ORP-70894
Revision 0

Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. 0

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

P.O. Box 450
Richland, Washington 99352

ORP-70894
Revision 0

Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. 0

I. Muller
Vitreous State Laboratory of The Catholic University of America

H. Gan
Vitreous State Laboratory of The Catholic University of America

I. L. Pegg
Vitreous State Laboratory of The Catholic University of America

Date Published
September 2024

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

Office of River Protection

P.O. Box 450
Richland, Washington 99352

APPROVED
By Sarah Harrison at 12:22 pm, Oct 02, 2024

Release Approval Date

TRADEMARK DISCLAIMER

Reference herein to any specific commercial product, process, or service by tradename, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors.

Printed in the United States of America

VSL-04R4480-2

Final Report

Phase 1 ILAW PCT and VHT Model Development

prepared by

Isabelle Muller, Hao Gan, and Ian L. Pegg[a]

Vitreous State Laboratory
The Catholic University of America
Washington, DC 20064

and

Scott K. Cooley and Greg F. Piepel[b]

Statistical Sciences
Battelle-Pacific Northwest Division
Richland, WA 99352

[a]For Duratek, Inc. and Bechtel National, Inc.
[b]For the Waste Treatment Plant Support Project for Bechtel National, Inc.

November 29, 2004

2/15/05

W. Tamosaitis

ACCEPTED FOR PROJECT USE

Rev. 0; 2/8/05

Document Title: **Phase 1 ILAW PCT and VHT Model Development**

Document Number and Revision: VSL-04R4480-2, Rev. 0
Issue Date: 2/8/05
Performing Organization: Vitreous State Laboratory, The Catholic University of America
Battelle-Pacific Northwest Division

Test Specifications: 24590-LAW-TSP-RT-01-013, Rev. 1
24590-WTP-TSP-RT-02-001, Rev. 0
Test Exceptions: None
Test Plans: VSL-02T4800-1, Rev. 1
TP-RPP-WTP-179, Rev. 1
R&T Focus Area(s): LAW Waste Form Qualification
Test Scoping Statement(s): VSL-21, LAW Glass Property Composition Modeling
VSL-22, LAW Processing Properties Models
B-66, Demonstrate Compliance with Glass Durability Requirements for ILAW

Completeness of Testing:

This report describes the results of work and testing specified by the above-listed Test Specification(s), Test Plan(s), and Text Exception(s). The work and any associated testing followed established quality assurance requirements and were conducted as authorized. The descriptions provided in this test report are an accurate account of both the conduct of the work and the data collected. Results required by the Test Plan are reported. Also reported are any unusual or anomalous occurrences that are different from the starting hypotheses. The test results and this report have been reviewed and verified.

I.L. Pegg: _____ **Date:** 2/8/05
VSL Program Director/Principal Investigator

I. Joseph: Innocent Joseph **Date:** 2/8/05
Duratek Sub-Contract Manager

TABLE OF CONTENTS

List of Tables

List of Figures

List of Appendices

List of Abbreviations

ANL-LRM	Argonne National Laboratory – Low Activity Reference Material
ASTM	American Society for Testing and Materials
BNFL	British Nuclear Fuels Limited
BNI	Bechtel National, Inc.
CSLM	Component Slope Linear Mixture
CUA	The Catholic University of America
DCP	Direct Current Plasma Emission Spectroscopy
DCP-AES	Direct Current Plasma Atomic Emission Spectroscopy
DOE	Department Of Energy
EGCR	Experimental Glass Composition Region
HLW	High Level Waste
IC	Ion Chromatography
ID	Identification
IHLW	Immobilized High Level Waste
ILAW	Immobilized Low Activity Waste
LAW	Low Activity Waste
LM	Linear Mixture
LOF	Lack of Fit
MAXR	Maximum R-squared Improvement
MSE	Mean Squared Error (from regression)
NIST	National Institute of Standards and Technology
ORP	Office of River Protection
PCT	Product Consistency Test
PI	Prediction Interval
PNWD	Pacific Northwest Division (Battelle)
PQM	Partial Quadratic Mixture
PSWP	Products and Secondary Wastes Plan
QA	Quality Assurance
QAPjP	Quality Assurance Project Plan for Testing Programs Generating Environmental Regulatory Data
QGCR	Qualified Glass Composition Regions
R&T	Research & Technology
RCRA	Resource Conservation and Recovery Act
RMSE	Root Mean Squared Error
RSD	Relative Standard Deviations
SD	Standard Deviation
SEM	Scanning Electron Microscopy
SRL-EA	Savannah River Laboratory-Environmental Assessment (Glass)
SUCI	Simultaneous Upper Confidence Intervals
TCLP	Toxicity Characteristic Leaching Procedure
TF COUP	Tank Farm Contractor Operation and Utilization Plan
UCI	Upper Confidence Intervals
ULS	Unweighted Least Squares
VHT	Vapor Hydration Test
VSL	Vitreous State Laboratory
WTP	Hanford Tank Waste Treatment and Immobilization Plant
WTPSP	Waste Treatment Plant Support Project
XRF	X-Ray Fluorescence

SUMMARY OF TESTING

A) Objectives

This report is one in a series of reports that presents the results from the Low Activity Waste (LAW) glass formulation development and testing work performed at the Vitreous State Laboratory (VSL) of the Catholic University of America (CUA) and the development of ILAW property-composition models performed jointly by Battelle-Pacific Northwest Division (PNWD) and VSL for the Waste Treatment and Immobilization Plant (WTP) Project. Specifically, this report presents results of glass testing and model development at PNWD and VSL for Phase I ILAW Product Consistency Test (PCT) and Vapor Hydration Test (VHT) models. The models presented in this report may be augmented and additional validation work performed during any future ILAW model development work. Completion of the test objectives is addressed in the table below.

Test Objective	Objective Met (Y/N)	Discussion
Develop property-composition models and supporting data that relate ILAW performance on the PCT to ILAW composition and are suitable for predicting the PCT performance of ILAW glasses to be produced in the WTP.	Yes	The PCT models are described in Section 6. The supporting data are described in Section 4. The experimental methods and test matrices are described in Sections 3 and 2, respectively.
Develop property-composition models and supporting data that relate ILAW performance on the VHT to ILAW composition and are suitable for predicting the VHT performance of ILAW glasses to be produced in the WTP.	Yes	The VHT models are described in Section 5. The supporting data are described in Section 4. The experimental methods and test matrices are described in Sections 3 and 2, respectively.

Other objectives in the Test Specifications and Test Plans for this work relate to the development of model for other properties; these are the subjects of separate reports.

B) Test Exceptions

None.

C) Results and Performance Against Success Criteria

The VHT results for the Test Matrix glasses varied from 0.11 g/m^2/day to 125 g/m^2/day, as compared to the contract requirement of < 50 g/m^2/day. The VHT results for the 21 Existing Matrix glasses ranged from less than 1 to 23 g/m^2/day. For a few of the Test Matrix glasses, the extent of VHT alteration was so high that no rate could be calculated because the entire glass coupon was altered. Five of the Test Matrix glasses were altered completely before the end of the 24-day test period. Another two glass samples had an alteration depth in excess of 700 μm (an alteration depth of ≈ 453 μm corresponds to an alteration rate of 50 g/m^2/day). These seven samples were not used in VHT modeling. During any future modeling work, efforts may be made to obtain more VHT data points near the contractual limit in order to improve predictive ability of the model in this range.

The PCT boron results varied from 0.08 g/m^2 to 17.84 g/m^2 for the Test Matrix glasses, and 0.19 g/m^2 to 0.87 g/m^2 for the Existing Matrix glasses. The 21 Existing Matrix glasses were designed to be compliant with ILAW performance requirements and, therefore, it was expected that their PCT boron results would be less than 2 g/m^2, which is the WTP contract limit. The Test Matrix glasses, however, were designed to cover a larger composition range and, accordingly, their PCT responses are expected to vary by a larger amount. Eight of the Test Matrix glasses showed PCT boron or sodium releases in excess of 2 g/m^2. These are mostly outer layer compositions, which were expected to provide a wider range of PCT values. However, these are not likely compositions to be selected for LAW processing at the WTP. Only those glasses with a PCT response of less than 2 g/m^2 were retained in the final regression set used for modeling, thereby reducing the Combined Matrix (Existing + Test Matrices) data set from 77 to 69 glasses. This is not an ideal solution, as preferably the modeling data set should have glasses with PCT releases near and somewhat beyond the specification limit. However, the model performance was found to be degraded when additional glasses were retained because their PCT responses were much higher than for the rest of the data set.

The WTP PCT specification requires that the normalized mass losses of boron, sodium, and silicon in a seven-day PCT at 90°C be less than 2 g/m^2. However, a review of the data from the present work showed that the normalized PCT mass losses for boron and sodium were *always* higher than the normalized PCT mass loss for silicon. Furthermore, for *every one* of the 77 glasses in the Combined Matrix, the normalized PCT mass loss for silicon was below the WTP contract limit of 2 g/m^2. These results suggest that: (i) if the boron and sodium mass losses are below the WTP limit, so too will be the silicon mass loss, and (ii) the silicon mass loss does not exceed the WTP limit over the LAW glass composition region of interest. We therefore concluded that a model for silicon PCT response is not needed. Accordingly, with concurrence from the WTP Project, only PCT boron and sodium releases were modeled.

The VHT and PCT data were fitted to linear mixture (LM) models and partial quadratic mixture (PQM) models and a variety of regression statistics were computed to assess the performance of the models. Validation of the models was performed in two ways. The primary method of validation was by data-splitting, in which a fraction of the data set is left out of the model regression and the ability of the resulting model to predict the responses for the omitted data is assessed. The secondary method of validation assessed the ability of the models to predict

the responses for a set of 59 glasses that composed the independent validation set (none of which were used in the model regression). The validation set was split into three sub-sets based on the closeness of the glass compositions to the composition region defined by the Combined Matrix. Validation statistics were then computed for each of the three subsets and the entire validation set.

For the VHT, reasonable LM and PQM models were identified (see Sections 5.3 and 5.4). However, the LM model showed significant lack-of-fit. This is likely a reflection of the complexity of the VHT process, which tends to accentuate non-linear effects of glass composition. Thus, it is reasonable that non-linear terms would be needed in the VHT model.

For PCT-Boron, an 11-term reduced LM model and a 14-term reduced PQM model were selected as the recommended ILAW Phase 1 models (see Section 6.3.4). It is recommended that both these ILAW PCT-Boron models be applied and their performances compared during any future ILAW glass formulation and waste form qualification work.

For PCT-Sodium, an 11-term reduced LM model and a 16-term reduced PQM model were selected as the recommended ILAW Phase 1 models (see Section 6.4.4). Although the 16-term reduced PQM model appears to have significant advantages over the 11-term reduced LM model, it is recommended that both these ILAW PCT-Sodium models be applied and their performances compared during any future ILAW glass formulation and waste form qualification work.

D) Quality Requirements

The portions of this work that were performed at VSL were conducted under a quality assurance program based on NQA-1 (1989) and NQA-2a (1990) Part 2.7 that is in place at the VSL. This program is supplemented by a Quality Assurance Project Plan for WTP work 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. This work was not subject to DOE/RW-0333P. This work was not subject to the requirements of WTP QAPjP for environmental regulatory data.

Five of the Existing Matrix glasses (LAWA44, LAWA54, LAWA56, LAWA88, and LAWA102) were prepared and characterized at VSL during Part B1 of the contract under British Nuclear Fuels Limited (BNFL). The remaining glasses were prepared and characterized during the Bechtel National Inc. (BNI) contract. An NQA-1 based QA program was in place during all of the work. Compositions of archived samples of Part B1 glasses were reanalyzed at the VSL as part of the present work and the results are presented in this report.

The QA requirements for the PNWD work were met through the Quality Assurance Project Plan for the PNWD Waste Treatment Plant Support Project (WTPSP). The WTPSP implementing procedures comply with the requirements of NQA-1 and NQA-2a Part 2.7.

E) R&T Test Conditions

The data set was based on a Combined Matrix of glasses that was composed of 21 existing glasses (the Existing Matrix) and 56 Test Matrix glasses. The compositions of the Test Matrix glasses were developed by applying statistical experimental design methods to optimally augment the set of Existing Matrix glasses. The 56 Test Matrix glasses were fabricated and characterized with respect to composition and VHT and PCT responses. The data for the Combined Matrix glasses are reported herein. In addition, a set of glasses from previous work in support of the WTP was selected to provide an independent data set for model validation. VHT- and PCT-glass composition models were developed by regression of the Combined Matrix glasses and validated by data-splitting using the regression set as well as by independent validation using the validation set. Based on the performance of the models that were investigated, recommended models were selected.

Crucibles melts of the 56 Test Matrix glasses (about 400 g) were prepared by melting mixtures of reagent grade or higher purity chemicals in platinum-gold crucibles at 1200°C for 75 minutes. Mixing of the melt was accomplished mechanically using a platinum stirrer, beginning 15 minutes after the furnace temperature reached 1200°C and continuing for the next 60 minutes. Samples of the resulting glasses were then analyzed for composition by XRF on solid samples, as well as by DCP-AES and IC on solutions resulting from microwave-assisted acid dissolution of solid samples. The PCT, at 90^{o}C for seven days, was performed on all of the glasses and the leachates were analyzed by DCP-AES. The VHT, at 200^{o}C for a nominal duration of 24 days, was performed on all of the glasses. The alteration layer thicknesses were measured by SEM.

F) Simulant Use

Waste simulants were not used in this work. All of the glasses were prepared from reagent chemicals in combinations designed to achieve the target compositions in the statistically-designed Test Matrix.

G) Discrepancies and Follow-On Tests

Follow-on efforts including additional model validation may be done as part of any future model development effort, which will provide the final WTP models.

SECTION 1
INTRODUCTION

The United States Department of Energy's (DOE's) Hanford site in the State of Washington is the current storage location for about 50 million gallons of high-level mixed waste. This waste is stored in underground tanks at the Hanford site. The Hanford Tank Waste Treatment and Immobilization Plant (WTP) will provide DOE with a means for treating this waste by vitrification for subsequent disposal. The tank waste will be partitioned 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 of in an engineered facility on the Hanford site while the IHLW product will be directed to the national deep geological disposal facility for high-level nuclear waste. The ILAW and IHLW products must meet a variety of requirements with respect to protection of the environment before they can be accepted for disposal.

This report is one in a series of reports that presents the results from the Low Activity Waste (LAW) glass formulation development and testing work performed at the Vitreous State Laboratory (VSL) of the Catholic University of America (CUA) and the development of ILAW property-composition models performed jointly by Battelle-Pacific Northwest Division (PNWD) and VSL for the Waste Treatment and Immobilization Plant (WTP) Project. Specifically, this report presents results of glass testing and model development at VSL and PNWD for Phase 1 ILAW Product Consistency Test (PCT) and Vapor Hydration Test (VHT) models. The modeling data presented in this report may be augmented and additional model validation performed during any future ILAW model development work.

This report is responsive to the Test Specifications [1, 2] and Test Plans [3, 4] for LAW property-composition modeling. The purpose of the work described in these documents is to develop property-composition models to support LAW waste form qualification and processing. The models are intended to provide the basis for defining the Qualified Glass Composition Regions (QGCRs), operating ranges, and target glass compositions for LAW processing at the WTP.

