CaO \times MgO$	-	0.958	-
CaO×Others	0.0055	<.0001	<.0001
$CaO \times SiO_2$	-	0.0134	-
$CaO \times TiO_2$	<.0001	0.0012	0.0003
$CaO \times ZrO_2$	-	<.0001	-
$K_2O \times Li_2O$	<.0001	0.0082	<.0001
$K_2O \times SnO_2$	0.0194	0.0007	0.001
$K_2O \times TiO_2$	-	0.0391	-
Li2O×MgO	-	0.0278	-
$Li_2O \times P_2O_5$	-	0.0433	-
$Li_2O \times ZrO_2$	-	0.0049	-
$MgO \times Na_2O$	-	0.0023	-
$MgO \times P_2O_5$	0.0279	0.1342	-
$Na_2O \times P_2O_5$	-	0.0048	-
$Na_2O \times TiO_2$	0.0595	-	-
$(Others)^2$	<.0001	-	0.0002
$P_2O_5 \times TiO_2$	0.0004	-	-
$SiO_2 \times P_2O_5$	<.0001	-	0.0011
$(TiO^2)^2$	0.0004	-	-
Number of Terms	32	36	24

- Empty data field.

Table 5.12. Coefficients and Performance Summary for Various Reduced Partial Quadratic Mixture Models on the Natural Logarithm of ILAW PCT-B.

Model	**1 [1]**		**2 [23]**		**3**		**4**		**5**		**6**	
Glass Count	244 (+20 outliers)		413 (+17 outliers +27 validation)		436 (+17 outliers +27 validation)		436 MRS, *p*-value thresholds: 0.025/0.025		436, MRS, *p*-value thresholds: 0.01/0.01		436 MRS, *p*-value thresholds: 0.005/0.005	
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_2O_3	-31.361	2.131	-9.063	1.252	-8.330	8.530	2.178	7.621	4.201	7.631	15.293	7.010
B_2O_3	11.810	2.550	18.482	1.268	14.086	1.589	15.317	1.426	15.205	1.435	11.695	1.211
CaO	-13.840	3.014	-22.305	1.858	-20.984	2.659	-12.456	1.683	-12.188	1.692	-16.280	1.287
Fe_2O_3	-16.595	3.216	-13.267	1.376	-10.138	4.145	3.833	2.652	4.088	2.668	-1.176	2.366
K_2O	7.969	1.745	112.383	17.487	33.383	6.097	34.103	5.963	34.416	6.002	33.607	6.207
Li_2O	83.304	8.489	-49.706	11.101	-80.080	20.145	-120.902	15.179	-120.900	15.282	-105.970	15.317
MgO	-21.234	8.249	24.264	1.723	21.396	3.754	17.773	3.289	17.157	3.303	13.819	3.233
Na_2O	46.160	5.214	15.164	0.661	29.079	4.755	16.294	1.130	15.873	1.125	13.077	0.874
P_2O_5	-19.254	2.818	-11.459	2.408	10.865	18.960	27.403	19.325	46.431	17.955	-11.999	2.474
SiO_2	-1.616	1.113	-7.674	0.440	-2.887	1.689	-7.041	1.190	-6.936	1.198	-4.943	0.986
SnO_2	-	-	-9.135	3.426	-25.843	4.662	-10.093	2.168	-9.989	2.183	-9.015	1.587
TiO_2	-	-	-	-	-29.161	5.629	-5.541	2.475	-5.491	2.492	-8.697	2.424
ZrO_2	-6.629	2.787	-10.105	2.293	-5.375	3.148	4.594	2.551	4.952	2.564	-4.131	2.070
Others[(a)]	-5.169	1.857	-3.175	1.205	-55.141	15.239	-54.990	15.152	-53.530	15.244	2.196	1.344
Al_2O_3×Fe_2O_3	-	-	-	-	102.474	32.772	-	-	-	-	-	-
Al_2O_3×K_2O	-	-	-277.876	57.221	-150.028	45.122	-144.450	43.251	-145.915	43.541	-183.545	43.685
Al_2O_3×Others	-	-	-	-	246.840	54.564	249.063	53.655	235.631	53.760		
Al_2O_3×SiO_2	-	-	-	-	-55.729	20.043	-62.684	19.143	-66.598	19.211	-67.701	18.844
Al_2O_3×SnO_2	-	-	-	-	155.235	50.468	-	-	-	-	-	-
B_2O_3 ×Li_2O	-374.954	72.145	-161.944	49.820	-	-	-	-	-	-	-	-
B_2O_3×K_2O	-	-	-270.939	58.868	-198.259	48.737	-194.095	49.147	-200.029	49.426	-192.894	50.667
B_2O_3×MgO	488.862	89.544	-	-	-	-	-	-	-	-	-	-
CaO×Fe_2O_3	212.095	46.097	278.781	20.570	106.402	26.110	75.273	21.886	71.166	21.975	98.163	21.113
CaO×Li_2O	-251.265	53.435	-	-	-	-	-	-	-	-	-	-
CaO×MgO	-	-	-	-	226.900	42.022	271.614	39.487	285.073	39.400	263.611	39.748
CaO×P_2O_5	-	-	-	-	414.812	141.212	371.677	145.382	-	-	-	-
CaO×SnO_2	-	-	99.796	56.039	-	-	-	-	-	-	-	-
CaO×TiO_2	-	-	-	-	185.924	59.745	-	-	-	-	-	-
CaO×ZrO_2	-	-	230.541	40.879	147.543	39.541	-	-	-	-	-	-
Fe_2O_3×K_2O	-	-	-	-	130.457	29.990	137.592	30.541	141.684	30.706	124.296	30.355
Fe_2O_3×Li_2O	-	-	-	-	317.816	43.955	368.875	43.386	379.687	43.473	289.411	40.298
Fe_2O_3×MgO	-	-	-	-	-239.231	49.556	-215.522	48.422	-225.394	48.596	-211.860	48.529
Fe_2O_3×TiO_2	-	-	-	-	274.167	78.321	-	-	-	-	-	-
Fe_2O_3×ZrO_2	-	-	-	-	-207.112	51.010	-253.214	46.663	-257.590	46.949	-173.193	45.721
K_2O×SiO_2	-	-	-131.361	34.008	-	-	-	-	-	-	-	-
K_2O×SnO_2	-	-	-284.835	67.949	-	-	-	-	-	-	-	-
Li_2O×Na_2O	-	-	-	-	72.906	22.539	71.793	22.702	77.329	22.752	67.832	23.359
Li_2O×SiO_2	-	-	209.400	22.592	156.410	43.856	250.832	28.857	247.644	29.026	228.319	28.810
Li_2O×SnO_2	-	-	-	-	286.182	68.354	204.851	66.672	184.431	66.642		
Li_2O×ZrO_2	-	-	-	-	518.034	75.552	539.125	77.615	533.996	78.116	422.815	75.668
Na_2O×SiO_2	-74.346	13.116	-	-	-33.282	12.428	-	-	-	-	-	-
SiO_2×Others	-	-	-	-	89.204	29.855	93.325	30.088	92.516	30.291	-	-
ZrO_2×P_2O_5	-	-	-	-	-1268.677	569.534	-1673.268	576.496	-1785.002	578.743	-	-

[(a)] "Others" components include the original "Others" component (which contains 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, SO_3, TiO_2, ZnO and V_2O_5, plus TiO_2 in Models 1 and 2, and SnO_2 in Model 1.

- Empty data field.

Table 5.12. Coefficients and Performance Summary for Various Reduced Partial Quadratic Mixture Models on the Natural Logarithm of ILAW PCT-B (continued).

PCT-B Model	Model Number					
	1 [1]	**2 [23]**	**3**	**4**	**5**	**6**
Number of Terms	17	22	37	31	30	26
Modeling Data Statistics						
R^2	0.866	0.865 / 0.790[(c)]	0.885	0.874	0.872	0.862
$R^2_{Adjusted}$	0.857	0.858/ 0.779[(c)]	0.875	0.865	0.863	0.853
$R^2_{Predict.}$	0.835	0.843	0.853	0.848	0.845	0.838
LOF	0.108	0.070	0.022	0.012	0.011	0.006
Validation Statistics on 27 Glasses Selected Over Full Data Range – 17 ORP-LAW and 10 WTP-LAW Glasses						
$R^2_{Validation}$	0.630[(b)]	0.825	0.825	0.813	0.748	0.797
$RMSE_{Validation}$	0.468 [(b)]	0.282	0.282	0.292	0.339	0.304

(a) "Others" components include the original "Others" component (which contains 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, SO_3, ZnO and V_2O_5, plus TiO_2 in Models 1 and 2, and SnO_2 in Model 1.

(b) Validation set was limited to 17 ORP-LAW glasses since 10 WTP-LAW glasses were already used in the model design [1] and none were set aside for independent validation.

(c) Statistics recalculated with the updated data set of 436 PCT-B including the LORPM glasses.

Table 5.13. Regression Coefficients' *p*-Values for PCT-B Model Quadratic Terms.

Model Terms	**3**	**3B**	**4**	**5**	**6**
	(436-MRS,5Fold)	(436-RS,5Fold)	436.MRS *p*-values thresholds: 0.025	436.MRS *p*-values thresholds: 0.01	436.MRS *p*-values thresholds: 0.005
$(Al_2O_3)^2$	-	<.0001	-	-	-
Al_2O_3×CaO	-	<.0001	-	-	-
Al_2O_3× Fe_2O_3	0.002	<.0001	-	-	-
Al_2O_3×K_2O	0.001	0.2806	0.0009	0.0009	<.0001
Al_2O_3×MgO	-	0.0005	-	-	-
Al_2O_3×Others	<.0001	<.0001	<.0001	<.0001	
Al_2O_3×SiO_2	0.006	0.0558	0.0011	0.0006	0.0004
Al_2O_3×SnO_2	0.002	<.0001	-	-	-
Al_2O_3×TiO_2	-	0.0031	-	-	-
B_2O_3×K_2O	<.0001	0.3294	<.0001	<.0001	0.0002
B_2O_3×TiO_2	-	0.0053	-	-	-
B_2O_3×ZrO_2	-	0.0007	-	-	-
CaO×CaO	-	0.0066	-	-	-
CaO×Fe_2O_3	<.0001	<.0001	0.0006	0.0013	<.0001
CaO×MgO	<.0001	0.0236	<.0001	<.0001	<.0001
CaO×Na2O	-	0.0001	-	-	-
CaO×P_2O_5	0.004	<.0001	0.0109	-	-
CaO×TiO_2	0.002	<.0001	-	-	-
CaO×ZrO_2	0.000	<.0001	-	-	-
$(Fe_2O_3)^2$	-	0.12	-	-	-
Fe_2O_3×K_2O	<.0001	<.0001	<.0001	<.0001	<.0001
Fe_2O_3×Li_2O	<.0001	<.0001	<.0001	<.0001	<.0001
Fe_2O_3×MgO	<.0001	<.0001	<.0001	<.0001	<.0001
Fe_2O_3×Na_2O	-	0.3469			
Fe_2O_3×TiO_2	0.001	<.0001			
Fe_2O_3×ZrO_2	<.0001	0.0003	<.0001	<.0001	0.0002
$(K_2O)^2$	-	<.0001	-	-	-
K_2O×Li_2O	-	0.0029	-	-	-
K_2O×MgO	-	<.0001	-	-	-
K_2O× Na_2O	-	0.0001	-	-	-
Li_2O×Li_2O	-	<.0001	-	-	-
Li_2O×MgO	-	0.0003	-	-	-
Li_2O× Na_2O	0.001	<.0001	0.0017	0.0007	0.0039
Li_2O×SiO_2	0.000	0.067	<.0001	<.0001	<.0001
Li_2O×SnO_2	<.0001	<.0001	0.0023	0.0059	-
Li_2O×ZrO_2	<.0001	0.1867	<.0001	<.0001	<.0001
MgO×ZrO_2	-	0.9192	-	-	-
Na_2O×Others	-	<.0001	-	-	-
Na_2O×SiO_2	0.008	<.0001	-	-	-
Na_2O×ZrO_2	-	0.0009	-	-	-
SiO_2×Others	0.003	-	0.0021	0.0024	-
SiO_2×TiO_2	-	0.1126	-	-	-
SnO_2× ZrO_2	-	0.0101	-	-	-
ZrO_2×P_2O_5	0.027	-	0.004	0.0022	-
Number of Terms	37	56	31	30	26

- Empty data field.

Table 5.14. PCT-Na and PCT-B Releases (g/L) for Glasses Tested at VSL and Outside Laboratories.

Formulation	Component	Simulant Test at VSL	Actual Waste Test at Outside Laboratory	Reference
LAWA44	B	0.371	0.366	WSRC-TR-2000-00322 [41]
	Na	0.358	0.396	
LAWC15	B	0.354	0.329	PNNL-13372 [42]
	Na	0.422	0.335	
LAWA88	B	0.654	0.569	PNNL-13372 [42]
	Na	0.639	0.589	
LAWA126	B	0.598	0.650	PNWD-3470 [44]
	Na	0.524	0.650	
LAWB83	B	0.233	0.260	PNWD-3464 [45]
	Na	0.232	0.250	
LAWB88	B	0.197	0.199	WSRC-TR-2003-00536 [46]
	Na	0.160	0.159	
LAWC21	B	0.327	0.298	WSRC-TR-2000-00371 [47]
	Na	0.357	0.350	

Table 5.15. 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 μm
ORPLA32	Outlying composition (MgO = 10.04 wt%)
LAWE3Cr2CCC	Non-representative composition & heat treatment
LAWE9HCr1CCC	Non-representative composition & heat treatment
LAWE9HCr2CCC	Non-representative composition & heat treatment
LAWE10HCr3CCC	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 5.16. 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
LAWE14	ORPLA31
10A-G-43B	ORPLB1
LAWA171	ORPLB1S4
LAWA172	ORPLC2
LAWA177	ORPLC3
LAWA178	ORPLC3S4
LAWA179	ORPLC4
LAWA181	ORPLC4S4
LAWA182	ORPLG13
LAWE17(T1)	ORPLG16
LAWE17(T2)	ORPLG17
ORPLA1	ORPLG18
ORPLA1S4	ORPLG19
ORPLA5S4	LORPM17R1

Table 5.17. Twenty-Seven Glasses Reserved from the VHT Dataset as Validation Set and Their VHT Alteration Depth.

Glass ID	VHT Alteration Depth (μm)	ln(Depth, μm)
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
LAWE11	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
LAWE13	615	6.4216
LAWA196	712	6.5681
ORPLA2S4	858	6.7546
ORPLA4	1031	6.9383

Table 5.18. 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).
NA – Not Applicable.

Table 5.18. 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) [(b)]	230	5.4381		
EWV-G-89B (LAWA187)	736	6.6012		
EWV-G-93B (LAWA187)	719	6.5779		
EWV93BCCC (LAWA187)[(c)]	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).
(b) Replicate of EWV-G-93B subjected to CCC heat-treatment.
(c) Replicate of EWV-G-89B subjected to CCC heat-treatment.

Table 5.18. 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)
NA – Not applicable

Table 5.19. Coefficients and Performance Summary for Various Reduced Partial Quadratic Mixture Models on the Natural Logarithm of VHT Alteration Depth.

VHT Model	Model Number									
	1 [1]		2 [23]		3		4		5	
Glass Count	165 (+16 outliers)		357 (+47 outliers + 27 validation)		377 (+47 outliers + 27 validation)		377 (+47 outliers + 27 validation)		377 (+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.
Al_2O_3	19.569	6.085	52.822	7.146	-5.746	7.225	1.307	5.210	38.911	14.634
B_2O_3	18.534	5.923	15.480	3.413	5.257	3.013	5.441	3.031	10.561	5.191
CaO	38.241	9.448	-127.339	19.772	-58.941	25.668	-65.357	25.027	54.411	32.943
Fe_2O_3	-8.413	4.722	5.015	3.137	-8.062	3.300	-8.263	3.331	-12.494	3.716
K_2O	-39.312	10.707	-109.334	16.281	-11.675	12.610	-15.498	12.968	-159.978	29.242
Li_2O	-17.825	20.067	-5.494	17.695	259.040	18.342	257.476	18.356	123.481	46.841
MgO	-8.307	8.041	-8.420	7.653	-	-	-	-	-	-
Na_2O	-20.652	10.476	-57.013	12.545	16.401	7.758	16.114	7.763	18.913	8.881
SiO_2	-0.514	2.287	-4.874	2.262	-10.702	1.870	-11.450	1.810	-12.143	2.215
SnO_2	-	-	-14.520	5.109	-30.339	6.412	-28.639	6.405	-7.808	8.337
TiO_2	-	-	-	-	-5.697	7.432	-5.909	7.474	-13.275	7.376
ZrO_2	-62.846	7.591	-44.557	4.428	-59.831	4.112	-62.236	4.100	-46.161	5.510
ZnO	-	-	-	-	-	-	5.911	4.843	2.396	4.651
Others[(a)]	-0.429	5.348	14.012	3.576	-17.251	7.657	-20.461	8.629	-46.621	9.055
$(K_2O)^2 \times Na_2O$	10138.3	1198.52	-	-	-	-	-	-	-	-
$(Na_2O)^3$	872.656	130.64	-	-	-	-	-	-	-	-
$Li_2O \times Na_2O \times SiO_2$	2139.80	387.60	-	-	-	-	-	-	-	-
$B_2O_3 \times CaO \times Na_2O$	-1943.1	773.36	-	-	-	-	-	-	-	-
$(CaO)^2$	-	-	219.306	57.309	215.117	65.505	225.201	65.212	225.197	64.796
$CaO \times SiO_2$	-	-	271.908	45.046	-	-				
$(K_2O)^2$	-	-	1374.019	234.831	1358.717	216.879	1412.054	220.451	1570.665	219.429
$K_2O \times MgO$	-	-	911.815	262.425	-	-	-	-	-	-
$Al_2O_3 \times Na_2O$	-	-	-149.973	43.427	-	-	-	-	-	-
$K_2O \times Na_2O$	-	-	444.083	70.439	-	-	-	-	745.963	125.337
$Li_2O \times Na_2O$	-	-	953.798	140.547	-	-	-	-	-	-
$(Na_2O)^2$	-	-	353.518	38.237	169.584	21.770	168.982	21.857	129.014	25.121
$CaO \times Li_2O$	-	-	-	-	-669.940	161.889	-618.401	160.616	-772.156	153.686
$CaO \times Na_2O$	-	-	-	-	-228.701	58.515	-216.084	57.551	-376.319	61.872
$K_2O \times Li_2O$	-	-	-	-	-1339.974	170.651	-1296.357	175.091	768.797	384.535
$(Li_2O)^2$	-	-	-	-	-1787.709	279.664	-1821.250	278.752	-1941.586	273.366
$CaO \times SiO_2$	-	-	-	-	202.247	43.294	207.205	43.284	37.773	53.162
$Fe_2O_3 \times SnO_2$	-	-	-	-	456.489	138.621	468.412	139.070	667.415	142.857
$Al_2O_3 \times$ Others	-	-	-	-	299.578	91.880	334.464	100.796	641.204	106.616
$(Al_2O_3)^2$	-	-	-	-	-	-	-	-	-311.666	91.524
$B_2O_3 \times CaO$	-	-	-	-	-	-	-	-	-209.104	81.800
$CaO \times SnO_2$	-	-	-	-	-	-	-	-	-544.020	146.011
$Fe_2O_3 \times K_2O$	-	-	-	-	-	-	-	-	236.939	116.770
$K_2O \times ZrO_2$	-	-	-	-	-	-	-	-	-636.169	167.267
$Li_2O \times SiO_2$	-	-	-	-	-	-	-	-	240.899	99.916

- Empty data field. [(a)] "Others" components include the original "Others" component (which contains 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, and V_2O_5, plus ZnO in Models 1,2 and 3, TiO_2 in Models 1 and 2, SnO_2 in Model 1 and MgO in Models 3-5.

Table 5.19. Coefficients and Performance Summary for Various Reduced Partial Quadratic Mixture Models on the Natural Logarithm of VHT Alteration Depth (continued).

VHT Model	Model Number				
	1 [1]	**2 [23]**	**3**	**4**	**5**
Number of terms	15	20	22	23	30
Modeling Data Statistic					
R^2	0.744	0.776	0.770	0.771	0.797
$R^2_{Adjusted}$	0.720	0.763	0.757	0.756	0.781
$R^2_{Predict}$	0.696	0.751	0.739	0.738	0.763
Validation Statistics on 27 Selected Glasses over Full Expanded Range – 16 from ORP Set and 11 from WTP Set					
$R^2_{Validation}$	-2.407[(b)]	0.724	0.724	0.708	0.765
$RMSE_{Validation}$	1.538[(b)]	0.790	0.790	0.812	0.730

[(a)] "Others" components include the original "Others" component (which contains 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, and V_2O_5, plus ZnO in Models 1,2 and 3, TiO_2 in Models 1 and 2, SnO_2 in Model 1 and MgO in Models 3-5

[(b)] 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 5.20. Thirty Glasses Reserved from the Electrical Conductivity Dataset as Validation Set and their Temperatures and EC Measurements.

Glass ID	Temp1 (ºC)	EC1 (S/cm)	Temp2 (ºC)	EC2 (S/cm)	Temp3 (ºC)	EC3 (S/cm)	Temp4 (ºC)	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 5.21. Variation in Electrical Conductivity Values for Near-Replicate Pairs.

Glass IDs of Replicate Pairs[a]	Electrical Conductivity Values at Measurement Temperatures								Pooled Over Temp.	
	950ºC		1050ºC		1150ºC		1250ºC		%RSD	SD
	T (ºC)	S/cm	T (ºC)	S/cm	T (ºC)	S/cm	T (ºC)	S/cm	S/cm	ln(S/cm)
LAWM1	959	0.052	1058	0.101	1156	0.169	1253	0.243		
LAWM53	945	0.074	1043	0.144	1141	0.241	1237	0.379		
%RSD[b], SD[c]	24.69%	0.249	24.82%	0.251	24.83%	0.251	30.92%	0.314	26.45%	0.268
LAWM9	963	0.027	1057	0.054	1154	0.097	1248	0.139		
LAWM54R1	949	0.023	1047	0.048	1146	0.092	1236	0.146		
%RSD[b], SD[c]	11.31%	0.113	8.32%	0.083	3.74%	0.037	3.47%	0.035	7.47%	0.075
LAWM12	973	0.249	1068	0.385	1161	0.553	1253	0.721		
LAWM55	944	0.248	1042	0.388	1139	0.588	1236	0.742		
%RSD[b], SD[c]	0.28%	0.003	0.55%	0.005	4.34%	0.043	2.03%	0.020	2.41%	0.024
LAWM35	961	0.126	1056	0.205	1152	0.306	1246	0.425		
LAWM56	947	0.123	1041	0.223	1138	0.331	1235	0.481		
%RSD[b], SD[c]	1.70%	0.017	5.95%	0.060	5.55%	0.056	8.74%	0.088	6.03%	0.060
LAWM50	947	0.101	1044	0.168	1143	0.26	1239	0.399		
LAWM51	939	0.091	1036	0.157	1133	0.245	1230	0.347		
%RSD[b], SD[c]	7.37%	0.074	4.79%	0.048	4.20%	0.042	9.86%	0.099	6.93%	0.069
LAWM52	942	0.176	1038	0.28	1137	0.421	1234	0.568		
LAWA88	949	0.248	1044	0.37	1143	0.554	1251	0.765		
%RSD[b], SD[c]	24.01%	0.242	19.58%	0.197	19.29%	0.194	20.90%	0.211	21.03%	0.212
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[b], SD[c]	3.51%	0.035	10.92%	0.109	0.86%	0.009	1.98%	0.020	5.83%	0.058
Pooled Over 7 Replicate Pairs										
%RSD[b], SD[c]	**14.06%**	**0.142**	**13.34%**	**0.134**	**12.37%**	**0.125**	**15.06%**	**0.152**	**13.74%**	**0.139**
Glass IDs of Replicate Pairs[a]	**Electrical Conductivity Values at Nominal Temperatures**								**Pooled Over Temp.**	
	950ºC		**1050ºC**		**1150ºC**		**1250ºC**		**%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)**
LAWM1	0.048	-3.03	0.097	-2.333	0.163	-1.813	0.241	-1.422		
LAWM53	0.077	-2.564	0.149	-1.906	0.255	-1.368	0.398	-0.921		
%RSD[b], SD[c]	32.81%	0.330	29.89%	0.302	31.13%	0.315	34.75%	0.354	32.20%	0.326
LAWM9	0.024	-3.735	0.053	-2.946	0.093	-2.374	0.141	-1.958		
LAWM54R1	0.023	-3.767	0.05	-3.005	0.093	-2.376	0.157	-1.85		
%RSD[b], SD[c]	3.01%	0.023	4.12%	0.042	0.00%	0.001	7.59%	0.076	4.57%	0.045
LAWM12	0.219	-1.517	0.359	-1.024	0.528	-0.638	0.717	-0.332		
LAWM55	0.255	-1.368	0.412	-0.887	0.591	-0.526	0.777	-0.253		
%RSD[b], SD[c]	10.74%	0.105	9.72%	0.097	7.96%	0.079	5.68%	0.056	8.74%	0.086
LAWM35	0.118	-2.134	0.199	-1.613	0.304	-1.191	0.43	-0.843		
LAWM56	0.126	-2.068	0.228	-1.477	0.356	-1.033	0.498	-0.697		
%RSD[b], SD[c]	4.64%	0.047	9.60%	0.096	11.14%	0.112	10.36%	0.103	9.29%	0.093
LAWM50	0.103	-2.273	0.171	-1.766	0.272	-1.303	0.415	-0.879		
LAWM51	0.097	-2.329	0.169	-1.779	0.261	-1.343	0.371	-0.993		
%RSD[b], SD[c]	4.24%	0.040	0.83%	0.009	2.92%	0.028	7.92%	0.081	4.74%	0.047
LAWM52	0.183	-1.696	0.297	-1.213	0.437	-0.828	0.597	-0.516		
LAWA88	0.248	-1.394	0.385	-0.955	0.558	-0.583	0.767	-0.265		
%RSD[b], SD[c]	21.33%	0.214	18.25%	0.182	17.20%	0.173	17.63%	0.177	18.67%	0.187
LAWC100R1	0.173	-1.753	0.27	-1.311	0.395	-0.93	0.549	-0.6		
WVY-G-95A	0.168	-1.784	0.285	-1.255	0.42	-0.868	0.566	-0.569		
%RSD[b], SD[c]	2.07%	0.022	3.82%	0.040	4.34%	0.044	2.16%	0.022	3.25%	0.033
Pooled Over 7 Replicate Pairs										
%RSD[b], SD[c]	**15.58%**	**0.156**	**14.37%**	**0.145**	**14.54%**	**0.147**	**15.96%**	**0.162**	**15.13%**	**0.152**

(a) Because glass compositions were renormalized based on analyzed (or estimates of analyzed) SO_3 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), calculated using the S/cm values.
(c) Calculated using ln(S/cm) values.

Table 5.22. 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 [23]**		**3**		**4**	
Data Count	171 (+10 outliers)		292 (+ LORPM13 outlier +30 validation)		317 (+ LORPM13 outlier +30 validation)		317 (+ LORPM13 outlier +30 validation)	
Model Terms	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.
Al_2O_3	4.229	6.207	2.213	2.897	2.409	2.307	1.401	2.275
B_2O_3	7.566	4.253	4.489	2.92	3.372	2.395	3.312	2.403
CaO	2.188	3.917	1.877	2.362	5.789	1.826	5.185	1.820
Fe_2O_3	3.983	4.020	6.882	2.62	6.047	2.066	6.135	2.073
K_2O	4.773	5.252	3.038	3.392	5.117	2.774	5.663	2.769
Li_2O	5.778	8.418	-2.52	6.727	1.478	5.327	-0.587	5.274
MgO	12.874	7.907	13.619	5.734	14.724	4.579	14.370	4.591
Na_2O	-1.653	2.458	-2.395	1.879	-1.049	1.573	-1.454	1.565
SiO_2	3.511	1.757	5.646	1.138	4.654	0.923	5.358	0.867
V_2O_5	-	-	-	-	-3.977	5.041	-	-
ZrO_2	10.237	8.121	13.955	4.593	12.062	3.700	12.029	3.713
Others[(a)]	12.840	5.089	5.528	3.069	8.644	2.526	6.021	2.202
CaO×Li_2O	145.252	22.879	177.415	14.196	150.551	10.801	153.995	10.736
CaO×Na_2O	79.122	7.579	39.402	4.549	32.128	3.551	32.859	3.552
Li_2O×Na_2O	-130.284	8.892	-55.557	5.496	-56.530	4.658	-55.261	4.637
Al_2O_3/(*T*/1000)	-11.571	8.400	-9.25	3.935	-9.667	3.144	-8.147	3.099
B_2O_3/(*T*/1000)	-10.551	5.749	-7.38	3.958	-5.822	3.251	-5.713	3.262
CaO/(*T*/1000)	-26.585	4.940	-21.062	2.956	-24.579	2.288	-23.929	2.278
Fe_2O_3/(*T*/1000)	-8.675	5.448	-11.759	3.556	-10.445	2.812	-10.548	2.821
K_2O/(*T*/1000)	-7.588	7.097	-5.878	4.608	-9.104	3.774	-9.914	3.768
Li_2O/(*T*/1000)	28.375	11.125	26.753	8.998	24.317	7.148	26.872	7.072
MgO/(*T*/1000)	-21.944	10.690	-23.195	7.784	-25.662	6.232	-25.108	6.249
Na_2O/(*T*/1000)	11.855	3.288	13.525	2.532	12.320	2.125	12.849	2.114
SiO_2/(*T*/1000)	-9.920	2.377	-12.734	1.544	-11.533	1.254	-12.561	1.178
V_2O5_3/(*T*/1000)	-	-	-	-	4.414	6.874		
ZrO_2/(*T*/1000)	-19.731	10.988	-24.479	6.229	-22.090	5.030	-21.995	5.048
Others/(*T*/1000)	-19.917	6.885	-9.456	4.169	-14.303	3.439	-10.377	3.002
Number of Terms	25		25		27		25	
Modeling Data Statistics								
R^2	0.951		0.952		0.961		0.961	
$R^2_{Adjusted}$	0.949		0.950		0.960		0.960	
$R^2_{Predict.}$	0.945		0.949		0.959		0.959	
LOF	No lack-of-fit data		0.386		0.696		0.685	
Validation Statistics on 30 Glasses Selected Over Full Range – 15 each from ORP-LAW and WTP-LAW Glasses								
$R^2_{Validation}$	0.800[(b)]		0.967		0.967		0.967	
$RMSE_{Validation}$	0.233 [(b)]		0.108		0.108		0.108	

(a) "Others" components include the original "Others" component (which contains 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, SO_3, TiO_2, SnO_2 and ZnO. In Models 1, 2 and 4, V_2O_5 is also added to "Others".

(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 5.23. Twenty-Eight Glasses Reserved from the Viscosity Dataset as a Validation Set and Their Temperatures and Viscosity Measurements.

Glass ID	Temp1 (ºC)	Vis1 (P)	Temp2 (ºC)	Vis2 (P)	Temp3 (ºC)	Vis3 (P)	Temp4 (ºC)	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
LAWE7H	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
LAWE2H	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 5.24. Variation in Melt Viscosity Values for Near-Replicate Pairs.

Glass IDs of Replicate Pairs[a]	T (ºC)	Viscosity (P)	T (ºC)	Viscosity (P)	T (ºC)	Viscosity (P)	T (ºC)	Viscosity (P)	Viscosity (P)	ln(Visc)
	Viscosity Values For Measurement Temperatures								Pooled Over Temp.	
	Near 950ºC		Near 1050ºC		Near 1150ºC		Near 1250ºC		%RSD	SD
LAWM1	953	376.96	1053	94.14	1152	35	1252	16.91		
LAWM53	958	314.34	1056	105.13	1150	39.95	1248	16.84		
%RSD[b], SD[c]	12.81%	0.128	7.80%	0.078	9.34%	0.094	0.29%	0.003	8.84%	0.089
LAWM9	946	2329.04	1048	462.35	1150	126.36	1252	43.77		
LAWM54R1	957	1659.86	1056	347.39	1155	105.91	1254	41.43		
%RSD[b], SD[c]	23.72%	0.240	20.08%	0.202	12.45%	0.125	3.88%	0.039	16.85%	0.170
LAWM12	951	90.07	1049	32.05	1148	14.24	1246	6.82		
LAWM55	956	65.9	1057	24.47	1158	11.23	1259	5.99		
%RSD[b], SD[c]	21.92%	0.221	18.97%	0.191	16.71%	0.168	9.16%	0.092	17.34%	0.175
LAWM35	950	269.85	1050	68.28	1149	25.02	1249	11.17		
LAWM56	956	262.73	1052	69.99	1148	25.79	1245	11.82		
%RSD[b], SD[c]	1.89%	0.019	1.75%	0.017	2.14%	0.021	4.00%	0.040	2.61%	0.026
LAWM50	953	721.01	1049	173.87	1146	60.43	1243	26.82		
LAWM51	966	624.53	1060	171.04	1154	59.03	1248	26.09		
%RSD[b], SD[c]	10.14%	0.102	1.16%	0.012	1.66%	0.017	1.95%	0.020	5.26%	0.053
LAWM52	955	531.45	1052	138.67	1149	51.5	1246	24.16		
LAWA88R1	931	750.05	1032	198.05	1133	71.1	1244	27.27		
%RSD[b], SD[c]	24.12%	0.244	24.94%	0.252	22.61%	0.228	8.55%	0.086	21.14%	0.213
LAWC100R1	946	250.25	1044	70.21	1142	26.60	1241	12.39		
WVY-G-95A	946	247.81	1044	69.08	1142	26.94	1241	13.01		
%RSD[a]	0.69%	0.007	1.15%	0.011	0.90%	0.009	3.45%	0.035	1.91%	0.019
Pooled Over 7 Replicate Pairs										
%RSD[b], SD[c]	**16.46%**	**0.166**	**14.40%**	**0.145**	**12.19%**	**0.123**	**5.40%**	**0.054**	**12.81%**	**0.129**

Glass IDs of Replicate Pairs[a]	Viscosity Values and Ln(Viscosity) at Nominal Temperatures								Pooled Over Temp.	
	950ºC		1050ºC		1150ºC		1250ºC		%RSD	SD
LAWM01	395.865	5.981	97.592	4.581	35.572	3.572	17.126	2.841		
LAWM53	347.297	5.85	110.907	4.709	40.436	3.7	16.483	2.802		
%RSD[b], SD[c]	9.24%	0.093	9.03%	0.091	9.05%	0.091	2.71%	0.028	8.00%	0.080
LAWM09	2169.88	7.682	449.653	6.108	126.308	4.839	44.611	3.798		
LAWM54R1	1882.91	7.541	379.032	5.938	111.184	4.711	42.918	3.759		
%RSD[b], SD[c]	10.01%	0.100	12.05%	0.120	9.01%	0.091	2.74%	0.028	9.14%	0.091
LAWM12	90.643	4.507	32.31	3.475	13.739	2.62	6.693	1.901		
LAWM55	70.436	4.255	26.04	3.26	11.858	2.473	6.304	1.841		
%RSD[b], SD[c]	17.74%	0.178	15.20%	0.152	10.39%	0.104	4.23%	0.042	12.96%	0.130
LAWM35	269.197	5.595	68.868	4.232	24.552	3.201	11.134	2.41		
LAWM56	288.933	5.666	71.826	4.274	25.268	3.23	11.425	2.436		
%RSD[b], SD[c]	5.00%	0.050	2.97%	0.030	2.03%	0.021	1.82%	0.018	3.21%	0.032
LAWM50	757.875	6.631	172.592	5.151	57.836	4.058	25.576	3.242		
LAWM51	809.817	6.697	191.577	5.255	62.245	4.131	25.548	3.241		
%RSD[b], SD[c]	4.69%	0.047	7.37%	0.074	5.19%	0.052	0.08%	0.001	5.08%	0.051
LAWM52	575.443	6.355	142.518	4.959	50.834	3.929	23.561	3.16		
LAWA88R1	569.817	6.345	163.696	5.098	59.826	4.091	26.211	3.266		
%RSD[b], SD[c]	0.69%	0.007	9.78%	0.098	11.49%	0.115	7.53%	0.075	8.44%	0.084
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]	0.77%	0.008	1.03%	0.010	0.96%	0.010	3.78%	0.038	2.06%	0.021
Pooled Over 7 Replicate Pairs										
%RSD[b], SD[c]	**8.85%**	**0.089**	**9.39%**	**0.094**	**7.88%**	**0.079**	**3.91%**	**0.039**	**7.81%**	**0.078**

(a) Near-replicates in which SO_3 values may not match exactly are treated here as replicate pairs for statistical data analyses.
(b) %RSD = 100×(Standard Deviation / Mean), calculated using the viscosity values in poise (P).
(c) Calculated using ln (P) values.