The test objectives and test overview are presented in Sections 1.2 and 1.3. The ILAW composition region of interest, the 21 Existing Matrix glasses, and development of the new Test Matrix are described in Section 2. Experimental procedures used in glass preparation, PCT sample preparation and analysis, and VHT sample preparation and analysis are described in Section 3. The PCT and VHT data and general features of their relationships to glass composition are discussed in Section 4. Models relating VHT alternation depth to LAW glass composition are presented and discussed in Section 5.0. Models relating PCT boron and sodium releases to LAW glass composition are presented and discussed in Section 6.0. Summary and conclusions from the ILAW PCT and VHT model development work are presented in Section 7.0. The quality assurance requirements applied to the work presented in this report are described in Section 8.0.

1.2 Test Objectives

The objectives of the ILAW property-composition modeling work as given in the Test Plans [3, 4] are given below along with the strategy to addresses them.

- *Develop property-composition models and supporting data that relate ILAW performance on the PCT to ILAW composition and are suitable for predicting the PCT performance of ILAW glasses to be produced in the WTP.*

- *Develop property-composition models and supporting data that relate ILAW performance on the VHT to ILAW composition and are suitable for predicting the VHT performance of ILAW glasses to be produced in the WTP.*

Development of the Phase 1 PCT and VHT property-composition models is presented in this report. PCT and VHT data for the 21 Existing Matrix glasses and 56 Test Matrix glasses were reported earlier [5].

- *Develop property-composition models that relate viscosity and electrical conductivity of glass melts to ILAW composition and are suitable for predicting the properties of ILAW glasses to be produced in the WTP.*

Viscosity and electrical conductivity data for 21 of the Test Matrix glasses were reported earlier [5]. Viscosity and electrical conductivity measurements of the remaining Test Matrix glasses have since been completed and preliminary property-composition models for viscosity and electrical conductivity have been developed [6].

- *Develop bounding models for ILAW TCLP response. Such models are expected to be appropriate for LAW glasses as a result of the very low levels of RCRA elements in the LAW streams.*

The bounding approach for ILAW TCLP response was developed and reported earlier [7].

- *Develop bounding models for ILAW liquidus temperature. Such models are expected to be appropriate for LAW glasses as a result of their consistently low liquidus values in comparison to the nominal melter operating temperature.*

Data on crystal content after heat treatment, which provide bounds on the liquidus temperature, for the Test Matrix glasses were reported earlier [5]. The bounding liquidus model will be developed and reported later.

- *Develop property-composition models that relate density of ILAW glasses to composition in order to predict overall volumes of ILAW that would be produced from a given waste feed.*

Density data for the Test Matrix glasses were reported earlier [5]. The density property-composition model may be developed and reported at a later date if so directed by the WTP Research and Technology (R&T) organization.

1.3 Test Overview

A set of 56 glass formulations based on a statistically-designed composition Test Matrix [8] was prepared and tested to support ILAW property-composition modeling. The glasses were prepared and characterized in a random order that was specified in the Test Matrix. The focus of the Test Matrix was the first 11 LAW streams for the WTP: AP-101, AZ-101, AZ-102, AN-102, AN-103, AN-104, AN-105, AN-107, AW-101, and AP-101/SY-104. Beryllium and mercury were not included in the ILAW Test Matrix at the direction of WTP. The waste composition information considered in the development of the ILAW Test Matrix included TF COUP Rev. 3A [9], TF COUP Rev. 2 [10], the WTP Test Specification for LAW melter testing [11] which also contained LAW actual waste characterization data, and prior VSL assessments of LAW waste composition [12, 13].

A set of 21 Existing Matrix glasses from previous [12] and ongoing work [14, 15] that are representative of the present range of working compositions was chosen as the starting point for the ILAW Test Matrix development. Preparation and characterization of five of the 21 existing glasses (LAWA44, LAWA54, LAWA56, LAWA88, and LAWA102) are reported in the Part B1 LAW glass formulation report [12]. Details of the preparation and characterization of the rest of the Existing Matrix glasses are presented in more recent reports [14, 15].

The 21 existing glass compositions for ILAW Test Matrix development were recommended by VSL and selected jointly by VSL, PNWD, and WTP [8]. The constraints for the statistically-designed composition Test Matrix were recommended by VSL and selected jointly by VSL, PNWD, and WTP [8]. The Test Matrix [8] was developed jointly by PNWD and VSL. Glass samples were prepared and PCT and VHT data were collected at VSL. Data were assessed and preliminary model forms were developed at VSL [16, 17] and provided to WTP and PNWD. The final model forms that are presented in this report were developed at PNWD.

The ILAW Test Matrix was designed to support the development of property-composition models for the PCT, VHT, melt viscosity, electrical conductivity, and density and to support bounding models for liquidus temperature. PCT and VHT data analysis and property-composition modeling are presented in this report. Toxicity Characteristic Leach Procedure (TCLP) testing and modeling, which is part of the Test Specification [1] and Test Plan [3] work scopes, were completed and reported earlier [7] using a separate composition matrix [18]. Because LAW glasses contain little or no RCRA metals, TCLP testing was limited to spiking a limited number of glasses with RCRA metals and subjecting the glasses to the TCLP in order to demonstrate that TCLP limits were not exceeded. Density and liquidus temperature data for the 56 Test Matrix glasses as well as viscosity and electrical conductivity of 21 of the Test Matrix glasses were reported earlier [5]. Viscosity and electrical conductivity have since been collected for all of the Test Matrix glasses and the data have been used to develop preliminary property-composition models [6]. A bounding model for liquidus temperature will be developed and reported later. A model for density may be developed at a later date if one is deemed necessary by WTP after a review of the data.

SECTION 2
DEVELOPMENT OF COMPOSITION TEST MATRIX

A total of 77 glass compositions were used in the development of Phase 1 ILAW PCT and VHT models. A set of 21 existing glasses that represent the range of current working glass compositions was used as the starting point for the work; these glasses are referred to as the *Existing Matrix* glasses. A statistically-designed composition matrix of 56 glasses was used to augment the existing glasses; these glasses are referred to as the *Test Matrix* glasses. Both matrices together are referred to as the *Combined Matrix*. The selection of the 21 Existing Matrix glasses and the development of the Test Matrix are discussed in this section.

2.1 Development of Composition Test Matrix

The design of the Test Matrix to support ILAW model development was reported previously [8]. For convenience, a summary of that information is presented in this section. Design of the ILAW Test Matrix began with the development of constraints to define the glass composition region to be covered by the Test Matrix. The development of the Test Matrix used a layered design approach [19] with one inner, one middle, and one outer layer.

The Test Matrix was developed based on information on Hanford LAW compositions, pretreatment and recycle assumptions, existing WTP glass formulation data, glass science knowledge and experience, and statistical experimental design methods. The composition constraints were developed based mainly on the compositions of glasses that have previously been developed and tested at the VSL. Target compositions for the seven LAW Sub-Envelopes that have undergone extensive melter testing formed a core data set on which to base the compositional region selected for testing. Another major factor in defining the composition region was the waste loading limit for each of the LAW Envelopes expressed as the Na_2O concentration in the glass. The Na_2O concentrations in the seven LAW Sub-Envelope target glass compositions, the Na_2O concentration boundaries for the three layers of the ILAW Test Matrix, and contractually required waste loading limits for the three LAW Envelopes are given in Figure 2.1. Component concentration ranges and mean concentrations for the glasses tested at VSL during Part A, Part B1, and Part B2 of the WTP program are given in Figure 2.2. These helped define the composition constraints for the Test Matrix.

2.1.1 Waste Composition Inputs Considered

The following waste composition inputs were considered in identifying glass compositions and ranges of glass component concentrations that form part of the definition of the ILAW experimental glass composition region (EGCR).

- TF COUP Rev. 3A [9]
- TF COUP Rev. 2 [10]

- Waste compositions estimates and flow-sheet impacts, including pretreatment and recycle, for LAW streams provided by the WTP [11]
- Data on WTP actual waste samples
- Vitreous State Laboratory (VSL) assessments performed during Part B1 [12, 13]

2.1.2 Basis for LAW Glass Composition Constraints

Component constraints for the ILAW Test Matrix are given in Table 2.1. The following glass formulation data bases and inputs were used in identifying glass components and constraints to define the ILAW EGCR of interest.

- Ongoing WTP glass formulation work
- Current WTP working compositions
- Part B1 WTP glass formulation work [12]
- Contract waste loading requirements [20]

Glass constituents were treated in the following ways:

- Major oxides significantly affecting glass properties were treated as design variables.
- Minor components were treated as a grouped variable referred to as "Others." Components in this group were maintained in fixed proportions with respect to each other, but the total wt% of this group in glass was a design variable.
- Radioactive and other trace components were excluded on the basis of small molar contributions to the glass composition and expected small effects on glass properties.

A total of 14 LAW glass components were chosen as design variables (including the Others component), as shown in Table 2.1.

2.1.3 LAW Waste Loading Constraints

Waste loading constraints for WTP LAW glasses were developed based on the following considerations.

- Contract Specification 2 [20]:
  - Envelope A: Waste $Na_2O > 14.0$ wt%

- Envelope B: Waste Na_2O > 5.0 wt%[1]
- Envelope C Waste Na_2O > 10.0 wt%

- Sulfate incorporation [12, 14, 21].

It is important to note that the preceding Na_2O minimums are for waste Na_2O in LAW glass, not total Na_2O. Waste loading credit cannot be taken for sodium added during pretreatment or via glass forming chemicals.

2.1.4 LAW Glass Property Constraints

Property constraints for the ILAW Test Matrix are given in Table 2.2. Model-based glass property constraints are given in Table 2.3. Glass property constraints used to help define the LAW EGCR were developed based on the following considerations.

- Part B1 data and property-composition models
- Viscosity and electrical conductivity constraints are based on processing limits
- The PCT constraint is based on the ILAW limit [20]
- A VHT constraint based on the ILAW limit [20] was not included because of the preliminary nature of the available models for that property and their generally poorer performance. Instead, the combination of the other glass property constraints and the composition constraints were judged to be sufficiently restrictive to constrain the VHT response to the general region of interest. To the extent that the preliminary VHT response models are reliable, this was confirmed by comparing the predicted VHT response [22] for each of the Test Matrix glasses to the corresponding ILAW limit to confirm that most of the glasses meet this requirement.

2.1.5 Experimental Design Approach for the ILAW Test Matrix

A layered design approach [19, 23] was chosen to generate the ILAW Test Matrix, with glass compositions on one outer layer, one middle layer, and one inner layer. It was also decided that the Test Matrix should include a center glass composition and some replicate data points. The layered design approach provides for covering the LAW glass composition region of interest by spreading data over the three layers and a center point. Property-composition models must be able to predict glass properties sufficiently to qualify as large a glass composition region as possible, and to discriminate between glasses with acceptable and unacceptable properties.

[1] Since this work was completed, the WTP contract was revised to allow a minimum waste sodium oxide loading for Envelope B waste from AZ-102 of 3 wt%. For Envelope B compositions sodium is added either from the waste or as glass formers to provide at least 5 wt% Na_2O in the glass.

Hence, data are needed on the boundary (outer layer) of the LAW glass composition region of interest covering a wider range of property values. Data on the outer layer of a design region also reduce the uncertainty of property-composition model predictions. However, data over more realistic composition regions (middle and inner layers) are also needed for property-composition models to be accurate with good precision over such regions. A layered design is an excellent choice for this type of problem.

The layered experimental design approach was used to cover an outer-layer composition region of LAW glass compositions with the lowest to highest waste loading (5 to 22 wt% Na_2O). This portion of the Test Matrix was chosen to provide data on the boundary (outer layer) of the LAW glass composition region of interest covering a wider range of property values. However, data over other composition regions (middle and inner layers) are also needed for property models to be accurate over such regions. Two inner-layer composition regions of intermediate waste loading glass compositions were defined (middle layer for 10 to 17 wt% Na_2O and inner layer for 12 to 14 wt% Na_2O). The outer-, middle-, and inner-layer composition regions were defined by: (i) lower and upper bound constraints on each of 14 glass components (including Na_2O), and (ii) several multi-component constraints. The 14 glass components varied in the ILAW Test Matrix are: Al_2O_3, B_2O_3, CaO, Fe_2O_3, K_2O, Li_2O, MgO, Na_2O, SiO_2, SO_3, TiO_2, ZnO, ZrO_2, and "Others". The single-component lower and upper constraints corresponding to the 14 components varied in the Test Matrix are listed in Table 2.1. "Others" was a group of components containing BaO, CdO, Cl, Cr_2O_3, F, NiO, PbO, and P_2O_5, which are present in the waste at minor levels and included in a fixed ratio. No component was kept constant. The region is 13-dimensional because the 14 oxide components varied in the Test Matrix must sum to 100%, and this constant-sum constraint reduces the dimensionality of the region. Additional information about how the 14 components were selected, the multi-component constraints involved in the definition of the glass composition region, and the statistical experimental design methods and software used to select test glasses is provided in the report by Cooley et al. [8].

2.1.6 Description of the ILAW Test Matrix

The ILAW Test Matrix contains 56 glasses: 1 center point, 15 outer-layer, 20 middle-layer, 14 inner-layer, and 6 replicates. Table 2.4 gives the target compositions of the 56 glasses in the ILAW Test Matrix. The composition of the grouped component "Others" is given in Table 2.5.

The Na_2O limits for each layer in the design are based on the presently expected approximate upper and lower limits for glasses in each waste envelope:

- Envelope A: 14 to 22 wt% Na_2O
- Envelope B: 5 to 7 wt% Na_2O
- Envelope C: 10 to 12 wt% Na_2O

These ranges are based on total Na_2O in LAW glass (i.e., from waste, added during pretreatment, or added via glass forming chemicals). Little-to-no sodium is expected to be added via glass

forming chemicals during LAW vitrification, with the possible exception of the highest sulfur tanks such as AZ-102. As a result of issues associated with the very high ratio of sulfate to sodium in the AZ-102 Envelope B waste [24], the WTP Project and DOE-ORP have agreed on the use of glass formulations for that stream that have less than 5 wt% waste Na_2O. However, the *total* Na_2O (waste plus additives) in those glasses is still above 5 wt% [24]. Na_2O values in excess of 22 wt% are not included in the Test Matrix because at higher alkali concentrations the leaching and refractory corrosion characteristics of the glasses become marginal to unacceptable. The outer layer, upper bound for K_2O in the ILAW Test Matrix is kept at 4 wt% to accommodate revisions to the LAW AP-101 waste composition data that show high concentrations of potassium [9, 11, 25]. Constraints for the remaining components are based mainly on existing LAW glass compositions and LAW glass formulation work previously completed by VSL. A description of the 21 existing glasses used in LAW PCT and VHT model development is given below. These glasses were used as the starting basis for the development of the ILAW Test Matrix.

2.2 Description of the 21 Existing Glasses

The compositions of the 21 Existing Matrix glasses used in LAW PCT and VHT model development are given in Table 2.6. Graphical displays of the 21 glass compositions with respect to the composition ranges that they represent are given in Figures 2.3 to 2.5. As can be seen from the figures, their compositions span most of the composition ranges explored in this work. Brief descriptions of each of the glasses are given below.

- LAWA44R10 is a glass sample with the same composition as that of LAWA44 that has been selected as the target composition for treating LAW Sub-Envelope A1 waste streams. These include LAW streams from tanks AN-103, AN-105, and SY-101/AP-104. The glass has one of the highest Na_2O and the lowest SO_3 concentrations among the seven LAW Sub-Envelope target compositions selected for waste processing. The K_2O concentration is relatively low for this composition. Due to its high Na_2O loading, Li_2O is not added and B_2O_3 additions are kept low compared to the other seven Sub-Envelope compositions selected for waste processing. The Fe_2O_3 concentration is relatively high (≈ 7 wt%). In the Test Matrix, LAWA44 is of interest because it represents the middle layer, lower bound for CaO concentration and close to the upper bound for Fe_2O_3. LAWA44 performs well in terms of processing and product quality.

- LAWA88R1 is a glass sample with the same composition as that of LAWA88 that has been selected as the target composition for treating LAW Sub-Envelope A2 waste streams. These include LAW streams from tanks AP-101 and AW-101 (TFCOUP Rev. 2 waste basis [10]). The glass has one of the highest Na_2O concentrations among the seven Sub-Envelope target compositions selected for waste processing. The K_2O concentration is one of the highest for this composition. The SO_3 concentration is higher than that for LAWA44. Due to its high Na_2O loading, Li_2O is not added. Compared to LAWA44, the Fe_2O_3, MgO, and SiO_2 concentrations are lower in order to accommodate the higher K_2O

concentration. In the Test Matrix, LAWA88 represents the middle layer, upper bound for K_2O. At moderate K_2O concentrations, LAWA88 performs well in terms of processing and product quality. However, its corrosion and leach characteristics are compromised to some extent when the potassium concentration in the waste stream is very high (> ≈ 2.75 wt% K_2O in the glass). Consequently, for very high potassium Sub-Envelope A2 waste streams, a different glass (LAWA126), at a lower Na_2O waste loading, is recommended.

- LAWA53 is a glass formulation designed immediately after sulfate removal was dropped from the Hanford LAW flow sheet. The glass composition was designed to test the effect of high CaO (≈ 7.8 wt%) and Fe_2O_3 (≈ 7.4 wt%) on sulfate solubility. In the Test Matrix, LAWA53 represents the middle layer, upper bound for CaO and the outer layer, upper bound for Fe_2O_3 concentration.

- LAWA56 is a glass formulation designed to test the effect of high B_2O_3 (≈ 12 wt%) and low CaO (≈ 2 wt%) on sulfate solubility. In the Test Matrix, LAWA56 represents the middle layer, lower bound for CaO and the upper bound for B_2O_3 concentration.

- LAWA102R1 is a glass sample with the same composition as that of LAWA102 that has been selected as the target composition for treating LAW Sub-Envelope A3 waste streams. This includes the LAW stream from tank AN-104. Sub-Envelope A3 has the highest SO_3 concentration among the LAW Envelope A waste streams and, therefore, LAWA102 has the lowest Na_2O loading of any of the LAWA glasses selected for waste processing. The glass contains about 14.5 wt% Na_2O and 2.50 wt% Li_2O is added to enhance sulfate solubility. In the Test Matrix, LAWA102 represents the inner layer, lower bounds for CaO at ≈ 5 wt% and Al_2O_3 at ≈ 6 wt% and the inner layer, upper bounds for Na_2O and Fe_2O_3 at about 14.5 wt% and 5 wt%, respectively.

- LAWA126 is the target glass composition selected for treating LAW Sub-Envelope A2 waste streams with high potassium concentrations. This includes the LAW stream from tank AP-101 per the composition data given in TFCOUP Rev. 3A [9]. As the composition basis for LAW AP-101 was changed from TFCOUP Rev. 2 [10] to TFCOUP Rev. 3A [9], the potassium concentration in the waste stream increased by about 80%. The old target composition, LAWA88, at 20 wt% Na_2O loading was no longer viable due to concerns about increased leaching and refractory corrosion as a result of the higher potassium concentration. Accordingly, the new glass composition, LAWA126, was developed at a lower Na_2O loading of 18.5 wt% and K_2O concentration of 3.9 wt%. This glass composition was used both in melter testing and actual waste vitrification of LAW AP-101. This glass composition is near the outer layer, upper bound for K_2O concentration.

- LAWA128 and LAWA130 are crucible melts prepared to determine the effect of lower B_2O_3 and Fe_2O_3 respectively, on the properties of glasses formulated for LAW AP-101. LAWA128, with about 7 wt% B_2O_3, is near the middle layer, lower bound, whereas LAWA130, with about 2.9 wt% Fe_2O_3, is near the inner layer, lower bound.

- LAWB65, LAWB66, and LAWB68 are part of a set of glass formulations investigated to identify a suitable composition for vitrification of LAW AZ-102 waste. Since LAW AZ-102 has the highest sulfate concentration among all LAW waste streams, the Na_2O loading in these glass compositions are kept low (about 5 wt%). The Li_2O additions are high (≈ 4.3 wt%) to maximize sulfate solubility. Consequently, these glasses represent the outer layer, lower bound for Na_2O and the outer layer, upper bound for Li_2O. LAWB65 and LAWB68 have ZnO concentrations of about 4.6 wt%, which is close to the inner layer, upper bound. LAWB66 and LAWB68 have CaO concentrations of about 8 wt%, which is close to the middle layer, upper bound.

- LAWB78, LAWB79, and LAWB80 are glass formulations prepared to test high-sodium-loading glasses for LAW AZ-101. The Na_2O concentrations in these glasses were 9.8 wt%, 8.6 wt%, and 6.6 wt%. LAWB78 with 9.8 wt% Na_2O is near the middle layer, lower bound, whereas LAWB80 with 6.6 wt% Na_2O is closer to the outer layer, lower bound. All glasses have B_2O_3 concentrations of about 12 wt%, which is close to the middle layer, upper bound. LAWB78 has a Li_2O concentration of about 3 wt%, which is the middle layer, upper bound. The K_2O concentration of about 2 wt% in LAWB80 is close to the middle layer, upper bound. The CaO concentration of ≈ 7.1 wt% in all three glasses is near the inner layer, upper bound and the Fe_2O_3 concentration of 3.25 wt% is close to the inner layer, lower bound.

- LAWB83, LAWB84, LAWB85, and LAWB86 are all glasses formulated at Na_2O concentrations of ≈ 5.5 wt% for the LAW AZ-101 stream. LAWB83 was used in melter testing and was selected as the target composition for processing of LAW AZ-101 waste. All four glasses have Li_2O concentrations close to the outer layer, upper bound of 4.5 wt%. The Fe_2O_3 concentration of ≈ 5.3 wt% in these glasses is close to the inner layer, upper bound. LAWB86 contains no TiO_2, which is the outer layer, lower bound. The B_2O_3 concentration of ≈ 12.4 wt% for LAWB86 is half way between the middle layer, upper bound and outer layer, upper bound. The CaO and Fe_2O_3 concentrations in LAWB83 are both close to the inner layer, upper bounds. The CaO concentration in LAWB85 of ≈ 5.3 wt% is close to the inner layer, lower bound.

- C100-G-136B is a DM100 melter test sample of the LAWC21 glass composition, which is the old target composition for processing LAW Sub-Envelope C1 waste stream from tank AN-102. The target glass composition for LAW AN-102 waste stream was recently revised to LAWC35 [15], which can accommodate higher

sulfate loading. The Na_2O concentration of ≈ 12 wt% in C100-G-136B is the inner layer, lower bound. The Fe_2O_3 concentration of ≈ 6.5 wt% is representative of the middle layer, upper bound. The Li_2O concentration of ≈ 2.7 wt% is half way between the inner layer, upper bound and middle layer, upper bound.

- LAWC27 and LAWC32 are glasses formulated for LAW material from tank AN-102. These were formulated to investigate low Fe_2O_3 glass compositions for LAW AN-102. LAWC27 contains almost no Fe_2O_3, which is the outer layer, lower bound. The B_2O_3 concentration of about 12.2 wt% in LAWC27 places it near the middle layer, upper bound. LAWC32 contains ≈ 9 wt% CaO and 2.4 wt% Fe_2O_3.

All of the 21 Existing Matrix glasses were designed to meet the contractual requirements and, therefore, their PCT and VHT responses are within the limits specified by the WTP contract. The PCT boron release for the 21 Existing Matrix glasses was on average 0.4 g/m^2, with a maximum of about 0.9 g/m^2, compared to the contract limit of 2 g/m^2. The VHT leach rates of the 21 Existing Matrix glasses ranged from less than 1 to 23 g/m^2/day, with an average of 1.7 g/m^2/day, compared to the contract limit of 50 g/m^2/day. Ranges of the VHT and PCT responses for the 21 Existing Matrix and 56 Test Matrix glasses are given in Figure 2.6.

2.3 Validation Data Sets

The VHT data set used in this work as the validation set was selected from results obtained from WTP LAW glass formulation work performed during Part B1 and subsequently [12, 14, 15, 24, 25, 26]. All of these glasses were "actively" rather than "statistically" designed[2] and, therefore, compositional correlations are almost certainly present in the data. Of the 66 glasses in the validation set, 12 glasses were developed during Part B1 [12], while the rest were developed during WTP work for BNI [14, 15, 24, 25, 26]. Overall, the LAW glasses in this validation set cover a slightly wider composition range than the Combined Matrix glasses. The VHT responses for this data set span a range comparable to that of the ILAW Test Matrix glasses. The compositions of the VHT validation glasses and their VHT results are given in Section 5 (Tables 5.4 and 5.5), where the results of VHT modeling are discussed.

The PCT data set used in this work as the validation set was selected from results obtained from WTP LAW glass formulation work performed during Part B1 and subsequently [12, 14, 15, 24, 25, 26]. As with the VHT validation set, all of these glasses were "actively" rather than "statistically" designed and, therefore, compositional correlations are almost certainly present in the data. Of the 59 glasses in the validation set, 10 glasses were developed during Part B1 [12], while the rest were developed during WTP work for BNI [14, 15, 24, 25, 26]. Overall,

[2] "Statistically designed" refers to a set of glass compositions designed 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.

the LAW glasses in this validation set cover a slightly wider composition range than the Combined Matrix glasses. The PCT responses for this data set span a range comparable to the ILAW Test Matrix glasses, with the exception of glasses exhibiting PCT boron and sodium releases in excess of the contract limit of 2 g/m^2. The compositions of the PCT validation glasses and their PCT releases are given in Section 6 (Tables 6.5 and 6.6), where the results of PCT modeling are discussed.

SECTION 3
EXPERIMENTAL PROCEDURES

The experimental procedures used in the preparation and characterization of the ILAW Test Matrix glasses are presented in this section. Preparation of batches, crucible glass melting, XRF analysis, and PCT and VHT test procedures are summarized below. New samples of some of the 21 Existing Matrix glasses were also prepared and characterized. XRF composition analysis of the 21 Existing Matrix glasses was also conducted during the course of this work.

3.1 Glass Batching and Preparation

All 56 Test Matrix glasses were prepared at VSL using reagent grade chemicals. Batching recipes were prepared to target the glass oxide compositions given in Table 2.4.

3.1.1 Batching of Starting Materials

Glass preparation began with a batching sheet that provided information on the required starting materials. The information included the chemicals needed, identification of the chemicals according to vendors and catalog numbers, the associated purity together with the necessary amounts to produce a given amount of glass. Chemicals were weighed and batched according to the batching sheets. The batching and preparation of some of the Test Matrix glasses was repeated as a result of the need for a larger amount of glass for extended testing and occasionally as a result of minor batching errors. Consequently, some glasses were prepared multiple times and are identified with an extension Rx (where x identifies the repetition number) before they were submitted for PCT and VHT analyses.

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. This information forms the basis of the compositions of the Test Matrix glasses prepared, which are identical to the target compositions provided in Tables 2.4 and 2.6.

3.1.2 Glass Preparation

Preparation of all Test Matrix glasses began with weighing and batching of chemicals according to the information in the batching sheets. The batches were prepared from reagent grade or higher purity chemicals to produce a batch size of approximately 400 to 450 g. A blender was used to mix and homogenize the starting materials before they were loaded into platinum/gold crucibles that were engraved with individual identification numbers in order to identify the melt.

For the ILAW Test Matrix, glass melts were prepared in the random order given in Table 2.4. After the melt order had been determined and the batching completed, the loaded

platinum/gold crucibles were placed inside a Deltech DT-28 (or DT-29) furnace with a Eurothem 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 1200°C and continuing for the next 60 minutes. The molten glass was poured at the end of 75 minutes onto a graphite plate to cool. Glass C100-G-136B was not prepared via crucible melt; it is a sample collected during DM100 melter tests using LAW Sub-Envelope C2 feed [27].

3.2 Analysis of Glass Compositions

The primary method used for glass composition analysis was x-ray fluorescence (XRF) on powdered glass samples. An ARL 9400 wavelength dispersive XRF spectrometer was used for this purpose. The XRF 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) and Savannah River Laboratory – Environmental Assessment Glass (SRL-EA).

Glass samples for direct current plasma atomic emission spectroscopy (DCP-AES) analysis were 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 were diluted to 50 ml and used for the dissolution. This procedure is similar to the ASTM Test Method C1412-99, which also employs a mixture of concentrated HF and HNO_3 in microwave digestion of pulverized glass samples; however, supplemental use of HCl/H_3BO_3 is not included in the VSL procedure since boron is normally one of the analytes. The resulting solutions were analyzed by DCP-AES for all constituents except sulfur, for which Dionex Ion Chromatography was used.

Appendix A presents the XRF analysis results for the 56 ILAW Test Matrix glasses and the 21 Existing Matrix glasses. XRF analysis does not provide composition information for lithium and boron. Consequently, these were determined by DCP-AES and the results are included in the XRF analysis tables. Complete DCP-AES analysis results of the Test Matrix and Existing Matrix glasses are given in Appendix B. The DCP-AES and XRF analyses are generally in good agreement with each other as well as with the target glass compositions given in Tables 2.4 and 2.6.

XRF analysis results and normalized DCP analysis results were compared to the target compositions. There are a total of 819 analysis results for components with target concentrations of 3.0 wt% or more in the glass. Of these, 98 showed more than ±10% deviations from the target; 38 of these 98 results are for iron oxide, which was traced to contamination from stainless steel during the grinding process for sample preparation for analyses. Of the remaining 60 results, *only 5 results* showed more than 10% deviation from the target by *both* DCP and XRF. These occurred once for K_2O and four times for ZrO_2. In all five cases, the absolute differences between analyzed and target compositions were less than 1.0 wt%. Fluorine, which is present in the glass in small concentrations (maximum of 0.3 wt%) is not expected to have a substantial

impact on glass properties and, therefore, was not analyzed. Fluorine analysis at these low levels requires additional, dedicated analysis and the information was not considered worth the significant additional effort that it would have taken to collect.

The detection limit for most components is about 0.01 wt%. The precision and accuracy of the analyses are about ± 10 relative percent for major components (> 3.0 wt% in the glass) or 1.0 wt% absolute, whichever is smaller. Note, however, that the batched (target) compositions are used for modeling since these data are derived from simple weighing of pure chemicals, which are believed to provide the best compositional data. Because target glass compositions are used in modeling, the principal role of the composition analysis is one of confirmation.