Table 5.25. Coefficients and Performance Summary for Various Mixture Models with Quadratic Terms on the Natural Logarithm of ILAW Viscosity.

Viscosity Model	Model Number									
Model	**1 [1]**		**2 [23]**		**3**		**4**		**5**	
Model Terms	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.	Coeff. Estimate	Std. Dev.
Al_2O_3	5.699	3.073	0.779	1.538	-12.637	2.964	2.862	1.432	-2.681	1.463
B_2O_3	-42.105	3.585	-24.167	2.074	-23.136	2.151	-23.208	2.043	-24.129	2.027
CaO	-10.823	1.781	-10.162	1.120	-18.859	2.104	-11.455	1.010	-10.636	0.987
Fe_2O_3	-4.755	1.887	-5.984	1.330	-13.598	2.607	-5.639	1.249	-4.674	1.223
K_2O	-0.904	0.489	-1.457	0.308	-1.172	0.311	-1.197	0.296	-0.276	0.302
Li_2O	11.231	4.481	10.506	3.693	57.970	6.705	12.435	3.429	-2.109	3.425
MgO	-6.463	4.535	-16.364	2.948	-27.954	5.845	-13.802	2.803	-12.804	2.738
Na_2O	0.919	1.186	0.763	0.970	7.782	1.944	0.194	0.937	-1.341	0.941
P_2O_5	-1.246	5.530	-1.929	6.027	-12.388	12.305	-0.459	5.903	-0.090	5.762
SiO_2	1.520	0.772	0.944	0.521	-12.853	0.984	0.394	0.483	0.860	0.472
SnO_2	-	-	-26.722	2.798	-57.273	5.317	-24.613	2.547	-23.834	2.485
ZrO_2	-11.599	3.886	-19.358	2.446	-49.962	4.928	-18.761	2.364	-18.676	2.307
Others[(a)]	-9.246	2.699	-6.404	1.992	-8.655	3.920	-4.600	1.880	-3.736	1.835
$Al_2O_3/(T/1000)^2$	24.234	5.421	32.327	2.789	-	-	29.032	2.599	28.978	2.538
$CaO/(T/1000)^2$	14.078	3.225	12.002	2.042	-	-	14.158	1.849	14.110	1.805
$Fe_2O_3/(T/1000)^2$	15.457	3.408	15.783	2.425	-	-	15.149	2.295	14.930	2.240
$Li_2O/(T/1000)^2$	-82.940	7.153	-82.262	6.197	-	-	-84.088	5.715	-84.066	5.579
$MgO/(T/1000)^2$	23.561	6.720	28.633	5.374	-	-	24.541	5.123	24.288	5.001
$Na_2O/(T/1000)^2$	-14.632	2.140	-14.561	1.756	-	-	-13.930	1.699	-13.868	1.659
$P_2O_5/(T/1000)^2$	24.785	10.107	27.110	11.041	-	-	25.863	10.839	26.286	10.580
$SiO_2/(T/1000)^2$	24.496	1.363	23.327	0.924	-	-	24.107	0.857	24.121	0.837
$SnO_2/(T/1000)^2$			68.348	5.120	-	-	64.691	4.704	64.596	4.592
$ZrO_2/(T/1000)^2$	47.267	7.055	60.167	4.460	-	-	59.153	4.325	58.938	4.222
$Others/(T/1000)^2$	17.008	4.900	11.052	3.636	-	-	8.477	3.445	8.644	3.363
$Al_2O_3 \times Li_2O$	-137.475	29.287	-84.640	12.648	-95.761	12.013	-96.333	11.412	-	-
$Al_2O_3 \times Na_2O$	-	-	-	-	-	-	-	-	29.338	3.227
$(B_2O_3)^2$	197.193	19.071	95.880	11.031	90.709	11.399	90.997	10.829	91.567	10.597
$(Li_2O)^2$	132.727	22.574	108.753	20.279	100.016	20.946	98.921	19.898	98.036	19.334
$(MgO)^2$	-169.558	53.834	-	-	-	-	-	-	-	-
$B_2O_3 \times Li_2O$	-	-	-	-	-	-	-	-	84.120	13.247
$Al_2O_3/(T/1000)$	-	-	-	-	42.564	4.032	-	-	-	-
CaO/(T/1000)	-	-	-	-	20.529	2.867	-	-	-	-
Fe2O3/(T/1000)	-	-	-	-	22.036	3.559	-	-	-	-
Li2O/(T/1000)	-	-	-	-	-124.339	8.881	-	-	-	-
MgO/(T/1000)	-	-	-	-	37.396	7.954	-	-	-	-
$Na_2O/(T/1000)$	-	-	-	-	-20.654	2.641	-	-	-	-
$P_2O_5/(T/1000)$	-	-	-	-	35.398	16.787	-	-	-	-
$SiO_2/(T/1000)$	-	-	-	-	35.852	1.330	-	-	-	-
$SnO_2/(T/1000)$	-	-	-	-	92.318	7.279	-	-	-	-
$ZrO_2/(T/1000)$	-	-	-	-	86.235	6.712	-	-	-	-
Others/(T/1000)	-	-	-	-	11.833	5.344	-	-	-	-

(a) "Others" components include the original "Others" component (which contains 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, SO_3, TiO_2, ZnO and V_2O_5. In Models 1 SnO_2 is also added to "Others" if it is not included in the model terms.

- Empty data field.

Table 5.25. Coefficients and Performance Summary for Various Mixture and Temperature Models with Quadratic Terms on the Natural Logarithm of ILAW Viscosity (continued).

Viscosity Model	1 [1]	2 [23]	3	4	5
Number of Terms	26	27	27	27	28
Modeling Data Statistics					
R^2	0.988	0.987	0.985	0.986	0.987
$R^2_{Adjusted}$	0.987	0.987	0.985	0.986	0.986
$R^2_{Predict.}$	0.986	0.986	0.984	0.986	0.986
LOF	-	-	0.043	0.082	0.108
Validation Statistics on 28 Glasses Selected over Full Range – 14 each ORP-LAW and WTP-LAW Glasses					
$R^2_{Validation}$	0.961	0.974	0.974	0.974	0.974
$RMSE_{Validation}$	0.259 (b)	0.224	0.226	0.224	0.223
Residuals Summary Statistics on fit of 1265 Viscosity/Temperature Measurements					
Mean Residual	-		4.4E-08	4.4E-08	4.5E-08
Std Dev			0.165	0.157	0.153
Std Err Mean			0.005	0.004	0.004
Upper 95% Mean			0.009	0.009	0.008
Lower 95% Mean			-0.009	-0.009	-0.008
Skewness			**0.157**	**0.081**	**0.137**

(a) "Others" components include the original "Others" component (which contains 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, SO_3, TiO_2, and ZnO. In Models 1 and 2, SnO_2 and V_2O_5 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.

Table 5.26. Regression Coefficients' *p*-Values for Melt Viscosity Model Quadratic Terms.

	Model Number				
Model Terms	**1 [1]**	**2 [23]**	**3**	**4**	**5**
$Al_2O_3/(T/1000)^2$	<.0001	<.0001	-	<.0001	<.0001
$CaO/(T/1000)^2$	<.0001	<.0001	-	<.0001	<.0001
$Fe_2O_3/(T/1000)^2$	<.0001	<.0001	-	<.0001	<.0001
$Li_2O/(T/1000)^2$	<.0001	<.0001	-	<.0001	<.0001
$MgO/(T/1000)^2$	0.0005	<.0001	-	<.0001	<.0001
$Na_2O/(T/1000)^2$	<.0001	<.0001	-	<.0001	<.0001
$P_2O_5/(T/1000)^2$	0.001	0.002	-	0.014	0.013
$SiO_2/(T/1000)^2$	0.015	0.014	-	0.017	<.0001
$SnO_2/(T/1000)^2$	Not included	<.0001	-	<.0001	<.0001
$ZrO_2/(T/1000)^2$	<.0001	<.0001	-	<.0001	<.0001
$Others/(T/1000)^2$	<.0001	<.0001	-	<.0001	0.010
$Al_2O_3 \times Li_2O$	<.0001	<.0001	<.0001	<.0001	-
$Al_2O_3 \times Na_2O$	-	-	-	-	<.0001
$(B_2O_3)^2$	<.0001	<.0001	<.0001	<.0001	<.0001
$(Li_2O)^2$	<.0001	<.0001	<.0001	<.0001	<.0001
$(MgO)^2$	0.0017	0.7622	-	-	-
$B_2O_3 \times Li_2O$	-	-	-	-	<.0001
$Al_2O_3/(T/1000)$	-	-	<.0001	-	-
$CaO/(T/1000)$	-	-	<.0001	-	-
Fe2O3/(T/1000)	-	-	<.0001	-	-
Li2O/(T/1000)	-	-	<.0001	-	-
$MgO/(T/1000)$	-	-	<.0001	-	-
$Na_2O/(T/1000)$	-	-	<.0001	-	-
$P_2O_5/(T/1000)$	-	-	0.0352	-	-
$SiO_2/(T/1000)$	-	-	<.0001	-	-
$SnO_2/(T/1000)$	-	-	<.0001	-	-
$ZrO_2/(T/1000)$	-	-	<.0001	-	-
Others/(T/1000)	-	-	0.027	-	-

- Empty data field.

Table 5.27. Summary of PCT Model Performance for Neural Network with One Inner Layer, 5 Nodes, Random Holdback, and Two Outputs: PCT-B and PCT-Na.

Ln(PCT-Na) Output		**Ln(PCT-B) Output**	
Training on 290 PCT-Na		**Training on 290 PCT-B**	
Ln(Na)	Measures	Ln(B)	Measures
R^2	**0.898**	R^2	**0.886**
RMSE	**0.209**	RMSE	**0.257**
Mean Abs Dev	0.167	Mean Abs Dev	0.200
SSE	12.608	SSE	19.218
Validation on 146 PCT-Na		**Validation on 146 PCT-B**	
Ln(Na)	Measures	Ln(B)	Measures
R^2	0.792	R^2	0.717
RMSE	0.266	RMSE	0.360
Mean Abs Dev	0.205	Mean Abs Dev	0.265
SSE	10.358	SSE	18.882
Generalized R^2			
Training	**0.988**		
Validation	**0.941**		
Validation on 27 VSL Glasses			
Model NN5	**PCT-Na**	**Model NN5**	**PCT-B**
R^2	**0.880**	**R^2**	**0.892**

Table 5.28. Neural Network Functions for PCT-B and PCT-Na Models.

Final Layer Formulas

Ln(PCT-Na) = -0.481712101235849×H1 + -0.0075162200465114 5×H2 + -1.09820917945233×H3 + -0.432451305180598×H4 + 0.482742745442285×H5 + -0.0376154353499791;

Ln(PCT-B) = -0.575773425084072×H1 + -0.193554981826724×H2 + -1.10337547741024×H3 + -0.654305867378834×H4 + 0.489710531640457×H5 + -0.112860067308696;

Hidden Layer Formulas

H1* = tanh(.5×(-12.6226386813106×Al2O3 + 4.30717924134255×B2O3 + 33.3471506310709×CaO + -32.457431440223×Fe2O3 + -13.4217140701885×K2O + -32.498022307795×Li2O + -86.0471296382991×MgO + -2.90290681217394×Na2O + 14.0926480608505×SiO2 + -11.6352039179707×SnO2 + -1.51742264117015×ZrO2 + 138.243517903265×P2O5 + 47.7876548733487×TiO2 + -65.2416378504747×V2O5 + -40.4484896600202×ZnO + 357.896203391433×SO3 + 483.925386158571×Cr2O3 + -205.086110818484×Others + -6.68396448222972));

H2 = tanh(.5×(-5.70998745930764×Al2O3 + 16.9605074274446×B2O3 + 52.2779259096742×CaO + 55.1777008482061×Fe2O3 + 6.4721512143419×K2O + 57.752401220343×Li2O + 63.4598509576019×MgO + -15.3076666638795×Na2O + 33.9920817335097×SiO2 + 3.32680291199081×SnO2 + -138.070296352039×ZrO2 + -395.201956885872×P2O5 + 70.5962457477059×TiO2 + 62.0950103353514×V2O5 + -116.57997606782×ZnO + 162.926810060882×SO3 + 49.2580204739592×Cr2O3 + -43.2023298263786×Others + -11.7354018653058));

H3 = tanh(.5×(50.040824000502×Al2O3 + 8.12620822110434×B2O3 + 8.71627164009128×CaO + 14.956639802812×Fe2O3 + 2.52789138050338×K2O + -48.0927428048769×Li2O + 17.9511912223143×MgO + -17.9741677813113×Na2O + 22.5783456000529×SiO2 + 27.188379870599×SnO2 + 32.2071072245611×ZrO2 + -19.6226847646879×P2O5 + 47.6729499837682×TiO2 + -1.19231540117757×V2O5 + 29.3269258237305×ZnO + -116.429699852542×SO3 + -42.2711950372897×Cr2O3 + 41.1542789263609×Others + -13.583259523694));

H4 = tanh(.5×(59.3344905639968×Al2O3 + -36.361557775019×B2O3 + 4.80856573136145×CaO + -27.7682320740259×Fe2O3 + -44.4372675404663×K2O + -57.9472313011341×Li2O + -240.410311469931×MgO + 6.93067394604581×Na2O + 2.46702832880878×SiO2 + -9.68928167715739×SnO2 + -19.6341489162444×ZrO2 + 120.274168019668×P2O5 + -90.1293467023497×TiO2 + -28.8733468852767×V2O5 + 28.5046028492715×ZnO + -66.6997448488929×SO3 + -40.1338333723819×Cr2O3 + -206.876208773847×Others + 5.16533711363785));

H5 = tanh(.5×(34.2272241436239×Al2O3 + 5.20415240640012×B2O3 + 22.6963030596901×CaO + -41.0328407367295×Fe2O3 + -3.9210609145016×K2O + -73.9981462366488×Li2O + -154.212186851902×MgO + 18.2774156010162×Na2O + -1.55117228662699×SiO2 + 27.5834245356606×SnO2 + -20.5416621833148×ZrO2 + 18.7643802279693×P2O5 + -32.053427560939×TiO2 + -166.178453288731×V2O5 + 38.6202084582876×ZnO + -226.363131001118×SO3 + 269.412330917945×Cr2O3 + -345.950478754937×Others + 0.44653229681034));

Table 5.29. Summary of VHT Neural Network Model Performance with One Inner Layer, 5 Nodes, and Random Holdback (377 Total VHT Data).

Training on 251 VHT		**Validation on 126 VHT**	
ln(VHT)	Measures	ln(VHT)	Measures
R^2	**0.917**	R^2	**0.700**
RMSE	0.504	RMSE	0.913
Mean Abs Dev	0.374	Mean Abs Dev	0.718
SSE	63.707	SSE	104.9986
Validation on VSL 27 Glasses		R^2	0.779

Table 5.30. Neural Network Functions for VHT Model.

Final Layer Formulas
Ln(VHT Alteration Depth) =2.9911604957273×H1 + 2.28972163050923×H2 + 2.09483995403266×H3 + 3.53375371163825×H4 + 1.78647258716057×H5 + 5.01779793651027;
Hidden Layer Formulas
H1* = tanh(.5×(-40.5584128159805×Al2O3 + 7.61143173691048×B2O3 + -32.492701380938×CaO + -23.0253533144501×Fe2O3 + 27.8588459341341×K2O + 26.0260842004554×Li2O + 17.5243073732781×MgO + 29.1656447051664×Na2O + -24.9676341205922×SiO2 + -23.9471486127042×SnO2 + -13.3430264256658×V2O5 + -30.3858627258288×ZrO2 + -39.5215127776644×SO3 + -58.5804711872221×TiO2 + -30.1643632431717×ZnO + -77.4538865097435×Cr2O3 + 4.63270103948018×P2O5 + -105.613450608711×Others + 11.7034074567139));
×
H2 = tanh(.5×(50.8994466969489×Al2O3 + -29.8169803638846×B2O3 + 21.7046589488252×CaO + -22.9818568669465×Fe2O3 + 14.12820091478×K2O + 65.2257201841918×Li2O + -95.3902120561685×MgO + 10.8885420453775×Na2O + -17.9454871999776×SiO2 + 42.1344396777906×SnO2 + -5.28290363385884×V2O5 + -126.022073996449×ZrO2 + -195.886518803905×SO3 + -65.4060961491633×TiO2 + -21.7160573518942×ZnO + -65.0324435462116×Cr2O3 + -95.4076265575522×P2O5 + -290.657912976921×Others + 15.2905251584086));
H3 = tanh(.5×(68.6868533300561×Al2O3 + 33.64149460478×B2O3 + 28.5773126902328×CaO + 15.1498578327272×Fe2O3 + -107.01812939841×K2O + 2.2530765914327×Li2O + -99.1235921376342×MgO + -6.34232598475454×Na2O + 1.01051192266354×SiO2 + 59.4640568624241×SnO2 + -68.5178981690653×V2O5 + -74.3746040486188×ZrO2 + 113.296627987266×SO3 + -41.2697869932065×TiO2 + 15.9766905731834×ZnO + 65.8911233090013×Cr2O3 + 137.980314113466×P2O5 + -84.1347441298669×Others + -4.46612459164599));
H4 = tanh(.5×(-36.2975716173225×Al2O3 + -10.0423950369186×B2O3 + -32.8994431064802×CaO + 4.14584452904624×Fe2O3 + 0.627442505919628×K2O + 16.1310178544679×Li2O + 45.2577933520534×MgO + 7.75201095252197×Na2O + -3.2027318641073×SiO2 + -49.0491619639946×SnO2 + 57.3196792474221×V2O5 + 28.3297666284559×ZrO2 + -64.8330014238934×SO3 + 58.8592152900871×TiO2 + -10.4799115873235×ZnO + 79.6293680373597×Cr2O3 + 32.0300092206782×P2O5 + 278.385674046195×Others + 1.14877417307589));
H5 = tanh(.5×(24.2278756851634×Al2O3 + -32.3353328362891×B2O3 + 36.7806843993129×CaO + -17.2712514360992×Fe2O3 + 53.2442333131239×K2O + 71.3486980230893×Li2O + 13.2572095839029×MgO + -15.1087852312112×Na2O + 3.76153651206376×SiO2 + -12.5302734512081×SnO2 + -143.172244592564×V2O5 + -9.7494710869843×ZrO2 + 377.823290140181×SO3 + -95.7041704305359×TiO2 + 37.4967970213976×ZnO + -74.4695265864648×Cr2O3 + -130.299341990048×P2O5 + -225.328071131829×Others + -1.23565568068421));

Table 6.1. Summary of Recommended Models for ILAW Glass Properties: PCT-Na, PCT-B, VHT, EC, Viscosity.

Model Terms	Ln (PCT-Na)	Model Terms	Ln (PCT-B)	Model Terms	Ln (VHT)	Model Terms	Ln (EC) Model	Model Terms	Ln (Viscosity) Model
Al_2O_3	-24.506	Al_2O_3	15.293	Al_2O_3	-5.746	Al_2O_3	1.401	Al_2O_3	2.862
B_2O_3	5.116	B_2O_3	11.695	B_2O_3	5.257	B_2O_3	3.312	B_2O_3	-23.208
CaO	-5.155	CaO	-16.28	CaO	-58.941	CaO	5.185	CaO	-11.455
-	-	Fe_2O_3	-1.176	Fe_2O_3	-8.062	Fe_2O_3	6.135	Fe_2O_3	-5.639
K_2O	41.243	K_2O	33.607	K_2O	-11.675	K_2O	5.663	K_2O	-1.197
Li_2O	43.578	Li_2O	-105.97	Li_2O	259.04	Li_2O	-0.587	Li_2O	12.435
MgO	15.98	MgO	13.819	MgO	-	MgO	14.37	MgO	-13.802
Na_2O	13.148	Na_2O	13.077	Na_2O	16.401	Na_2O	-1.454	Na_2O	0.194
P_2O_5	80.051	P_2O_5	-11.999	SiO_2	-10.702	SiO_2	5.358	P_2O_5	-0.459
SiO_2	-4.949	SiO_2	-4.943	SnO_2	-30.339	ZrO_2	12.029	SiO_2	0.394
SnO_2	-2.325	SnO_2	-9.015	TiO_2	-5.697	Others[(a)]	6.021	SnO_2	-24.613
TiO_2	-16.527	TiO_2	-8.697	ZrO_2	-59.831	$CaO \times Li_2O$	153.995	ZrO_2	-18.761
ZrO_2	-3.871	ZrO_2	-4.131	Others[(a)]	-17.251	$CaO \times Na_2O$	32.859	Others[(a)]	-4.600
Others[(a)]	7.314	Others[(a)]	2.196	$(CaO)^2$	215.117	$Li_2O \times Na_2O$	-55.261	$Al_2O_3/(T/1000)^2$	29.032
$(Al_2O_3)^2$	108.571	$Al_2O_3 \times K_2O$	-183.545	$(K_2O)^2$	1358.717	$Al_2O_3/(T/1000)$	-8.147	$CaO/(T/1000)^2$	14.158
$Al_2O_3 \times K_2O$	-126.849	$Al_2O_3 \times SiO_2$	-67.701	$(Na_2O)^2$	169.584	$B_2O_3/(T/1000)$	-5.713	$Fe_2O_3/(T/1000)^2$	15.149
$Al_2O_3 \times Li_2O$	-187.784	$B_2O_3 \times K_2O$	-192.894	$CaO \times Li_2O$	-669.94	$CaO/(T/1000)$	-23.929	$Li_2O/(T/1000)^2$	-84.088
$B_2O_3 \times K_2O$	-223.153	$CaO \times Fe_2O_3$	98.163	$CaO \times Na_2O$	-228.701	$Fe_2O_3/(T/1000)$	-10.548	$MgO/(T/1000)^2$	24.541
$CaO \times Li_2O$	-116.819	$CaO \times MgO$	263.611	$K_2O \times Li_2O$	-1339.974	$K_2O/(T/1000)$	-9.914	$Na_2O/(T/1000)^2$	-13.93
CaO×Others	67.777	$Fe_2O_3 \times K_2O$	124.296	$(Li_2O)^2$	-1787.709	$Li_2O/(T/1000)$	26.872	$P_2O_5/(T/1000)^2$	25.863
$CaO \times TiO_2$	159.881	$Fe_2O_3 \times Li_2O$	289.411	$CaO \times SiO_2$	202.247	$MgO/(T/1000)$	-25.108	$SiO_2/(T/1000)^2$	24.107
$K_2O \times Li_2O$	-207.756	$Fe_2O_3 \times MgO$	-211.86	$Fe_2O_3 \times SnO_2$	456.489	$Na_2O/(T/1000)$	12.849	$SnO_2/(T/1000)^2$	64.691
$K_2O \times SnO_2$	-158.678	$Fe_2O_3 \times ZrO_2$	-173.193	$Al_2O_3 \times$Others	299.578	$SiO_2/(T/1000)$	-12.561	$ZrO_2/(T/1000)^2$	59.153
$SiO_2 \times P_2O_5$	-212.005	$Li_2O \times Na_2O$	67.832			$ZrO_2/(T/1000)$	-21.995	Others/$(T/1000)^2$	8.477
$(Others)^2$	-61.29	$Li_2O \times SiO_2$	228.319	-		Others/$(T/1000)$	-10.377	$Al_2O_3 \times Li_2O$	-96.333
-		$Li_2O \times ZrO_2$	422.815			-		$(B_2O_3)^2$	90.997
		-						$(Li_2O)^2$	98.921
R^2	*0.866*	R^2	*0.862*	R^2	*0.770*	R^2	*0.961*	R^2	*0.986*
$R^2_{Adjusted}$	*0.858*	$R^2_{Adjusted}$	*0.853*	$R^2_{Adjusted}$	*0.757*	$R^2_{Adjusted}$	*0.960*	$R^2_{Adjusted}$	*0.986*
$R^2_{Predict.}$	*0.849*	$R^2_{Predict.}$	*0.838*	$R^2_{Predict.}$	*0.739*	$R^2_{Predict.}$	*0.959*	$R^2_{Predict.}$	*0.986*
$R^2_{Validation}$	*0.890*	$R^2_{Validation}$	*0.797*	$R^2_{Validation}$	*0.724*	$R^2_{Validation}$	*0.967*	$R^2_{Validation}$	*0.974*

- Empty data field

Table 6.2. Centroid Compositions for the Recommended Models for ILAW Glass Properties: PCT-Na, PCT-B, VHT, EC, Viscosity (also shown in Figure 6.1).

Component Oxides (wt%)	Centroid PCT(Na)	Centroid PCT(B)	Centroid VHT	Centroid EC	Centroid Viscosity
Al_2O_3	7.443	7.443	7.745	7.564	7.525
B_2O_3	9.808	9.808	9.591	9.708	9.727
CaO	5.272	5.272	5.19	5.366	5.444
Fe_2O_3	–	3.428	3.09	3.469	3.458
K_2O	1.43	1.43	1.492	1.472	1.417
Li_2O	1.646	1.646	1.514	1.783	1.748
MgO	1.677	1.677	–	1.761	1.732
Na_2O	16.015	16.015	16.782	15.552	15.712
P2O5	0.2449	0.2449	–	–	0.209
SiO_2	42.962	42.962	42.329	42.881	42.963
SnO_2	0.658	0.658	0.798	–	0.583
TiO_2	0.9169	0.9169	0.843	–	–
ZrO_2	3.547	3.547	3.726	3.506	3.506
Others	8.381	4.952	6.9	6.939	5.977
Sum	100.00	100	100	100.00	100.00
Predicted Value	Ln(PCT-Na) = -0.053	Ln(PCT-B) = -0.169	Ln(VHT) = 3.595	Pred Ln(EC at 1150ºC) = -1.064	Pred Ln(Visc at 1150ºC) = 3.710
				Pred Ln(EC at 950ºC) = -1.961	Pred Ln(Visc at 950ºC) = 6.088

- Empty data field (component included in "Others")

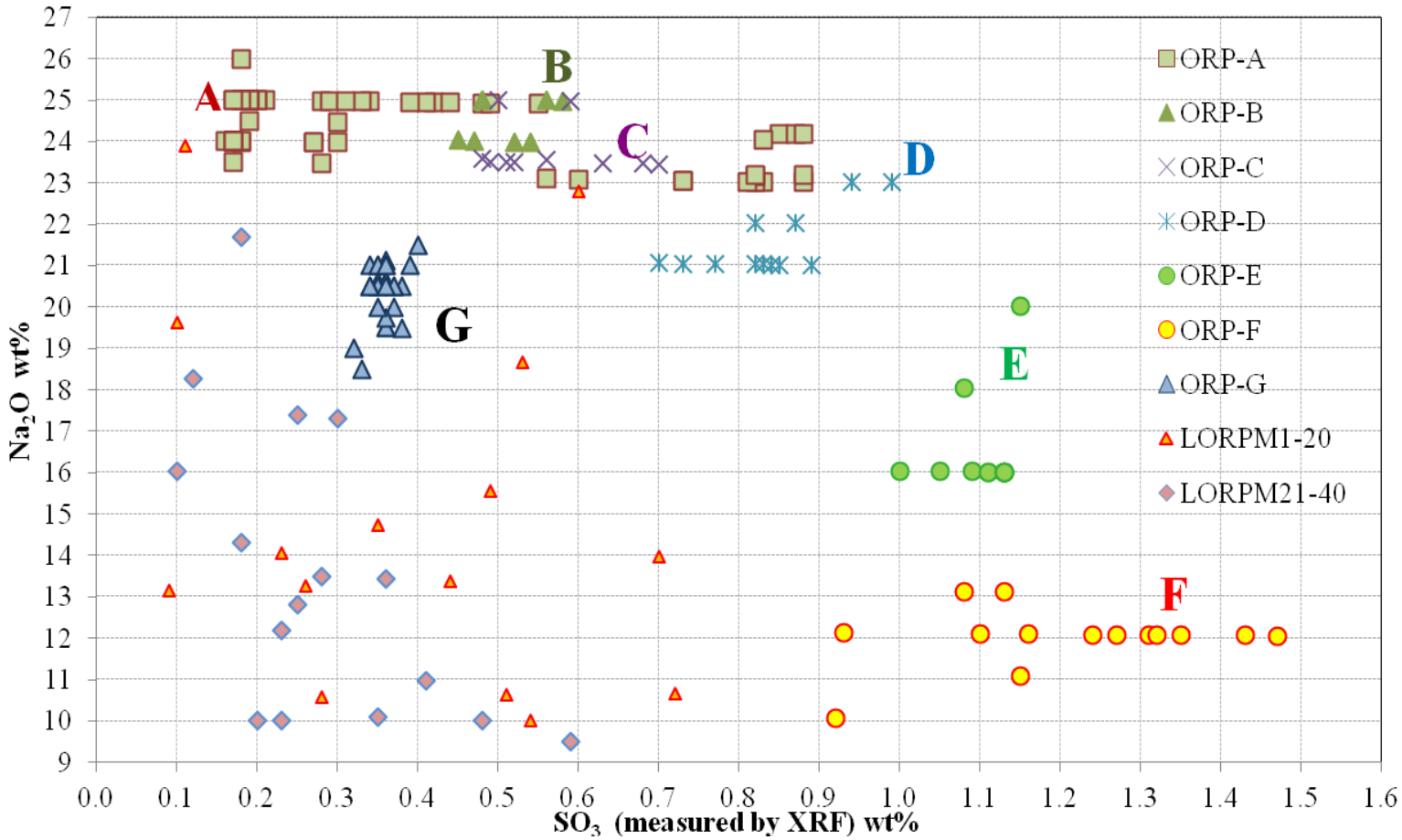


Figure 2.1. Na_2O and SO_3 concentrations for 153 high waste loading ORP-LAW glasses and 40 LORPM glasses.

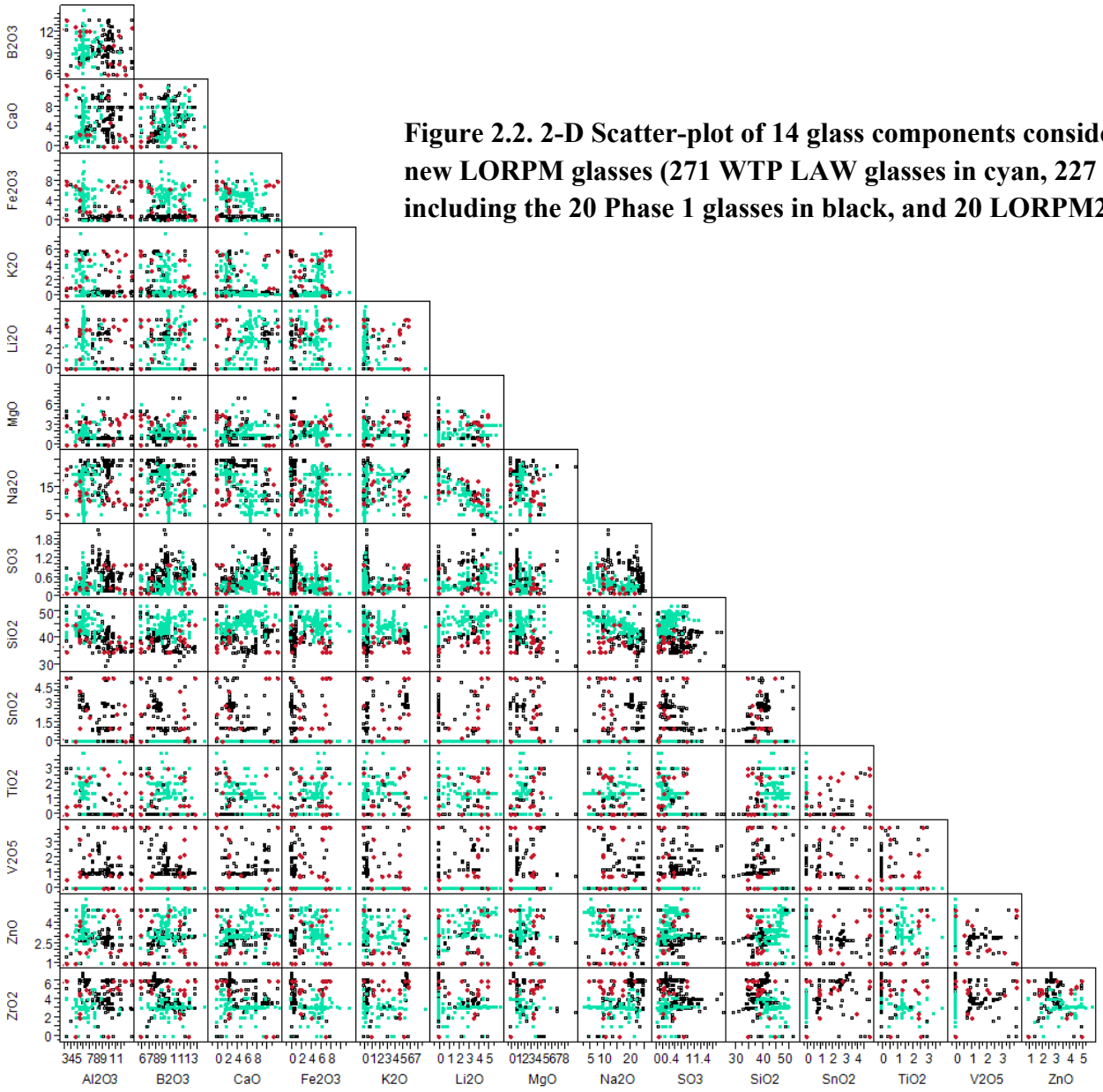


Figure 2.2. 2-D Scatter-plot of 14 glass components considered in the selection of 20 new LORPM glasses (271 WTP LAW glasses in cyan, 227 ORP LAW glasses including the 20 Phase 1 glasses in black, and 20 LORPM21-40 glasses in red).

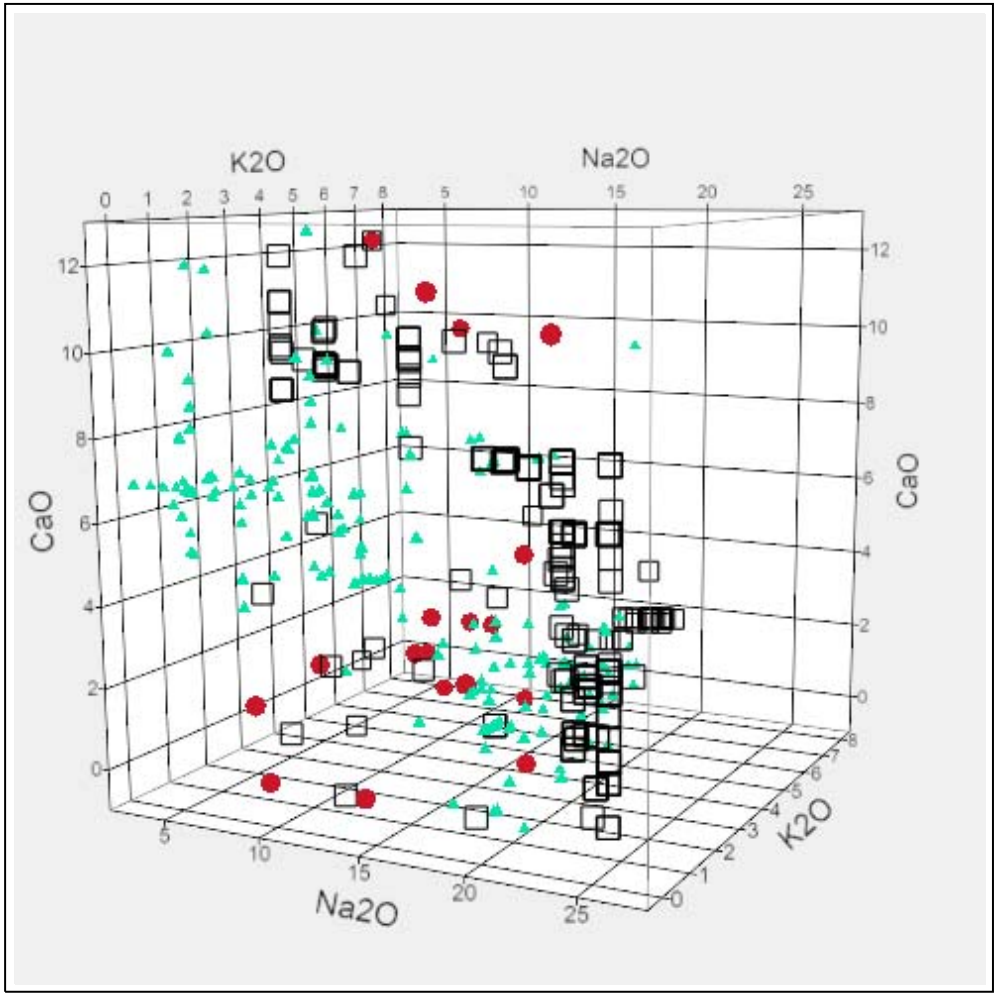


Figure 2.3. Na_2O-K_2O-CaO scatter-plot showing the WTP glasses (green triangles), the ORP glasses (black squares) and the 20 LORPM21-40 glasses (red circles).