3.3 Vapor Hydration Test

The vapor hydration tests are 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 procedure given in Appendix A of the PSWP [28]. Glass coupons are fashioned about 5 to 10 mm square, about 2 mm thick, and with one cut and one fractured surface. A hole approximately 1.6 mm in diameter is drilled near one corner of the coupon to allow it to be suspended from a hanger made of 24 gauge stainless steel wire. Dimensional measurements are made to permit calculation of the area and the coupon is weighed before and after the VHT on a balance having a resolution of 100 μg. The coupon is suspended vertically from the hanger in the pressure vessel and enough deionized water is 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. The pressure vessels are flushed with argon, sealed, weighed, and placed in an oven held at 200ºC. The temperature is monitored continuously with an independent thermocouple. At the completion of the test, the pressure vessels are removed and immediately partially immersed in an ice/water bath to condense the water vapor near the bottom of the vessel. Once cool, the vessels are weighed and opened, and then the coupons are removed and weighed. If the difference in the mass of the sealed pressure vessel before and after the test indicated a water loss in excess of 50% of the original amount, the test results are discarded. Otherwise, the coupons are examined using low-power optical microscopy and an X-ray diffraction pattern is taken directly off the surface of the coupon. Next, the coupons are sectioned and the pieces mounted separately to allow SEM examination both of the cross section of the leached coupon and the leached surface itself. For consistency with existing data, the nominal test duration was 24 days.

All of the VHT data used in this report were collected at VSL from tests performed at 200^{o}C for a nominal duration of 24 days. The reacted glass samples were sectioned and examined by scanning electron microscopy (SEM) to determine the altered layer thickness. The altered layer thickness, which (given certain assumptions) relates directly to the mean glass alteration rate over the test interval, was the variable that was used in the present analysis. Thus, the dependence of the altered layer thickness on glass composition was investigated.

WTP Contract Specification 2 [20] requires that the VHT alteration rate determined from tests of seven days or longer duration must be below 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:

$$r = \rho D/t, \tag{3.1}$$

where ρ is the glass density in g/cm^3 and t is the test duration. Under this assumption, for a typical 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.

It should be noted that, in contrast to previous VHT modeling work in which the test duration was included as a modeling variable [22], the present work is restricted to an assessment of VHT results obtained at a single test duration because that is the nature of the new data that have been collected.

3.4 Product Consistency Test

The Product Consistency Test (PCT; ASTM C 1285-94) was conducted on 4 g of 100-200 mesh crushed glass (75-149 μm) placed in 40 ml of test solution (deionized water in this case). PCT tests were performed at 90ºC, in accordance with the current WTP contract requirement. The ratio of the glass surface area to the solution volume for this test is about 2000 m^{-1} (4 g of 100-200 mesh glass is immersed in 40 ml deionized water). All tests were conducted in triplicate, in 304L stainless steel vessels, and in parallel with the ANL-LRM standard glass included in each test set. The leachates were sampled at seven days. One milliliter of sampled leachate is mixed with 20 ml of 1M HNO_3 and the resulting solution is analyzed by DCP-AES; another 3 ml of sampled leachate is used for pH measurement.

In addition to the leachate concentrations themselves, 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 is calculated from the elemental concentrations c_i measured in the leachate (in ppm) as:

$$C_i = \frac{c_i}{f_i}\ , \tag{3.2}$$

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 (PCT-A). 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 is then obtained from:

$$L_i = \frac{C_i}{(S/V)}, \tag{3.3}$$

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 (since 1 g/L = 1000 g/m^3). Specification 2.2.2.17.2 in the WTP Contract [20] sets limits of 2 g/m^2 for the normalized mass losses of Na, B, and Si on the PCT. 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.

SECTION 4
PCT AND VHT RESULTS

PCT and VHT results for the 56 ILAW Test Matrix glasses and the 21 Existing Matrix glasses are presented and discussed in this section. In addition, general compositional trends in the data with respect to the expected roles of glass constituents (glass formers, modifiers, etc.) on the PCT and VHT responses are discussed.

4.1 VHT Results

The VHT results for the 56 Test Matrix glasses and the 21 Existing Matrix glasses are presented in Tables 4.1 and 4.2, respectively. The VHT results for the Test Matrix glasses vary from 0.11 g/m^2/day to 125 g/m^2/day, as compared to the contract requirement of < 50 g/m^2/day. For a few of the Test Matrix glasses, the extent of VHT alteration was so high that no rate could be calculated because the entire glass coupon was altered. VHT results for the 21 Existing Matrix glasses ranged from less than 1 to 23 g/m^2/day. The Existing Matrix glasses were actively designed to meet contract and processing requirements and their VHT results are expected to be within the contract requirements.

4.1.1 Selection of Data Set for VHT Modeling

The initial data set for ILAW VHT modeling included composition and VHT results for 77 glasses, consisting of 56 Test Matrix and 21 Existing Matrix glasses. The target glass compositions were used for all of the Test Matrix glasses. For the Existing Matrix glasses, the same SO_3 values that were used as the basis for the Test Matrix design were used. A minor error was made in the case of LAWA44R10, for which a SO_3 value of 0.41 wt% instead of 0.09 wt% was used in the modeling work. However, since the modeling work showed no correlation between VHT results and SO_3 concentration, this error should not have any significant effect on the modeling results. This error was identified and corrected prior to performing the modeling of the PCT data. In addition, some time after the VHT modeling work was started, the WTP Project decided to use analyzed SO_3 values for all future modeling efforts. Accordingly, VSL completed new XRF analysis of all 21 Existing Matrix glasses using archived samples and the results were used in PCT modeling. The same composition data for the 21 Existing Matrix glasses that was used in PCT modeling will be used in all future modeling that use these glasses. Repetition of the VHT modeling work using the revised composition data was not deemed necessary because any effects are expected to be small, the current modeling efforts may not be final, and the revised compositions will be used in any future VHT modeling. The target glass compositions are given in Tables 2.4 and 2.6. The normalized compositions used in VHT modeling are given in Table 5.1. The VHT results for the Test Matrix and Existing Matrix glasses are given in Tables 4.1 and 4.2, respectively.

Five of the Test Matrix glasses were altered completely before the end of the 24-day test period. Another two glass samples had an alteration depth in excess of 700 μm (an alteration depth of ≈ 453 μm corresponds to an alteration rate of 50 g/m^2/day). These seven samples were not used in VHT modeling. These glasses are LAWM11, LAWM12, LAWM13, LAWM14, LAWM15, LAWM32, and LAWM55. During any future modeling work, efforts may be made to obtain more VHT data points near the contractual limit in order to improve predictive ability of the model in this range.

4.1.2 Discussion of VHT Results

In order to examine compositional trends in the VHT data with respect to the expected roles of the glass components, it is convenient to consider the glass compositions on a molar basis. The compositions of the 56 Test Matrix glasses and the 21 Existing Matrix glasses in mol% are given in Tables 4.3 and 4.4, respectively. Components such as SiO_2, B_2O_3, and P_2O_5 are known to be glass formers and contribute to the network structure of the glass matrix. Depending on the glass composition, components such as Al_2O_3, Fe_2O_3, and ZrO_2 can also contribute with the glass formers and strengthen the glass network. In silicate glasses, trivalent species require charge compensation by cations such as alkalis in order to go into four-fold coordination and contribute to the network structure. However alkali oxides, such as Li_2O, Na_2O, and K_2O, also act as network modifiers (fluxes) by breaking Si-O-Si bonds and depolymerizing the network structure. Alkaline earth oxides (CaO, MgO), play a similar role to the alkalis but generally to a lesser extent since their higher field strength and higher valence leads to more covalence in the glass network. In general, glasses that are high in network formers are more durable and those high in modifiers are more leachable. Among glass network formers, SiO_2 in higher concentration makes the glass more durable. Similar effects are seen for Al_2O_3 and ZrO_2 and, to a lesser extent, also for B_2O_3. Although boron, in the presence of sufficient alkali, does contribute to the network, it is highly soluble; much of its beneficial effect on glass leaching is instead associated with buffering of the leachant.

The VHT results were reviewed in terms of the molar concentrations of glass network formers and modifiers to examine the extent to which general trends or relationships may be evident. This is made somewhat challenging by the fact that the ILAW Test Matrix was designed to cover a composition space and, therefore, employs "many-at-a-time" variations in glass components; systematic variation of the concentrations of a single component or a set of similar components (e.g. alkali oxides) was not the purpose. In addition, the VHT is designed to assess relatively late-stage features of the glass corrosion in which the leachate is dominated by glass corrosion products, which significantly modify the leachate properties, and in which secondary phases are formed as reaction products. Consequently, VHT alteration is a complex process expected to exhibit complex dependences on glass composition.

Figure 4.1 shows the VHT alteration depth as a function of the alkali oxide concentration. The seven glasses with the highest VHT alteration depth occur at the high end of the alkali oxide concentration. There are, however, other glasses with similar alkali oxide concentrations that show much lower alteration rates, so no clear trend is evident in this figure. Figure 4.2 shows VHT alteration depth as a function of the sum of the alkali and alkaline earth oxide

concentrations. Again, no clear trend in VHT alteration rate is evident in this figure. VHT alteration depth as a function of the glass network former oxide concentration is given in Figure 4.3 in both linear and logarithmic scales. The highest VHT alteration depths are observed for glasses that are towards the low end of the range in glass network former oxide concentration, which is consistent with expectations. In the logarithmic plot, a slight trend of decreasing VHT alteration depth with increasing glass network former oxide concentration is visible. Figure 4.4 shows VHT alteration depth as a function of the ratio of alkali oxide to glass network former oxide concentration on both linear and logarithmic scales. The highest VHT alteration depths occur at high ratios of alkali oxides to glass network former oxides, which is as would be expected. A clear increasing trend in VHT alteration depth as the ratio increases is evident in Figure 4.4, especially in the logarithmic plot.

The VHT alteration depth data do not show simple correlations with either glass alkali oxide or network former oxide concentrations. However, there is a noticeable correlation between the logarithm of VHT alteration depth and the ratio of alkali oxide concentration to glass network former oxide concentration. This correlation is generally consistent with 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. As discussed above, however, the overall VHT alteration mechanism is complex and a useful simple correlation to glass structural roles would seem to be unlikely.

4.2 PCT Results

PCT results for the 56 Test Matrix glasses and the 21 Existing Matrix glasses are given in Tables 4.5 and 4.6, respectively. The PCT boron results vary from 0.08 g/m^2 to 17.84 g/m^2 for the Test Matrix glasses, and 0.19 g/m^2 to 0.87 g/m^2 for the Existing Matrix glasses. The 21 Existing Matrix glasses were designed to be compliant with ILAW performance requirements and, therefore, it is expected that their PCT boron results will be less than 2 g/m^2, which is the contract limit. The Test Matrix glasses, however, were designed to cover a larger composition range and, accordingly, their PCT responses are expected to vary by a larger amount. Eight of the Test Matrix glasses show PCT boron or sodium releases in excess of 2 g/m^2. These are mostly outer-layer compositions, which were expected to provide a wider range of PCT values but which are not likely compositions to be selected for LAW processing at the WTP.

4.2.1 Selection of Data Set for PCT Modeling

The initial data set for ILAW PCT modeling included compositions and PCT boron, sodium, and silicon releases for 77 glasses consisting of 56 Test Matrix and 21 Existing Matrix glasses. The target glass compositions were used for all components except SO_3, for which XRF analyzed data were used. After substituting target SO_3 concentrations with XRF analyzed SO_3 concentrations, the compositions were renormalized to 100%. The target compositions are given in Tables 2.4 and 2.6. The normalized compositions for PCT modeling are given in Table 6.1.

The PCT boron, sodium, and silicon releases for the Test Matrix and Existing Matrix glasses are given in Tables 4.5 and 4.6, respectively.

As stated earlier, eight of the glasses exceeded the WTP contract specification for PCT release, which corresponds to 4 g/L (or 2 g/m^2), by considerable amounts. These are LAWM12, LAWM13, LAWM17, LAWM33R1, LAWM34, LAWM35, LAWM55 and LAWM56. For modeling, only those glasses with a PCT response of less than 4 g/L were used, thereby reducing the data set from 77 to 69 glasses. Based on the distribution of PCT responses, the value of 4 g/L appears to be a reasonable dividing point; however, the use of somewhat higher cutoffs was also investigated during the modeling work in attempts to improve the predictive capabilities of the model near the contract limit.

As can be seen from Table 4.5, the normalized PCT mass losses for boron and sodium are *always* higher than the normalized PCT mass loss for silicon. Furthermore, for *every one* of the 77 glasses in the Combined Matrix, the normalized PCT mass loss for silicon is below the WTP contract limit of 2 g/m^2. These results suggest that: (i) if the boron and sodium mass losses are below the WTP limit, so too will be the silicon mass loss, and (ii) the silicon mass loss does not exceed the WTP limit over the region of interest. We therefore concluded that a model for silicon PCT response is not needed. Accordingly, with concurrence from the WTP Project, only PCT boron and sodium releases were modeled.

4.2.2 Discussion of PCT Results

The PCT results were reviewed with respect to general trends with glass composition, as was done for the VHT data in Section 4.1.2. The compositions of the 56 Test Matrix glasses and the 21 Existing Matrix glasses in mol% are given in Tables 4.3 and 4.4, respectively. The PCT results were reviewed in terms of the molar concentrations of glass network formers and modifiers to examine the extent to which general trends or relationships may be evident. This is made somewhat challenging by the fact that the ILAW Test Matrix was designed to cover a composition space and, therefore, employs "many-at-a-time" variations in glass components; systematic variation of the concentrations of a single component or a set of similar components (e.g., alkali oxides) was not the purpose.

Boron forms few secondary phases that precipitate from the leachate and, consequently, its concentration in solution provides one of the best measures of the extent of the reaction of the glass with the leachant. For glasses that show little leaching (less than 2 g/m^2), the observed sodium and boron releases are approximately congruent, as can be seen in Figure 4.5. With increased leaching (extent of reaction), sodium-containing secondary phases are more likely to form, which causes a deviation from congruent behavior. Glass LAWM13 (see Figure 4.5) with 22 wt% Na_2O and comparatively low concentrations of Al_2O_3 and SiO_2 is an exception. In these types of glasses, sodium release is higher than that of boron or any other glass constituent. Sodium (and other alkalis) can be released into solution by ion exchange and diffusion processes, in addition to matrix hydrolysis, which, depending on their relative rates, can lead to normalized leachate concentrations higher than that of boron.

The leachate pH is not only a symptom of the glass-water reaction, it is also a factor in determining the rate and path of subsequent reactions. Alkali ion exchange tends to rapidly increase the pH from neutral to basic. In addition, the rate of hydrolysis of the silicate matrix increases as the pH increases. Furthermore, the stability of alteration phases can be dependent on the solution pH. Certain glass constituents, such as boron, tend to buffer the solution and moderate the pH rise. It is therefore natural to examine the relationships between the measured leachate pH values, the glass composition, and PCT boron and sodium releases.

As expected, leachate pH increases as the alkali concentration in the glass increases, as can be seen in Figure 4.6. PCT boron release as a function of leachate pH is given in Figure 4.7. The boron release increases with pH. PCT boron release as a function of alkali concentration in the glass is given in Figure 4.8. In general, the PCT boron release increases as the alkali concentration increases. A similar trend is observed for PCT sodium release as a function of alkali concentration, as shown in Figure 4.9. PCT boron release as a function of alkali and alkaline earth oxides concentration is shown in Figure 4.10. As the sum of the alkali and alkaline earth oxides increases, the PCT release also increases. The data point at about 40 mol% combined alkali and alkaline earth oxides and 0.4 g/m^2 PCT boron release is LAWM3, which contains about 19 mol% alkaline earth oxides and about 21 mol% alkali oxides. As mentioned previously, alkaline earth oxides are far less effective than alkali oxides in disrupting the glass network structure and, therefore, degrade glass durability to a lesser extent. PCT boron release as a function of the molar concentration of the glass network former oxides is shown in Figure 4.11. As expected, the PCT boron release decreases as the concentration of network formers in the glass increases. PCT boron release is plotted as a function of the ratio of the concentration of alkali oxides to the concentration of network former oxides in Figure 4.12. As is evident from the figure, the PCT boron release increases as this ratio increases. This is as expected because the ratio increases as the alkali oxide concentration increases or the glass network former oxide concentration decreases. Figure 4.13 shows PCT boron release as a function of the ratio of the sum of the concentrations of alkali and alkaline earth oxides to the concentration of network former oxides. Again, the PCT boron release increases as this ratio increases.

The PCT releases of the Test Matrix and Existing Matrix glasses, in general, increase as the glass modifier content increases and as the glass former network content decreases. A clear increasing trend of PCT boron release is observed as the alkali oxide content increases. This is expected because alkali oxides are the most effective modifiers in breaking up the glass structure. An increasing trend in PCT releases with increase in alkaline earth oxide concentration is less clear. Again, this is not unexpected because alkaline earth oxides have a lesser tendency to depolymerize the glass structure as a result of their greater tendency towards covalent bonding. Finally, as expected, increases in the glass network former oxide concentrations lead to a decreasing trend in the PCT releases.

SECTION 5
MODELS RELATING VHT ALTERATION DEPTH TO LAW GLASS COMPOSITION

This section documents the development and validation of property-composition models and corresponding uncertainty expressions for predicting the alteration depth for Low Activity Waste (LAW) glasses when subjected to the vapor hydration test (VHT). The property-composition models and corresponding uncertainty expressions for VHT alteration depth presented in this section were developed and validated using glass composition and VHT data collected on simulated LAW glasses.

The simulated LAW glasses used for VHT model development and validation are discussed briefly in Section 5.1, but are addressed in further detail in Section 2. Section 5.2 presents the model forms for VHT modeling that were investigated. Sections 5.3 and 5.4 summarize the results for the selected linear and quadratic VHT model forms, respectively. Section 5.5 summarizes the recommended VHT models and provides suggestions for future VHT modeling. Section 5.6 illustrates the calculation of VHT alteration depth predictions and the uncertainties in those predictions using the recommended VHT models and corresponding uncertainty equations. Section 5.7 discusses other modeling techniques that were investigated during this phase of VHT model development. Appendix C discusses the statistical methods and summary statistics used to develop, evaluate, and validate the several VHT model forms investigated, as well as statistical equations for quantifying the uncertainties in VHT alteration depth models.

5.1 VHT Alteration Depth Data Used for Model Development and Validation

The data used for developing VHT alteration depth models are discussed in Section 5.1.1. The two approaches and data used for validating the models are discussed in Sections 5.1.2 and 5.1.3.

5.1.1 VHT Alteration Depth Model Development Data

As described in Section 2, data for 77 ILAW glasses were available for the development of property-composition models for PCT and VHT. The compositions for these 77 glasses are referred to collectively as the Combined Matrix. The Combined Matrix is comprised of the Existing Matrix (21 glasses) and the Test Matrix (56 glasses). Section 2.1 describes the Test Matrix and Section 2.2 describes the Existing Matrix glasses. The Test Matrix glasses were selected from outer-, middle-, and inner-layer glass composition regions so as to optimally augment the 21 Existing Matrix glasses using statistical optimal experimental design methods and software. The LAW glass composition region defined by the outer-layer constraints for the Test Matrix is larger than the glass composition region corresponding to the Existing Matrix. It is larger because the ranges of some components were widened in anticipation of future waste composition and recycle assumption changes, potential new glass composition ranges, and

potential variations in concentrations of specific glass components during production due to process variability. Additional details of the Phase 1 ILAW modeling data are given in Section 4.

Table 5.1 lists the normalized glass compositions from the 21 Existing Matrix and the 56 Test Matrix glasses in the forms used for VHT model development. The Layer column of Table 5.1 indicates the design layer containing each of the Test Matrix glasses. The Existing Matrix glasses are labeled "Existing" in the Layer column of Table 5.1. The glass compositions in Table 5.1 are the normalized weight percents (wt%) of the 14 components varied in the Combined matrix, Al_2O_3, B_2O_3, CaO, Fe_2O_3, K_2O, Li_2O, MgO, Na_2O, SO_3, SiO_2, TiO_2, ZnO, ZrO_2, and Others. The wt% values of the 14 components shown in Table 5.1 were "normalized" so that they sum to 100% for each of the glasses in the Combined Matrix. However, for model development and validation purposes, the compositions were converted to mass fractions so that each composition summed to 1.0 rather than 100%. The mass fractions x_i were calculated using the equation

$$x_i = \frac{W_i}{\sum_{i=1}^{q} W_i}, \tag{5.1}$$

where W_i denotes the wt% of the i^{th} glass oxide or halide component. The number of components varied in the Combined Matrix is $q = 14$. There are two main reasons why normalized mass fractions are used in mixture experiment models. First, the theory of mixture experiment models indicates that properties of a mixture should depend only on the relative proportions of those components that actually affect the property [29]. Second, normalized mass fractions maintain the mixture experiment literature convention of component proportions summing to 1.

For the VHT modeling, the glass compositions used were "target" compositions. In preliminary modeling work [16], VSL investigated using analyzed as well as target values of SO_3, which showed some differences due to volatilization. However, Perez-Cardenas et al. [16] concluded SO_3 did not have a large effect on VHT results, so it was decided to use target SO_3 values in the VHT modeling work summarized in this document. Thus, the SO_3 values listed in Table 5.1 (and subsequently, Table 5.4) are target values. As explained earlier in Section 4.1.1 and also later in Section 6, analyzed rather than target values of SO_3 were used for PCT modeling. Table 5.1 identifies several pairs of replicate glasses contained in the Combined Matrix. These replicates allow for assessing model lack-of-fit during model development.

Table 5.2 contains VHT alteration depths (in microns) for the 77 glasses of the Combined Matrix. Table 5.2 also includes a column designating the data-splitting validation subsets for VHT modeling. These subsets and the data-splitting validation approach are discussed in Section 5.1.2.

Of the 77 simulated LAW glasses in the Combined Matrix, 7 had alteration depths $D >$ 700 microns, with five of the glasses being completely altered ($D >$ 1100 microns). After considering several model forms based on data sets that included or excluded these seven glasses, it was decided that they would be dropped from the model development. Thus, 70

simulated LAW glasses and their corresponding VHT alteration depth values remained for use in developing VHT models. The glasses dropped were LAWM11, LAWM12, LAWM13, LAWM14, LAWM15, LAWM32, and LAWM55.

Table 5.3 lists the replicate pairs of glasses in the ILAW VHT modeling data set, the corresponding VHT alteration depths, and pairwise as well as two pooled estimates of percent relative standard deviations (%RSDs) based on the replicate pairs. A pooled %RSD combines the separate pairwise %RSDs so that a more accurate, combined estimate of the %RSD is obtained. Two pooled %RSDs are summarized in Table 5.3, one over the five pairs of replicates retained in the VHT modeling data set, and the other over four pairs of replicates remaining in the VHT modeling data set when ignoring one pair that are actually near-replicates. These pooled %RSDs include variations due to fabricating glasses, performing the VHT, and measuring alterations.

The magnitudes of the pooled %RSDs in Table 5.3 are quite large. However, the magnitude is inflated significantly by the results for a single replicate pair (LAWM09 and LAW54R1), which have measured layer thicknesses of 1 and 3 μm, respectively. These thicknesses (which correspond to alteration rates of about 0.3% of the WTP contract limit) are approaching the resolution of the test. Furthermore, the relative error of the layer thickness measurement is larger for small layer thicknesses because of the effects of poor layer definition; i.e., the boundaries of the layer are not sharp and, on a relative basis, this diffuseness is increasingly important for thin layers. If this replicate pair is removed, the pooled %RSD for the five remaining pairs decreases to about 33%; the limited results from a previous study (based on replicates having alteration rates that are significantly greater than those for LAWM09 and LAW54R1) suggest %RSDs that are about the same as this value [30].

5.1.2 Primary Model Validation Approach and Data

The primary model validation approach was based on splitting the 70 Combined Matrix data points remaining for ILAW VHT model development into five modeling/validation partitions. Of the 77 model development glasses, 12 were intended to be replicates (6 replicate pairs). Of the 70 glasses remaining for VHT modeling after dropping the 7 glasses mentioned previously, 10 were intended to be replicates (5 replicate pairs, although one pair were actually near-replicates). These 10 glasses were included in each of the five modeling splits. The remaining 60 glasses were divided to finish forming the five modeling/validation splits as follows.

- The five pairs of ‘replicates’ were set aside so they would always be included in each of the five model development data sets. This was done so that there would always be some replicates in the modeling splits to allow for statistically testing model lack-of-fit (see Appendix C). It was also done so that replicate pairs would not be split between modeling and validation subsets, thus negating the intent to have validation glasses different than model development glasses. Because there were only 4 pairs of true replicates in each of the modeling splits, the lack-of-fit tests for the modeling splits are based on 4 degrees of freedom for pure error.

- The remaining 70 – 10 = 60 data points were ordered from smallest to largest according to their VHT alteration depths. The 60 data points were numbered 1, 2, 3, 4, 5, 1, 2, 3, 4, 5, etc. All of the 1's formed the first model validation set, while all of the remaining points formed the first model development data set. Similarly, all of the 2's, 3's, 4's, and 5's respectively formed the second, third, fourth, and fifth model validation sets. In each case, the remaining non-2's, non-3's, non-4's, and non-5's formed the second, third, fourth, and fifth model development data sets. Accordingly, each of the splits contained 12 glasses for validation and 48 glasses for modeling.

- The 10 'replicate' glasses were added to each of the modeling splits so that each of the five splits contained 58 glasses for modeling and 12 glasses for validation. The last column of Table 5.2 specifies the validation subsets for the five modeling/validation splits for primary validation approach for VHT model development.

Data splitting was chosen as the primary validation approach because other VHT-composition data available for model validation purposes that satisfied all of the constraints defining the ILAW composition region and meeting quality assurance (QA) requirements were very limited, and because statistical comparisons indicated differences exist between the modeling data and separate validation data (discussed in the next section).

5.1.3 Secondary Model Validation Approach and Data

As discussed previously in Section 5.1.2, the validation data were not part of the experimental design for Phase 1 LAW modeling. Because they were collected at different times and locations than the LAW modeling data, some differences exist between the modeling and validation data sets. Therefore, subsets of the validation data were formed that were based on the individual component ranges for the 14 components represented in the modeling data and on the multi-component constraints that helped define the composition region for the LAW modeling design matrix [8]. The compositions for the 59 validation glasses are given in Table 5.4, listed as weight percents summing to 100%. The corresponding VHT alteration depth data are given in Table 5.5.

Compositions of the validation glasses were converted into the same compositional form employed by the Combined Matrix used for VHT model development. That is, the same 14 components were used for the validation data compositions. The components Ag_2O, Cl, Cr_2O_3, Cs_2O, F, MnO, NiO, P_2O_5, PbO, and Re_2O_7 from the validation data (see Table 5.4) were added to form the Others component. Furthermore, the target values of sulfate (SO_3) were used for validation data compositions, and validation compositions were normalized to sum to 1 for computational purposes during software applications. This follows the compositional form used with the ILAW Combined Matrix glasses for VHT model development (see Section 5.1.1).

In the tables and plots generated to describe VHT model validation results, the set consisting of all 59 validation glasses was labeled 'All'. The validation subset V1 contains the 37 validation glasses that satisfy upper and lower limits obtained by extending the outer layer

single-component limits by 10%, for all 14 components. The validation subset V2 contains the 24 validation glasses that satisfy the upper and lower limits of the outer layer for all 14 components of the modeling data (as listed in Table 2.1).

The data splitting approach discussed in Section 5.1.2 is considered the primary validation approach because the Combined Matrix data used by that approach are from the ILAW composition region and satisfy the full QA requirements. The separate validation data set and subsets thereof are used as a secondary validation approach because the validation glasses are not from the ILAW Combined Matrix. In fact, many of the validation glasses do not all fall in the ILAW composition region.

5.2 VHT Alteration Depth Model Forms

Ideally, a property-composition model for VHT would utilize known mechanisms of VHT alteration as a function of glass composition and aspects of the VHT. However, no such mechanisms are known, so that mechanistic and semi-empirical model forms are not available. Hence, several empirical model forms with parameters to be estimated from model development data were considered. These model forms are from the general class of *mixture experiment models*. Section 5.2.1 discusses mixture experiments and the two general forms of mixture experiment models used in this work. Section 5.2.2 discusses the use of transformed VHT alteration depths as the response variable for VHT modeling.

5.2.1 Mixture Experiment Model Forms

Linear mixture (LM) and partial quadratic mixture (PQM) model forms introduced in Section C.1.1 of Appendix C were chosen for use in modeling VHT alteration depths. The specific LM model form is given by

$$\ln(D) = \sum_{i=1}^{q} b_i x_i + \varepsilon \tag{5.2}$$

while the specific PQM model form is given by

$$\ln(D) = \sum_{i=1}^{q} b_i x_i + \text{Selected}\left\{ \sum_{i=1}^{q} b_{ii} x_i^2 + \sum_{i<}^{q-1} \sum_{j}^{q} b_{ij} x_i x_j \right\} + \varepsilon \ , \tag{5.3}$$

In Equations (5.2) and (5.3): $\ln(D)$ denotes the natural logarithm of the VHT alteration depth, D, in microns; the x_i (i = 1, 2, …, q) are proportions of q components such that $\sum_{i=1}^{q} x_i = 1$; the b_i (i = 1, 2, …, q), the b_{ii} (selected), and the b_{ij} (selected) are coefficients to be estimated from data; and ε is a random error for each data point. Many statistical methods exist for the case where the ε are independent (i.e., not correlated) and normally distributed with mean 0 and standard

deviation σ. In Equation (5.3), "Selected" means that only some of the terms in curly brackets are included in the model. The subset is selected using standard stepwise regression or similar methods [31, 32]. PQM models are discussed in more detail and illustrated by Piepel et al. [23].

Cornell [29] discusses many other empirical mixture model forms that could have been considered but were not because of time constraints. However, models of the form in Equations (5.2) and (5.3) are widely used in many application areas (including waste glass property modeling) and have been shown to perform very well.

Use of the natural logarithm transformation of VHT alteration depths will be discussed further in the next section.