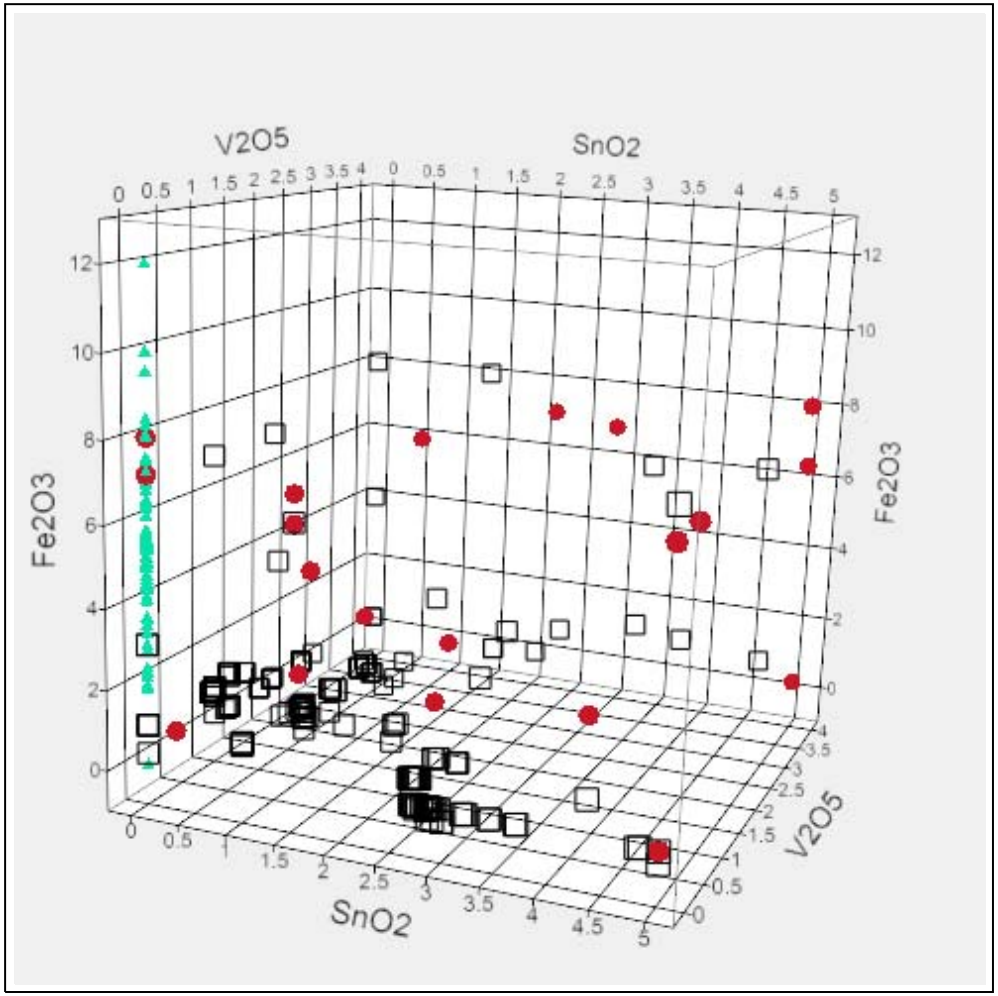


Figure 2.4. SnO_2-V_2O_5-Fe_2O_3 scatter-plot showing the WTP glasses (green triangles), the ORP glasses (black squares) and the 20 LORPM21-40 glasses (red circles).

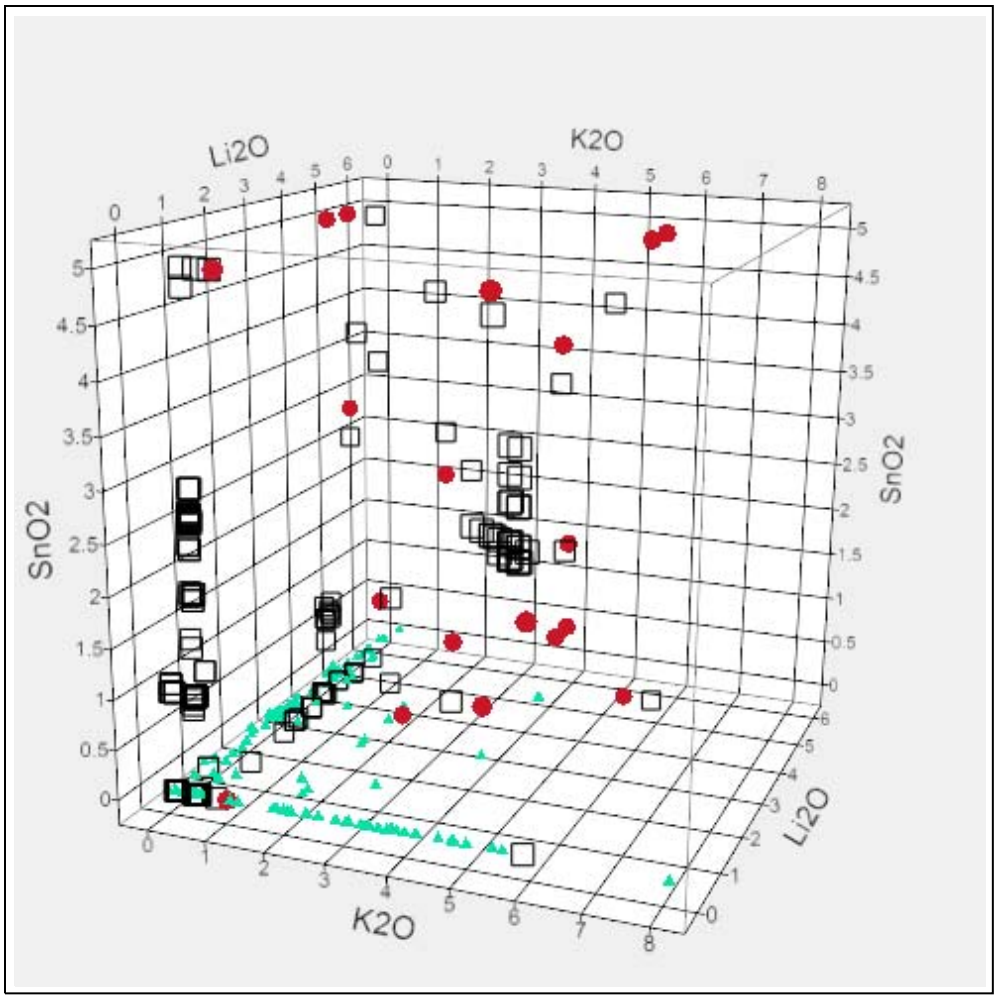


Figure 2.5. K_2O-Li_2O-SnO_2 scatter-plot showing the WTP glasses (green triangles), the ORP glasses (black squares) and the 20 LORPM21-40 glasses (red circles).

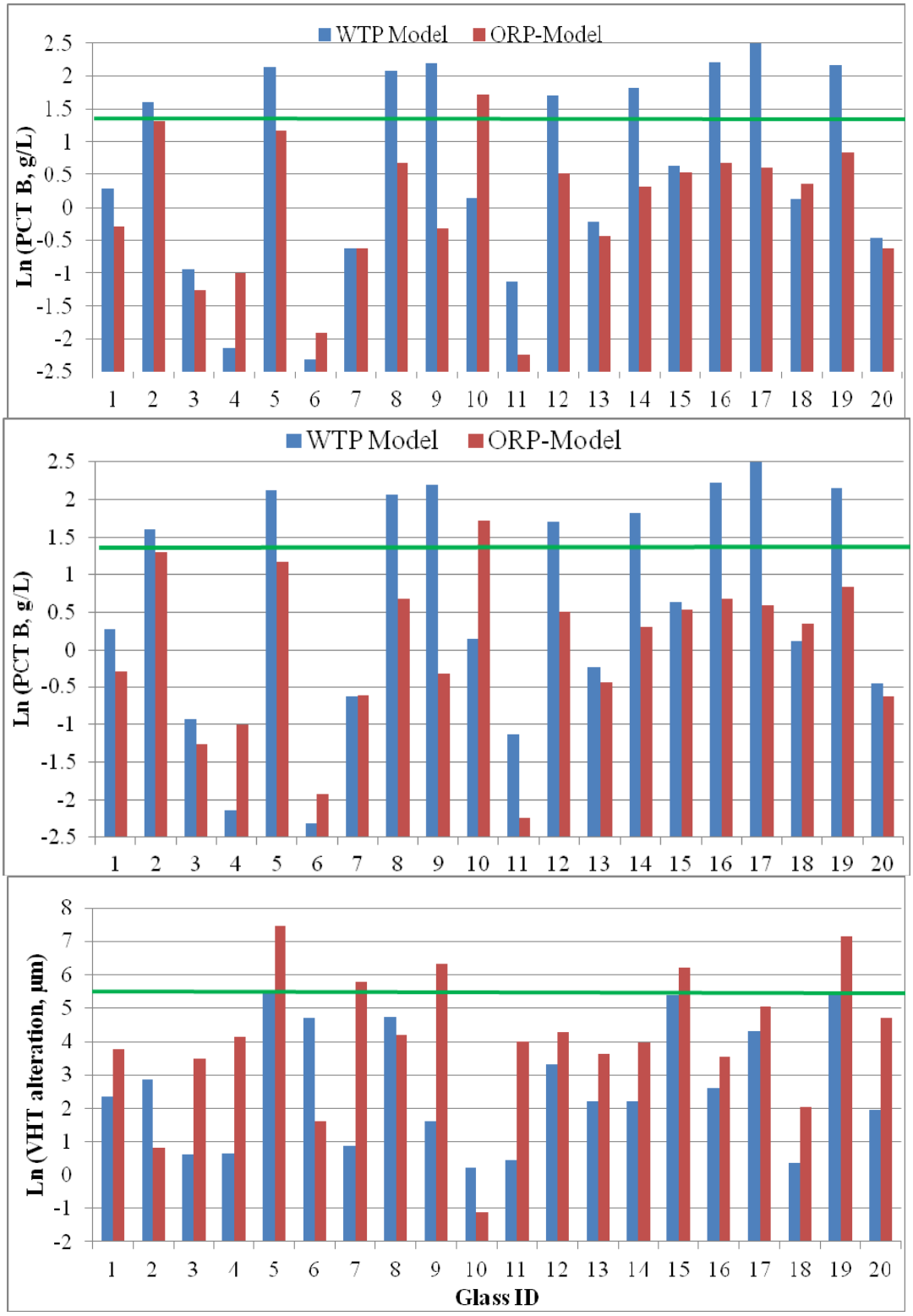


Figure 2.6. Comparison of predicted PCT and VHT responses for the 20 LORPM21-40 glasses using the baseline WTP models and the Phase 1 ORP models. Green lines indicate contractual limit.

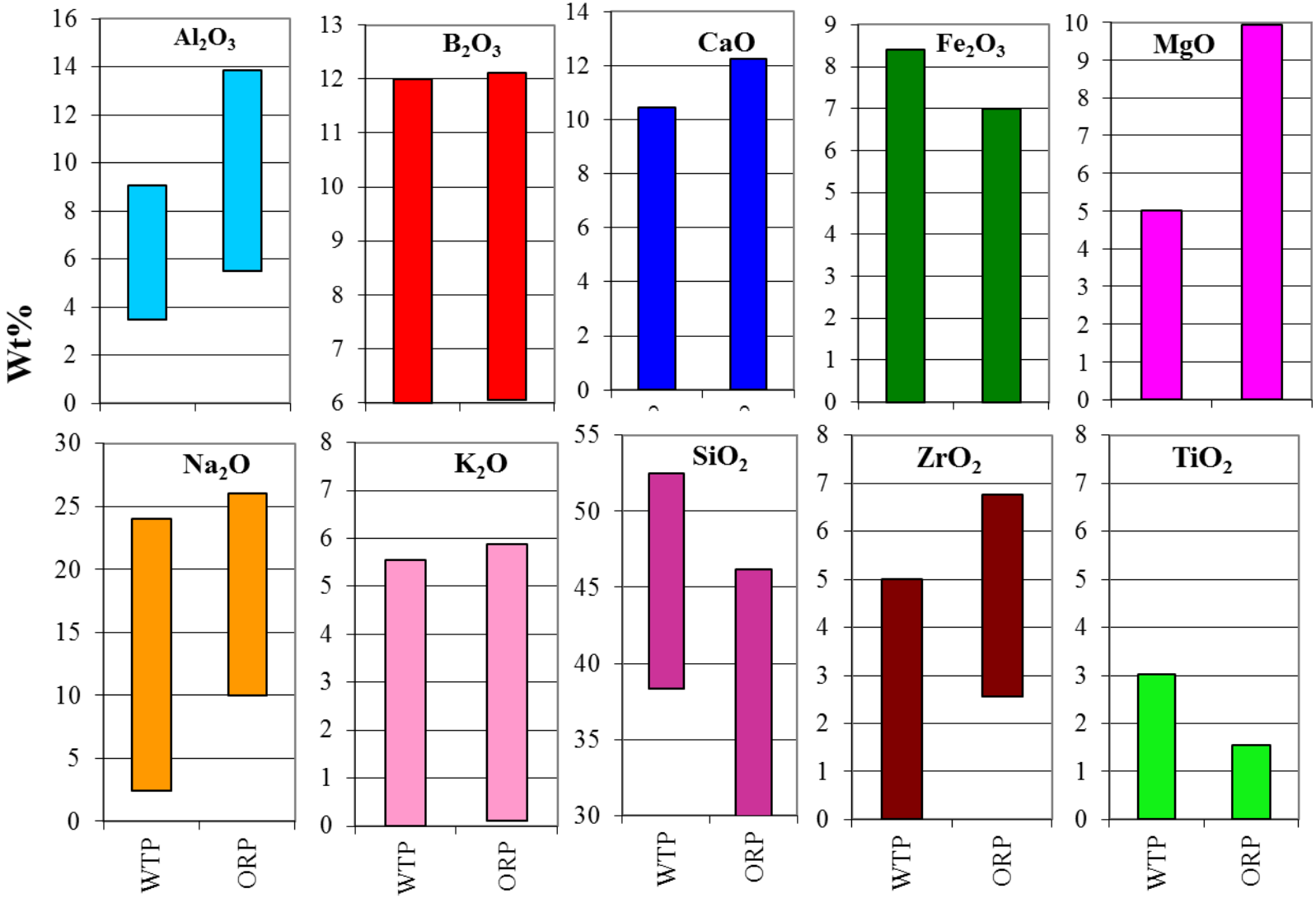


Figure 2.7. Range of concentrations for major components in the combined LAW glass dataset (537 glass samples).

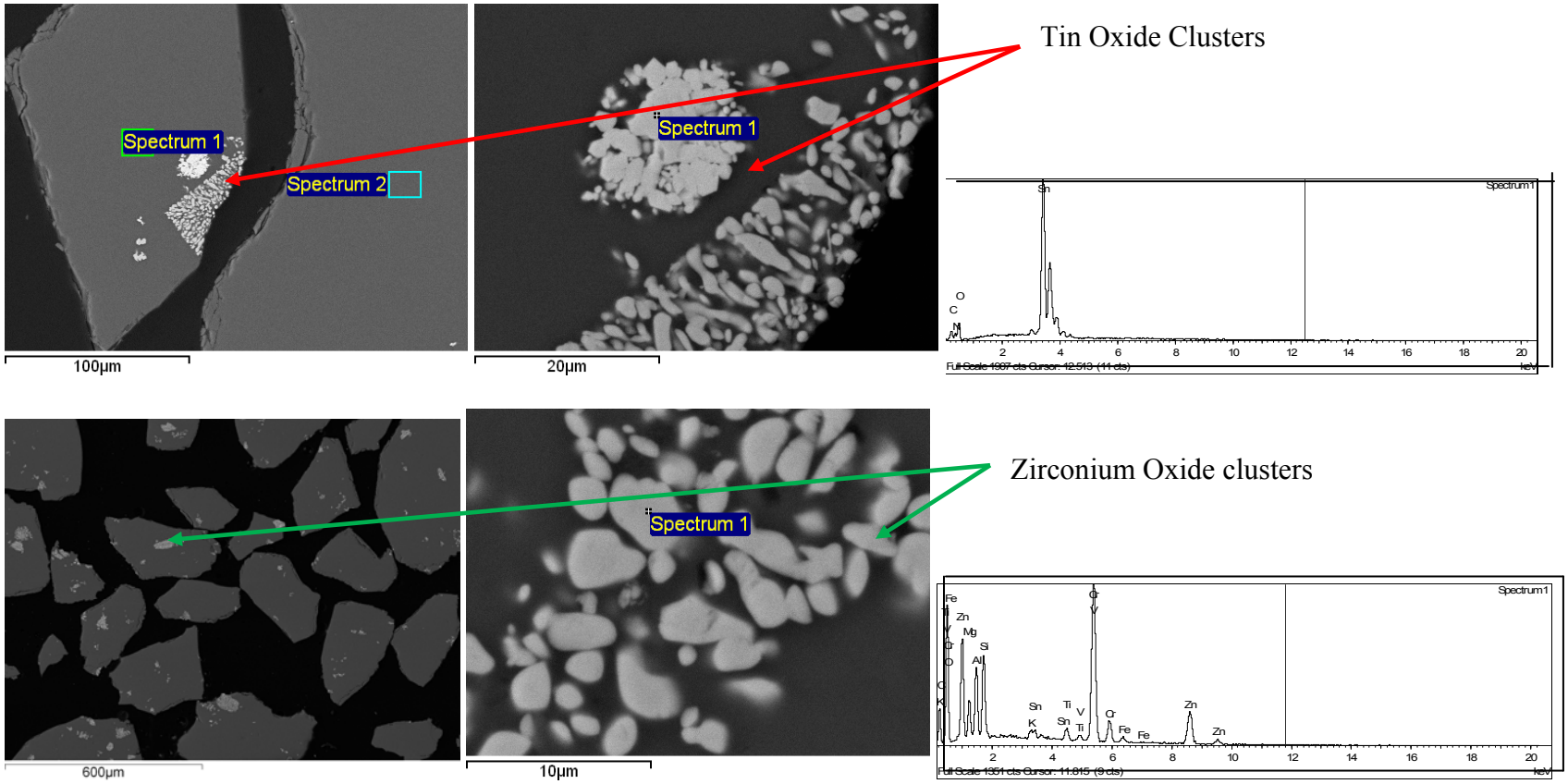


Figure 4.1. SEM images and EDS spectra of two types of crystals observed in LORPM24: 0.1 vol% of 0.2 to 1 micron size tin oxide crystals in clusters (top) and 1.1 vol% of elongated Zr-oxide crystals 0.1-2 µm in size homogeneously dispersed in the glass (bottom).

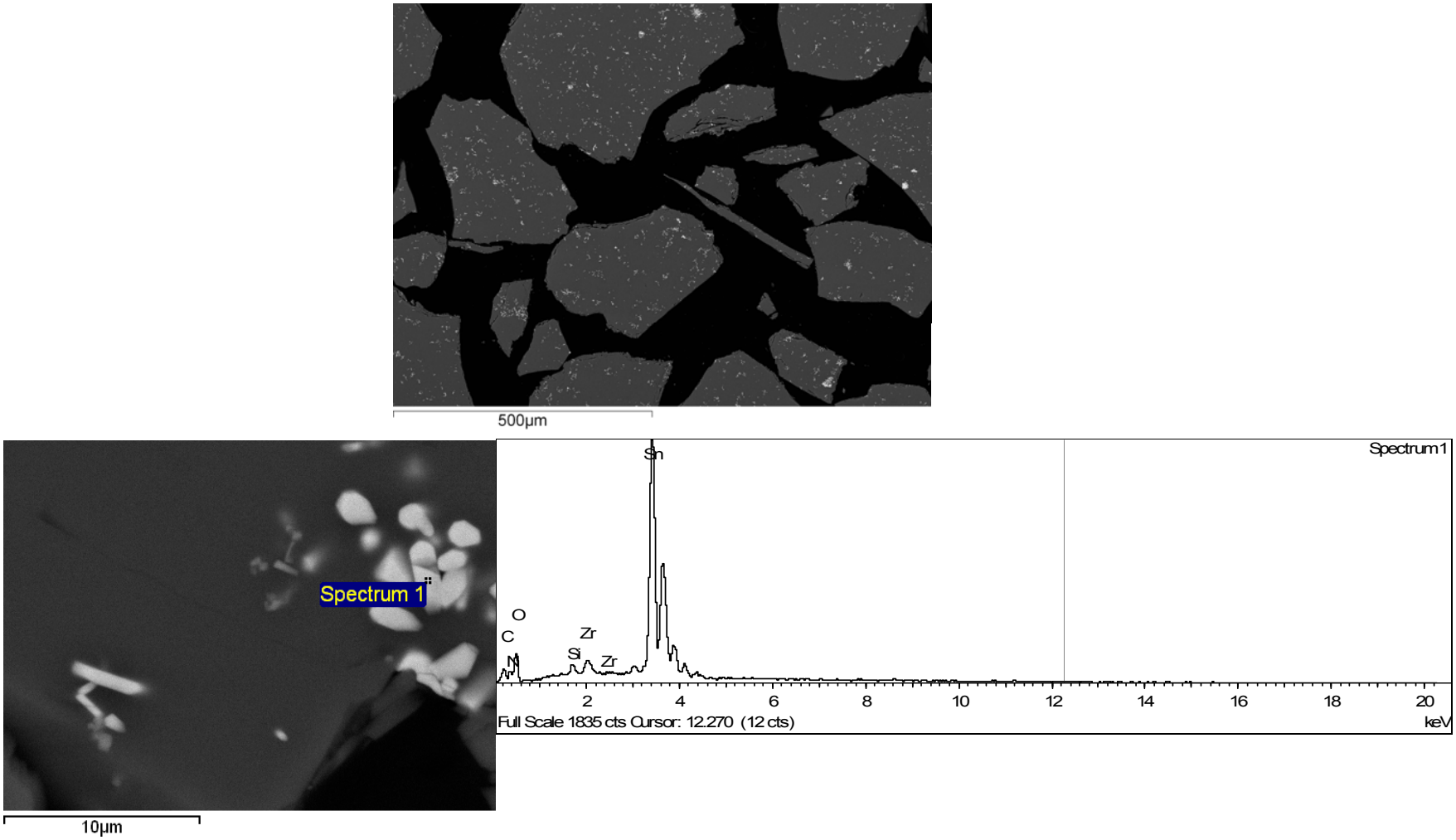


Figure 4.2. SEM images and EDS spectra of crystals observed in LORPM29: 1.5 vol% of 0.2-1 µm by 1-5 µm, subhedral, clustered, and heterogeneously distributed Sn-oxide crystals.

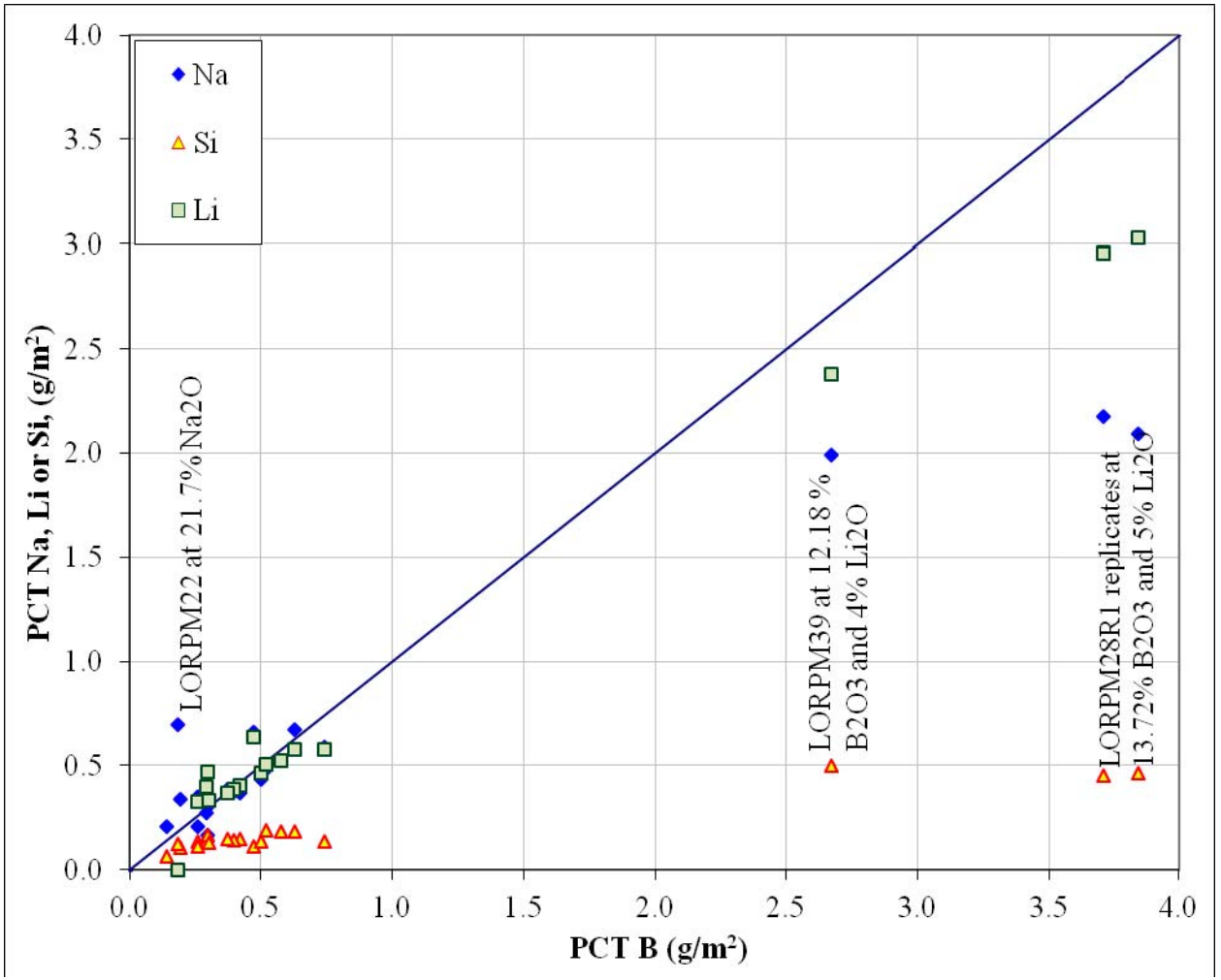


Figure 4.3. PCT sodium, lithium and silicon releases (g/m^2) as a function of PCT boron release for 20 LORPM21-40 glasses.

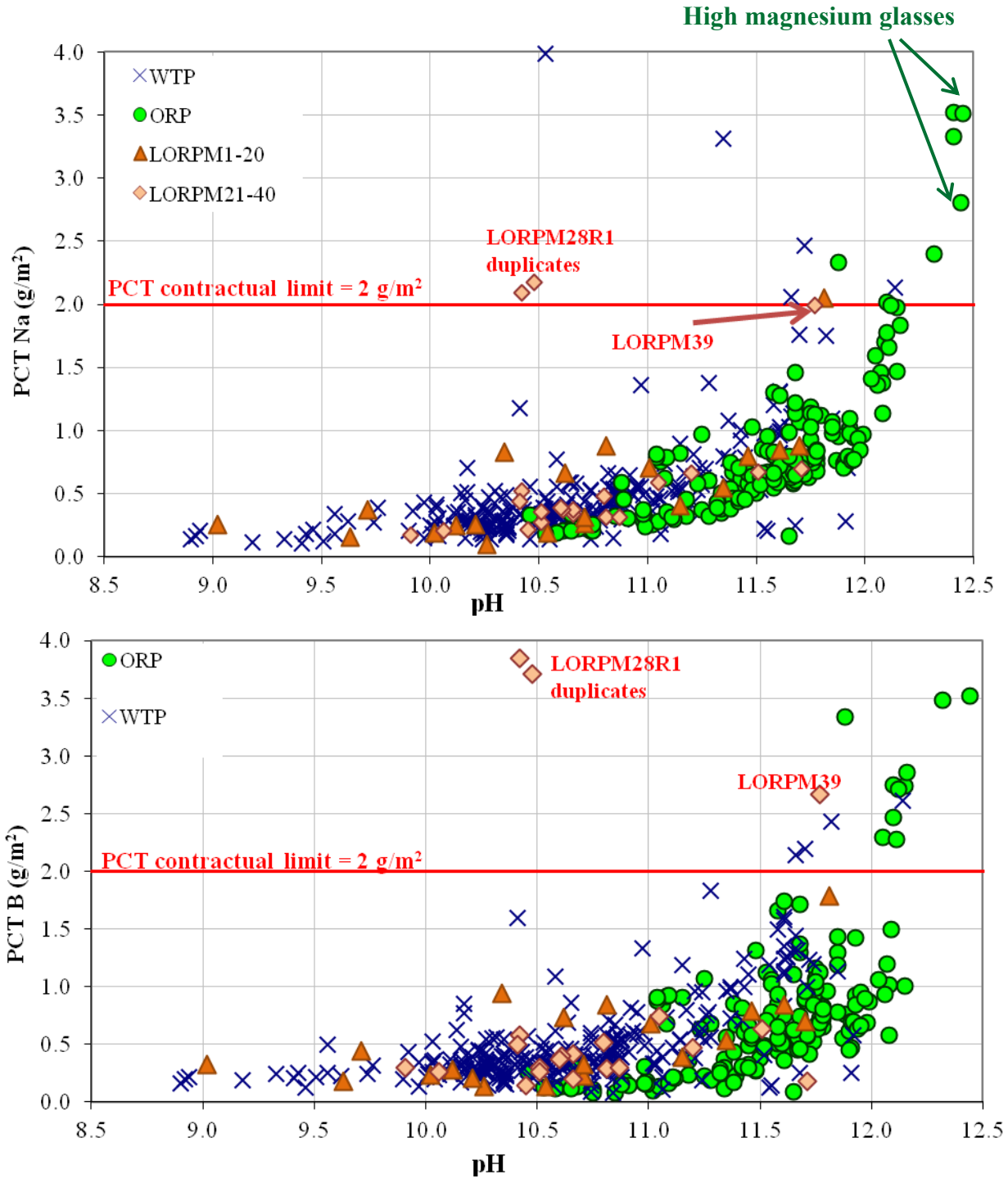


Figure 4.4. PCT sodium and boron releases as a function of the pH measured at 20°C in the 7-day PCT leachate.

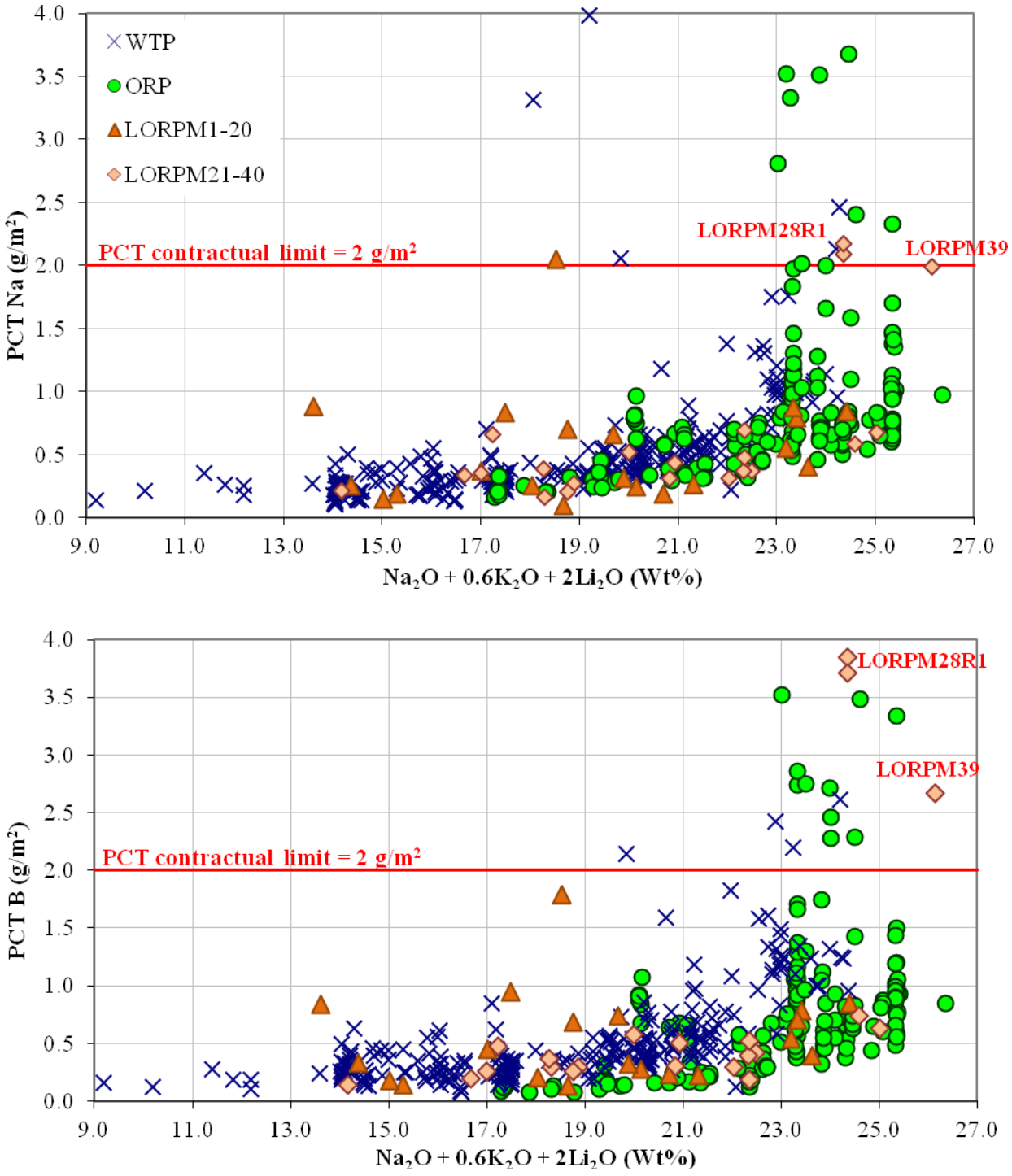


Figure 4.5. PCT sodium and boron releases (g/m^2) as a function of glass alkali concentration.

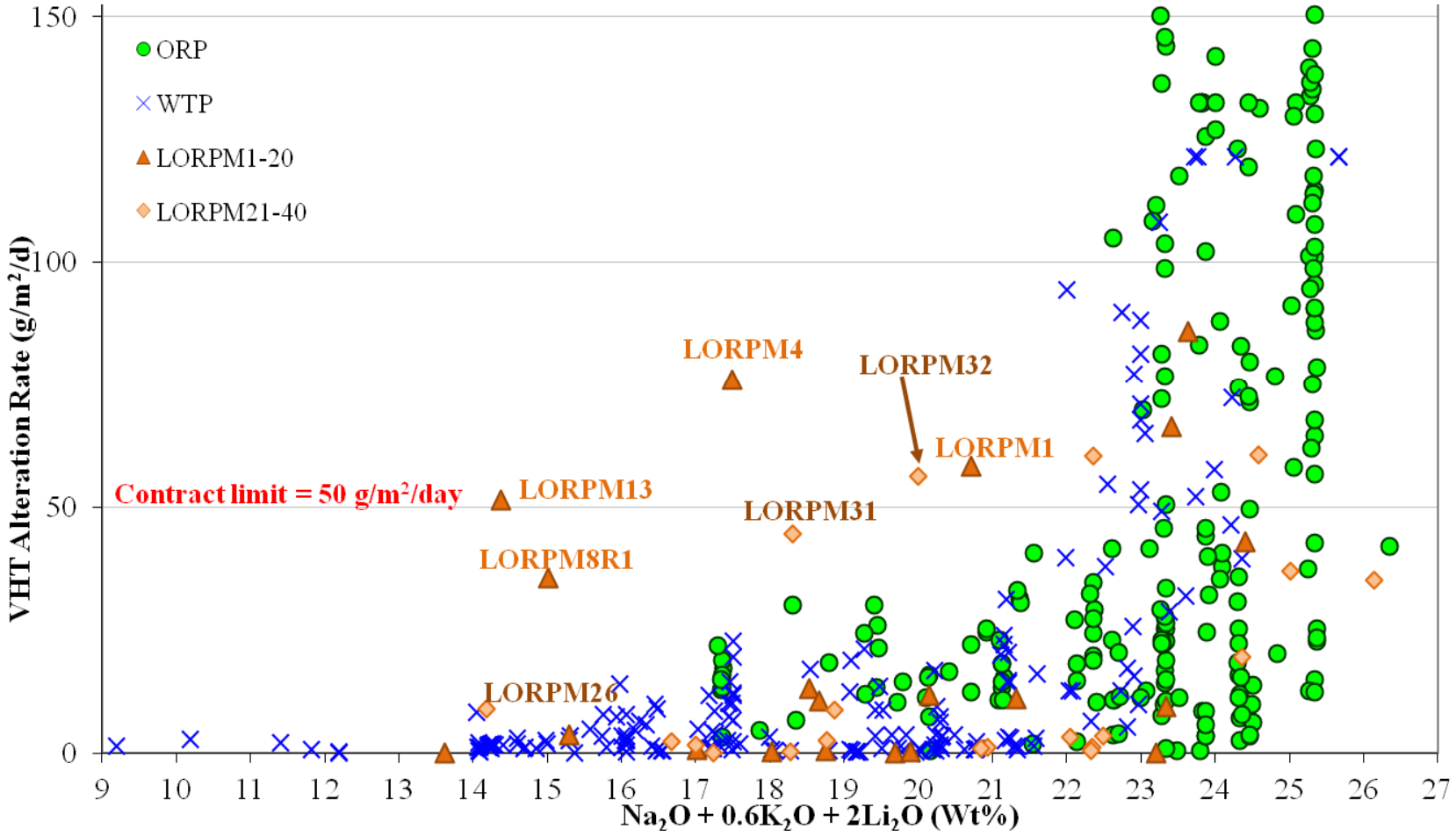


Figure 4.6. VHT alteration rate (g/m^2/day) as a function of glass alkali concentration.