5.2.2 Transformation of VHT Alteration Depth

In modeling VHT alteration depths, it is advantageous to transform the alteration depths to the natural logarithm of the alteration depths. The advantages of this transformation include:

- The VHT alteration depths for the 77 glasses of the Combined Matrix range from 1 to 1100 microns. For the 70 Combined Matrix glasses used for VHT modeling, the alteration depths varied from 1 to 420 microns. This is a range of over 2 orders of magnitude difference. In such cases, typically the uncertainty in making glasses, performing the VHT, and measuring the alteration depths leads to smaller absolute uncertainties for smaller alteration depths and larger absolute uncertainties for larger alteration depths. Hence, the unweighted least squares (ULS) regression assumption of equal variances for all response variable values (see Section C.2 of Appendix C) is violated. After a logarithmic transformation, variances of response values tend to be approximately equal as required for ULS regression.

- A logarithmic transformation tends to linearize the compositional dependence of corrosion and leach test data and reduce the need for non-linear terms in the model form.

- A natural logarithm transformation is preferred over a common logarithm (or other base logarithm) transformation because of the approximate relationship

$$\mathrm{SD}\,[\ln(y)] \cong \mathrm{RSD}\,(y) \tag{5.4}$$

  where SD denotes standard deviation, and RSD denotes relative standard deviation (i.e., the standard deviation divided by the mean). The relationship in Equation (5.4) is very useful, in that uncertainties of the natural logarithm of the response variable y can be interpreted as RSDs of the untransformed response variable y.

For these reasons, the natural logarithmic transformation was employed for all VHT release model forms.

5.3 Linear Mixture Model Results for LAW VHT Alteration Depth

This section discusses the results of fitting a LM model using natural logarithms of LAW VHT alteration depths, denoted ln(*D*), as the response variable. The model contained linear terms for each of the 14 components included in the LAW design matrix, as specified in Equation (5.2). Section 5.3.1 presents the results for the LM model fit to the 70 glasses of the modeling data set. Section 5.3.2 presents the validation results for the LM model.

5.3.1 Results for VHT LM Model Fit to Modeling Data

Table 5.6 lists the coefficients and coefficient standard deviations for the LM model terms. Table 5.6 also includes summary statistics that describe how well the LM model fits the modeling data. The $R^2 = 0.6408$, $R^2_A = 0.5574$, and $R^2_P = 0.2982$ values indicate that the LM model offers only marginal performance even when fitted to the modeling data. The root mean squared error (RMSE) value of 0.8741 in Table 5.6 is quite large. Based on Equation (5.4), this value suggests that either: (i) the experimental error in fabricating glasses, performing the VHT, and measuring the alteration layer is quite large at approximately 87 %RSD, and/or (ii) the LM model has a large lack-of-fit. The lack-of-fit (LOF) test p-value = 0.0744 included in Table 5.6 indicates that the LM model could have a statistically significant lack-of-fit. Thus, model lack-of-fit appears to at least partially explain the large differences between measured and predicted VHT alteration depths. The analysis of replicate pairs in Table 5.3 indicates that the inherent uncertainty in fabricating a glass, performing the VHT, and measuring alteration depth is in the range of 39 to 43 %RSD based on the VHT alteration depths in microns. The pooled estimates of standard deviation given in Table 5.3, calculated using the natural logarithms of VHT alteration depths, can also be viewed as approximations of %RSD. Expressed as percentages, these pooled estimates of standard deviation range from 42.28% to 46.34%. Any of these %RSD approximations indicate very large inherent uncertainty, and that it will be difficult to model VHT alteration depths. See Appendix C for further explanations of the statistics and LOF test discussed in this paragraph.

Figures 5.1 through 5.4 provide several regression diagnostic plots for assessing the fit of LM model to the modeling data. Figures 5.1 and 5.2 do not suggest any significant departures from normality for the distribution of standardized residuals[3] from the LM model. Figure 5.3 displays significant scatter about the line of ideal prediction, corresponding to the relatively low R^2 value. Figure 5.4 does not show any significant departure from the assumption of equal uncertainty in ln(*D*) values over the modeling data set. In summary, the ULS regression techniques should be appropriate for the LM model development and evaluation.

[3] Standardized residuals are residuals [measured minus predicted ln(*D*) values], divided by their standard deviations.

5.3.2 Validation Results for the VHT LM Model

Table 5.6 lists the R^2, R^2_A, R^2_P, RMSE, and SSE (sum of squared error) values for each of the five modeling splits as well as the validation R^2 value for each of the five validation splits used in the primary validation approach (data-splitting approach) discussed in Section 5.1.2. The columns in the lower portion of the table are labeled DS# to represent the five data-splitting subsets. The last column presents averages of the modeling $R^2 = 0.7103$, $R^2_A = 0.5996$, $R^2_P = 0.1718$, RMSE = 0.7986, and validation $R^2 = 0.1174$ statistics over the five data-splits. The marginal performance of the LM model fitted to all of the modeling data is reinforced by the model's relatively poor validation performance for the five modeling/validation splits.

Table 5.6 also lists the R^2 values obtained by applying the LM model to the validation data set (denoted All) and two subsets thereof (denoted V1 and V2) according to the secondary validation approach (separate validation data approach) discussed in Section 5.1.3. The validation R^2 for all 59 validation points is 0.2337, which increases to 0.5105 for the V1 validation data set of 37 glasses (some of which have compositions not too far outside the glass composition region of interest), and then decreases to 0.3779 for the V2 validation subset of 24 glasses (which are all within the composition region of interest). The poor R^2 for all validation glasses is explainable by the fact that some glasses are significantly outside the composition region covered by the modeling data set. It is also understandable that the validation performance improves for the V1 subset when attention is restricted to glasses within or not too far outside the composition region of interest. The decrease in validation performance of the LM model from the V1 to the V2 validation subset may be due to the restricted region of variation represented by the V2 compositions.

Figures 5.5 through 5.7 are predicted versus measured plots for the separate validation data and subsets thereof. The line segments in Figures 5.5 through 5.7 are error bars that represent 95% prediction intervals (see Sections C.5 and C.6 of Appendix C for an explanation of prediction intervals) for each of the validation glasses. The diagonal lines in these figures represent perfect agreement between observed and predicted VHT alteration depths. Note that the points in the figures generally follow more horizontal patterns than the diagonal line. This indicates that the LM model represented in these figures tends to overpredict ln(D) for validation glasses with low VHT alteration depths and underpredict ln(D) for validation glasses with high VHT alteration depths.

In summary, the validation performance of the full LM model (i.e., using all 14 components varied in the Combined Matrix) is marginal to poor, most likely owing to the rather large uncertainty inherent in the VHT results, and the lack-of-fit of the LM model.

5.4 Partial Quadratic Mixture Model Results for LAW VHT Alteration Depth

As seen in the previous section, the VHT full LM model in the 14 components offered only marginal performance, and there were indications of model lack-of-fit suggesting that a model containing quadratic terms might perform better. Therefore, PQM models of the general form in Equation (5.3) were considered for LAW VHT modeling. Section 5.4.1 presents the

results for the PQM model fit to the 70 glasses of the modeling data set. Section 5.4.2 presents the validation results for the PQM model.

5.4.1 Results for VHT PQM Model Fit to Modeling Data

Stepwise regression was used to search for quadratic terms (squared and two-component crossproduct terms) that would result in a better fitting model than the LM model discussed in Section 5.3. The stepwise selection was conducted using tight limits (full-versus-reduced model F-test significance levels of 0.05) for terms to enter and remain in the model. There were eight crossproduct terms identified, that when added to the full LM model, resulted in a PQM model with significantly improved fit over the full LM model. The crossproduct terms included in the PQM model were $MgO*TiO_2$, $Al_2O_3*K_2O$, $CaO*Fe_2O_3$, K_2O*ZnO, B_2O_3*CaO, $B_2O_3*SO_3$, MgO*Others, and $CaO*SiO_2$. As with the full LM model, the response variable for the PQM model was the natural logarithm of LAW VHT alteration depth, ln(*D*).

Before discussing the PQM modeling results, we note that due to practical as well as budget considerations, the more comprehensive PQM model development methods discussed in Section 6 (e.g., MAXR and more significance levels for stepwise regression) for the PCT models were not applied during the VHT model development. Additional PQM model development methods could be explored as part of any future VHT model development that might arise. Given the relatively high uncertainty in VHT data, it was judged not worthwhile to return to VHT modeling and invest the additional time and resources at this time.

Table 5.7 lists the fitted model coefficients and coefficient standard deviations for the terms in the PQM model. Table 5.7 also includes the summary statistics obtained by applying the model to the modeling data set. The model fits the 70-point modeling data set with $R^2 = 0.8727$, meaning that 87.27% of the variation in ln(*D*) values is accounted for by the model. $R^2_A = 0.8170$ is somewhat less than R^2, indicating that the model may have a small number of unnecessary terms (possibly linear terms). $R^2_P = 0.7496$ being somewhat less than R^2_A suggests that one or more of the 70 modeling data points are influential. Data points are influential if they impact the calculated values of the regression coefficients more than other points in the modeling data set. That is, the calculated values of regression coefficients can differ significantly depending on whether influential data points (considered individually) are included or excluded when fitting the model. Influential data points in a statistically designed test matrix are usually outliers and are generally considered undesirable in model fitting because their presence in the model fitting data set can lead to calculated model coefficients that are not representative of the majority of the data.

Table 5.7 shows that RMSE = 0.5620. If the model does not have a statistically significant lack-of-fit, RMSE provides an estimate of the experimental error standard deviation in VHT ln(*D*) test results. Because of the natural logarithm transformation of *D*, the RMSE can be interpreted (per Equation (5.4)) as a VHT experimental error of approximately 56 %RSD for alteration depth (*D*) results if there is no model LOF. The RMSE value is somewhat larger than the pooled estimate of standard deviation of 0.4228 (see Table 5.3) obtained using the natural

logarithm of VHT alteration depths for the four pairs of exact replicate VHT results included in the modeling data set. The pooled standard deviation estimate can also be viewed as an approximate %RSD, although the corresponding pooled %RSD estimate from Table 5.3 is not as close to the pooled estimate of standard deviation in ln(*D*) units as would typically be expected. Expressed as %RSDs, these values are 39.02% and 42.28%, respectively (see bottom row of Table 5.3). In any case, such high experimental error in the measured VHT alteration depths indicates the relatively large uncertainty of the VHT testing procedure and results.

Included in Table 5.7 is the p-value from an F-test to assess model lack-of-fit. The p-value is ~0.30, which indicates that the PQM model does not have a statistically significant LOF. The non-significant model LOF result indicates that the prediction errors of the model in Table 5.7 are comparable in magnitude to the differences in ln(*D*) results for replicate VHT tests, as discussed in the previous paragraph.

Figures 5.8 and 5.9, respectively, show a histogram and normal probability plot of the standardized residuals for the fit of the model in Table 5.7 to the 70-point modeling data set. These two plots do not show any significant departure from normality, which is required to utilize statistical interval formulas based on the model.

Figure 5.10 shows a predicted versus measured plot for the fit of the model in Table 5.7 to the 70-point modeling data set. The plotted points in Figure 5.10 show a relatively even scatter about the 45º line corresponding to perfect prediction. Also, the scatter is much smaller for the PQM model than that shown in Figure 5.3 for the full LM model.

Figure 5.11 displays a graph of the standardized residuals plotted versus the data index (a sequential numbering of the modeling data points) with different plotting symbols representing different types of glasses (i.e., existing, outer-layer, middle-layer, inner-layer, and center-point). Typically, few if any standardized residuals beyond ±2.5 or ±3.0 is desirable. Noticeable in Figure 5.11 are the wider spread of standardized residuals for inner-layer glasses, and standardized residuals < -2.5 for the center-point glass replicates. These observations suggest that the model in Table 5.7 may not approximate the true VHT ln(*D*)-composition relationship as well in the interior of the glass composition region of interest.

5.4.2 Validation Results for the VHT PQM Model

Performance statistics for the VHT PQM model when applied to the five modeling/validation splits formed from the modeling data set are given in Table 5.7. The columns in the lower portion of the table are labeled DS# to represent the five data-splitting subsets. The last column presents averages of the modeling R^2, R^2_A, R^2_P, RMSE, SSE, and R^2_V statistics over the five data-splits. The average data-splitting R^2, R^2_A, R^2_P, and RMSE statistics are similar to those statistics calculated from the full modeling data set. The average R^2_V statistic is slightly larger than the average R^2_P statistic for the data-splitting approach. In general, the data-splitting results show that the PQM model in Table 5.7 maintains the level of its predictive performance when applied to validation data within the same composition region as used to develop the model.

Table 5.7 shows the validation R^2 statistics for the VHT PQM model when applied to each of the three separate validation sets: $R^2_{All} = 0.0307$, $R^2_{V1} = 0.5542$, and $R^2_{V2} = 0.3553$. The R^2_{V1} and R^2_{V2} statistics are considerably smaller than the R^2, R^2_A, and R^2_P statistics shown in Table 5.7 for the modeling data. A reason for this outcome is given in the following paragraph.

Figures 5.12 through 5.14 display predicted versus measured plots for the PQM model in Table 5.7 applied to the validation sets. The error bars on the plotted points in Figures 5.12 through 5.14 represent 95% prediction intervals (see Sections C.5 and C.6 of Appendix C). If the error bar for a validation point overlaps the 45º line, that means the predicted and measured ln(*D*) values are within model and measurement uncertainty of each other. However, the 95% prediction intervals are quite wide, because of the relatively large uncertainty in the VHT test results, and hence the predictions made by the PQM model in Table 5.7 are fairly uncertain. Figures 5.13 and 5.14 help to explain why R^2_{V1} and R^2_{V2} statistics are considerably smaller than the R^2, R^2_A, and R^2_P statistics for the modeling data. These figures indicate that this occurs because the model in Table 5.7 tends to overpredict ln(*D*) for the V1 and V2 subsets of the validation data, except possibly for glasses with higher VHT alteration depths. This observation is consistent with the results of statistical comparisons of the modeling and validation data sets that found statistically significant differences in some cases (see Section 5.7.2). The very low $R^2_{All} = 0.0307$ statistic for the full validation data set occurs because of several plotted points being significantly removed from the 45º line (i.e., because of ln(*D*) predictions being significantly different than measured values). Many of these correspond to glasses that are significantly outside the LAW glass composition region corresponding to the modeling data set, and thus involve significant model extrapolation. Generally, significant extrapolation of regression-based models should be avoided.

5.5 Summary of Recommended VHT Models

The LM model in Table 5.6 and the PQM model in Table 5.7 appear to be reasonable VHT-composition models given the relatively high uncertainty in the VHT data available for model development. Despite the high data uncertainty, the LM model has a statistically significant model lack-of-fit. The VHT alteration of LAW glasses clearly depends nonlinearly on LAW glass composition. Thus, the PQM model offers a better fit than the LM model for the modeling data. There are indications that the nonlinear dependence may be more "local" in nature, such that "global" nonlinear terms in a model (e.g., the quadratic terms in the selected PQM model) may be insufficient. Alternately, it may be that the nonlinear dependence involves higher than quadratic effects. The LM model is included as a recommended VHT model because it may outperform the PQM model on other LAW VHT data sets. It is possible that the selection of quadratic terms for the PQM model was influenced by certain glasses included in the modeling data set. These quadratic terms may not be as important in the prediction of VHT alteration depths for other data sets.

If any experimental work is planned in the future to generate additional VHT data, two suggestions are made. First, consideration should be given to obtaining more data for LAW

glasses with moderately high VHT alterations, closer to and somewhat above the 453 micron alteration depth that corresponds to the 50 g/m^2/day limit specified in the WTP contract. Such data are needed to provide for models that can predict whether glasses have VHT alteration above or below the limit. Second, spreading glass compositions more evenly over the composition region of interest would provide good support for more advanced non-parametric modeling approaches that can better capture higher-order and/or local nonlinear composition effects (should such more advanced models be necessary to more accurately predict VHT alteration).

5.6 Example Illustrating Model Predictions and Statistical Intervals

This section contains examples to illustrate the use of the 14-term LM model and 22-term PQM model to obtain predicted VHT alteration depths and corresponding 90% upper confidence intervals (UCIs) and 95% simultaneous upper confidence intervals (SUCIs) as described in Section C.6 of Appendix C. A specific LAW glass composition was selected for use in the examples.

The glass composition used in the examples is that of LAWA126, which is one of the glasses in the ILAW Test Matrix. The composition of LAWA126 for VHT modeling is given in Table 5.1 in normalized weight percent format. The VHT LM model contains only linear terms for each of the components of the ILAW design matrix. Thus, the LAWA126 composition from Table 5.1 need only be converted to normalized mass fractions summing to 1.0 (by dividing by 100) in order to be used in the LM model. Normalized mass fractions from the linear terms are then multiplied to obtain the quadratic components corresponding to the quadratic terms of the PQM model. Table 5.8 contains the composition for LAWA126 prepared for use in the two ILAW VHT models.

For each of the VHT models, predicted ln(VHT alteration depths) are obtained by multiplying the composition in the format needed for the specific models by the coefficients for the models (see Tables 5.6 and 5.7), then summing the results. That is, the predicted values are calculated by

$$\hat{y}(\boldsymbol{a}) = \boldsymbol{a}^T\boldsymbol{b}$$

where $\boldsymbol{a}$ is the composition of LAWA126 formatted to match the terms in a given model (from Table 5.8), T represents a matrix transpose (or vector transpose in this case), and $\boldsymbol{b}$ is the vector of model coefficients for a given model. The predicted ln(VHT alteration depth) values from each of the ILAW VHT models are listed in the second column of Table 5.9. The predicted ln(VHT alteration depths) in ln(micron) units are easily converted to the usual VHT alteration depths in microns by exponentiation. The third column of Table 5.9 contains the predicted VHT alteration depths in microns. However, as discussed in Section C.6 of Appendix C, these back-transformed VHT alteration depth predictions in microns should be considered estimates of the true median of the distribution of alteration depths that would result if the VHT were repeated multiple times using coupons of the LAWA126 glass, not estimates of the true mean.

Equation (C.13) can be used to calculate a 90% UCI for the true mean of ln(VHT alteration depths) from the LAWA126 glass composition for each of the ILAW VHT models. In the notation of Equation (C.13):

- $100(1-\alpha)\% = 90\%$, so that $\alpha = 0.10$.
- The vector $\boldsymbol{a}$ is the composition of LAWA126 formatted to match the terms in a given model.
- The matrix $\boldsymbol{A}$ is the design matrix of normalized linear components and selected quadratic components derived from the linear components (in the case of the PQM model) formatted to match the terms in a given model.

To obtain an 90% UCI in ln(VHT alteration depth) units of ln(microns), the quantity $t_{1-\alpha,n-p} RMSE \sqrt{\boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{a}}$ is added to the predicted VHT alteration depth $\hat{y}(\boldsymbol{a})$ described above, as indicated by Equation (C.13). The $MSE[\boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{a}]$ portion of this expression is the variance-covariance matrix for the estimated model coefficients, as discussed near the end of Section C.6 of Appendix C. The variance-covariance matrices for the VHT models are listed in Appendix D. The quantity *MSE* is the mean squared error from regression, *RMSE* is the square root of *MSE*.

The 90% UCI values for the true mean ln(VHT alteration depth) in units of ln(microns) for the LAWA126 composition based on the ILAW VHT models are given in the fourth column of Table 5.9. Exponentiating the resulting 90% UCIs for the mean in ln(micron) units yields 90% UCIs for the median in microns. For example, the 14-term LM model for VHT has 2.4845 ln(microns) as the upper limit of the 90% UCI on the true mean ln(VHT alteration depth) for LAWA126, whereas $e^{2.4845} = 11.9952$ microns is the upper limit of the 90% UCI on the true median VHT alteration depth. The fifth column of Table 5.9 contains 90% UCIs for the true median VHT alteration depth from the LAWA126 glass composition based on the ILAW VHT models. Note that the 90% UCI values of 2.4845 and 2.8532 microns for the ILAW VHT models are more than two orders of magnitude below the VHT alteration depth limit of ≈ 453 microns for 24-day VHT and a glass density of 2.65 g/cm^3.

As discussed in Appendix C, there are times when a SUCI may be preferred rather than an UCI. This is particularly true when the regression model (composition-property model) is to be used a large number of times for various glass compositions from a specified composition region. Equation (C.15) can be used, in much the same way as how Equation (C.13) is used to obtain UCIs, to calculate a 95% SUCI for the true mean of ln(VHT alteration depth) for glasses having a specified composition. The 95% SUCI values for the true mean ln(VHT alteration depth) in units of ln(microns) for the LAWA126 composition based on the ILAW VHT models are given in the fifth column of Table 5.9. Exponentiating the resulting 95% SUCIs for the mean in ln(micron) units yields 95% SUCIs for the median in microns. The sixth column of Table 5.9 contains 95% SUCIs for the true median VHT alteration depth from the LAWA126 glass composition based on the ILAW VHT models. Note that the 95% SUCI values of 36.9156 and

56.3761 microns for the ILAW VHT models are nearly an order of magnitude below the VHT alteration depth limit of ≈ 453 microns for 24-day VHT and a glass density of 2.65 g/cm^3.

5.7 Other Model Development Techniques Considered

Because the VHT LM and PQM models had inadequacies when applied to the validation data, and the LM model was less than adequate even for the modeling data, other models and modeling approaches were investigated during this phase of VHT model development. Unfortunately, none of these investigations led to models that performed any better than the LM and PQM models described in Sections 5.3 and 5.4. However, the investigations are briefly summarized for documentation purposes.

Section 5.7.1 discusses reduced LM and PQM models that were considered. Section 5.7.2 discusses attempts to develop VHT models using the ILAW Test Matrix glasses and the separate validation glasses combined as a modeling data set. Section 5.7.3 discusses the use of classification trees and regression trees for VHT modeling.

5.7.1 Reduced LM and PQM Models for VHT Modeling

This section describes investigations to reduce the number of glass components appearing in the LM model, and develop PQM models using the reduced LM model as a starting point.

Reduced Linear Mixture Model

Models containing unnecessary terms often suffer from inflated prediction variance. For this reason, model reduction methods can lead to improved models. Two model reduction methods appropriate for LM models were used to reduce the full LM model (that is, omit terms that do not significantly contribute to the model's predictive ability). The first method was the Component Slope Linear Mixture (CSLM) model approach [33]. The second model reduction method was a sequential full-versus-reduced model F-test approach (see Section C.4.1 of Appendix C). Each of these methods has various options available when conducting model reduction. Use of different options can lead to different reduced model forms. However, the reduced LM model obtained using the F-test approach where non-significant components were always normalized out, and with a stopping limit of 0.10 resulted in the same reduced model obtained using the CSLM reduction approach where non-significant terms were always normalized out and the reference composition was either the center glass or the centroid composition. This reduced LM model contains linear terms for the components Al_2O_3, B_2O_3, CaO, Fe_2O_3, Li_2O, Na_2O, SiO_2, ZrO_2, and Others. The reduced LM model offered similar performance as the full LM model. Because the reduced LM model did not show clear improvement over the 14-term full LM model given in Table 5.6 and discussed in Section 5.3, it was decided that all 14 components should be retained for the recommended LM model for

VHT. However, model reduction methods may be worth exploring as part of any future VHT modeling work that might arise.

Reduced Linear Mixture Model with Selected Quadratic Terms

The reduced LM model discussed above was also augmented with selected quadratic terms to form a reduced PQM model. Quadratic terms available for selection were all squared and two-component crossproduct terms involving the 9 linear terms contained in the reduced linear model. The reduced PQM model performed better than the reduced LM model, but it did not perform as well as the full PQM model given in Table 5.7 and discussed in Section 5.4. As with the selection of quadratic terms to augment the full LM model, the stepwise selection routine in PROC REG of SAS [34] was used to select the quadratic terms to augment the linear terms of the reduced model. With 0.05 as the stepwise significance level for entry into the model and to stay in the model, only three quadratic terms were selected to include in the reduced PQM model: Al_2O_3*B_2O_3, Na_2O*ZrO_2, and CaO*SiO_2.

5.7.2 VHT Models Based on Combining LAW Test Matrix and Validation Glass Data

This section describes a statistical comparison of the modeling and validation data sets, as well as work using the combined modeling and validation data sets as a model development data set.

Comparing Modeling and Validation Data Sets

Prior to investigating VHT model development based on the combined modeling and validation data sets, the two data sets were compared to determine if combining them would be appropriate. Several methods were used to assess the appropriateness of combining the two data sets. These methods included: (1) the addition of a single model term to the full LM model that was an indicator for whether glasses came from the modeling or validation data sets, (2) the addition of a separate indicator term for each linear term in the full LM model, and (3) forming regression tree models that included a single indicator term.

The first approach used the model form given in Equation (C.6) in Appendix C, with B = 0 for the modeling data and B = 1 for the validation data. The results indicated that marginally significant differences may exist between the modeling and validation data sets, because the p-value on the indicator term was 0.13067.

The second approach used the model form given in Equation (C.7) in Appendix C, again with B = 0 for the modeling data and B = 1 for the validation data. The results of this approach indicated that the influence of some components differed significantly between the modeling and validation data sets. Component plots indicate that differences in the influence of certain components could be due in part to differences in the ranges of those components over the modeling versus validation glasses.

The third approach, binary regression tree models, attempts to build models by performing successive binary splits of predictor variables. The indicator variable (B = 0 for modeling data and B = 1 for validation data) was a candidate for splitting as were the 14 oxide glass components. This approach did not indicate that significant differences exist between the modeling and validation data sets because the algorithm did not split on the indicator term. However, the relatively small data set available is not conducive to this approach given the larger number of predictor variables, so its failure to identify a difference between modeling and validation data sets may be more a function of the approach rather than an actual lack of difference.

Combining Data Sets for Model Development

Some attempts were made to generate a VHT model using the modeling (ILAW Combined Matrix) and validation data sets combined. This was done with caution because of the indications that differences may exist between the modeling and validation data sets, and such indications generally imply that such data sets should not be combined. Use of the full 77-glass LAW Combined Matrix as well as the subset of 70 glasses used to develop the LM and PQM models from Section 5.3 and 5.4, respectively, were considered for inclusion with the validation glasses.

Also, because the V2 validation subset contains compositions more like the ILAW Test Matrix glasses, model development was investigated using the modeling (LAW Combined Matrix) and V2 data sets combined. None of the combinations of modeling and validation glasses led to better fitting models than those presented in Sections 5.3 and 5.4. This outcome would be expected if indeed there are differences between the modeling and validation data sets.

5.7.3 Classification and Regression Tree Models

Classification tree and/or regression tree models can often perform better than parametric models when the response takes on more “localized” patterns. As mentioned in Section 5.5, there were indications that the VHT alteration depths may exhibit such behavior, where the response can change dramatically in certain small regions of the composition space. For this reason, classification and regression tree methods were considered during this phase of VHT model development.

Classification Trees

This approach involves modeling a binary response based on recursive partitioning (using binary splits) on the components of the composition space. The binary response was obtained by dividing the VHT alteration depths into two groups, those falling below a specified alteration level, and those above that level. Various VHT alteration depths were considered for forming the binary response. For example, 200, 100, 50, 25, 20, 15, and 10 microns were all considered for the binary cutoff point. Other considerations to make under the classification tree approach include ‘tree growing’ strategies. Certain parameter inputs are used by the software to determine

how extensive the tree branching system becomes, and whether or not the tree is to be pruned. For this initial classification tree modeling attempt, tree pruning was not conducted. However, one tree growing parameter was employed in the R script [35] used to generate the classification tree models. This parameter specifies the minimum number of points that must be allocated to a particular node in order for that node to be split further. Higher values for this parameter work to prevent tree growing, while setting this parameter to 2 implements no constraints, and allows unrestricted tree growth. Three settings were considered for this parameter, 2, 3, and 5.

The statistical measure used to assess the quality of the classification model fit was the miss-classification rate. Miss-classification rates were calculated for the modeling and validation data sets. Similar to the parametric models (LM and PQM models) discussed previously, the classification tree models performed quite well on the modeling data set, but showed obvious problems when applied to the validation data. Additionally, use of a classification tree model would most likely have the classification cut-off set at the VHT regulatory limit of approximately 400 microns. Of the 70 glasses used for this phase of VHT modeling, only one glass had a VHT alteration depth above 400 microns. This does not provide adequate support to develop reliable classification tree models based on a classification cut-off at 400 microns. Further pursuit of VHT classification tree models would require additional LAW VHT data where more glasses have VHT alterations above 400 microns. However, there is still the issue of poor classification tree model performance for the validation data. Regression tree models do not require a classification cut-off and were therefore considered for VHT modeling.

Regression Trees

Regression trees are similar to classification trees in that they involve recursive partitioning of the components in the composition space, but the response is continuous. In this case, the response was the natural logarithm of VHT alteration depth, ln(D), just like the response for the usual regression models discussed in Sections 5.3 and 5.4. Because the response is continuous, predicted values from the regression tree model are also continuous. Thus, an R^2 value can be calculated to assess model fit for both the modeling and validation data sets. Because the response is not binary, no binary cutoff point is needed for the regression tree algorithm. Like the classification tree algorithm, the regression tree algorithm does allow the specification of the minimum number of points that must exist at a particular node in order for the algorithm to attempt further splits at that node. The same minimum node sizes were considered for the regression tree approach as for the classification tree approach, 2, 3, and 5. Additionally, 10 was used as a minimum node size value for the regression tree approach. Furthermore, some tree pruning was investigated with the regression tree approach. The regression tree algorithm in R requires that a complexity parameter be specified. The complexity parameter controls the extent of tree pruning. Several values were considered for the complexity parameter, 0.02, 0.05, and 0.10. Larger values for the complexity parameter generally lead to more tree pruning, while setting the complexity parameter to zero results in no tree pruning.

The regression tree results were much like the classification tree results. The R^2 values from the regression tree approach were very promising when regression tree models were applied to the modeling (ILAW Combined Matrix) glasses. However, the R^2 values were far from adequate when the regression tree models were applied to the validation data. The R^2

values for the modeling data set do indicate that the regression tree approach could hold some potential for future VHT modeling work. It is possible that the validation glasses are significantly different from the intended glasses of the LAW composition region, and model performance for the validation glasses is actually misleading.