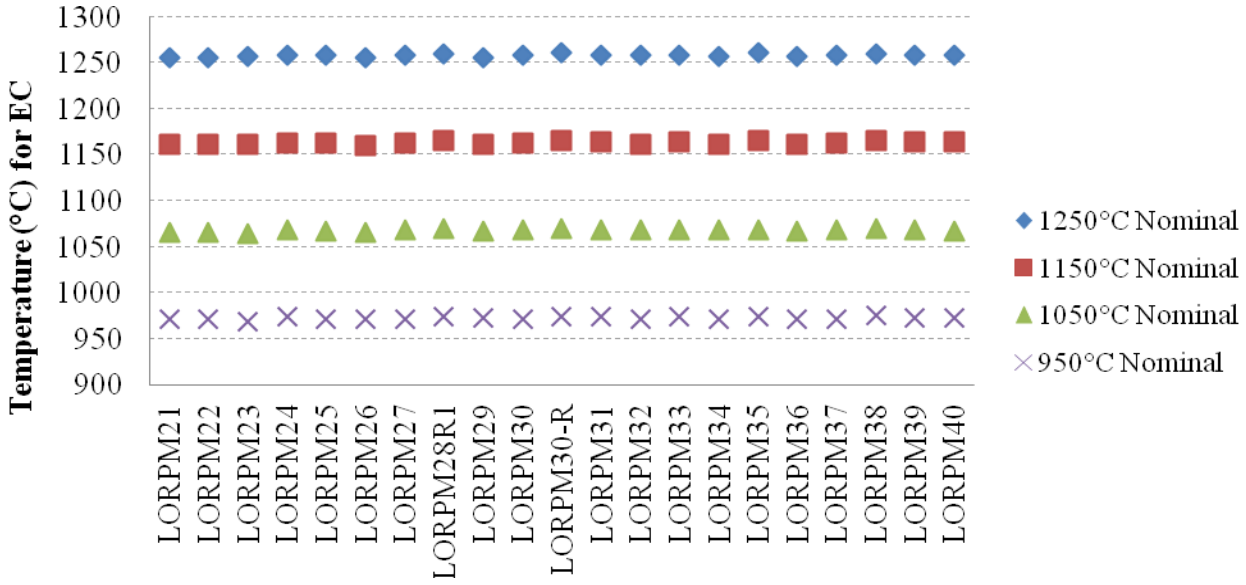


Figure 4.7. Distribution of temperature values at which melt electrical conductivity was measured for the 20 LORPM21-40 glasses.

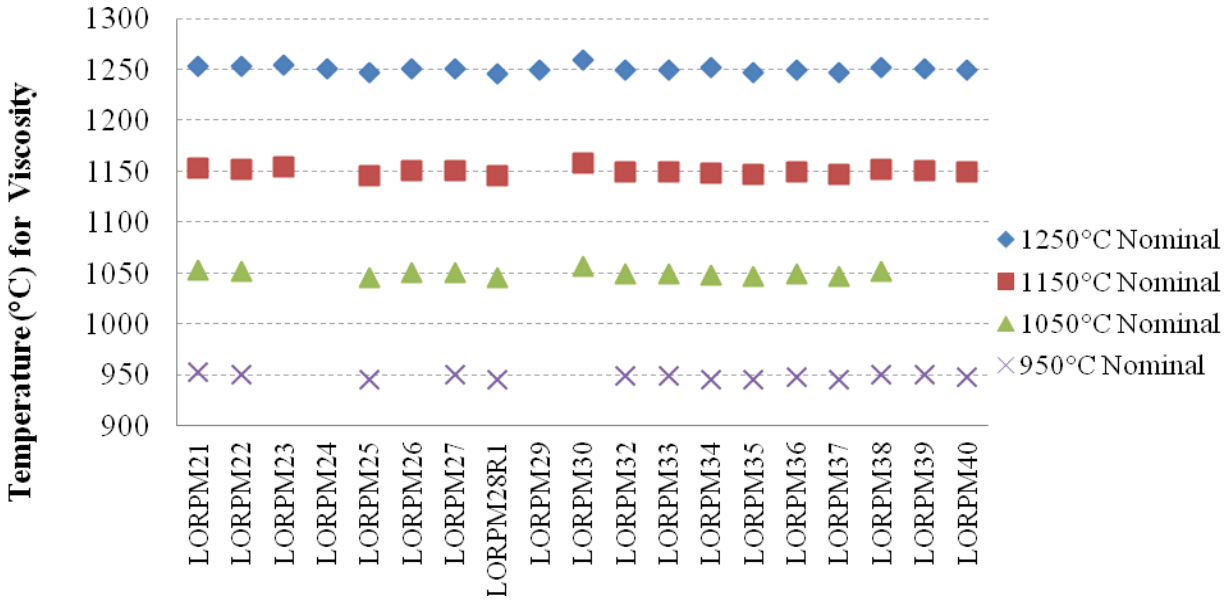


Figure 4.8. Distribution of temperature values at which melt viscosity was measured for the 20 LORPM21-40 glasses.

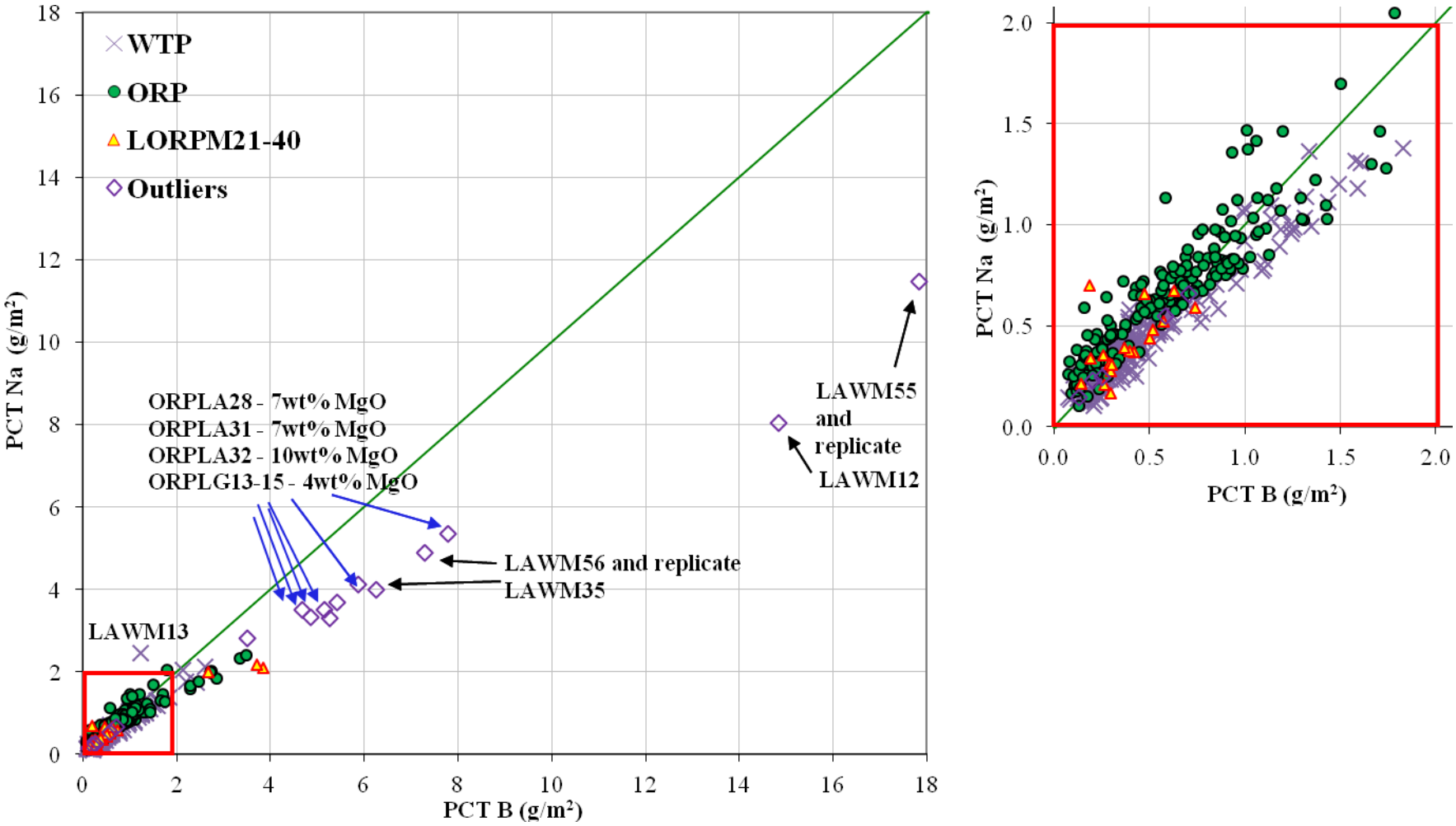


Figure 5.1. PCT sodium release as a function of PCT boron release (g/m^2) for 477 LAW glasses considered in new models.

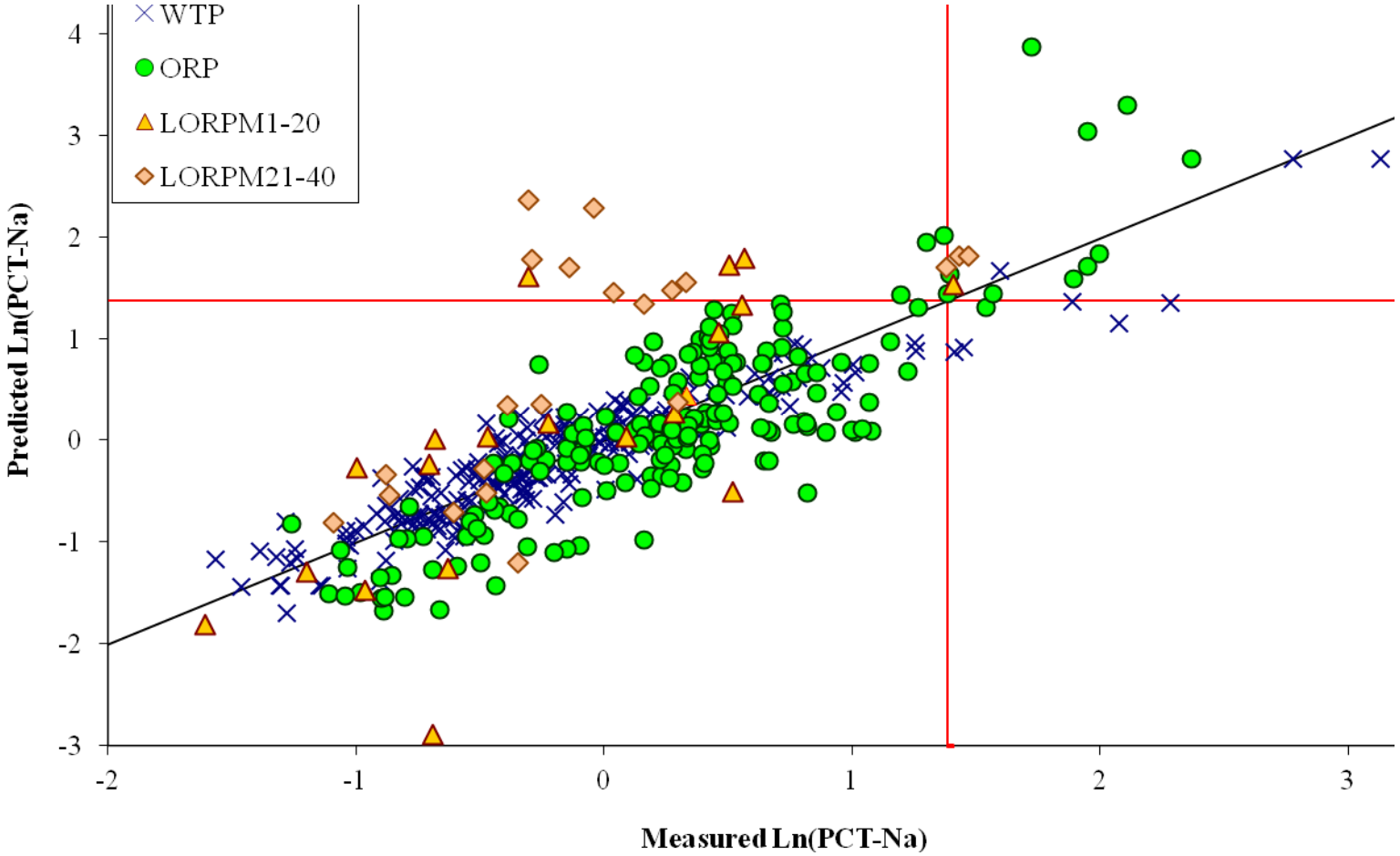


Figure 5.2. Comparison of predicted versus measured PCT-Na for the WTP-LAW (including outliers), ORP-LAW, twenty Phase 1 LORPM glasses, and the twenty LORPM21-40 glasses using the WTP baseline 17-term reduced partial quadratic mixture PCT-Na model [1]. The red lines represent the WTP contract limit (4 g/L) for PCT-Na release.

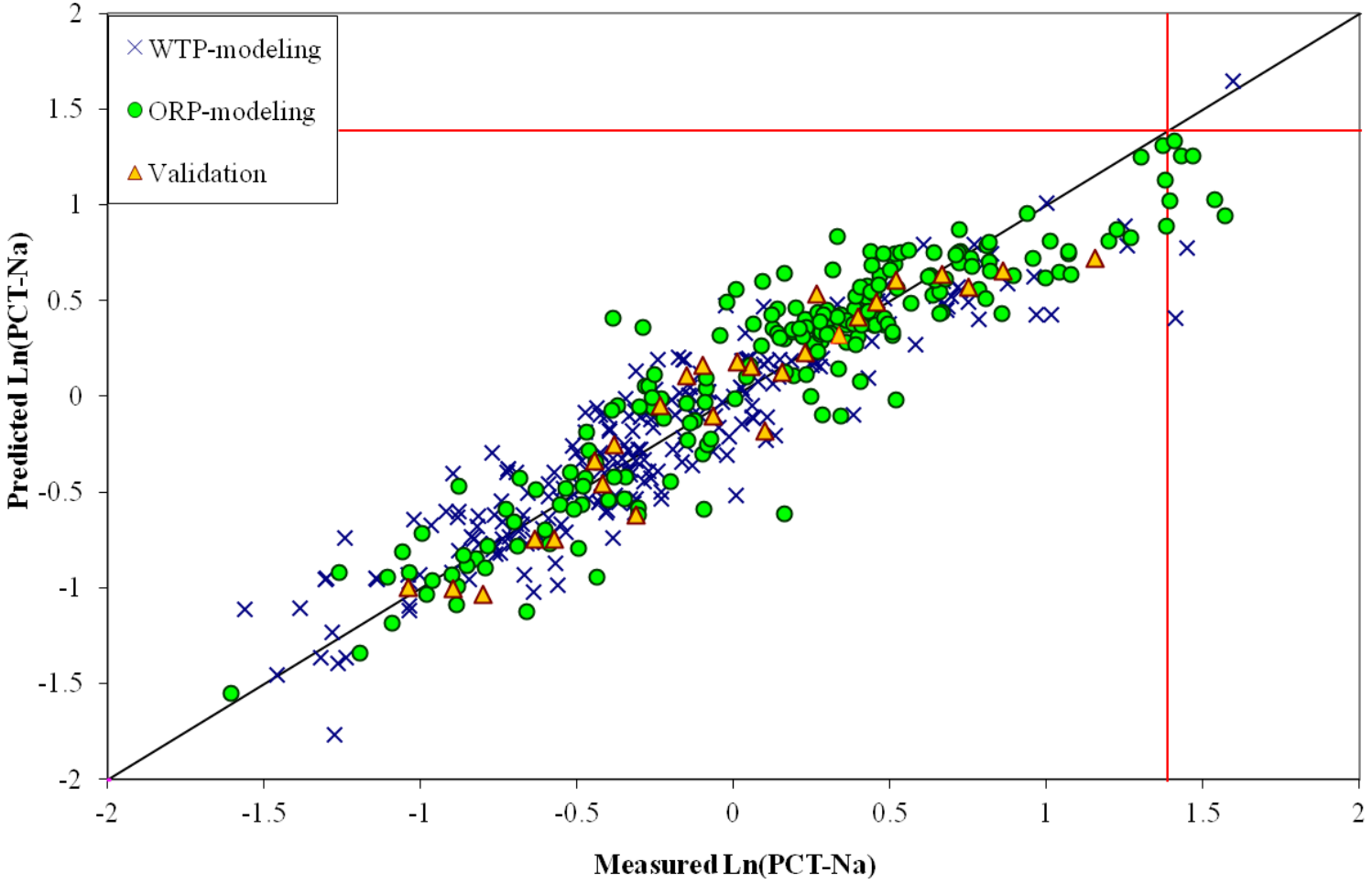


Figure 5.3. Predicted versus measured plot for 24-term mixture model (Model 4) on PCT-Na. The red lines represent the WTP contract limit (4 g/L) for PCT-Na release.

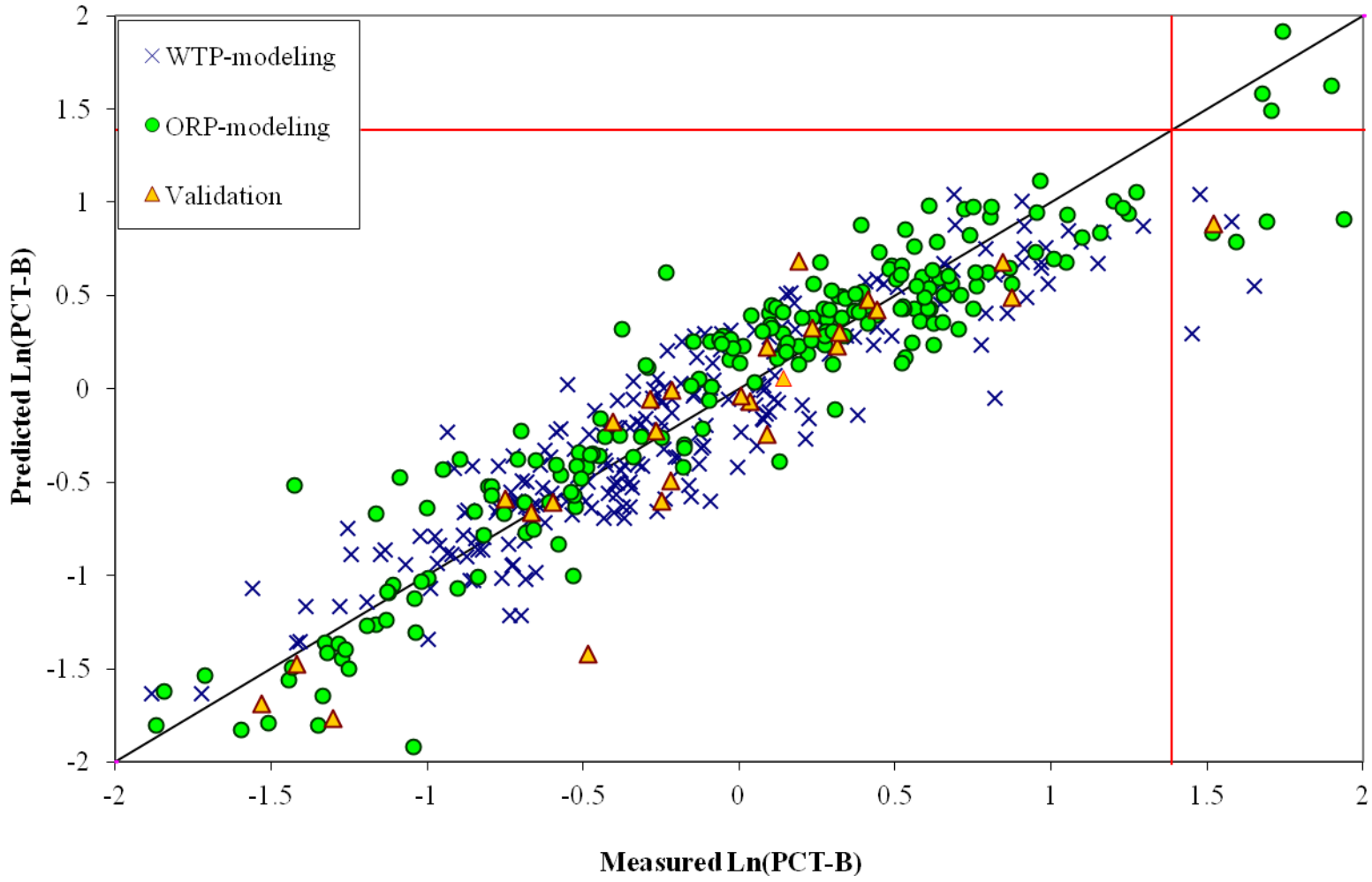


Figure 5.4. Predicted versus measured plot for 26-term mixture model (Model 6) on PCT-B. The red lines represent the WTP contract limit (4 g/L) for PCT-B release.

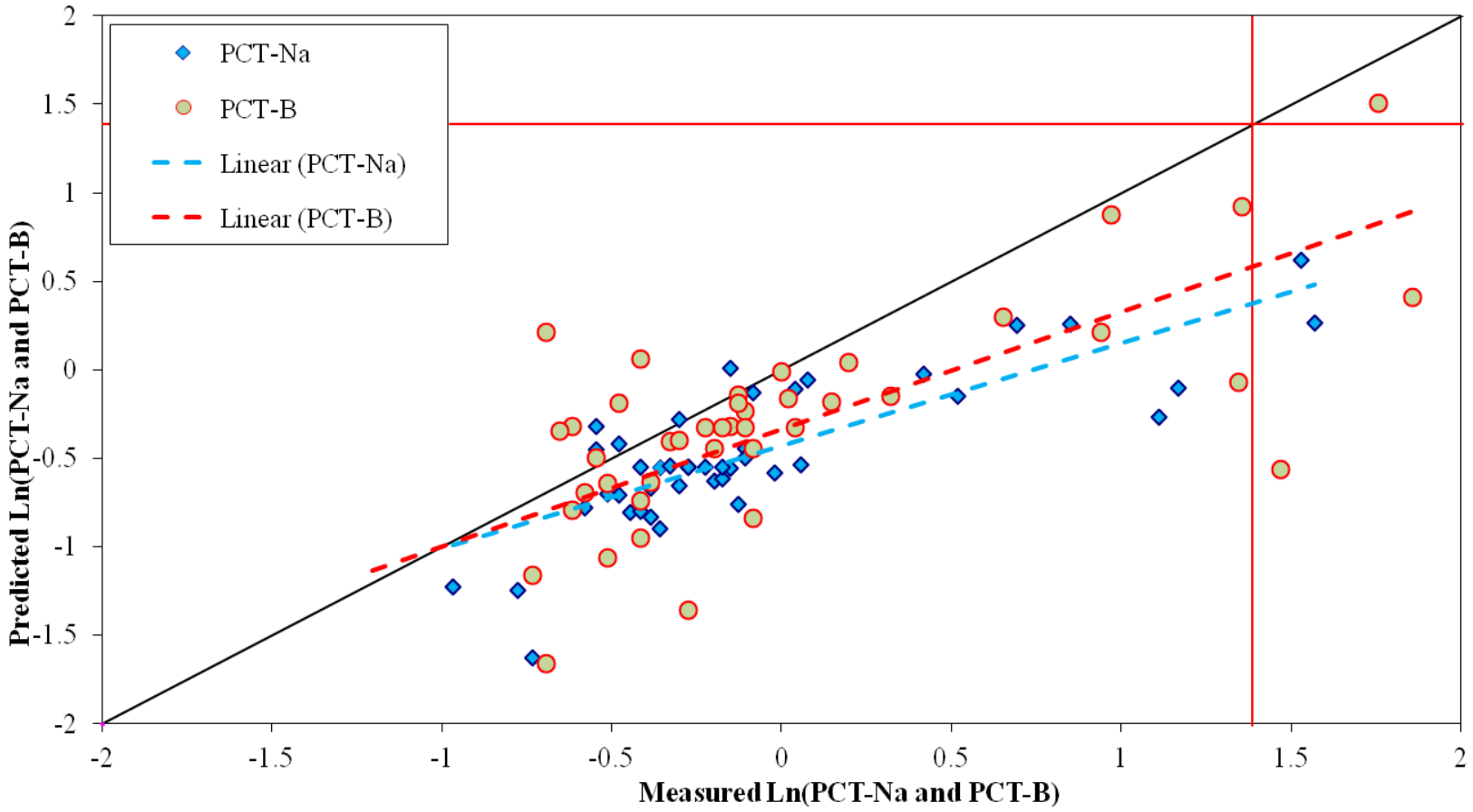


Figure 5.5. Predicted versus measured plot applying the selected mixture models on PCT-Na (Model 4) and PCT-B (Model 6) to glasses from the HLP series with compositions falling inside the composition regions of the LAW models.

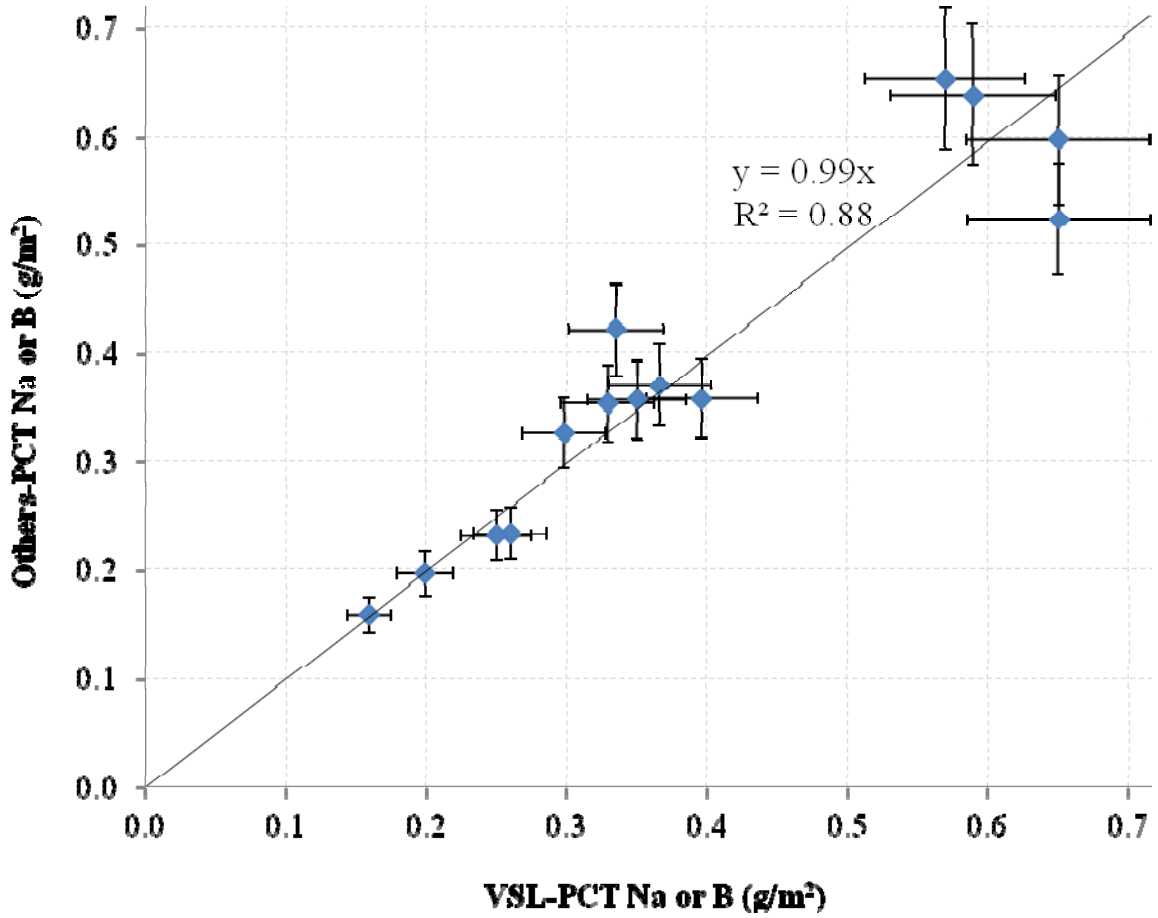


Figure 5.6. PCT sodium and PCT boron releases from measurements at VSL versus measurements at other laboratories (g/m^2) for seven pairs of LAW glasses considered in the current model (with 10% error bars).

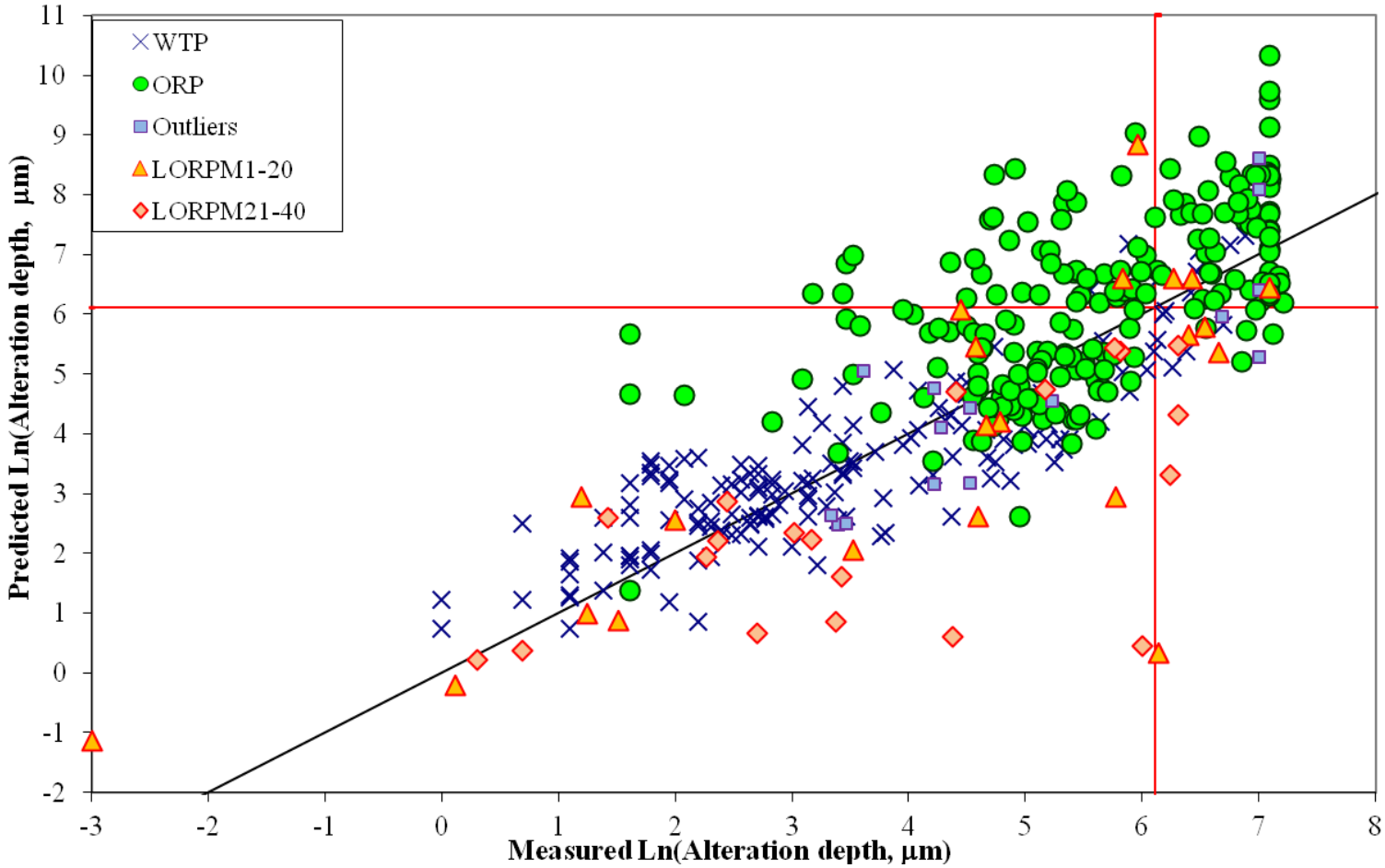


Figure 5.7. Comparison of predicted versus measured VHT for the WTP-LAW, ORP-LAW, twenty Phase 1 LORPM1-20 glasses, and the twenty LORPM21-40 glasses using the WTP baseline 15-term reduced partial quadratic mixture model [1] on the natural logarithm of VHT alteration depth. The red lines represent the WTP contract limit (50 g/m^2/day alteration rate).

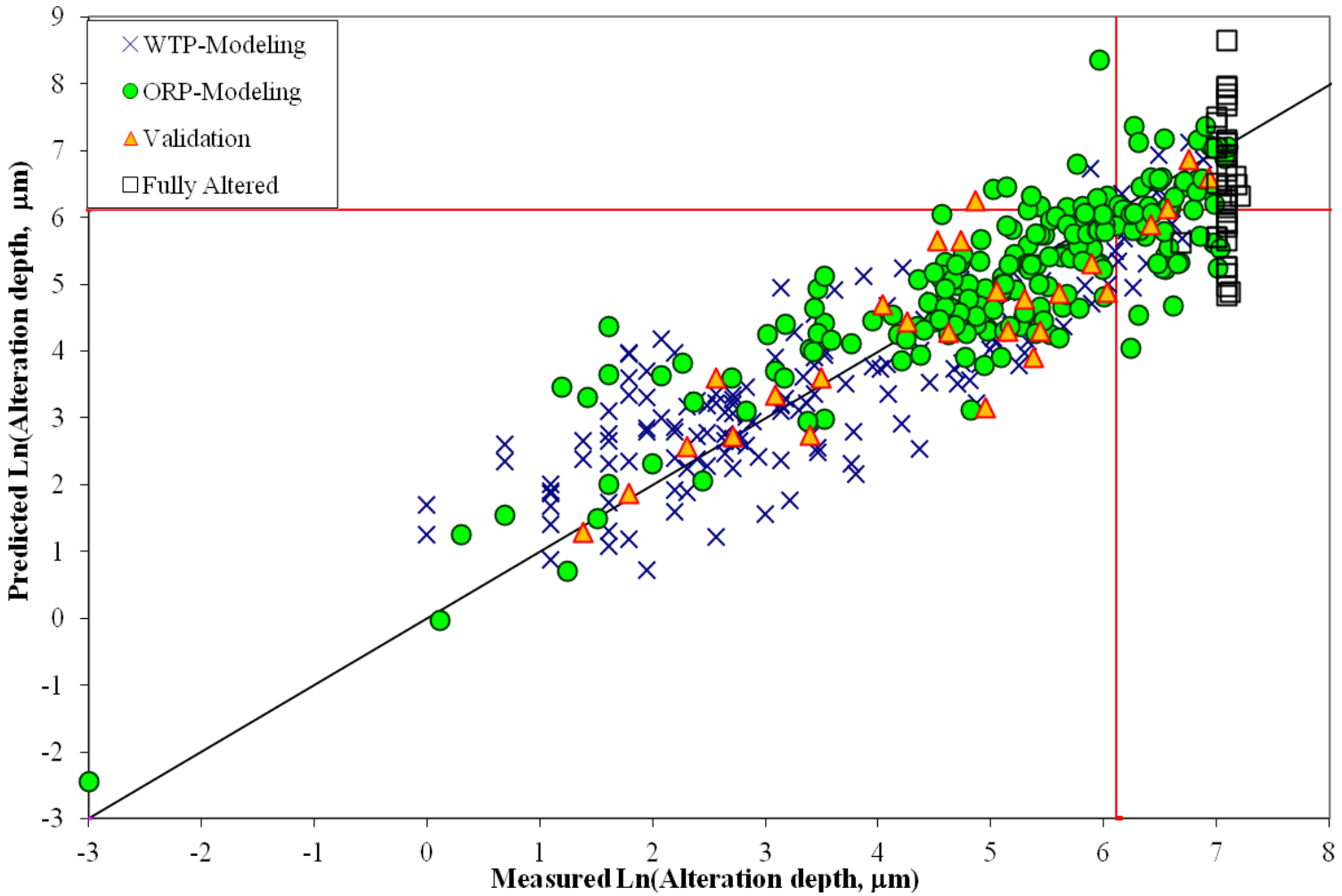


Figure 5.8. Predicted versus measured plot for 22-term mixture model (Model 3) on VHT alteration depth (*D*). The red lines represent the WTP contract limit corresponding to 50 g/m^2/day (*D* = 453 µm).

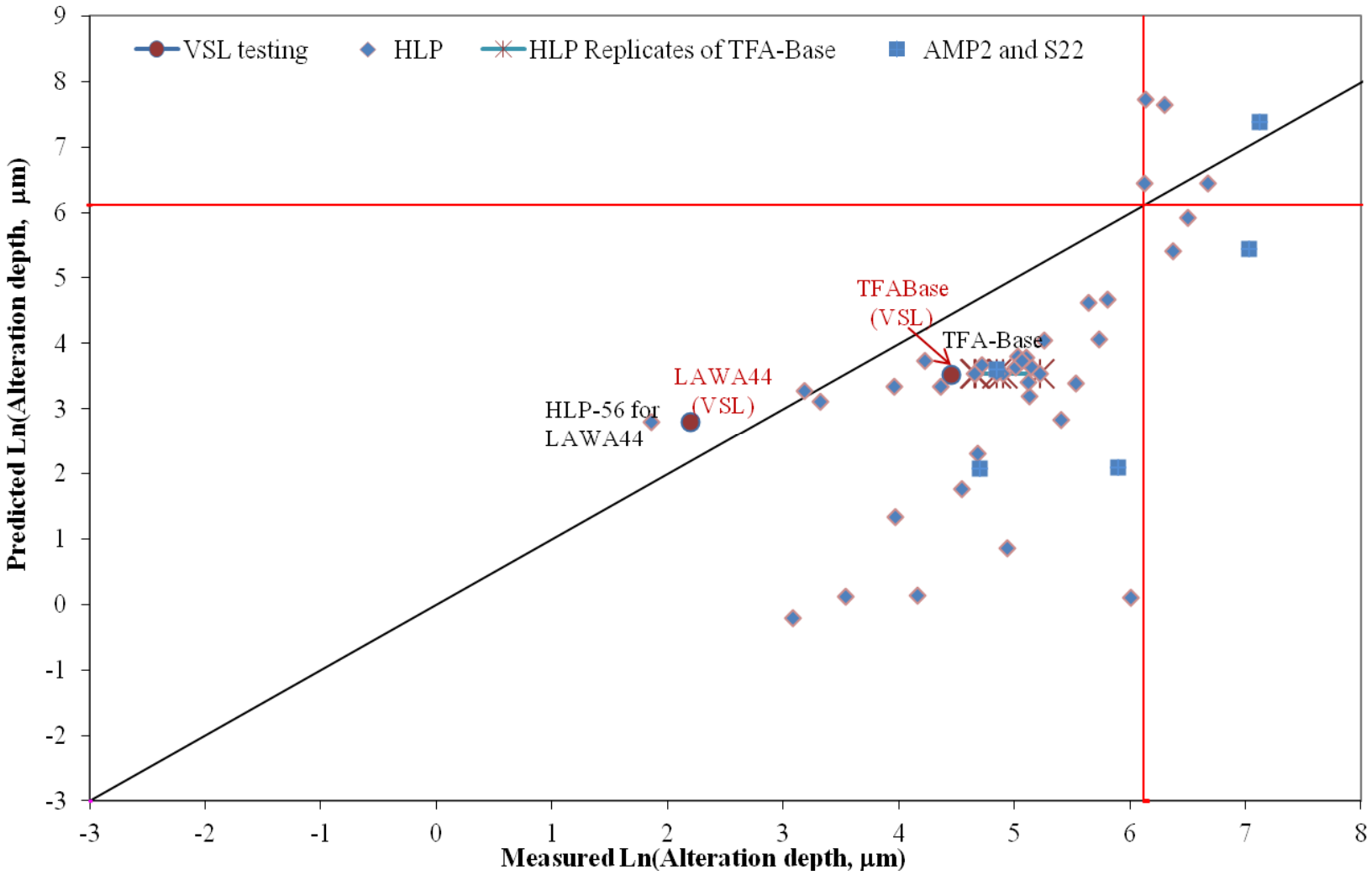


Figure 5.9. Predicted versus measured plot for 22-term mixture model (Model 3) on extrapolated VHT alteration depth (*D*) from published rate values. The red lines represent the WTP contract limit corresponding to 50 g/m^2/day (*D* = 453 µm).

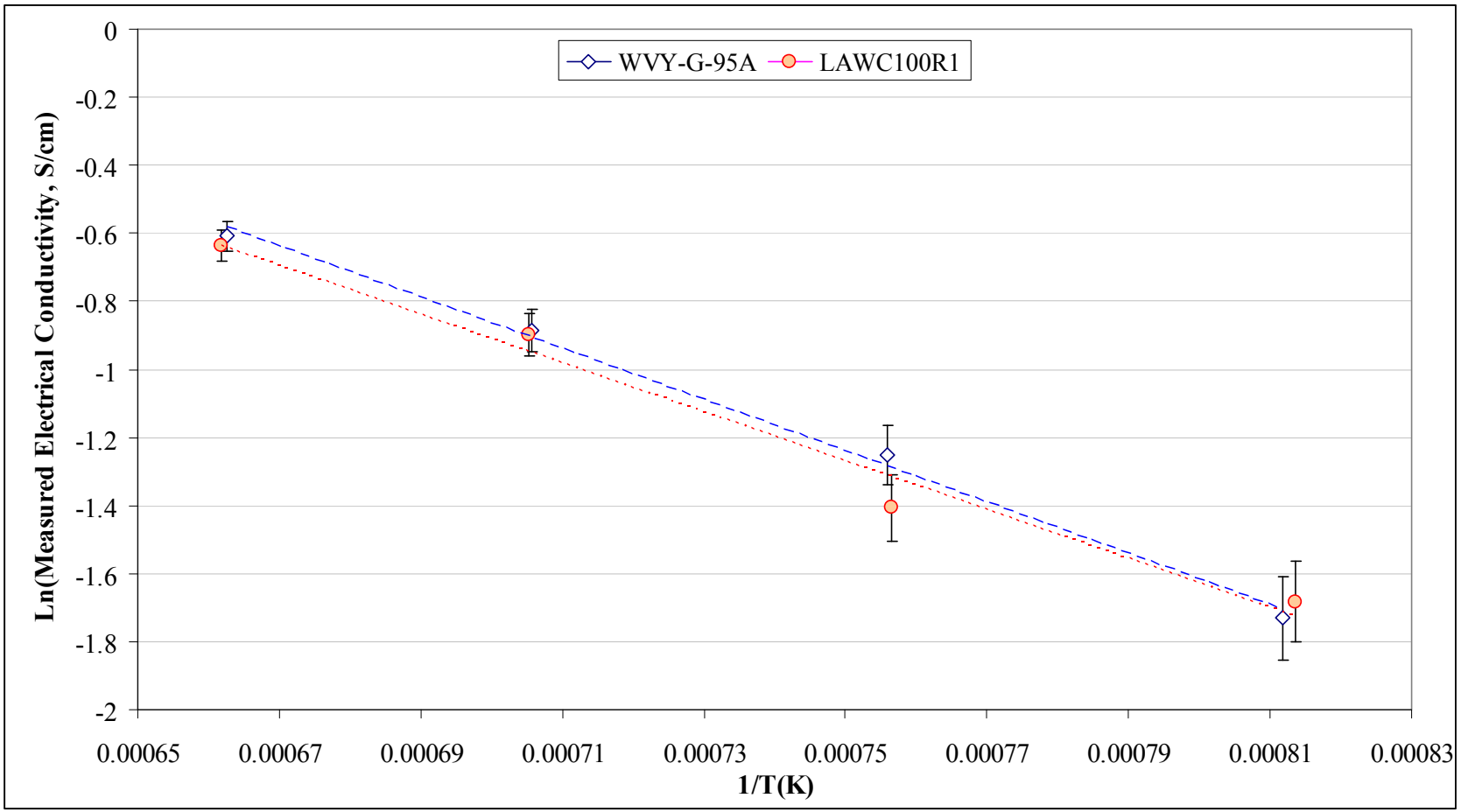


Figure 5.10. Melt electrical conductivity data measured on near-replicate glasses LAWC100R1 (crucible) and WVY-G-95A (DM100 melter glass).

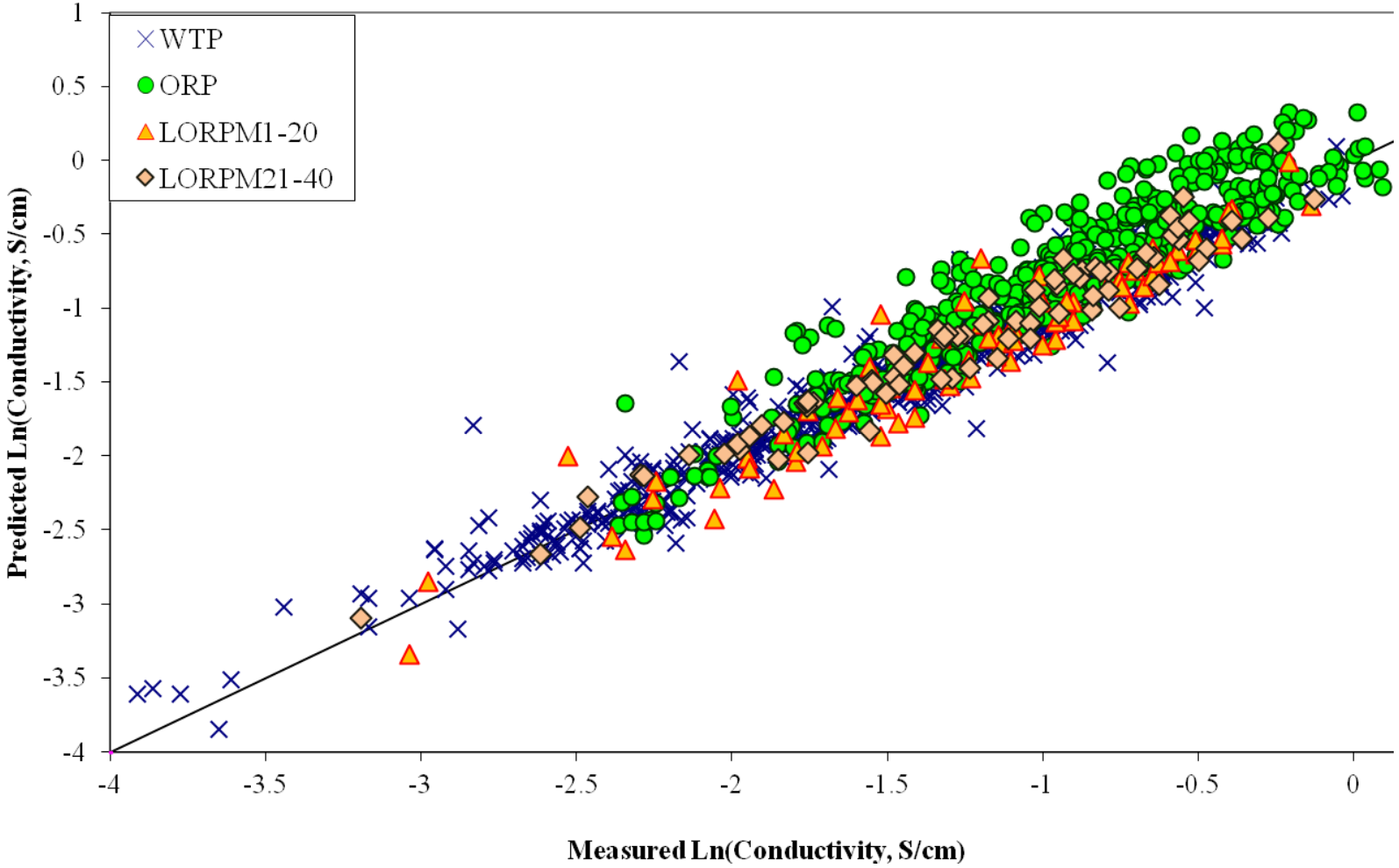


Figure 5.11. Comparison of predicted versus measured electrical conductivity for the WTP-LAW, ORP-LAW, and twenty LORPM glasses using the WTP baseline 25-Term reduced Arrhenius linear mixture model with three cross product terms [1] on the natural logarithm of electrical conductivity.

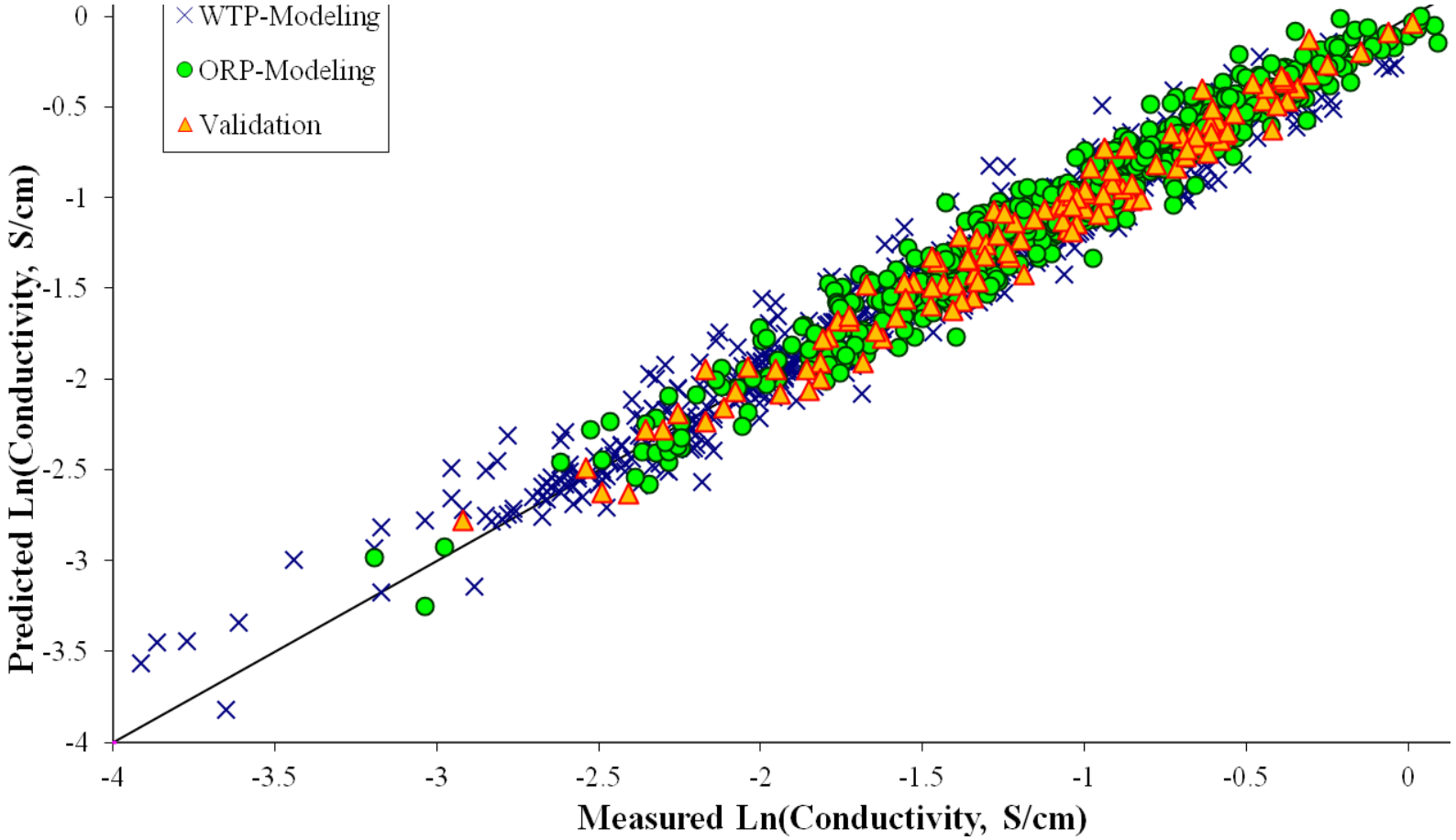


Figure 5.12. Predicted versus measured plot for 25-term Arrhenius-linear mixture model (Model 4) with three cross product terms on ILAW electrical conductivity.

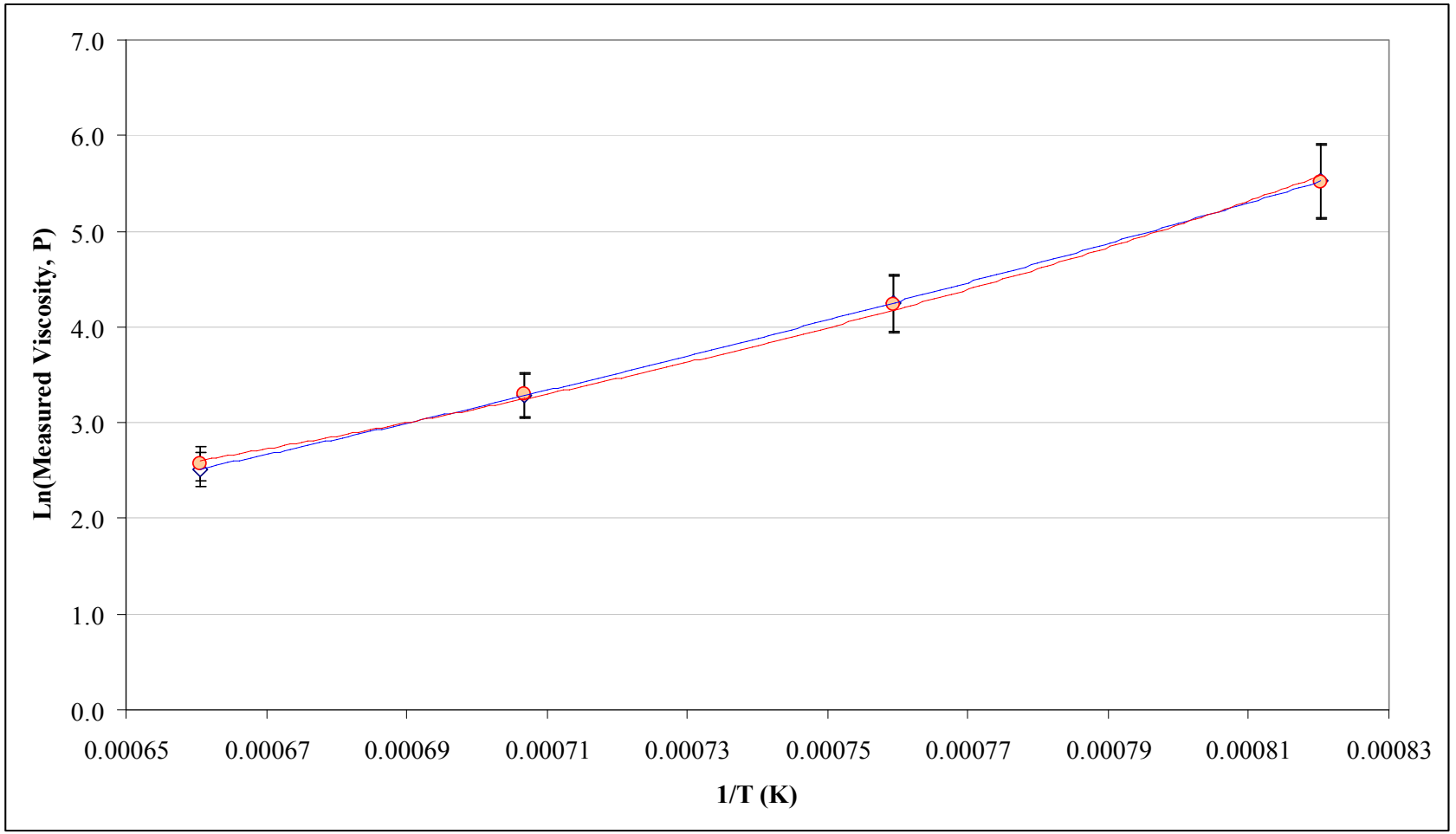


Figure 5.13. Melt viscosity data measured on near-replicate glasses LAWC100R1 (crucible) and WVY-G-95A (DM100 melter glass).

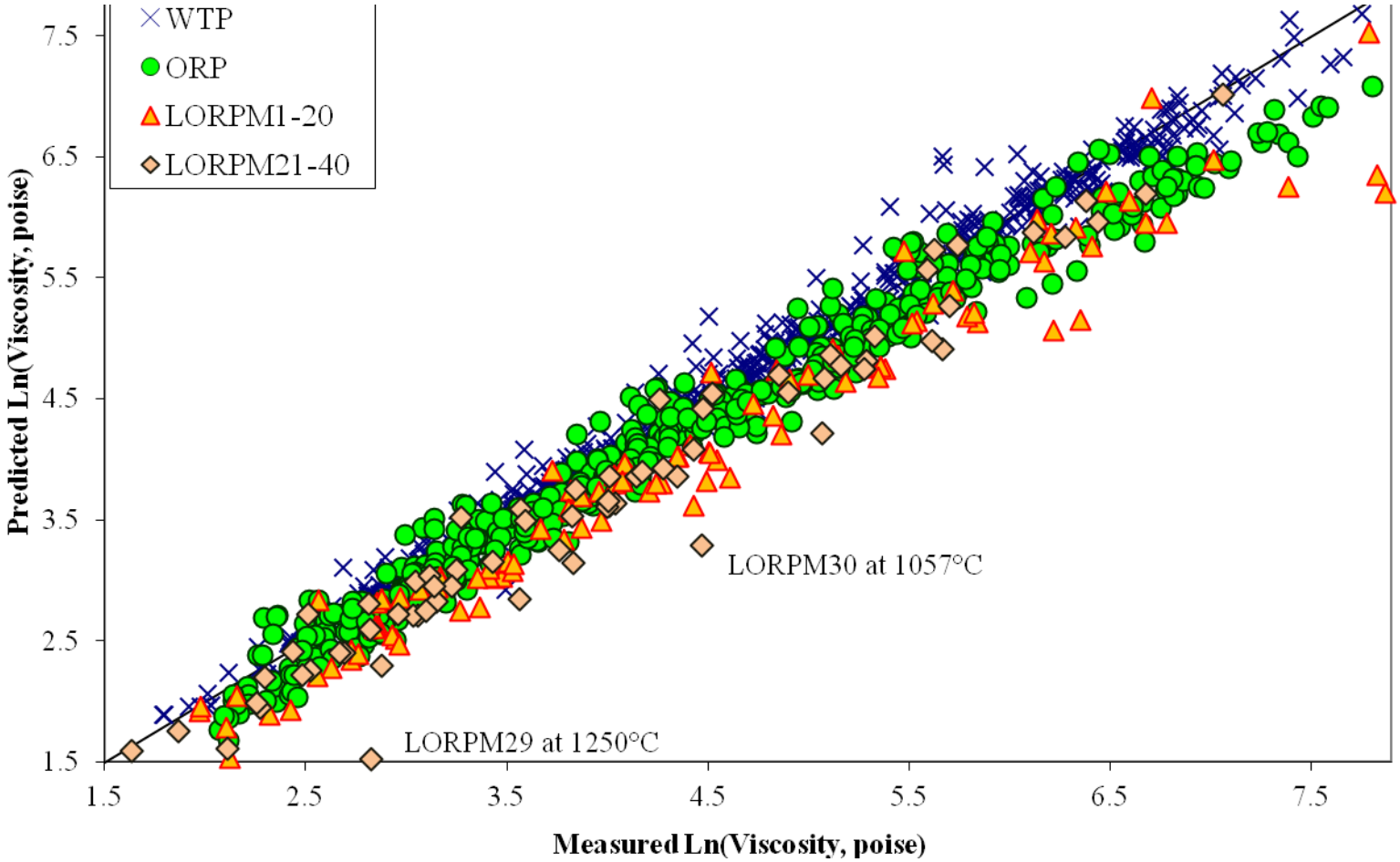
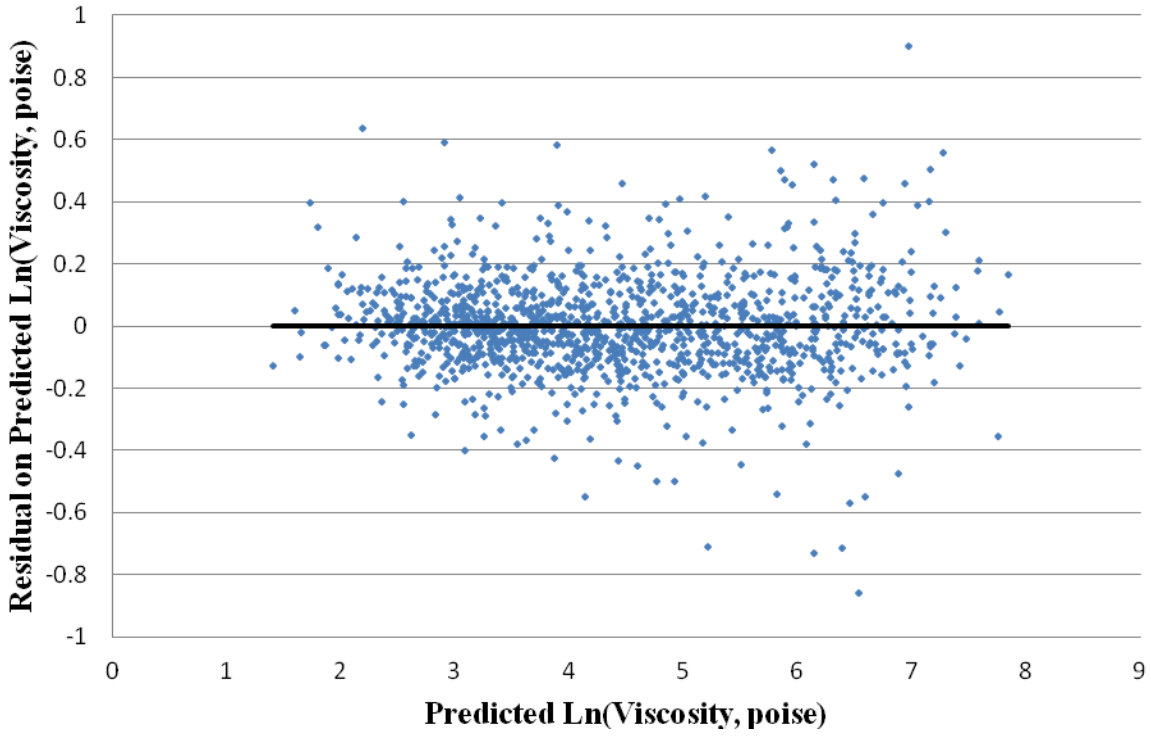


Figure 5.14. Comparison of predicted versus measured melt viscosity for the WTP-LAW, ORP-LAW, eighteen Phase 1 LORPM glasses, and nineteen LORPM21-40 glasses using the WTP baseline 26-term reduced truncated T2-linear mixture model with four quadratic terms on the natural logarithm of viscosity.



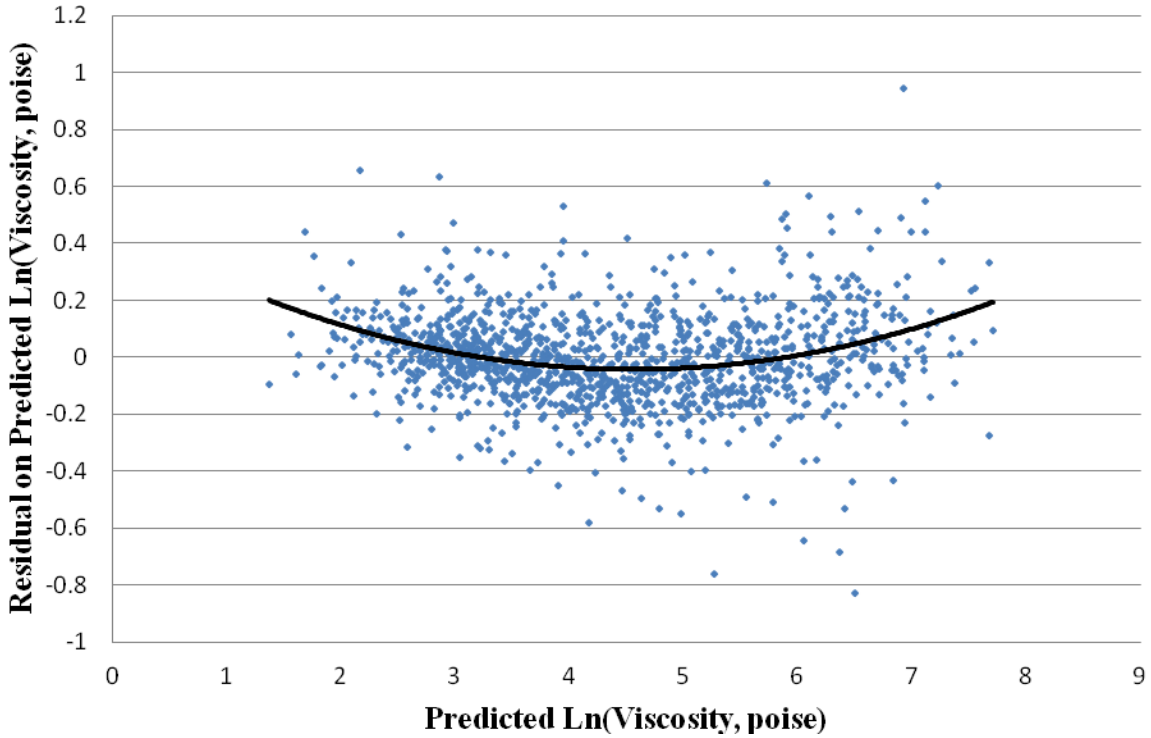


Figure 5.15. Plot of residuals on predicted ln (viscosity) comparing model forms in $1/T^2$ (top: Model 4) and in 1/T (bottom: Model 3) illustrating the skewed response with 1/T.

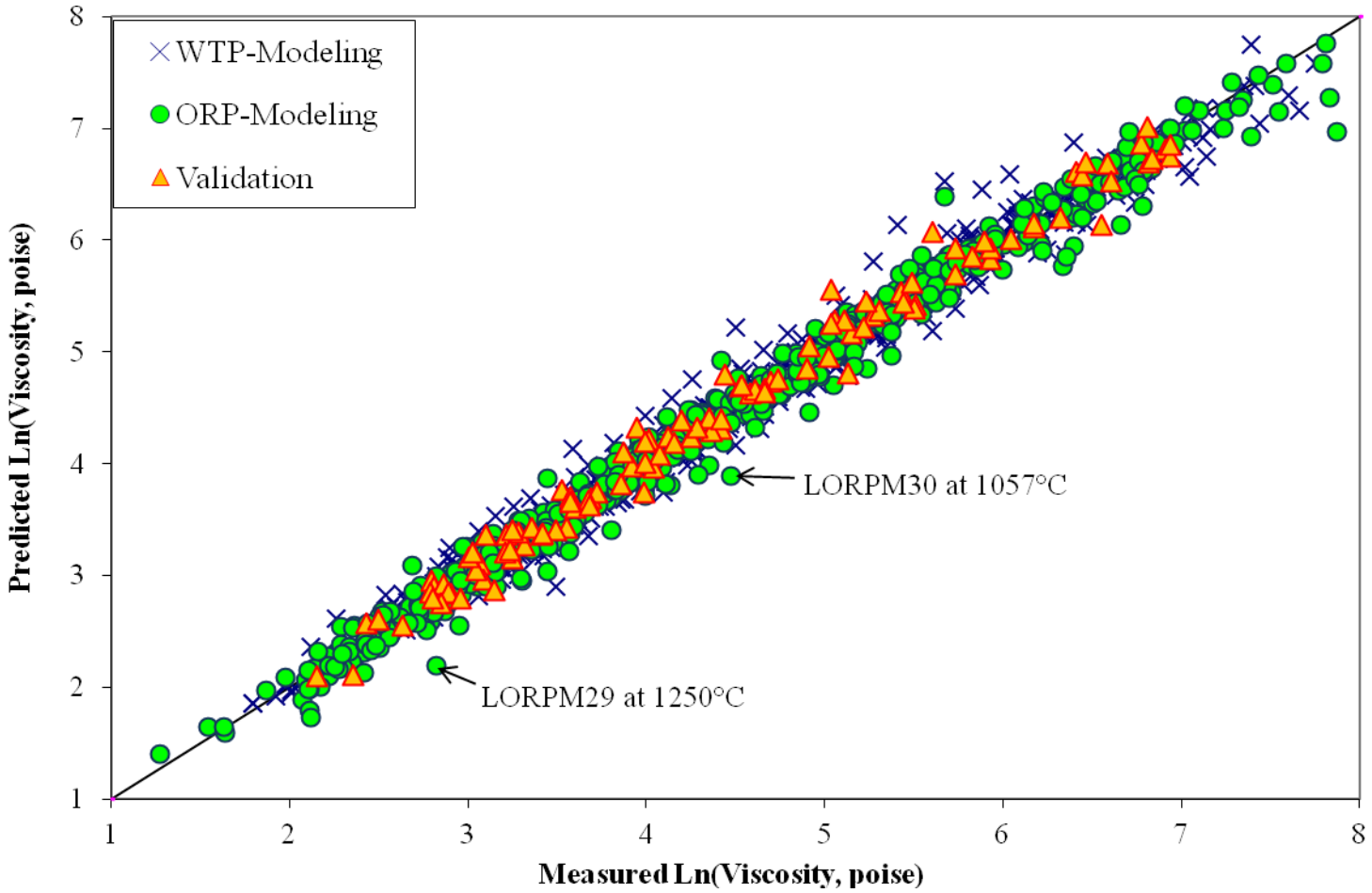


Figure 5.16. Predicted versus measured plot for 27-term reduced truncated T2-linear mixture model (Model 4) with three quadratic terms on ILAW viscosity.

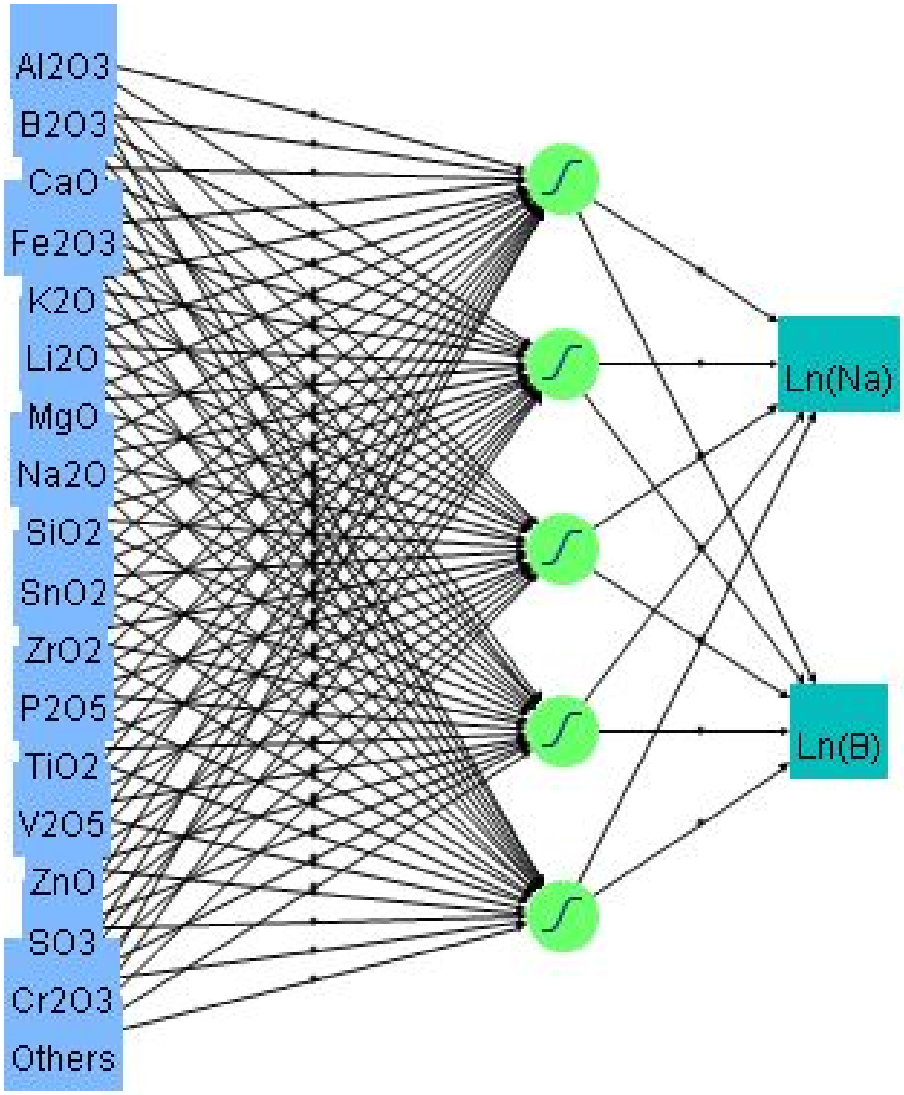


Figure 5.17. Block diagram of the Neural Network PCT-B/PCT-Na models.

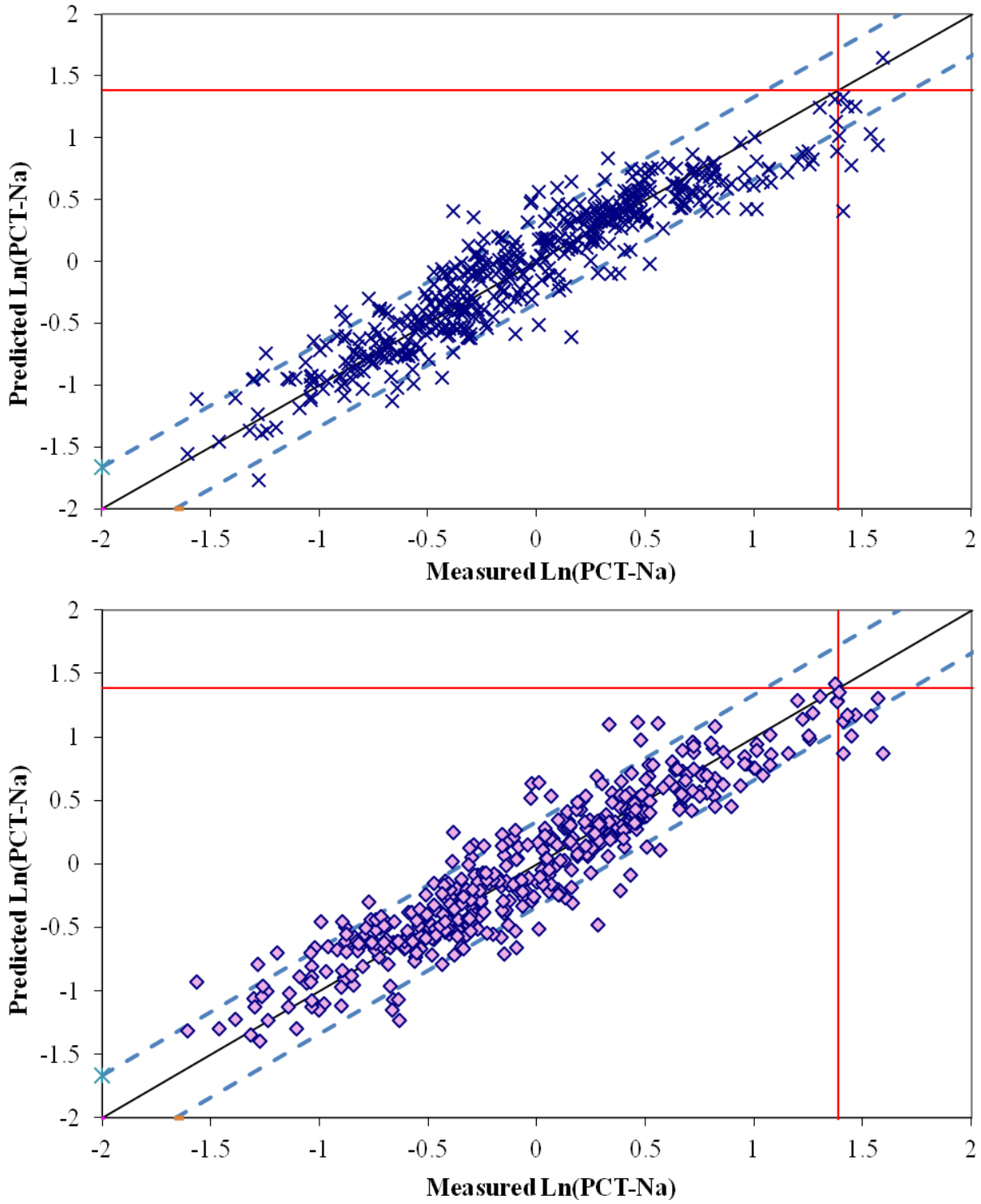


Figure 5.18. Comparison of PQM model (top) and Neural Network model (bottom) on combined PCT-Na data from WTP-LAW and ORP-LAW glasses.

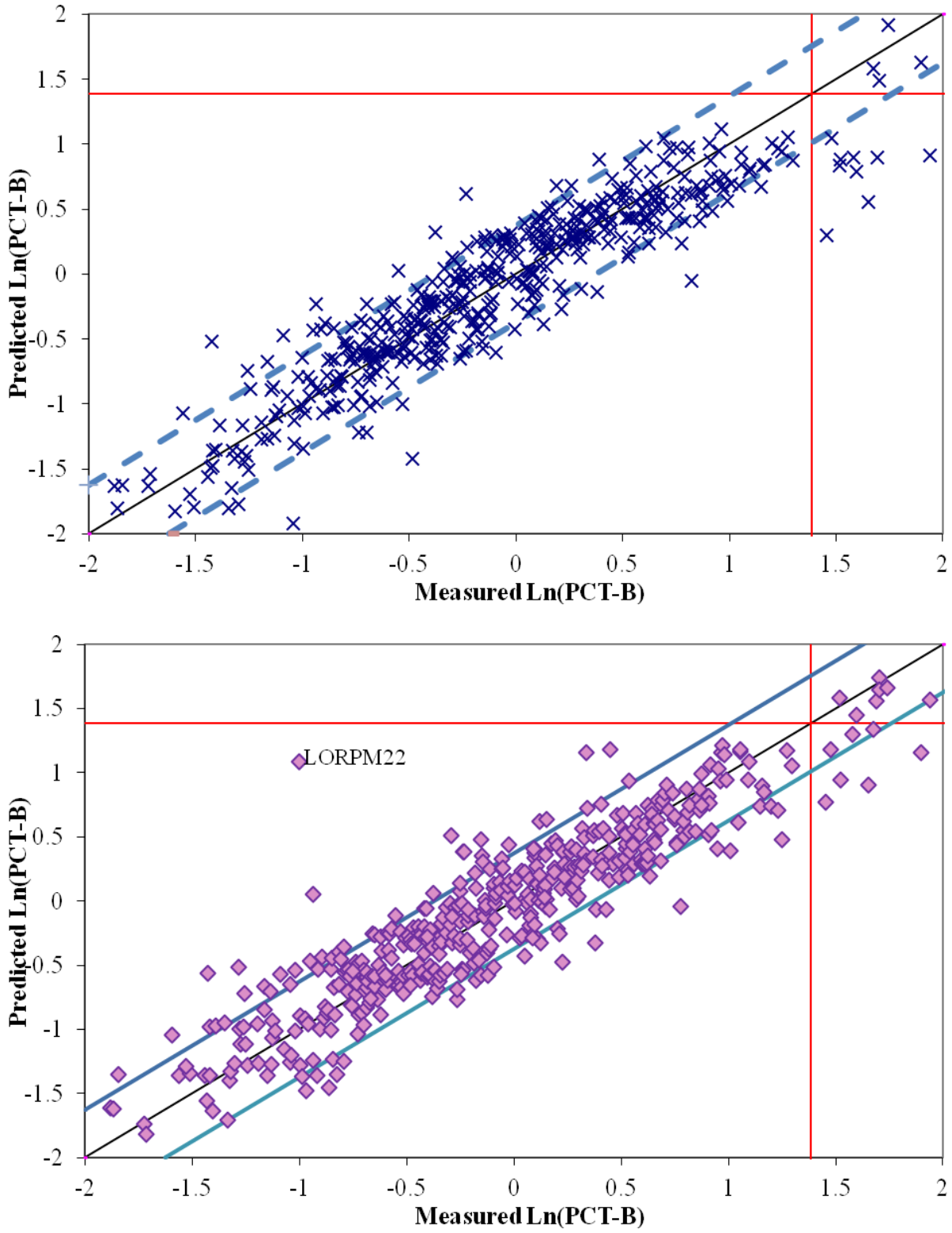


Figure 5.19. Comparison of PQM model (top) and Neural Network model (bottom) on combined PCT-B data from WTP-LAW and ORP-LAW glasses.

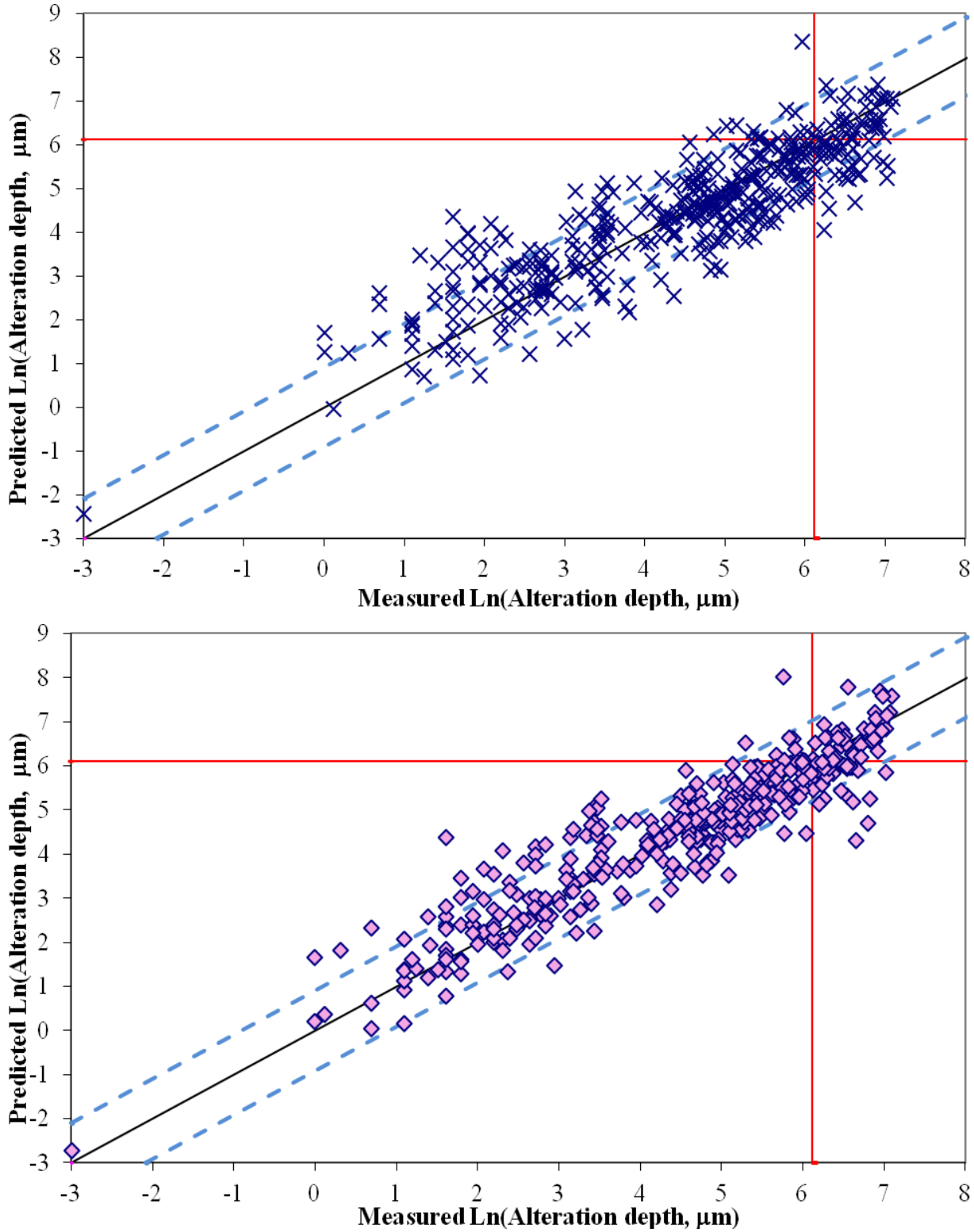


Figure 5.20. Comparison of PQM model (top) and Neural Network model (bottom) on combined VHT data from WTP-LAW and ORP-LAW glasses.

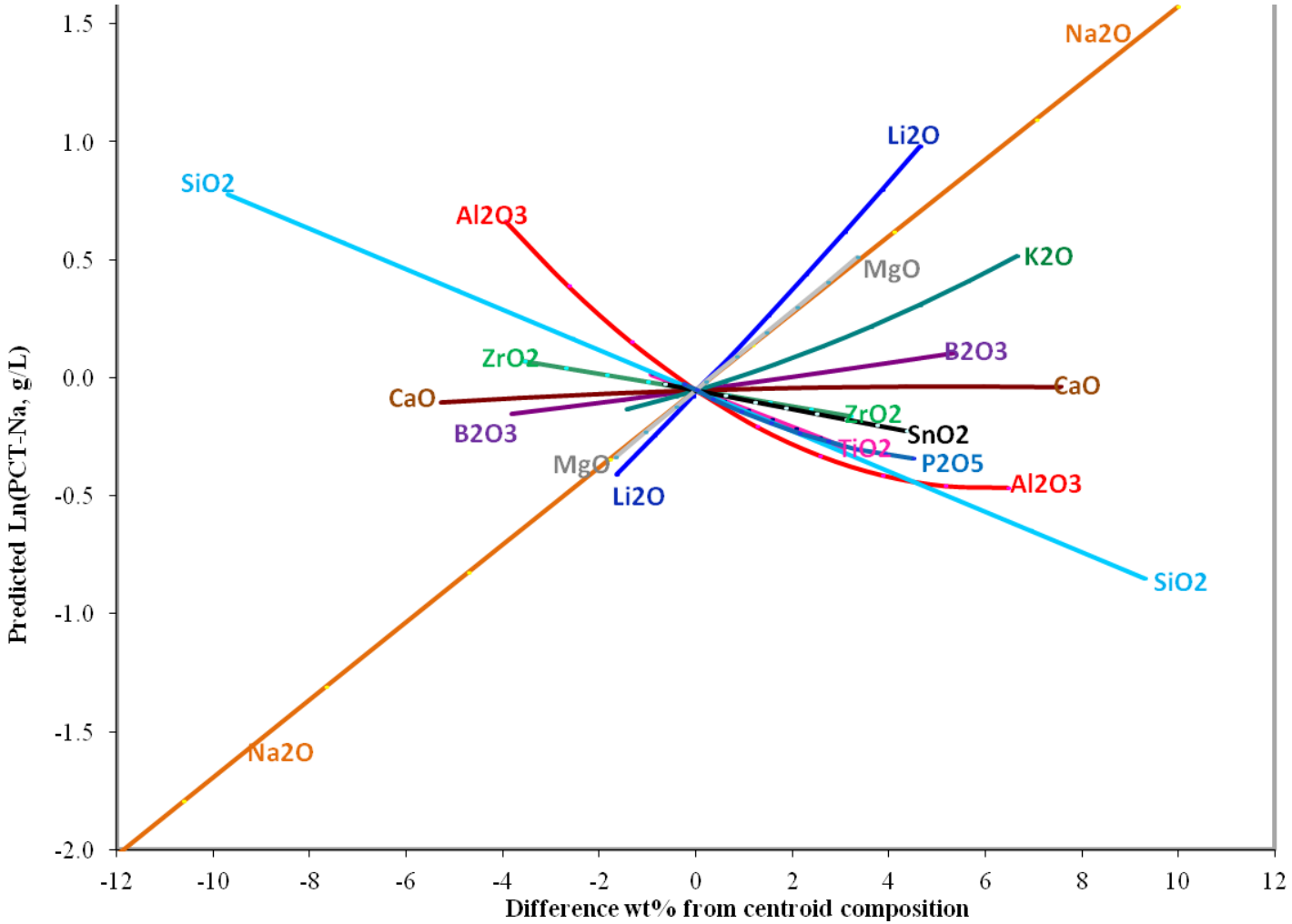


Figure 6.1. Effect of component concentration changes on predicted PCT-Na release at the composition region centroid.

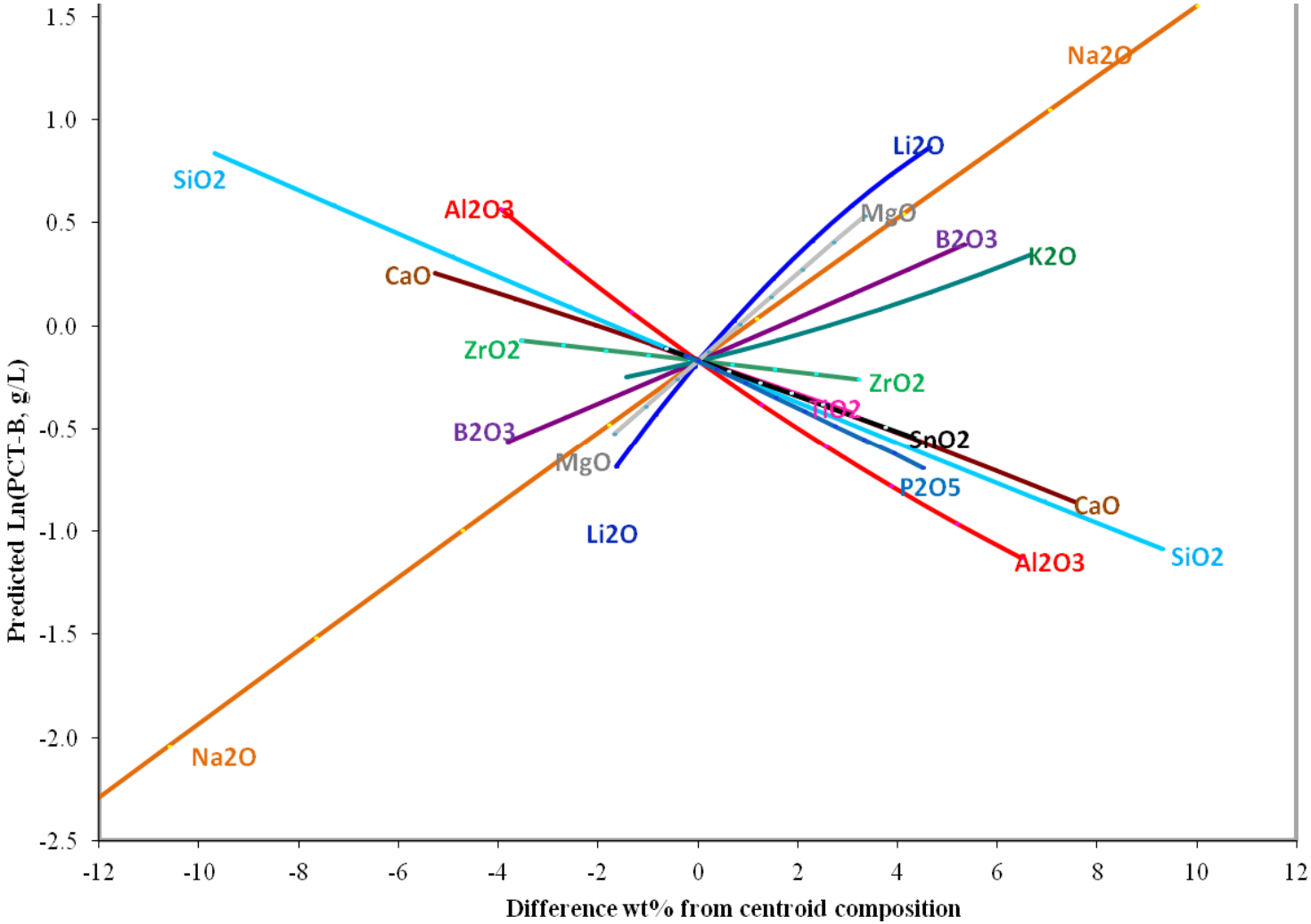


Figure 6.2. Effect of component concentration changes on predicted PCT-B release at the composition region centroid.

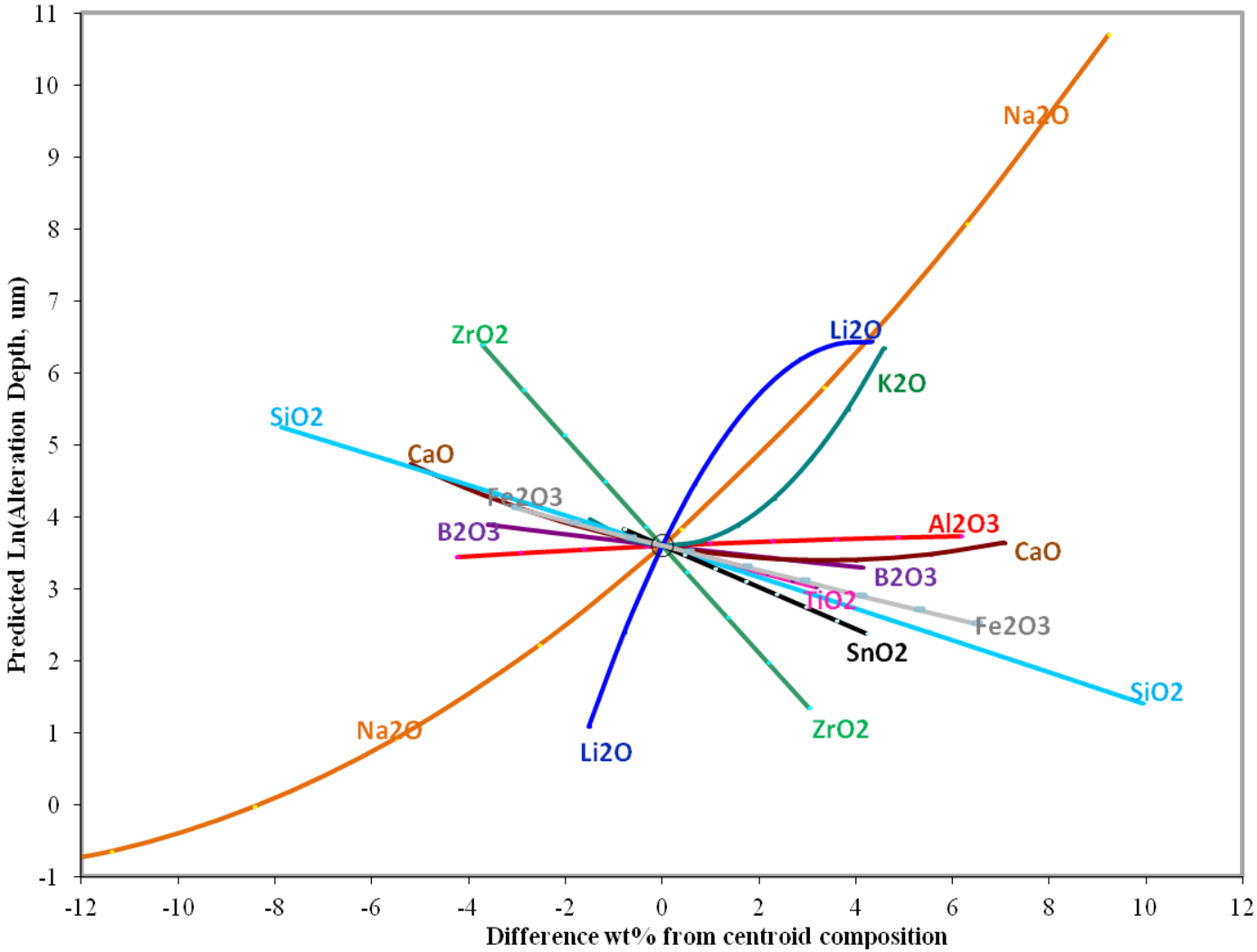


Figure 6.3. Effect of component concentration changes on predicted VHT response at the composition region centroid.

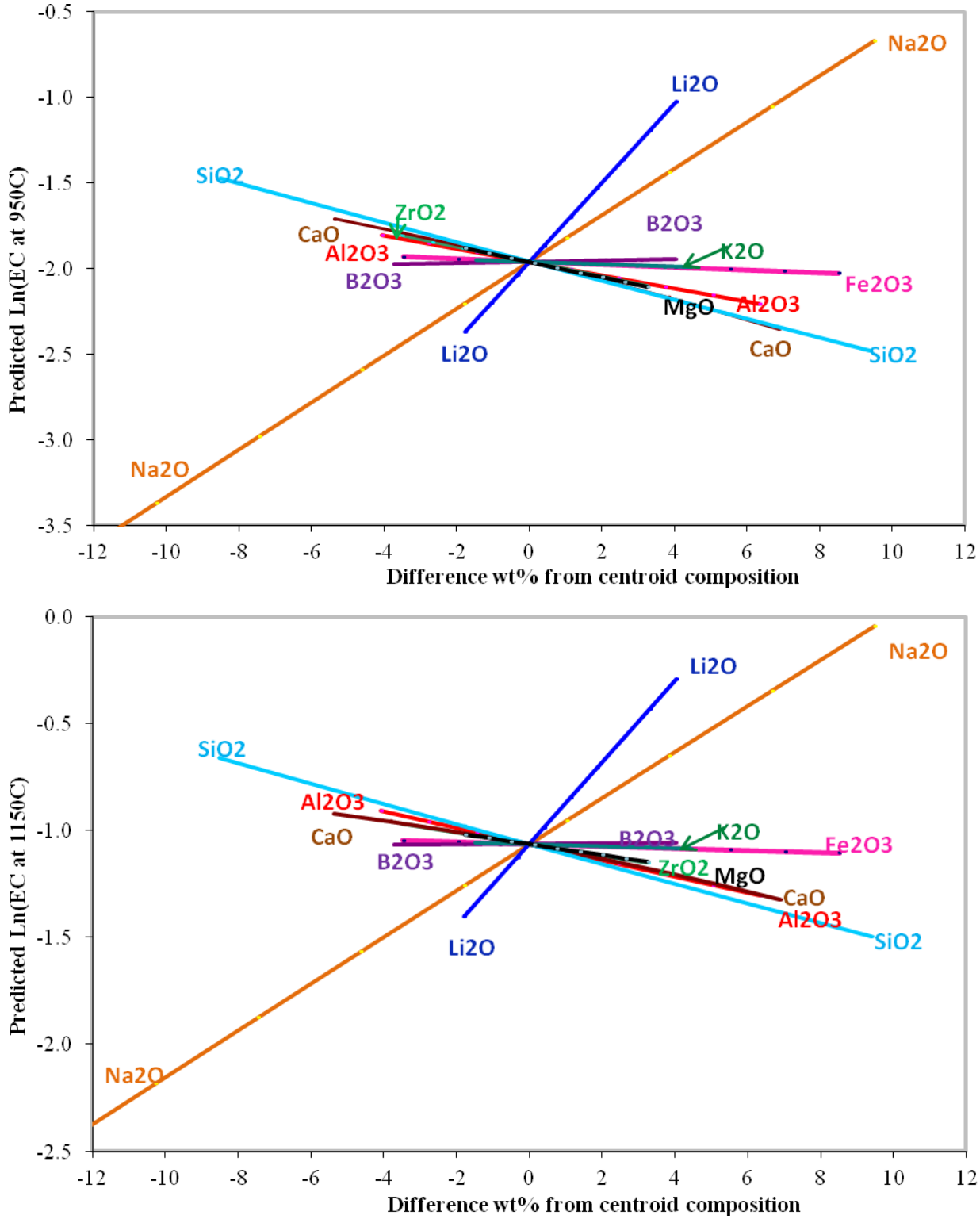


Figure 6.4. Effect of component concentration changes on predicted melt electrical conductivity for temperatures of 950 and 1150°C at the composition region centroid.

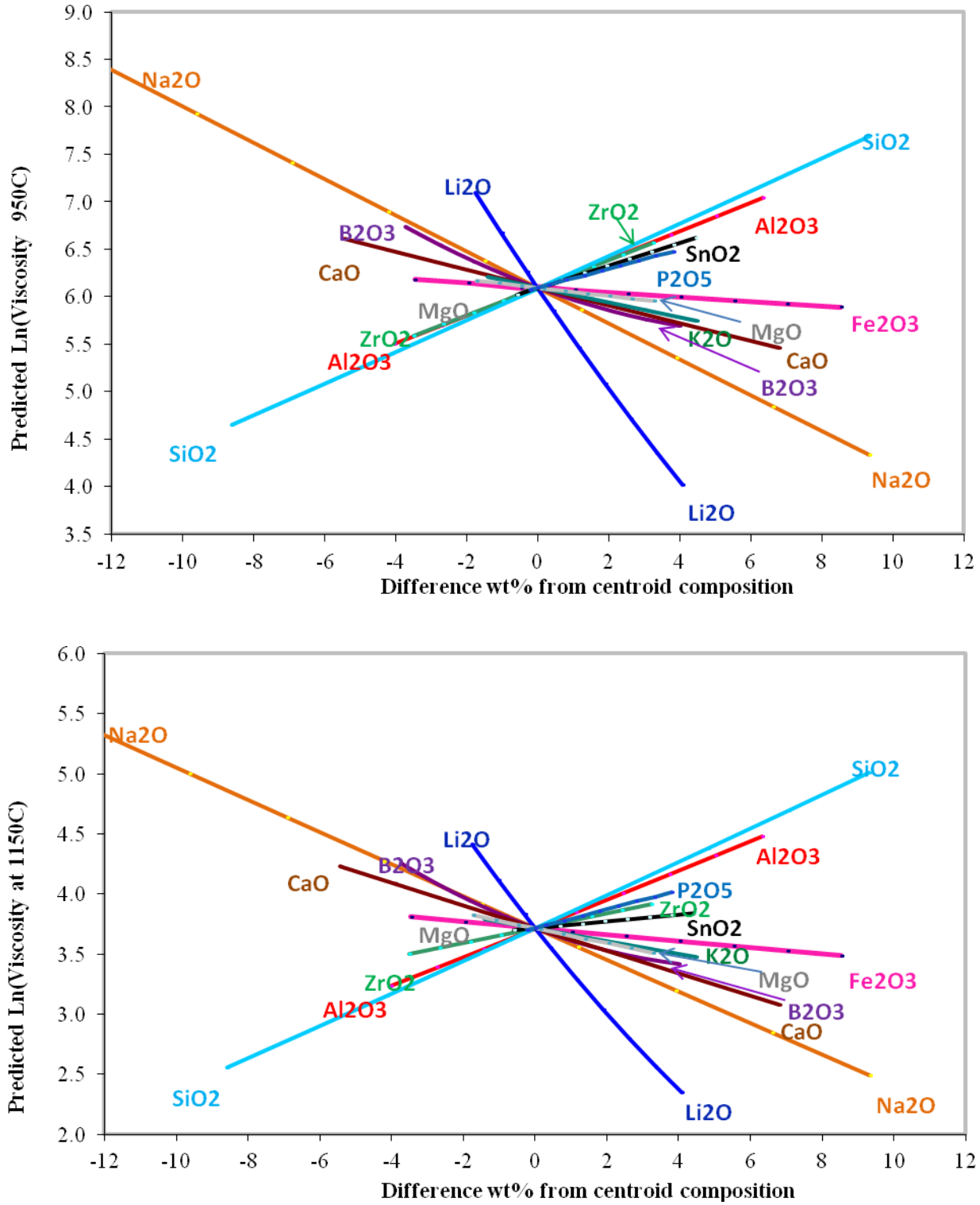


Figure 6.5. Effect of component concentration changes on predicted melt viscosity for temperatures of 950 and 1150°C at the composition region centroid.

APPENDIX A

EVALUATION OF SIGNIFICANT LINEAR TERMS IN PCT-Na, PCT-B, VHT VISCOSITY AND EC MODEL DEVELOPMENT

The process of seeking the optimum model set of terms rests on the best balance between model fit and complexity. The objective is to achieve simplicity and parsimony in number of terms, while minimizing the possible loss of information from a model in which a model term is removed [A1]. As described in Section 5, a *p*-value stopping criterion was used within JMP as part of the selection process for quadratic model terms. However, this approach is incorrectly implemented in JMP for the case of linear mixture model terms because the *p*-value is tested against zero (which is appropriate for interaction terms) instead of the mean response, which is required for linear mixture terms; this issue has been noted previously [A2, A3] and we confirmed with the makers of JMP that that is still the case [A4]. Consequently, alternative approaches were used for the selection of the linear terms in this work.

Two commonly used model selection criteria are the Akaike Information Criterion value [A5, A6] – corrected to relax the large-population requirement (AICc [A7, A8]) – and the Bayesian Information Criterion value (BIC [A6, A9]), both of which are calculated in JMP. For both of these criteria, lower values indicate more desirable models. For the selection of the linear terms in the PCT-Na, PCT-B, and VHT models these two criteria were also complemented by checking whether the confidence interval of the parameter estimates for the linear mixture terms contain the mean response, which indicates that the property is not significantly affected by the model term [A1, A3]. The results from this process are presented in Exhibits A1 – A3, respectively.

For the PCT-Na model, the AICc and BIC selection approaches indicated that the full 18-term linear model should be reduced to 12 terms (Exhibit A1). This was generally consistent with the results from the confidence interval approach except that that approach also indicated removal of the Others term, which was not accepted, and retention of the CaO term, which was accepted (Exhibit A1). The suggested reduction from 13 terms to 12 terms by removal of the CaO term was rejected for several reasons: (i) CaO is expected to affect glass leaching; (ii) Removal of the CaO term was not similarly supported for the PCT-B model; (iii) The decrease in AICc and BIC by removal of the CaO term was small; (iv) The confidence interval approach supported retention of the CaO term; and (v) Quadratic terms involving CaO were significant, as discussed in Section 5. Thus, the 13-term model including CaO was selected as the starting point for evaluation of quadratic terms in the development of the PCT-Na model.

For the PCT-B model, the AICc and BIC selection approaches indicated that the full 18-term linear model should be reduced to 14 terms with the CaO term retained; this was generally consistent with the results from the confidence interval approach except that that approach also indicated removal of the Others term and the SnO_2 term (marginally), which was not accepted (Exhibit A2). This 14-term model was selected as the starting point for evaluation of quadratic terms in the development of the PCT-B model.

For the VHT model, the AICc and BIC selection approaches indicated that the full 18-term linear model should be reduced to 11 terms, without a CaO term (Exhibit A1). This was generally consistent with the results from the confidence interval approach except that that approach also indicated retention of the CaO term. The suggested reduction from 12 terms to 11 terms by removal of the CaO term was rejected for the same reasons listed above for the PCT-Na model. This 12-term model was selected as the starting point for evaluation of quadratic terms in the development of the VHT model.

The melt viscosity and electrical conductivity models involve both composition- and composition-temperature terms. For these models the AICc and BIC criteria were used as selection criteria to evaluate the significance of SnO_2 and V_2O_5 terms in comparison to the previous models in which these components were not used. Both of these terms were rejected in the case of the electrical conductivity model (Exhibit A4) while only the SnO_2 term was accepted in the case of the viscosity model (Exhibit A5).

References

[A1] "Experiments with Mixtures: Designs, Models, and the Analysis of Mixture Data," J.A. Cornell, 3rd Edition, John Wiley and Sons, Inc., New York (2002).

[A2] "Tips on JMP®ing into Mixture Experimentation," D.J. Obermiller, in Proceedings of the Twenty-First Annual SAS User's Group International Conference, Cary, NC; SAS Institute Inc., pp 799-804 (1996).

[A3] E-mail communications with D.J. Obermiller.

[A4] E-mail communications with JMP Software support.

[A5] "A New Look at the Statistical Model Identification," H. Akaike, IEEE Transactions on Automatic Control, 19, 716-723, (1974).

[A6] "Multimodel Inference. Understanding AIC and BIC in Model Selection," K.P. Burnham and D.R. Anderson, Sociological Methods and Research, 33, 261-304 (2004).

[A7] "Further Analysis of the Data by Akaike's Information Criterion and the Finite Corrections," N. Sugiura, Communications in Statistics, A 7, 13- 26 (1978).

[A8] "Regression and Time Series Model Selection in Small Samples," C.M. Hurvich and C.L. Tsai, Biometrika 76, 297-307 (1989).

[A9] "Estimating the Dimension of a Model," G. Schwarz, Annals of Statistics, 6, 461-464 (1978).

Exhibit A1: Selection of Significant Main Components in PCT-Na Model.

Main Term Selection for PCT-Na Model 3	Lower 95% Confidence Interval	Upper 95% Confidence Interval	Is Mean Response Inside Confidence Interval?	Are AICc and BIC Above Minimum?	Main Components Selected or Out?
Model Terms	Mean Ln(PCT-Na measured in g/L) = -0.045				
Al_2O_3	-13.911	-10.713	N	Minimum	Selected
B_2O_3	2.626	5.928	N	Minimum	Selected
CaO	0.556	3.033	N	Near minimum and in cross terms	Selected
Cr_2O_3	-6.207	30.543	Y	Y*	Out
Fe_2O_3	-0.132	2.921	Y	Y*	Out
K_2O	6.435	10.132	N	Minimum	Selected
Li_2O	16.182	23.826	N	Minimum	Selected
MgO	11.596	17.931	N	Minimum	Selected
Na_2O	12.181	14.386	N	Minimum	Selected
P_2O_5	-18.887	-8.803	N	Minimum	Selected
SiO_2	-5.726	-4.419	N	Minimum	Selected
SnO_2	-7.085	-0.699	N	Minimum	Selected
SO_3	-27.175	2.596	Y	Y*	Out
TiO_2	-17.041	-8.133	N	Minimum	Selected
V_2O_5	-1.236	6.374	Y	Y*	Out
ZnO	-2.359	4.227	Y	Y*	Out
ZrO_2	-7.407	-1.955	N	Minimum	Selected
Others	-9.548	9.241	Y	Minimum	Selected

* Eliminated in the "13 components" as shown in graph below.

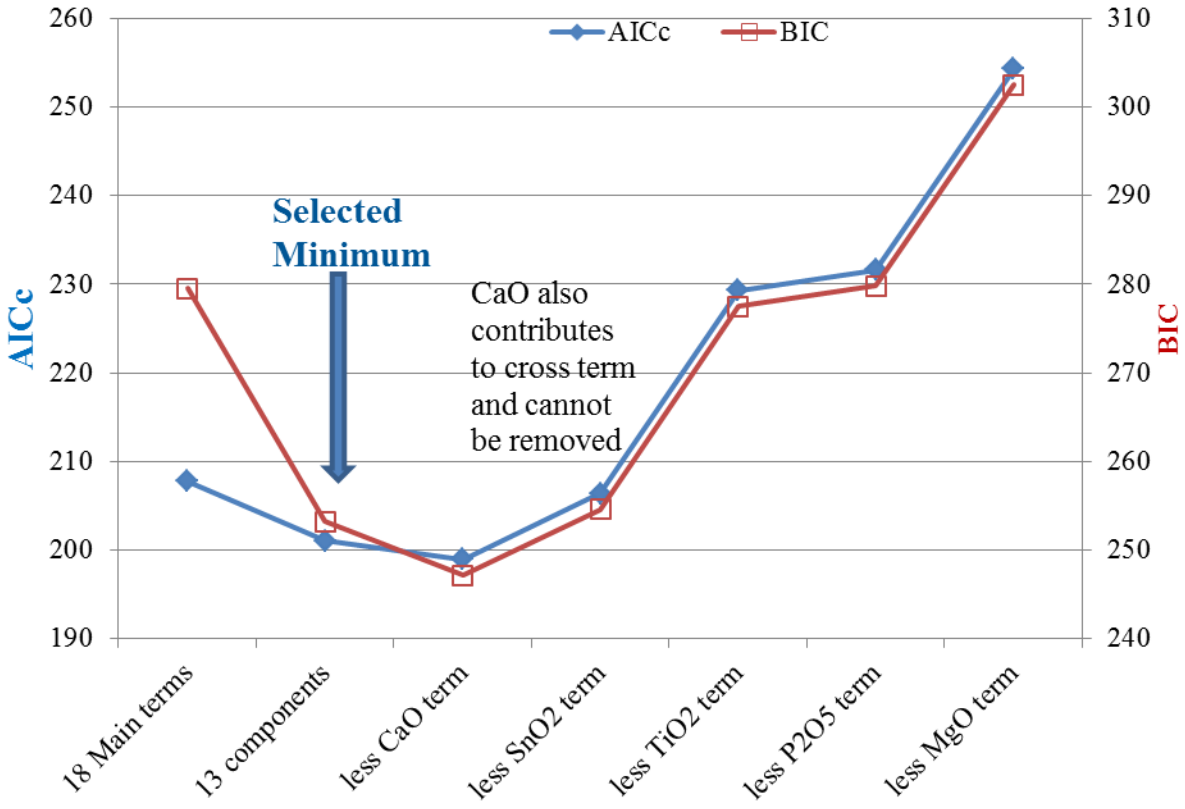


Exhibit A2: Selection of Significant Main Components in PCT-B Model.

Main Term Selection for PCT-B Model 3	Lower 95% Confidence Interval	Upper 95% Confidence Interval	Is Mean Response Inside Confidence Interval	Are AICc and BIC Above Minimum?	Main Components Selected or Out?
Model Terms	Mean Ln(PCT- B measured in g/L) = -0.0863				
Al_2O_3	-16.607	-12.303	N	Minimum	Selected
B_2O_3	8.564	13.007	N	Minimum	Selected
CaO	-6.224	-2.890	N	Minimum	Selected
Cr_2O_3	-22.928	26.530	Y	Y*	Out
Fe_2O_3	0.861	4.970	N	Minimum	Selected
K_2O	4.702	9.678	N	Minimum	Selected
Li_2O	17.258	27.546	N	Minimum	Selected
MgO	17.020	25.546	N	Minimum	Selected
Na_2O	11.912	14.880	N	Minimum	Selected
P_2O_5	-18.726	-5.155	N	Minimum	Selected
SiO_2	-6.920	-5.162	N	Minimum	Selected
SnO_2	-8.594	0.000	Y	Minimum	Selected
SO_3	-32.820	7.244	Y	Y*	Out
TiO_2	-24.732	-12.744	N	Minimum	Selected
V_2O_5	-4.707	5.534	Y	Y*	Out
ZnO	-1.459	7.405	Y	Y*	Out
ZrO_2	-8.327	-0.989	N	Minimum	Selected
Others	-2.988	22.298	Y	Minimum	Selected

* Eliminated in the "14 components" as shown in graph below.

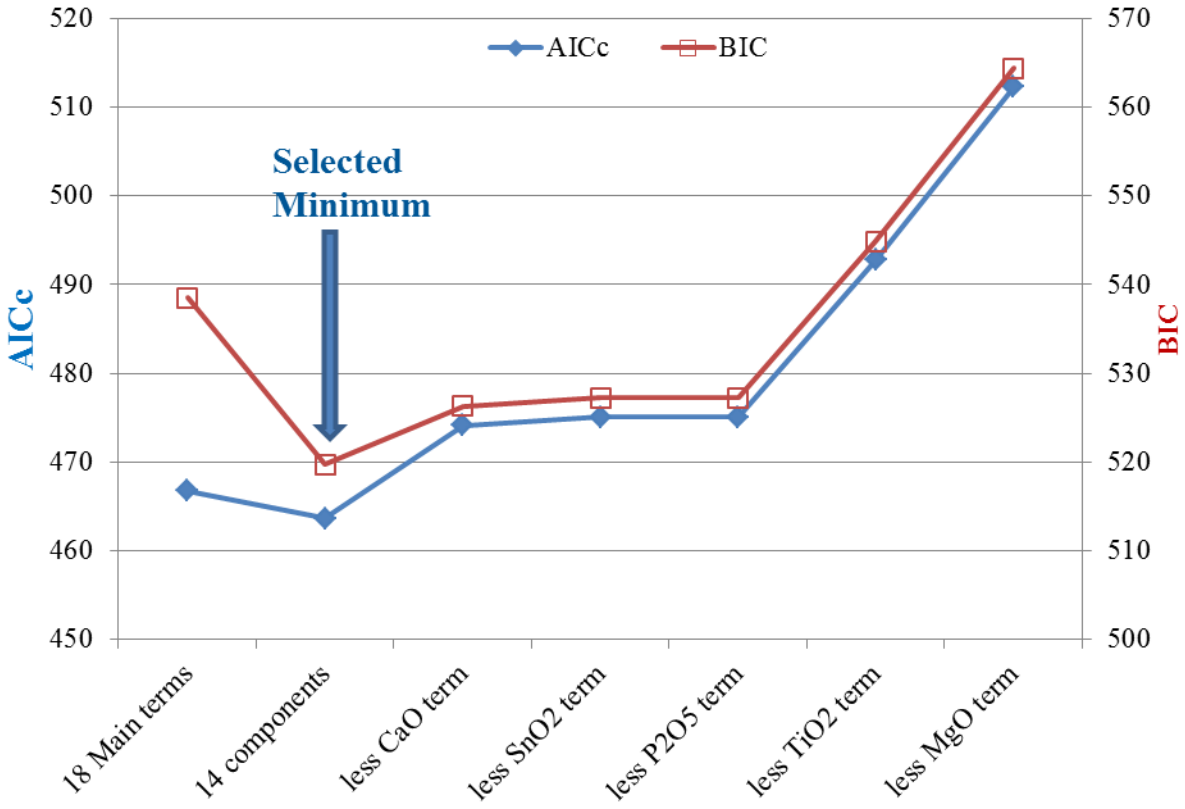


Exhibit A3: Selection of Significant Main Components in VHT Model.

Main Term Selection for VHT Model 3	Lower 95% Confidence Interval	Upper 95% Confidence Interval	Is Mean Response Inside Confidence Interval	Are AICc and BIC Above Minimum?	Main Components Selected or Out?
Model Terms	Mean Ln(VHT measured in µm) = 4.4274				
Al_2O_3	6.716	19.125	N	Minimum	Selected
B_2O_3	-15.676	-2.824	N	Minimum	Selected
CaO	-9.926	-0.250	N	Near minimum and in cross terms	Selected
Cr_2O_3	-41.561	118.629	Y	Y*	Out
Fe_2O_3	-17.066	-3.668	N	Minimum	Selected
K_2O	18.842	32.958	N	Minimum	Selected
Li_2O	74.487	106.088	N	Minimum	Selected
MgO	-10.307	14.475	Y	Y*	Out
Na_2O	33.063	42.275	N	Minimum	Selected
P_2O_5	-28.060	43.553	Y	Y*	Out
SiO_2	-5.126	-0.125	N	Minimum	Selected
SnO_2	-28.594	-5.334	N	Minimum	Selected
SO_3	-51.842	72.088	Y	Y*	Out
TiO_2	-43.840	-5.480	N	Minimum	Selected
V_2O_5	-13.629	15.480	Y	Y*	Out
ZnO	-2.878	21.228	Y	Y*	Out
ZrO_2	-60.819	-40.229	N	Minimum	Selected
Others	-102.510	-29.195	N	Minimum	Selected

* Eliminated in the "12 components" as shown in graph below.

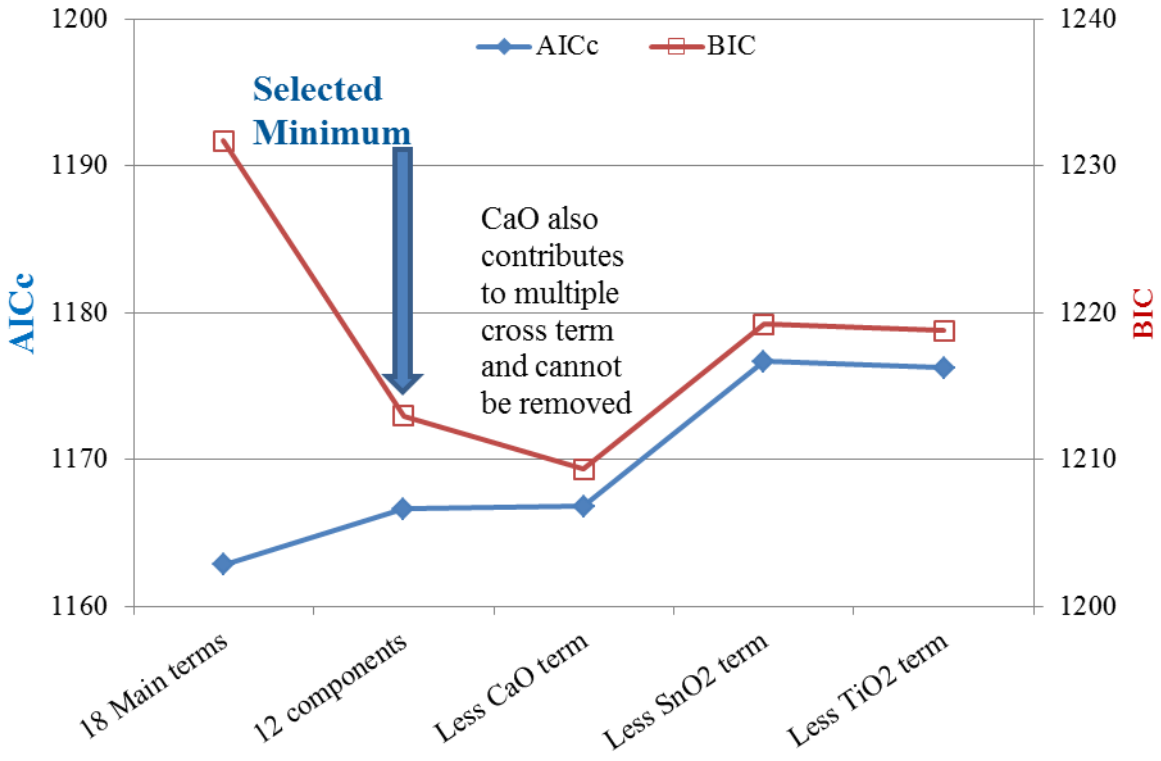
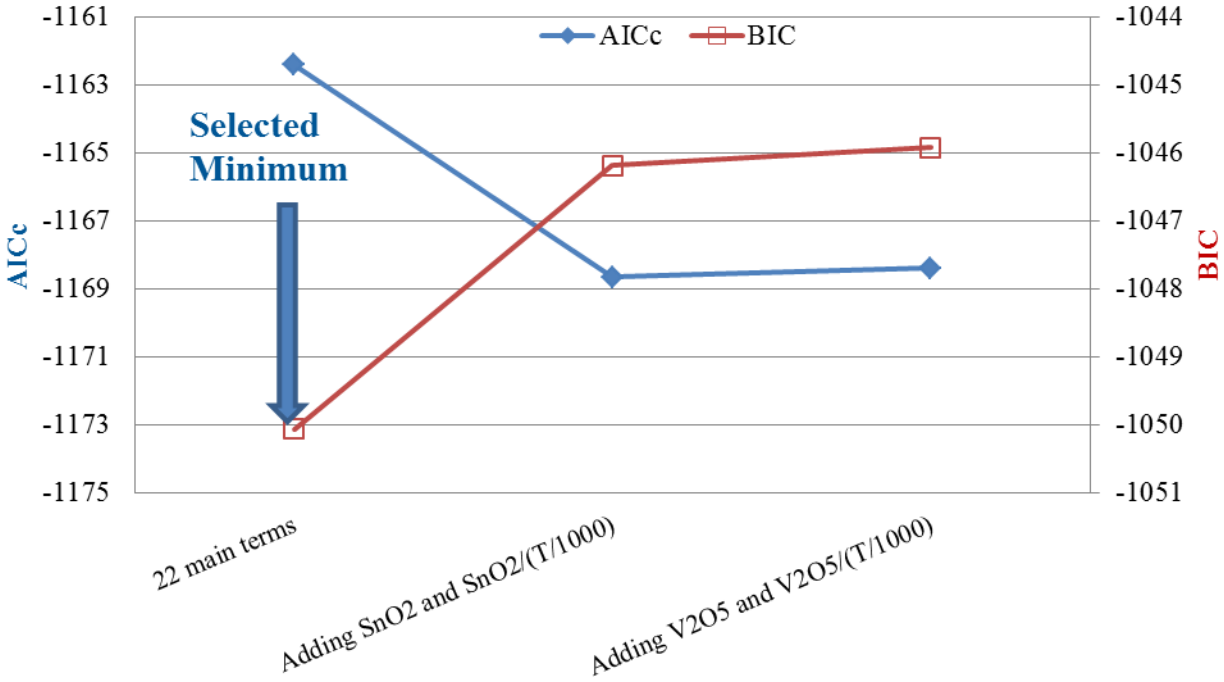
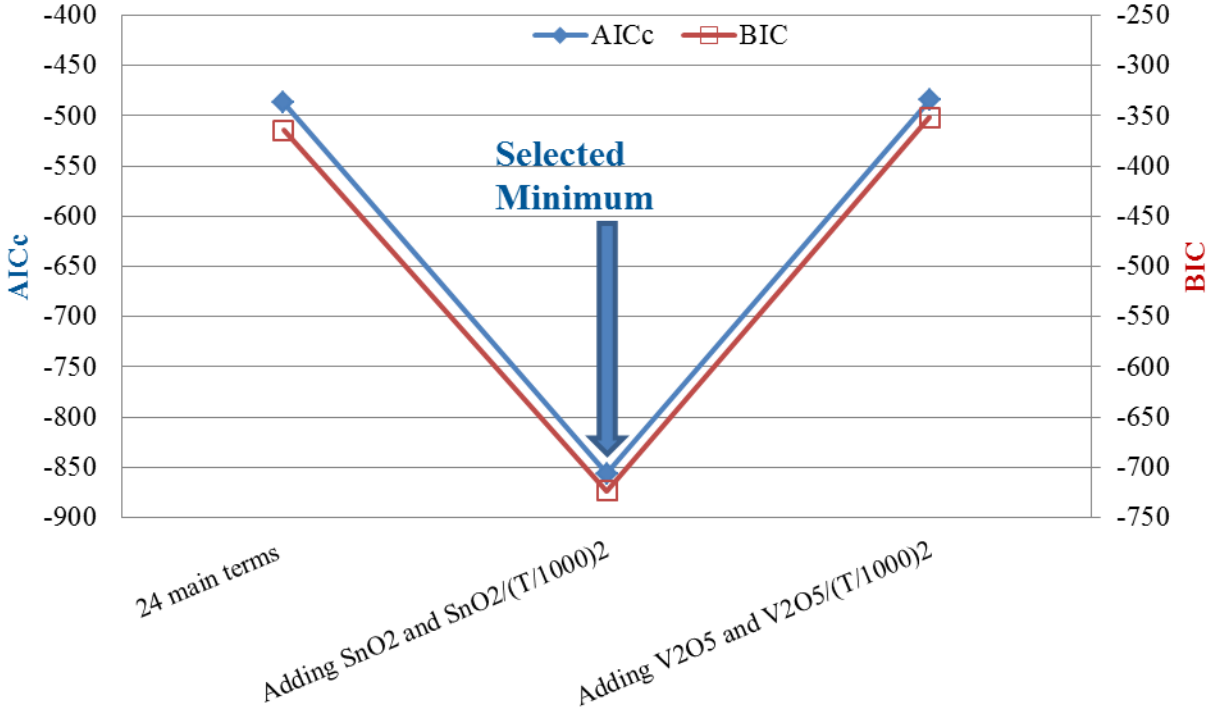


Exhibit A4. Selection of Significant Main Components in EC Model.



Exhbit A5. Selection of Significant Main Components in Viscosity Model.



APPENDIX B

VARIANCE-COVARIANCE MATRICES FOR SELECTED MODELS

Table B.1. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 24 -Term Model (Model 4) for ln(PCT-Na, g/L) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset.

Term	Al_2O_3	B_2O_3	CaO	K_2O	Li_2O	MgO	Na_2O	SiO_2	SnO_2	ZrO_2
Al_2O_3	17.2809	-0.9781	-0.5024	4.0234	3.5549	0.0776	-0.7495	-0.6740	0.2192	-0.7492
B_2O_3	-0.9781	0.8408	-0.4290	1.4432	-0.8477	0.0512	0.0765	-0.0490	0.1601	-0.0092
CaO	-0.5024	-0.4290	1.9857	-0.4210	0.9142	-0.1168	-0.1095	-0.0082	0.0053	0.0994
K_2O	4.0234	1.4432	-0.4210	25.8048	2.5538	0.9836	-0.3838	-0.5253	0.7551	-1.1949
Li_2O	3.5549	-0.8477	0.9142	2.5538	12.3256	-0.4704	0.3133	-0.3339	-0.7787	-0.3608
MgO	0.0776	0.0512	-0.1168	0.9836	-0.4704	1.7823	0.1256	-0.0527	0.0777	-0.1528
Na_2O	-0.7495	0.0765	-0.1095	-0.3838	0.3133	0.1256	0.2689	-0.0111	-0.1724	-0.1357
SiO_2	-0.6740	-0.0490	-0.0082	-0.5253	-0.3339	-0.0527	-0.0111	0.1219	-0.0411	-0.0072
SnO_2	0.2192	0.1601	0.0053	0.7551	-0.7787	0.0777	-0.1724	-0.0411	2.5451	-0.3276
ZrO_2	-0.7492	-0.0092	0.0994	-1.1949	-0.3608	-0.1528	-0.1357	-0.0072	-0.3276	1.2577
P_2O_5	-1.4167	-2.7691	-1.4293	7.6048	9.0697	-0.7922	-1.9004	2.5208	-3.5909	-0.9466
TiO_2	1.7013	0.3194	-0.1803	1.6953	3.1914	-0.8058	0.0426	-0.1490	0.5664	0.4276
Others	-2.5479	-0.4907	0.8387	0.7295	-1.3313	-0.3899	-0.4697	-0.3522	0.5992	0.2054
$Al_2O_3 \times Al_2O_3$	-99.8651	4.5475	2.2225	-16.8254	-16.8704	-1.1649	3.1163	4.1567	-1.1245	4.3143
$Al_2O_3 \times K_2O$	-30.6284	3.3820	0.7266	-100.2635	11.4044	-7.7216	5.0256	1.2928	2.8085	2.3459
$B_2O_3 \times K_2O$	-17.3617	-18.4603	4.4603	-194.0784	-20.1124	-4.0616	1.2707	4.0949	-6.9414	9.7783
$Al_2O3 \times Li_2O$	-36.4658	8.5152	-10.0394	-7.3192	-92.5555	6.9336	4.7755	2.0359	-4.0438	-0.7139
$CaO \times Li_2O$	-25.7457	5.8016	-10.3061	-18.7750	-45.9978	1.0481	0.1387	-0.0007	10.3052	0.1639
$K_2O \times Li_2O$	12.0445	-1.4055	7.2039	-31.7500	-48.7031	-5.5748	-4.8182	2.7497	-2.9060	2.2024
$K_2O \times SnO_2$	-40.3858	-3.4786	3.7158	-71.5797	-22.6261	-6.1275	3.1527	1.1637	-47.1857	3.1159
$SiO_2 \times P_2O_5$	2.1978	5.9590	3.3435	-18.2799	-19.7018	1.2901	4.5025	-5.6267	8.3287	2.2974
$CaO \times TiO_2$	-30.2098	-0.2654	3.1277	-15.7875	-44.4100	5.9035	-0.3617	-0.3898	-6.3779	2.5129
CaO×Others	5.8946	3.7784	-19.4739	-2.0254	-1.6262	1.2861	2.2336	0.4001	-0.0978	-0.2852
Others×Others	9.0800	1.7703	0.2516	-10.4489	5.6477	1.5771	2.3938	1.8231	-3.8043	-0.3695

Table B.1. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 24 -Term Model (Model 4) for ln(PCT-Na, g/L) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset (continued).

Term	P_2O_5	TiO_2	Others	Al_2O_3× Al_2O_3	Al_2O_3× K_2O	B_2O_3× K_2O	Al_2O_3× Li_2O	CaO× Li_2O
Al_2O_3	-1.4167	1.7013	-2.5479	-99.8651	-30.6284	-17.3617	-36.4658	-25.7457
B_2O_3	-2.7691	0.3194	-0.4907	4.5475	3.3820	-18.4603	8.5152	5.8016
CaO	-1.4293	-0.1803	0.8387	2.2225	0.7266	4.4603	-10.0394	-10.3061
K_2O	7.6048	1.6953	0.7295	-16.8254	-100.2635	-194.0784	-7.3192	-18.7750
Li_2O	9.0697	3.1914	-1.3313	-16.8704	11.4044	-20.1124	-92.5555	-45.9978
MgO	-0.7922	-0.8058	-0.3899	-1.1649	-7.7216	-4.0616	6.9336	1.0481
Na_2O	-1.9004	0.0426	-0.4697	3.1163	5.0256	1.2707	4.7755	0.1387
SiO_2	2.5208	-0.1490	-0.3522	4.1567	1.2928	4.0949	2.0359	-0.0007
SnO_2	-3.5909	0.5664	0.5992	-1.1245	2.8085	-6.9414	-4.0438	10.3052
ZrO_2	-0.9466	0.4276	0.2054	4.3143	2.3459	9.7783	-0.7139	0.1639
P_2O_5	841.2113	-5.0914	-5.1691	18.4339	-75.4558	-25.4429	-84.4147	-71.1735
TiO_2	-5.0914	8.8600	-3.2322	-7.7908	12.8166	-20.4224	-23.6716	-8.7580
Others	-5.1691	-3.2322	9.6030	16.0066	-8.9500	-7.4757	-8.9542	17.2566
Al_2O_3×Al_2O_3	18.4339	-7.7908	16.0066	611.7614	77.6819	108.9833	131.2985	162.2931
Al_2O_3×K_2O	-75.4558	12.8166	-8.9500	77.6819	1258.4874	200.7271	-183.0149	106.3432
B_2O_3×K_2O	-25.4429	-20.4224	-7.4757	108.9833	200.7271	1936.2619	127.2690	83.1400
Al_2O3×Li_2O	-84.4147	-23.6716	-8.9542	131.2985	-183.0149	127.2690	1260.1176	60.6650
CaO×Li_2O	-71.1735	-8.7580	17.2566	162.2931	106.3432	83.1400	60.6650	650.9685
K_2O×Li_2O	-4.7941	-39.3715	10.8245	-110.6761	8.4019	103.4440	69.2254	122.1163
K_2O×SnO_2	-93.8529	-25.2298	22.5335	239.2402	-122.4950	554.1851	306.6681	33.6542
SiO_2×P_2O_5	-1865.2180	12.9675	10.1787	-34.0143	175.4336	73.7034	184.6979	169.3193
CaO×TiO_2	-59.5355	-103.5097	52.3114	166.7312	-248.9387	229.1292	362.7332	159.4754
CaO×Others	5.9035	17.5187	-22.0817	-38.0122	67.7608	-2.8198	115.4286	-14.2603
Others×Others	13.9004	11.6518	-47.5115	-60.2929	49.3673	98.8962	38.7696	-77.8867

Table B.1. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 24 -Term Model (Model 4) for ln(PCT-Na, g/L) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset (continued).

Term	$K_2O \times Li_2O$	$K_2O \times SnO_2$	$SiO_2 \times P_2O_5$	$CaO \times TiO_2$	CaO×Others	Others×Others
Al_2O_3	12.0445	-40.3858	2.1978	-30.2098	5.8946	9.0800
B_2O_3	-1.4055	-3.4786	5.9590	-0.2654	3.7784	1.7703
CaO	7.2039	3.7158	3.3435	3.1277	-19.4739	0.2516
K_2O	-31.7500	-71.5797	-18.2799	-15.7875	-2.0254	-10.4489
Li_2O	-48.7031	-22.6261	-19.7018	-44.4100	-1.6262	5.6477
MgO	-5.5748	-6.1275	1.2901	5.9035	1.2861	1.5771
Na_2O	-4.8182	3.1527	4.5025	-0.3617	2.2336	2.3938
SiO_2	2.7497	1.1637	-5.6267	-0.3898	0.4001	1.8231
SnO_2	-2.9060	-47.1857	8.3287	-6.3779	-0.0978	-3.8043
ZrO_2	2.2024	3.1159	2.2974	2.5129	-0.2852	-0.3695
P_2O_5	-4.7941	-93.8529	-1865.2180	-59.5355	5.9035	13.9004
TiO_2	-39.3715	-25.2298	12.9675	-103.5097	17.5187	11.6518
Others	10.8245	22.5335	10.1787	52.3114	-22.0817	-47.5115
$Al_2O_3 \times Al_2O_3$	-110.6761	239.2402	-34.0143	166.7312	-38.0122	-60.2929
$Al_2O_3 \times K_2O$	8.4019	-122.4950	175.4336	-248.9387	67.7608	49.3673
$B_2O_3 \times K_2O$	103.4440	554.1851	73.7034	229.1292	-2.8198	98.8962
$Al_2O3 \times Li_2O$	69.2254	306.6681	184.6979	362.7332	115.4286	38.7696
$CaO \times Li_2O$	122.1163	33.6542	169.3193	159.4754	-14.2603	-77.8867
$K_2O \times Li_2O$	1856.0626	60.6253	-2.7053	352.9159	-175.0028	-20.7899
$K_2O \times SnO_2$	60.6253	2281.8490	192.8314	456.0991	-97.5879	-51.1492
$SiO_2 \times P_2O_5$	-2.7053	192.8314	4155.8930	117.0706	-11.0296	-24.1699
$CaO \times TiO_2$	352.9159	456.0991	117.0706	1911.4492	-286.2710	-207.7256
CaO×Others	-175.0028	-97.5879	-11.0296	-286.2710	278.5443	53.9361
Others×Others	-20.7899	-51.1492	-24.1699	-207.7256	53.9361	260.5230

Table B.2. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 26-Term Model (Model 6) for ln(PCT-B, g/L) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset

Term	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SiO_2	SnO_2
Al_2O_3	49.147	-4.699	-4.496	-2.419	-3.690	23.359	-9.120	-4.643	6.134	-2.439
B_2O_3	-4.699	1.466	0.132	-0.232	3.066	-1.942	0.613	0.371	-0.734	0.190
CaO	-4.496	0.132	1.655	0.877	-0.725	-5.278	2.001	0.376	-0.568	0.772
Fe_2O_3	-2.419	-0.232	0.877	5.596	0.931	-9.022	2.695	0.110	-0.672	0.108
K_2O	-3.690	3.066	-0.725	0.931	38.522	-14.781	3.661	0.223	-1.623	-1.199
Li_2O	23.359	-1.942	-5.278	-9.022	-14.781	234.607	-10.958	-2.312	6.383	-4.752
MgO	-9.120	0.613	2.001	2.695	3.661	-10.958	10.452	0.779	-1.411	0.427
Na_2O	-4.643	0.371	0.376	0.110	0.223	-2.312	0.779	0.763	-0.647	0.103
SiO_2	6.134	-0.734	-0.568	-0.672	-1.623	6.383	-1.411	-0.647	0.973	-0.258
SnO_2	-2.439	0.190	0.772	0.108	-1.199	-4.752	0.427	0.103	-0.258	2.518
ZrO_2	-2.618	0.382	0.332	2.300	-0.793	-5.974	1.404	-0.171	-0.662	-0.565
P_2O_5	-3.802	0.083	0.491	0.276	-0.330	-6.697	0.137	0.540	-0.655	0.314
TiO_2	-4.483	0.989	0.411	-0.956	2.179	-12.219	-1.031	0.418	-0.954	0.453
Others	-4.750	0.326	0.305	0.716	-0.201	-6.396	0.555	0.404	-0.706	-0.073
$CaO \times Fe_2O_3$	-17.172	5.805	-12.348	-23.103	10.575	26.726	-0.491	3.489	-2.987	-7.215
$Al_2O_3 \times K_2O$	-13.540	1.149	3.150	-17.768	-171.940	159.889	-29.752	6.027	5.821	-2.554
$B_2O3 \times K_2O$	-0.643	-30.206	11.538	9.793	-258.693	-43.600	-11.876	-0.067	4.294	10.864
$Fe_2O3 \times K_2O$	3.978	-0.882	-1.520	-9.681	-65.934	-11.886	1.657	-2.031	3.513	9.186
$Fe_2O3 \times Li_2O$	-29.922	-1.849	17.033	10.166	-33.513	-180.623	14.104	0.232	-0.242	8.252
$CaO \times MgO$	48.263	-4.029	-29.136	-1.888	-10.240	26.248	-76.379	-2.326	6.072	-4.017
$Fe_2O_3 \times MgO$	7.732	4.852	6.904	-50.898	-21.162	36.947	-60.238	-0.728	3.196	3.407
$Li_2O \times Na_2O$	-2.622	3.375	-0.161	5.601	28.403	-240.441	6.847	-3.191	-4.126	3.249
$Al_2O_3 \times SiO_2$	-130.114	12.263	11.274	7.107	18.136	-78.566	24.697	11.814	-16.874	6.865
$Li_2O \times SiO_2$	-53.144	5.334	9.622	16.004	31.129	-424.529	20.699	7.673	-14.603	7.832
$Fe_2O_3 \times ZrO_2$	-8.531	6.231	-4.810	-79.757	10.149	135.744	-31.881	4.145	2.115	10.585
$Li_2O \times ZrO_2$	-93.067	-9.273	15.315	46.168	22.961	-583.255	35.281	15.323	-11.945	9.210

Table B.2. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 26-Term Model (Model 6) for ln(PCT-B, g/L) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset (continued)

Term	ZrO_2	P_2O_5	TiO_2	Others	CaO× Fe_2O_3	Al_2O_3× K_2O	B_2O_3× K_2O	Fe_2O_3× K_2O	Fe_2O_3× Li_2O
Al_2O_3	-2.618	-3.802	-4.483	-4.750	-17.172	-13.540	-0.643	3.978	-29.922
B_2O_3	0.382	0.083	0.989	0.326	5.805	1.149	-30.206	-0.882	-1.849
CaO	0.332	0.491	0.411	0.305	-12.348	3.150	11.538	-1.520	17.033
Fe_2O_3	2.300	0.276	-0.956	0.716	-23.103	-17.768	9.793	-9.681	10.166
K_2O	-0.793	-0.330	2.179	-0.201	10.575	-171.940	-258.693	-65.934	-33.513
Li_2O	-5.974	-6.697	-12.219	-6.396	26.726	159.889	-43.600	-11.886	-180.623
MgO	1.404	0.137	-1.031	0.555	-0.491	-29.752	-11.876	1.657	14.104
Na_2O	-0.171	0.540	0.418	0.404	3.489	6.027	-0.067	-2.031	0.232
SiO_2	-0.662	-0.655	-0.954	-0.706	-2.987	5.821	4.294	3.513	-0.242
SnO_2	-0.565	0.314	0.453	-0.073	-7.215	-2.554	10.864	9.186	8.252
ZrO_2	4.284	0.395	1.091	0.620	-1.931	-3.950	9.680	7.856	-3.712
P_2O_5	0.395	6.123	1.042	0.267	0.721	-2.530	12.438	3.959	-0.571
TiO_2	1.091	1.042	5.876	0.629	3.560	-5.066	-12.022	-4.881	8.763
Others	0.620	0.267	0.629	1.807	2.400	1.451	8.846	-4.063	6.433
CaO×Fe_2O_3	-1.931	0.721	3.560	2.400	445.763	18.741	-92.192	-74.884	-456.585
Al_2O_3×K_2O	-3.950	-2.530	-5.066	1.451	18.741	1908.406	363.866	191.093	41.511
B_2O3×K_2O	9.680	12.438	-12.022	8.846	-92.192	363.866	2567.169	210.491	307.620
Fe_2O3×K_2O	7.856	3.959	-4.881	-4.063	-74.884	191.093	210.491	921.429	255.268
Fe_2O3×Li_2O	-3.712	-0.571	8.763	6.433	-456.585	41.511	307.620	255.268	1623.949
CaO×MgO	-8.405	4.275	8.717	-2.929	-10.961	62.302	33.984	61.871	-58.641
Fe_2O_3×MgO	-7.825	-2.698	11.531	2.011	96.271	235.332	94.537	-49.221	-274.071
Li_2O×Na_2O	12.916	4.039	13.989	4.225	-14.279	-269.267	-71.587	65.421	186.280
Al_2O_3×SiO_2	7.151	10.967	13.269	12.290	54.691	-64.592	-3.176	-24.645	62.255
Li_2O×SiO_2	12.930	15.258	25.365	12.028	-4.286	-252.959	40.458	-11.112	155.689
Fe_2O_3×ZrO_2	-47.105	2.391	17.528	-9.477	282.032	216.915	-198.291	-177.116	-414.811
Li_2O×ZrO_2	-33.688	15.094	-1.140	21.019	-111.966	-555.862	459.319	-69.061	1009.371

Table B.2. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 26-Term Model (Model 6) for ln(PCT-B, g/L) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset (continued)

Term	CaO× MgO	Fe_2O_3×MgO	Li_2O× Na_2O	Al_2O_3×SiO_2	Li_2O×SiO_2	Fe_2O_3×ZrO_2	Li_2O×ZrO_2
Al_2O_3	48.263	7.732	-2.622	-130.114	-53.144	-8.531	-93.067
B_2O_3	-4.029	4.852	3.375	12.263	5.334	6.231	-9.273
CaO	-29.136	6.904	-0.161	11.274	9.622	-4.810	15.315
Fe_2O_3	-1.888	-50.898	5.601	7.107	16.004	-79.757	46.168
K_2O	-10.240	-21.162	28.403	18.136	31.129	10.149	22.961
Li_2O	26.248	36.947	-240.441	-78.566	-424.529	135.744	-583.255
MgO	-76.379	-60.238	6.847	24.697	20.699	-31.881	35.281
Na_2O	-2.326	-0.728	-3.191	11.814	7.673	4.145	15.323
SiO_2	6.072	3.196	-4.126	-16.874	-14.603	2.115	-11.945
SnO_2	-4.017	3.407	3.249	6.865	7.832	10.585	9.210
ZrO_2	-8.405	-7.825	12.916	7.151	12.930	-47.105	-33.688
P_2O_5	4.275	-2.698	4.039	10.967	15.258	2.391	15.094
TiO_2	8.717	11.531	13.989	13.269	25.365	17.528	-1.140
Others	-2.929	2.011	4.225	12.290	12.028	-9.477	21.019
CaO×Fe_2O_3	-10.961	96.271	-14.279	54.691	-4.286	282.032	-111.966
Al_2O_3×K_2O	62.302	235.332	-269.267	-64.592	-252.959	216.915	-555.862
B_2O3×K_2O	33.984	94.537	-71.587	-3.176	40.458	-198.291	459.319
Fe_2O3×K_2O	61.871	-49.221	65.421	-24.645	-11.112	-177.116	-69.061
Fe_2O3×Li_2O	-58.641	-274.071	186.280	62.255	155.689	-414.811	1009.371
CaO×MgO	1579.910	-541.338	91.979	-109.973	-61.500	231.931	-85.500
Fe_2O_3×MgO	-541.338	2355.081	-61.831	-40.815	-33.944	290.375	-384.720
Li_2O×Na_2O	91.979	-61.831	545.657	32.878	389.791	-101.879	116.373
Al_2O_3×SiO_2	-109.973	-40.815	32.878	355.092	170.396	28.560	275.708
Li_2O×SiO_2	-61.500	-33.944	389.791	170.396	830.025	-163.296	827.478
Fe_2O_3×ZrO_2	231.931	290.375	-101.879	28.560	-163.296	2090.367	-1243.660
Li_2O×ZrO_2	-85.500	-384.720	116.373	275.708	827.478	-1243.660	5725.676

Table B.3. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 22-Term Model (Model 3) for ln(VHT Alteration Depth, μm) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset

Term	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	Na_2O
Al_2O3	52.2000	1.9504	-87.4399	3.7315	4.8924	-11.9666	-13.0044
B_2O_3	1.9504	9.0770	-33.5238	2.9192	-0.8092	0.9836	-9.6957
CaO	-87.4399	-33.5238	658.8473	-32.8669	-18.4492	66.7129	65.0395
Fe_2O_3	3.7315	2.9192	-32.8669	10.8910	-3.5331	-4.7336	-7.5966
K_2O	4.8924	-0.8092	-18.4492	-3.5331	159.0083	14.1318	-14.8410
Li_2O	-11.9666	0.9836	66.7129	-4.7336	14.1318	336.4308	-20.2783
Na_2O	-13.0044	-9.6957	65.0395	-7.5966	-14.8410	-20.2783	60.1917
SiO_2	-4.1099	-0.7848	12.4363	-0.6869	-0.9196	-6.9455	-7.1393
SnO_2	7.0691	4.6825	-45.0939	12.4757	0.6064	-20.1456	-9.0385
ZrO_2	-3.1312	1.5460	-14.0370	1.7111	3.8991	-16.3055	-4.8968
TiO_2	1.1383	2.0442	-22.0325	-5.5576	-1.1339	16.3167	-6.8267
Others	47.4862	2.2284	-94.2964	4.2021	11.1419	-8.2719	-12.0173
CaO×CaO	135.2615	54.7858	-983.2777	58.3247	20.6503	187.4342	-205.2160
K_2O×K_2O	-28.9885	58.2847	-105.7703	73.3629	-2591.2364	420.0778	47.7864
CaO×Li_2O	275.0995	162.4177	-1551.6142	195.1112	-52.6680	-1466.8709	-531.4085
K_2O×Li_2O	-120.3353	-20.3599	-167.7641	-48.8272	-681.4999	-1504.3173	353.1012
Li_2O×Li_2O	-263.0771	-224.8834	685.5395	-104.6608	-56.4244	-3795.9135	1113.5040
CaO×Na_2O	155.7491	64.5772	-1057.2407	84.9684	53.7170	-321.0220	-303.9412
Na_2O×Na_2O	7.8803	25.1867	-118.8580	15.8923	39.0371	184.4039	-151.5903
CaO×SiO_2	101.6905	36.7832	-916.7990	29.5041	28.3884	-39.3080	25.7627
Fe_2O_3×SnO_2	-57.0871	20.1301	-65.1135	-225.4410	6.9919	63.0561	27.2093
Al_2O_3×Others	-617.0260	-14.8096	874.7177	-19.0723	-99.1750	38.7610	121.8230

Table B.3. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 22-Term Model (Model 3) for ln(VHT Alteration Depth, μm) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset (continued)

Term	SiO_2	SnO_2	ZrO_2	TiO_2	Others	CaO×CaO	K_2O×K_2O	CaO×Li_2O
Al_2O3	-4.1099	7.0691	-3.1312	1.1383	47.4862	135.2615	-28.9885	275.0995
B_2O_3	-0.7848	4.6825	1.5460	2.0442	2.2284	54.7858	58.2847	162.4177
CaO	12.4363	-45.0939	-14.0370	-22.0325	-94.2964	-983.2777	-105.7703	-1551.6142
Fe_2O_3	-0.6869	12.4757	1.7111	-5.5576	4.2021	58.3247	73.3629	195.1112
K_2O	-0.9196	0.6064	3.8991	-1.1339	11.1419	20.6503	-2591.2364	-52.6680
Li_2O	-6.9455	-20.1456	-16.3055	16.3167	-8.2719	187.4342	420.0778	-1466.8709
Na_2O	-7.1393	-9.0385	-4.8968	-6.8267	-12.0173	-205.2160	47.7864	-531.4085
SiO_2	3.4968	-0.6918	0.7389	-1.5412	-5.6627	10.2894	-3.7717	91.1509
SnO_2	-0.6918	41.1102	-1.3894	2.6208	5.8519	59.9343	-76.4813	430.4531
ZrO_2	0.7389	-1.3894	16.9068	6.9244	-2.5438	30.1396	-113.8781	84.2718
TiO_2	-1.5412	2.6208	6.9244	55.2304	-3.4540	54.9129	87.3587	21.5357
Others	-5.6627	5.8519	-2.5438	-3.4540	58.6253	122.9814	-127.5327	252.7417
CaO×CaO	10.2894	59.9343	30.1396	54.9129	122.9814	4290.9443	620.8344	415.6996
K_2O×K_2O	-3.7717	-76.4813	-113.8781	87.3587	-127.5327	620.8344	47036.5874	-361.6365
CaO×Li_2O	91.1509	430.4531	84.2718	21.5357	252.7417	415.6996	-361.6365	26208.0159
K_2O×Li_2O	25.4969	-93.0040	29.7512	-318.3250	-101.9166	-2526.3452	5414.6457	4044.5105
Li_2O×Li_2O	-37.1303	-133.9467	115.1071	-196.4074	-273.6593	-4398.5073	-7011.5245	-4522.9239
CaO×Na_2O	32.9141	130.8645	55.0501	45.2265	159.5457	1598.3911	-289.3499	7009.0741
Na_2O×Na_2O	12.8033	9.4221	-0.1522	25.7735	11.8017	510.2525	156.7561	510.3335
CaO×SiO_2	-49.9188	36.4752	5.1803	30.5983	122.4524	683.4729	170.8902	7.7097
Fe_2O_3×SnO_2	12.7793	-571.4074	10.0316	42.0317	-56.7838	-1028.8075	919.9561	-1950.1348
Al_2O_3×Others	56.9211	-42.4156	41.7080	23.0111	-655.0950	-1431.2220	1139.8105	-2042.2379

Table B.3. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 22-Term Model (Model 3) for ln(VHT Alteration Depth, µm) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset (continued)

Term	K_2O×Li_2O	Li_2O×Li_2O	CaO×Na_2O	Na_2O×Na_2O	CaO×SiO_2	Fe_2O_3×SnO_2	Al_2O_3×Others
Al_2O3	-120.3353	-263.0771	155.7491	7.8803	101.6905	-57.0871	-617.0260
B_2O_3	-20.3599	-224.8834	64.5772	25.1867	36.7832	20.1301	-14.8096
CaO	-167.7641	685.5395	-1057.2407	-118.8580	-916.7990	-65.1135	874.7177
Fe_2O_3	-48.8272	-104.6608	84.9684	15.8923	29.5041	-225.4410	-19.0723
K_2O	-681.4999	-56.4244	53.7170	39.0371	28.3884	6.9919	-99.1750
Li_2O	-1504.3173	-3795.9135	-321.0220	184.4039	-39.3080	63.0561	38.7610
Na_2O	353.1012	1113.5040	-303.9412	-151.5903	25.7627	27.2093	121.8230
SiO_2	25.4969	-37.1303	32.9141	12.8033	-49.9188	12.7793	56.9211
SnO_2	-93.0040	-133.9467	130.8645	9.4221	36.4752	-571.4074	-42.4156
ZrO_2	29.7512	115.1071	55.0501	-0.1522	5.1803	10.0316	41.7080
TiO_2	-318.3250	-196.4074	45.2265	25.7735	30.5983	42.0317	23.0111
Others	-101.9166	-273.6593	159.5457	11.8017	122.4524	-56.7838	-655.0950
CaO×CaO	-2526.3452	-4398.5073	1598.3911	510.2525	683.4729	-1028.8075	-1431.2220
K_2O×K_2O	5414.6457	-7011.5245	-289.3499	156.7561	170.8902	919.9561	1139.8105
CaO×Li_2O	4044.5105	-4522.9239	7009.0741	510.3335	7.7097	-1950.1348	-2042.2379
K_2O×Li_2O	29121.6273	14933.1045	-48.9299	-1368.2893	856.2864	2505.1374	1422.1121
Li_2O×Li_2O	14933.1045	78212.0088	-2446.5183	-3790.0460	714.3590	-666.7959	3258.1771
CaO×Na_2O	-48.9299	-2446.5183	3424.0579	501.5386	649.3023	-634.3151	-1506.4593
Na_2O×Na_2O	-1368.2893	-3790.0460	501.5386	473.9547	-33.9312	53.1140	-60.0079
CaO×SiO_2	856.2864	714.3590	649.3023	-33.9312	1874.3713	643.3545	-1012.7562
Fe_2O_3×SnO_2	2505.1374	-666.7959	-634.3151	53.1140	643.3545	19215.6707	273.8325
Al_2O_3×Others	1422.1121	3258.1771	-1506.4593	-60.0079	-1012.7562	273.8325	8441.8462

Table B.4. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 25-Term Model (Model 4) for ln(Electrical Conductivity, S/cm) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset

Term	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SiO_2
Al_2O_3	5.1734	-0.5274	-0.8213	0.3024	0.1520	-2.7164	-1.4781	-1.5160	0.2138
B_2O_3	-0.5274	5.7762	-0.6034	0.4872	0.4742	-1.1498	-0.7954	-0.5273	-0.9997
CaO	-0.8213	-0.6034	3.3106	0.4891	0.5147	-1.2351	1.4200	0.3272	-0.3231
Fe_2O_3	0.3024	0.4872	0.4891	4.2969	-0.5930	0.6085	-1.1381	0.1783	-0.8607
K_2O	0.1520	0.4742	0.5147	-0.5930	7.6700	1.9696	0.1384	0.3483	-0.2133
Li_2O	-2.7164	-1.1498	-1.2351	0.6085	1.9696	27.8148	0.6764	6.6450	-2.0139
MgO	-1.4781	-0.7954	1.4200	-1.1381	0.1384	0.6764	21.0734	1.6630	-0.8050
Na2O	-1.5160	-0.5273	0.3272	0.1783	0.3483	6.6450	1.6630	2.4483	-0.6535
SiO2	0.2138	-0.9997	-0.3231	-0.8607	-0.2133	-2.0139	-0.8050	-0.6535	0.7519
ZrO2	-1.2867	0.2738	0.3977	1.8892	-1.7957	-5.2299	-0.2602	-2.1429	-0.1370
Others	-0.6175	0.3494	0.2539	0.6815	-1.6075	-1.9856	-1.9304	-0.4043	-0.4970
CaO*Li_2O	0.0987	0.8446	-6.8161	0.5486	-0.0233	-5.4044	-0.1660	-1.1679	0.2263
CaO*Na_2O	0.0207	0.0404	-2.5029	0.1867	-0.0550	-0.9133	-0.1084	-0.4798	0.1577
Li_2O*Na_2O	0.0436	-0.1096	0.2987	0.1088	-0.1773	-3.4911	0.1888	-0.2923	0.1124
Al_2O_3/(T/1000)	-7.0244	0.7252	1.0961	-0.4089	-0.2163	3.6124	2.0188	2.0486	-0.2889
B_2O_3/(T/1000)	0.7229	-7.8114	0.7841	-0.6598	-0.6505	1.4811	1.0899	0.7056	1.3553
CaO/(T/1000)	1.1170	0.7907	-3.8421	-0.7140	-0.6888	1.9987	-1.8953	-0.3208	0.4005
Fe_2O_3/(T/1000)	-0.4114	-0.6594	-0.7138	-5.8283	0.8034	-0.8571	1.5470	-0.2466	1.1721
K_2O/(T/1000)	-0.2142	-0.6525	-0.7274	0.8064	-10.4024	-2.6598	-0.2128	-0.4685	0.2940
Li_2O/(T/1000)	3.6542	1.4804	2.1486	-0.8758	-2.6299	-36.6793	-0.9970	-8.8553	2.7001
MgO/(T/1000)	2.0187	1.0935	-1.9629	1.5519	-0.2130	-1.0232	-28.5941	-2.2780	1.0942
Na_2O/(T/1000)	2.0542	0.7098	-0.2843	-0.2507	-0.4565	-8.8694	-2.2648	-3.2765	0.8721
SiO_2/(T/1000)	-0.2905	1.3535	0.3974	1.1729	0.2898	2.7126	1.0905	0.8748	-1.0163
ZrO_2/(T/1000)	1.7380	-0.3711	-0.6014	-2.5675	2.4216	6.9784	0.3538	2.8790	0.1967
Others/(T/1000)	0.8442	-0.4695	-0.4133	-0.9320	2.1749	2.6279	2.6304	0.5333	0.6811

Table B.4. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 25-Term Model (Model 4) for ln(Electrical Conductivity, S/cm) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset (continued)

Term	ZrO_2	Others	$CaO*Li_2O$	$CaO*Na_2O$	Li_2O*Na_2O	Al_2O_3/(T/1000)	B_2O_3/(T/1000)
Al_2O_3	-1.2867	-0.6175	0.0987	0.0207	0.0436	-7.0244	0.7229
B_2O_3	0.2738	0.3494	0.8446	0.0404	-0.1096	0.7252	-7.8114
CaO	0.3977	0.2539	-6.8161	-2.5029	0.2987	1.0961	0.7841
Fe_2O_3	1.8892	0.6815	0.5486	0.1867	0.1088	-0.4089	-0.6598
K_2O	-1.7957	-1.6075	-0.0233	-0.0550	-0.1773	-0.2163	-0.6505
Li_2O	-5.2299	-1.9856	-5.4044	-0.9133	-3.4911	3.6124	1.4811
MgO	-0.2602	-1.9304	-0.1660	-0.1084	0.1888	2.0188	1.0899
Na2O	-2.1429	-0.4043	-1.1679	-0.4798	-0.2923	2.0486	0.7056
SiO2	-0.1370	-0.4970	0.2263	0.1577	0.1124	-0.2889	1.3553
ZrO2	13.7898	0.2182	0.9315	0.4224	0.1665	1.7420	-0.3673
Others	0.2182	4.8483	0.7443	0.1663	0.1821	0.8483	-0.4721
$CaO*Li_2O$	0.9315	0.7443	115.2548	28.6368	3.7925	0.4302	-0.2424
$CaO*Na_2O$	0.4224	0.1663	28.6368	12.6193	-2.3065	0.0737	0.0562
Li_2O*Na_2O	0.1665	0.1821	3.7925	-2.3065	21.4973	0.1524	0.1972
Al_2O_3/(T/1000)	1.7420	0.8483	0.4302	0.0737	0.1524	9.6021	-0.9954
B_2O_3/(T/1000)	-0.3673	-0.4721	-0.2424	0.0562	0.1972	-0.9954	10.6395
CaO/(T/1000)	-0.6371	-0.4001	0.7670	0.2394	-0.0454	-1.5346	-1.0774
Fe_2O_3/(T/1000)	-2.5668	-0.9321	-0.0088	-0.0280	-0.0856	0.5638	0.9034
K_2O/(T/1000)	2.4311	2.1759	0.2621	0.2265	0.1537	0.3062	0.9000
Li_2O/(T/1000)	6.9634	2.5934	-1.9504	-0.5367	0.7904	-4.9690	-1.9905
MgO/(T/1000)	0.3615	2.6368	0.8812	0.3388	-0.1480	-2.7694	-1.5019
Na_2O/(T/1000)	2.8673	0.5301	-0.3374	-0.1373	0.1462	-2.8042	-0.9637
SiO_2/(T/1000)	0.1987	0.6817	0.0443	-0.0008	-0.1048	0.3969	-1.8464
ZrO_2/(T/1000)	-18.6824	-0.2834	-0.3797	-0.2342	0.0612	-2.3616	0.5052
Others/(T/1000)	-0.2829	-6.5865	0.1035	0.0410	-0.2090	-1.1609	0.6468

Table B.4. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 25-Term Model (Model 4) for ln(Electrical Conductivity, S/cm) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset (continued)

Term	CaO/(T/1000)	Fe_2O_3/(T/1000)	K_2O/(T/1000)	Li_2O/(T/1000)	MgO/(T/1000)
Al_2O_3	1.1170	-0.4114	-0.2142	3.6542	2.0187
B_2O_3	0.7907	-0.6594	-0.6525	1.4804	1.0935
CaO	-3.8421	-0.7138	-0.7274	2.1486	-1.9629
Fe_2O_3	-0.7140	-5.8283	0.8064	-0.8758	1.5519
K_2O	-0.6888	0.8034	-10.4024	-2.6299	-0.2130
Li_2O	1.9987	-0.8571	-2.6598	-36.6793	-1.0232
MgO	-1.8953	1.5470	-0.2128	-0.9970	-28.5941
Na2O	-0.3208	-0.2466	-0.4685	-8.8553	-2.2780
SiO2	0.4005	1.1721	0.2940	2.7001	1.0942
ZrO2	-0.6371	-2.5668	2.4311	6.9634	0.3615
Others	-0.4001	-0.9321	2.1759	2.5934	2.6368
CaO*Li_2O	0.7670	-0.0088	0.2621	-1.9504	0.8812
CaO*Na_2O	0.2394	-0.0280	0.2265	-0.5367	0.3388
Li_2O*Na_2O	-0.0454	-0.0856	0.1537	0.7904	-0.1480
Al_2O_3/(T/1000)	-1.5346	0.5638	0.3062	-4.9690	-2.7694
B_2O_3/(T/1000)	-1.0774	0.9034	0.9000	-1.9905	-1.5019
CaO/(T/1000)	5.1880	0.9807	0.9455	-2.7914	2.5836
Fe_2O_3/(T/1000)	0.9807	7.9606	-1.0972	1.1727	-2.1179
K_2O/(T/1000)	0.9455	-1.0972	14.1992	3.5717	0.3267
Li_2O/(T/1000)	-2.7914	1.1727	3.5717	50.0120	1.4328
MgO/(T/1000)	2.5836	-2.1179	0.3267	1.4328	39.0479
Na_2O/(T/1000)	0.4218	0.3328	0.6097	12.0808	3.1060
SiO_2/(T/1000)	-0.5411	-1.6036	-0.3992	-3.6946	-1.4884
ZrO_2/(T/1000)	0.8664	3.5176	-3.2965	-9.4649	-0.4863
Others/(T/1000)	0.5595	1.2891	-2.9609	-3.5415	-3.6091

Table B.4. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 25-Term Model (Model 4) for ln(Electrical Conductivity, S/cm) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset (continued)

Term	Na_2O/(T/1000)	SiO_2/(T/1000)	ZrO_2/(T/1000)	Others/(T/1000)
Al_2O_3	2.0542	-0.2905	1.7380	0.8442
B_2O_3	0.7098	1.3535	-0.3711	-0.4695
CaO	-0.2843	0.3974	-0.6014	-0.4133
Fe_2O_3	-0.2507	1.1729	-2.5675	-0.9320
K_2O	-0.4565	0.2898	2.4216	2.1749
Li_2O	-8.8694	2.7126	6.9784	2.6279
MgO	-2.2648	1.0905	0.3538	2.6304
Na2O	-3.2765	0.8748	2.8790	0.5333
SiO2	0.8721	-1.0163	0.1967	0.6811
ZrO2	2.8673	0.1987	-18.6824	-0.2829
Others	0.5301	0.6817	-0.2834	-6.5865
CaO*Li_2O	-0.3374	0.0443	-0.3797	0.1035
CaO*Na_2O	-0.1373	-0.0008	-0.2342	0.0410
Li_2O*Na_2O	0.1462	-0.1048	0.0612	-0.2090
Al_2O_3/(T/1000)	-2.8042	0.3969	-2.3616	-1.1609
B_2O_3/(T/1000)	-0.9637	-1.8464	0.5052	0.6468
CaO/(T/1000)	0.4218	-0.5411	0.8664	0.5595
Fe_2O_3/(T/1000)	0.3328	-1.6036	3.5176	1.2891
K_2O/(T/1000)	0.6097	-0.3992	-3.2965	-2.9609
Li_2O/(T/1000)	12.0808	-3.6946	-9.4649	-3.5415
MgO/(T/1000)	3.1060	-1.4884	-0.4863	-3.6091
Na_2O/(T/1000)	4.4688	-1.1897	-3.9041	-0.7211
SiO_2/(T/1000)	-1.1897	1.3870	-0.2788	-0.9367
ZrO_2/(T/1000)	-3.9041	-0.2788	25.4857	0.3771
Others/(T/1000)	-0.7211	-0.9367	0.3771	9.0148

Table B.5. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 27-Term Model (Model 4) for ln(Viscosity, poise) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset

Term	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O
Al_2O_3	2.0504	-0.1689	-0.3589	0.1936	0.0131	-0.9832	-0.5421	-0.6540
B_2O_3	-0.1689	4.1737	-0.1481	-0.0954	-0.1691	-0.3664	-0.1775	-0.2170
CaO	-0.3589	-0.1481	1.0210	0.2177	0.0065	-0.6583	0.4979	0.0821
Fe_2O_3	0.1936	-0.0954	0.2177	1.5594	-0.0033	0.3156	-0.4746	0.0488
K_2O	0.0131	-0.1691	0.0065	-0.0033	0.0875	0.0820	0.0074	0.0171
Li_2O	-0.9832	-0.3664	-0.6583	0.3156	0.0820	11.7595	0.1493	2.3452
MgO	-0.5421	-0.1775	0.4979	-0.4746	0.0074	0.1493	7.8586	0.5790
Na_2O	-0.6540	-0.2170	0.0821	0.0488	0.0171	2.3452	0.5790	0.8771
P_2O_5	0.6276	-0.0397	0.1406	0.2370	0.0258	1.1326	-0.9783	0.1359
SiO_2	0.0488	-0.2455	-0.0939	-0.2714	0.0061	-0.7474	-0.2546	-0.2200
SnO_2	0.2741	0.0301	0.4311	0.4890	-0.0472	-0.8924	-0.2285	-0.2191
ZrO_2	-0.5477	-0.2193	0.1474	0.6824	-0.0088	-1.3673	-0.2990	-0.6592
Others	-0.0753	-0.1431	-0.1218	0.1506	-0.0103	-0.9419	-1.1187	-0.2766
$B_2O_3 \times B_2O_3$	0.8508	-21.9818	0.7711	0.5487	0.9028	1.6279	0.8827	1.1221
$Li_2O \times Li_2O$	-1.2299	3.5252	0.7825	-0.3750	-0.5377	-22.3250	-0.1562	-0.1808
$Al_2O_3 \times Li_2O$	-2.3454	-0.6119	0.5932	-0.0807	-0.1566	-11.8974	0.1031	0.2918
$Al_2O_3/(T/1000)^2$	-3.6290	-0.0483	0.6498	-0.3503	-0.0036	2.1705	1.0021	1.1962
$CaO/(T/1000)^2$	0.6534	0.0056	-1.8379	-0.3948	0.0075	1.1318	-0.8802	-0.1321
$Fe_2O_3/(T/1000)^2$	-0.3435	-0.0773	-0.3921	-2.8217	0.0020	-0.5142	0.8519	-0.0706
$Li_2O/(T/1000)^2$	2.1862	0.0982	1.0642	-0.5076	-0.0314	-17.7703	-0.2901	-4.2228
$MgO/(T/1000)^2$	0.9849	0.0912	-0.8807	0.8474	-0.0054	-0.3573	-14.1688	-1.0365
$Na_2O/(T/1000)^2$	1.1872	0.0247	-0.1328	-0.0728	-0.0085	-4.2265	-1.0336	-1.5594
$P_2O_5/(T/1000)^2$	-1.1149	0.0225	-0.2561	-0.4309	-0.0021	-2.0192	1.7650	-0.2351
$SiO_2/(T/1000)^2$	-0.0716	0.0033	0.1882	0.5026	0.0015	1.3523	0.4865	0.4183
$ZrO_2/(T/1000)^2$	1.0127	-0.0460	-0.2543	-1.2284	0.0123	2.4793	0.5118	1.2042
$Others/(T/1000)^2$	0.1160	-0.0024	0.2293	-0.2835	0.0099	1.6241	2.0278	0.5137
$SnO_2/(T/1000)^2$	-0.5307	-0.0581	-0.7982	-0.9146	0.0069	1.6218	0.4147	0.4038

Table B.5. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 27-Term Model (Model 4) for ln(Viscosity, poise) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset (continued)

Term	P_2O_5	SiO_2	SnO_2	ZrO_2	Others	$B_2O_3 \times B_2O_3$	$Li_2O \times Li_2O$	$Al_2O_3 \times Li_2O$
Al_2O_3	0.6276	0.0488	0.2741	-0.5477	-0.0753	0.8508	-1.2299	-2.3454
B_2O_3	-0.0397	-0.2455	0.0301	-0.2193	-0.1431	-21.9818	3.5252	-0.6119
CaO	0.1406	-0.0939	0.4311	0.1474	-0.1218	0.7711	0.7825	0.5932
Fe_2O_3	0.2370	-0.2714	0.4890	0.6824	0.1506	0.5487	-0.3750	-0.0807
K_2O	0.0258	0.0061	-0.0472	-0.0088	-0.0103	0.9028	-0.5377	-0.1566
Li_2O	1.1326	-0.7474	-0.8924	-1.3673	-0.9419	1.6279	-22.3250	-11.8974
MgO	-0.9783	-0.2546	-0.2285	-0.2990	-1.1187	0.8827	-0.1562	0.1031
Na_2O	0.1359	-0.2200	-0.2191	-0.6592	-0.2766	1.1221	-0.1808	0.2918
P_2O_5	34.8435	-0.2156	-0.0341	0.2821	-1.2631	0.2292	0.5453	-0.4867
SiO_2	-0.2156	0.2335	0.0297	-0.1689	-0.3219	1.2673	0.0241	0.2034
SnO_2	-0.0341	0.0297	6.4848	-1.6819	0.0003	-0.0566	-0.8013	0.5375
ZrO_2	0.2821	-0.1689	-1.6819	5.5887	0.6358	1.2094	-0.1414	0.1327
Others	-1.2631	-0.3219	0.0003	0.6358	3.5331	0.7816	-0.0303	0.4361
$B_2O_3 \times B_2O_3$	0.2292	1.2673	-0.0566	1.2094	0.7816	117.2746	-17.8676	5.8675
$Li_2O \times Li_2O$	0.5453	0.0241	-0.8013	-0.1414	-0.0303	-17.8676	395.9275	44.8501
$Al_2O_3 \times Li_2O$	-0.4867	0.2034	0.5375	0.1327	0.4361	5.8675	44.8501	130.2411
$Al_2O_3/(T/1000)^2$	-1.1140	-0.0691	-0.5478	1.0070	0.1187	0.2105	0.7586	0.2445
$CaO/(T/1000)^2$	-0.2552	0.1870	-0.8023	-0.2573	0.2252	-0.0257	-0.7678	-0.4144
$Fe_2O_3/(T/1000)^2$	-0.4261	0.5076	-0.9158	-1.2238	-0.2780	0.3906	0.4199	-0.1370
$Li_2O/(T/1000)^2$	-1.9927	1.3385	1.6343	2.4481	1.6495	-0.4325	0.1834	1.7225
$MgO/(T/1000)^2$	1.7629	0.4811	0.4171	0.5057	2.0253	-0.4092	0.5490	0.5028
$Na_2O/(T/1000)^2$	-0.2388	0.4170	0.4107	1.2024	0.5140	-0.0963	-0.3808	0.2772
$P_2O_5/(T/1000)^2$	-63.1267	0.3882	0.0266	-0.5064	2.2652	-0.1721	0.8572	0.0317
$SiO_2/(T/1000)^2$	0.3891	-0.3954	-0.0475	0.3320	0.6030	-0.0186	0.0106	-0.1318
$ZrO_2/(T/1000)^2$	-0.4995	0.3353	3.0295	-10.0764	-1.1175	0.1861	-0.1253	-0.2656
$Others/(T/1000)^2$	2.2700	0.6047	-0.0355	-1.1201	-6.3816	-0.0233	0.4762	0.0075
$SnO_2/(T/1000)^2$	0.0380	-0.0422	-11.7914	3.0383	-0.0263	0.2512	0.9009	-0.6928

Table B.5. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 27-Term Model (Model 4) for ln(Viscosity, poise) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset (continued)

	$Al_2O_3/(T/1000)^2$	$CaO/(T/1000)^2$	$Fe_2O_3/(T/1000)^2$	$Li_2O/(T/1000)^2$	$MgO/(T/1000)^2$
Term	-3.6290	0.6534	-0.3435	2.1862	0.9849
Al_2O_3	-0.0483	0.0056	-0.0773	0.0982	0.0912
B_2O_3	0.6498	-1.8379	-0.3921	1.0642	-0.8807
CaO	-0.3503	-0.3948	-2.8217	-0.5076	0.8474
Fe_2O_3	-0.0036	0.0075	0.0020	-0.0314	-0.0054
K_2O	2.1705	1.1318	-0.5142	-17.7703	-0.3573
Li_2O	1.0021	-0.8802	0.8519	-0.2901	-14.1688
MgO	1.1962	-0.1321	-0.0706	-4.2228	-1.0365
Na_2O	-1.1140	-0.2552	-0.4261	-1.9927	1.7629
P_2O_5	-0.0691	0.1870	0.5076	1.3385	0.4811
SiO_2	-0.5478	-0.8023	-0.9158	1.6343	0.4171
SnO_2	1.0070	-0.2573	-1.2238	2.4481	0.5057
ZrO_2	0.1187	0.2252	-0.2780	1.6495	2.0253
Others	0.2105	-0.0257	0.3906	-0.4325	-0.4092
$B_2O_3 \times B_2O_3$	0.7586	-0.7678	0.4199	0.1834	0.5490
$Li_2O \times Li_2O$	0.2445	-0.4144	-0.1370	1.7225	0.5028
$Al_2O_3 \times Li_2O$	6.7552	-1.2103	0.6708	-4.1267	-1.8676
$Al_2O_3/(T/1000)^2$	-1.2103	3.4197	0.7410	-1.9814	1.6144
$CaO/(T/1000)^2$	0.6708	0.7410	5.2662	0.9035	-1.5506
$Fe_2O_3/(T/1000)^2$	-4.1267	-1.9814	0.9035	32.6590	0.6161
$Li_2O/(T/1000)^2$	-1.8676	1.6144	-1.5506	0.6161	26.2458
$MgO/(T/1000)^2$	-2.2226	0.2435	0.1196	7.8134	1.9241
$Na_2O/(T/1000)^2$	2.0644	0.4872	0.7930	3.6153	-3.2654
$P_2O_5/(T/1000)^2$	0.1311	-0.3506	-0.9397	-2.4842	-0.9152
$SiO_2/(T/1000)^2$	-1.8708	0.4780	2.2944	-4.4975	-0.8566
$ZrO_2/(T/1000)^2$	-0.1799	-0.4167	0.5568	-3.0461	-3.7480
$Others/(T/1000)^2$	1.0751	1.5125	1.7806	-3.0884	-0.7825

Table B.5. Variance-Covariance Matrix Associated With the Estimated Coefficients of Terms in the 27-Term Model (Model 4) for ln(Viscosity, poise) for Combined WTP-LAW, ORP-LAW and LORPM Glass Dataset (continued)

	$Na_2O/(T/1000)^2$	$P_2O_5/(T/1000)^2$	$SiO_2/(T/1000)^2$	$ZrO_2/(T/1000)^2$	Others/$(T/1000)^2$	$SnO2/(T/1000)^2$
Term	1.1872	-1.1149	-0.0716	1.0127	0.1160	-0.5307
Al_2O_3	0.0247	0.0225	0.0033	-0.0460	-0.0024	-0.0581
B_2O_3	-0.1328	-0.2561	0.1882	-0.2543	0.2293	-0.7982
CaO	-0.0728	-0.4309	0.5026	-1.2284	-0.2835	-0.9146
Fe_2O_3	-0.0085	-0.0021	0.0015	0.0123	0.0099	0.0069
K_2O	-4.2265	-2.0192	1.3523	2.4793	1.6241	1.6218
Li_2O	-1.0336	1.7650	0.4865	0.5118	2.0278	0.4147
MgO	-1.5594	-0.2351	0.4183	1.2042	0.5137	0.4038
Na_2O	-0.2388	-63.1267	0.3891	-0.4995	2.2700	0.0380
P_2O_5	0.4170	0.3882	-0.3954	0.3353	0.6047	-0.0422
SiO_2	0.4107	0.0266	-0.0475	3.0295	-0.0355	-11.7914
SnO_2	1.2024	-0.5064	0.3320	-10.0764	-1.1201	3.0383
ZrO_2	0.5140	2.2652	0.6030	-1.1175	-6.3816	-0.0263
Others	-0.0963	-0.1721	-0.0186	0.1861	-0.0233	0.2512
$B_2O_3 \times B_2O_3$	-0.3808	0.8572	0.0106	-0.1253	0.4762	0.9009
$Li_2O \times Li_2O$	0.2772	0.0317	-0.1318	-0.2656	0.0075	-0.6928
$Al_2O_3 \times Li_2O$	-2.2226	2.0644	0.1311	-1.8708	-0.1799	1.0751
$Al_2O_3/(T/1000)^2$	0.2435	0.4872	-0.3506	0.4780	-0.4167	1.5125
$CaO/(T/1000)^2$	0.1196	0.7930	-0.9397	2.2944	0.5568	1.7806
$Fe_2O_3/(T/1000)^2$	7.8134	3.6153	-2.4842	-4.4975	-3.0461	-3.0884
$Li_2O/(T/1000)^2$	1.9241	-3.2654	-0.9152	-0.8566	-3.7480	-0.7825
$MgO/(T/1000)^2$	2.8867	0.4244	-0.7717	-2.2185	-0.9558	-0.7859
$Na_2O/(T/1000)^2$	0.4244	117.4897	-0.7154	0.9111	-4.1921	-0.0521
$P_2O_5/(T/1000)^2$	-0.7717	-0.7154	0.7349	-0.6240	-1.1315	0.0659
$SiO_2/(T/1000)^2$	-2.2185	0.9111	-0.6240	18.7095	2.0503	-5.5973
$ZrO_2/(T/1000)^2$	-0.9558	-4.1921	-1.1315	2.0503	11.8657	0.1426
Others/$(T/1000)^2$	-0.7859	-0.0521	0.0659	-5.5973	0.1426	22.1294