The regression tree approach was also used with the response being residuals that resulted from an initial least squares regression fit of a LM model. That is, an ordinary least squares regression for a LM model was conducted using the compositions and natural logarithms of VHT alteration depths from the modeling data set. The residuals from this regression were then used to serve as the response for the regression tree model development. The idea behind this approach was to fit the main linear effects of the glass components with a LM model, and then use a regression tree to capture nonlinear blending effects of the components in a different way than occurs with PQM models. This approach yielded slightly better results than the regression tree models based on the natural logarithms of VHT alteration depths as the response variable. However, the results were still no better than those for the recommended LM and PQM models presented in Section 5.3 and 5.4. Therefore, regression tree modeling was not pursued further at this time, but may be an effective modeling approach for any future VHT modeling.

SECTION 6
MODELS RELATING PCT BORON AND SODIUM RELEASES TO LAW GLASS COMPOSITION

This section documents the development and validation of property-composition models and corresponding uncertainty expressions for predicting the PCT-Boron and PCT-Sodium releases from Low -Activity Waste (LAW) glasses. Specification 2.2.2.17.2 in the WTP Contract [20] sets a 2 g/m^2 limit on PCT releases of boron, sodium, and silicon from LAW glasses. However, as discussed in Section 4.2, PCT-Silicon releases were less than PCT-Boron and PCT-Sodium releases for all of the simulated LAW glasses to be used for developing models. Because PCT-Boron and PCT-Sodium releases dominate PCT-Silicon releases, it was agreed with the WTP Project that only PCT-Boron and PCT-Sodium releases need be modeled. The property-composition models and corresponding uncertainty expressions for PCT-Boron and PCT-Sodium releases presented in this section were developed and validated using composition and PCT release data collected on simulated LAW glasses.

The simulated LAW glasses used for PCT model development and validation are discussed in Section 6.1, and in further detail in Sections 2.1 and 2.2. Section 6.2 presents the model forms for PCT-Boron and PCT-Sodium releases that were investigated. Sections 6.3 and 6.4 summarize the results for the selected PCT-Boron and PCT-Sodium model forms, respectively. Using the recommended PCT models and corresponding uncertainty equations for each of PCT-Boron and PCT-Sodium, Section 6.5 illustrates the calculation of PCT release predictions and the uncertainties in those predictions. Section 6.6 briefly discusses the consequences of lack-of-fit and prediction uncertainties in the recommended PCT-Boron and PCT-Sodium models. Appendix C discusses the statistical methods and summary statistics used to develop, evaluate, and validate the several model forms investigated, as well as statistical equations for quantifying the uncertainties in PCT release predictions made with the selected models.

6.1 PCT Release Data Used for Model Development and Validation

The data used for developing PCT-Boron and PCT-Sodium release models are discussed in Section 6.1.1. The two approaches and data used for validating the models are discussed in Sections 6.1.2 and 6.1.3.

6.1.1 PCT Release Model Development Data

The data available for developing property-composition models for PCT-Boron and PCT-Sodium releases consist of composition and PCT release data from two matrices of simulated LAW glasses. The two matrices were developed using information about Hanford LAW compositions, previous WTP glass formulation work, glass science knowledge and experience, and statistical experimental design methods. The first matrix, referred to as the *Existing Matrix*, consists of 21 LAW glass compositions from previous work that were within (or close to) the composition region of interest (see Section 2.2). The second matrix, referred to as the *Test Matrix*, consists of 56 simulated LAW glasses selected by statistical experimental design methods to optimally augment the Existing Matrix. Both matrices together are referred to as the *Combined Matrix* for Phase 1 LAW model development [8]. The glasses of the Combined Matrix were used for both ILAW VHT and ILAW PCT model development. Details of the Phase 1 ILAW modeling data are given in Section 4.2.

Table 6.1 lists the normalized glass compositions for the 21 Existing Matrix glasses and the 56 Test Matrix glasses in the forms used for PCT model development. The Layer column of Table 6.1 indicates the design layer containing each of the Test Matrix glasses. The Existing Matrix glasses are labeled "Existing" in the Layer column of Table 6.1. The glass compositions in Table 6.1 are the normalized weight percents (wt%) of the 14 components varied in each of the design matrices. These are the same 14 components involved in VHT model development, Al_2O_3, B_2O_3, CaO, Fe_2O_3, K_2O, Li_2O, MgO, Na_2O, SO_3, SiO_2, TiO_2, ZnO, ZrO_2, and Others. The wt% values of the 14 components shown in Table 6.1were "normalized" so that they sum to 100% for each of the glasses in the Combined Matrix. However, for model development and validation purposes, the compositions were converted to mass fractions so that each composition summed to 1.0 rather than 100%.

For the PCT modeling, the analyzed values of SO_3 obtained by XRF (labeled SO_3.XRF in Tables 6.1 and 6.3) were used rather than the target values. The analyzed SO_3.XRF values are less than the target SO_3 values to varying degrees because SO_3 can be partially volatilized during glass melting. The decision to use analyzed SO_3 values and normalize the compositions was different than the decision for the LAW VHT modeling (Section 5), which used target values of all components including SO_3. Thus, the normalized ILAW compositions used for the PCT modeling are slightly different than the unnormalized ILAW compositions used for the VHT modeling.

As discussed previously in Sections 4.1.1 and 5.1.1, the decision to use target SO_3 values for VHT models was based on the idea that during operation of the WTP LAW vitrification facility, the estimated glass compositions to be used in the models will be obtained from process samples and measurements prior to the melter. Such estimates of glass composition would not reflect partial volatility of SO_3. So, at the time the VHT modeling was done, it was decided to use glass compositions based on target SO_3 values, which would be more representative of estimated glass compositions during production of WTP LAW glasses. However, when it subsequently came time to do the PCT modeling, the WTP Project position on this issue had changed. It was decided that models should be based on property-composition data having the most accurate glass compositions possible. This meant using simulated LAW glass compositions

based on analyzed rather than target SO_3 values. It was decided that during production of WTP LAW glass, SO_3 volatility factors could be applied in calculating the estimated glass composition from process samples and measurements. For the purposes of this ILAW property-composition modeling work, it was decided not to redo the VHT models using the renormalized glass compositions based on analyzed SO_3.XRF values. However, future modeling work will consistently use such glass compositions for property-composition model development.

The changes to the LAW glass compositions caused by the renormalization associated with the use of SO_3.XRF resulted in replicates not being equal in composition. This resulted in the inability to conduct the usual statistical tests for model lack-of-fit using routines available in many statistical software packages. Instead, customized lack-of-fit tests were conducted based on near-replicate pairs, the pairs of glasses that were intended to be replicates.

Table 6.2 contains columns of non-normalized (given in ppm units) and normalized (given in g/L units) versions of the as-measured PCT-Boron and PCT-Sodium releases for the 77 glasses of the Combined Matrix. The normalized releases were calculated as described previously in Section 4.2. Table 6.2 also includes columns for PCT-Silicon data. However, a PCT-Silicon model was not needed as discussed in the opening remarks of Section 6, so these columns were not used in the model development effort.

Of the 77 simulated LAW glasses in the Combined Matrix, some had PCT releases (for boron, sodium, or both) that exceeded the limit of 4 g/L [equivalent to 2 g/m^2, as required by Specification 2.2.2.17.2 in the WTP Contract]. It is desirable to have some glasses in the modeling data set that have PCT releases at or slightly above the limit. This allows for more confident use of the model in discerning between acceptable and unacceptable glasses. However, glass formulations that have PCT releases far beyond the limit are not desirable for model development, because including such glasses could adversely affect model performance for the majority of the glasses. For this reason, dropping certain glasses from the modeling data set was investigated. The number of glasses to be dropped was determined based on the performance of the models considered during model development. The results of this investigation are summarized in Table 6.3. As a result of this investigation, it was decided that 8 glasses would be deleted from the modeling data set, thus leaving 69 of the 77 Combined Matrix glasses for model development. The glasses dropped were LAWM12, LAWM13, LAWM17, LAWM33R1, LAWM34, LAWM35, LAWM55, and LAWM56. The 69 glasses remaining for model development had PCT-Boron and PCT-Sodium releases less than the limit of 4 g/L. As mentioned above, it would have been desirable to have some glasses in the modeling data set that had PCT release at or slightly above the limit. However, dropping fewer glasses in order to retain some glasses having PCT releases at or above the limit resulted in noticeably poorer model performance for the validation data, as shown in Table 6.3.

Table 6.4 lists the replicate pairs of glasses in the ILAW PCT modeling data set, the corresponding PCT-Boron and PCT-Sodium normalized releases, and pairwise as well as two pooled estimates of percent relative standard deviations (%RSDs) based on the replicate pairs. A pooled %RSD combines the separate pairwise %RSDs so that a more accurate, combined estimate of the %RSD is obtained. Two pooled %RSDs are summarized in Table 6.4, one over all six pairs of replicates, and the other over the four pairs of replicates remaining in the PCT

modeling data set. These pooled %RSDs include variations due to fabricating glasses, performing the PCT, and chemically analyzing leachates.

The magnitudes of the pooled %RSDs in Table 6.4 are roughly twice the approximately 10 %RSD values for PCT-Boron and PCT-Sodium reported in Table F.5 of Hrma et al. [36]. The results from that Table F.5 were based on replicate pairs of the same glasses fabricated and tested several times over several years. Hence, the approximately 10% RSD values for PCT-Boron and PCT-Sodium reported by Hrma et al. [36] include an additional source of variation not included in the replicate data of Table 6.4. This suggests that the PCT-Boron and PCT-Sodium data for the ILAW Combined Matrix in Table 6.3 were subject to more experimental, testing, and measurement uncertainty than in this previous glass composition variation study.

6.1.2 Primary Model Validation Approach and Data

As with the VHT modeling, the primary model validation approach for PCT modeling was based on splitting the Combined Matrix data points remaining for model development into five modeling/validation partitions. The data-splitting for PCT modeling was conducted much like that for the VHT modeling (see Section 5.1.2). However, the number of glasses used for PCT model development was 69 rather than 70, so the modeling/validation splits were different. Of the 77 model development glasses, 12 were intended to be replicates (6 replicate pairs). Of the 69 glasses remaining for PCT modeling after dropping the 8 glasses mentioned previously, 8 were intended to be replicates (4 replicate pairs, or actually 'near-replicate' pairs due to the renormalization associated with the use of analyzed SO_3 values). These 8 glasses were included in each of the five modeling splits. The remaining 61 glasses were divided to finish forming the five modeling/validation splits as follows.

- The 4 pairs of 'replicates' were set aside so they would always be included in each of the five model development data sets. This was done so that there would always be 4 degrees of freedom for "pure error" in the model development data set for statistically testing model lack-of-fit (see Appendix C). It was also done so that replicate pairs would not be split between modeling and validation subsets, thus negating the intent to have validation glasses different than model development glasses.

- The remaining 69 – 8 = 61 data points were ordered from smallest to largest according to their values of normalized PCT-Boron or PCT-Sodium release (g/L). The 61 data points were numbered 1, 2, 3, 4, 5, 1, 2, 3, 4, 5, etc. All of the 1's formed the first model validation set, while all of the remaining points formed the first model development data set. Similarly, all of the 2's, 3's, 4's, and 5's respectively formed the second, third, fourth, and fifth model validation sets. In each case, the remaining non-2's, non-3's, non-4's, and non-5's formed the second, third, fourth, and fifth model development data sets. Accordingly, four of these splits contained 12 glasses for validation and 49 glasses for modeling, and one of the splits contained 13 glasses for validation and 48 glasses for modeling.

- The 8 'replicate' glasses were added to each of the modeling splits yielding 4 splits with 57 glasses for modeling and 12 glasses for validation, and one split with 56 glasses for modeling and 13 glasses for validation. The last two columns of Table 6.2 specify the validation subsets for the five modeling/validation splits for primary validation approach for both PCT-Boron and PCT-Sodium model development.

Data splitting was chosen as the primary validation approach because other PCT-composition data available for model validation purposes that satisfied all of the constraints defining the ILAW composition region and meeting quality assurance (QA) requirements were very limited.

6.1.3 Secondary Model Validation Approach and Data

The same 59 validation glasses described in Section 5.1.3 were available for PCT model validation. Again, use of these glasses was considered a secondary model validation approach because the 59 glasses were not part of the ILAW experimental design work discussed by Cooley et al. [8].

The compositions for the 59 validation glasses are given in Table 6.5, listed as weight percents summing to 100%. The corresponding PCT release data (unnormalized and normalized) are given in Table 6.6. Note that the validation compositions listed in Table 6.5 were converted into the same compositional form employed by the Combined Matrix used for PCT model development. That is, the same 14 components were used from the validation data compositions. Furthermore, as with the PCT model development data, the analyzed values of sulfate (SO_3.XRF) were used for PCT model validation data compositions. Finally, the components Ag_2O, Cl, Cr_2O_3, Cs_2O, F, MnO, NiO, P_2O_5, PbO, and Re_2O_7 from the validation data (Table 6.5) were added to form the Others component. Validation compositions were normalized to sum to 1 for computational purposes during software applications.

As with the VHT model validation work, different subsets of the validation data were formed to investigate PCT model performance on validation data that fall inside or are "close" to the ILAW glass composition region discussed in Section 2. In the tables and plots generated to describe PCT model validation results, the set consisting of all 59 validation glasses was labeled 'All'. A "trimmed" validation data set was formed by dropping three specific validation glasses, leaving 56 glasses. The three glasses were dropped because they were clear outliers in one of the components. These three glasses were: (1) LAWA33, which was an outlier in Al_2O_3, (2) LAWC25, which was an outlier in K_2O (including LAWC25 more than doubles the K_2O range for the validation glasses), and (3) LAWB67, which was an outlier in Others (including LAWB67 nearly triples the range of Others for the validation glasses). This trimmed validation subset was labeled V1. Another subset contains those validation glasses (40 glasses) that satisfy upper and lower limits obtained by extending the outer-layer single-component limits by 10%, for all 14 components. This validation subset was labeled V2. A third subset contains those validation glasses (26 glasses) that satisfy the upper and lower limits of the outer layer for all 14 components of the composition region for the modeling data. This validation subset was labeled V3. The PCT validation subsets V2 and V3 are defined the same way as the VHT validation subsets V1 and V2, respectively, were formed. However, the number of validation glasses in

these subsets differ for PCT versus VHT validation because of the slight compositional differences that result from normalizing compositions based on analyzed SO_3.XRF (PCT modeling) versus target SO_3 values (VHT modeling). Finally, a subset was formed that contains those validation glasses (22 glasses) that satisfy the single-component constraints for all 14 components as well as the nine multi-component constraints that were used to define the glass composition region represented by the Test Matrix (see Table 3.1). This validation subset was labeled V4.

The data-splitting approach discussed in Section 6.1.2 is considered the primary validation approach because the Combined Matrix data used by that approach are from the ILAW composition region and satisfy the full QA requirements. The separate validation data set and subsets thereof are used as a secondary validation approach because the validation glasses are not from the ILAW Combined Matrix. In fact, many of the validation glasses do not all fall in the ILAW glass composition region.

6.2 PCT Release Model Forms

Ideally, a property-composition model for PCT would utilize known mechanisms of PCT release as a function of glass composition and aspects of the PCT. However, no such mechanisms are known, so that mechanistic and semi-empirical model forms are not available. Hence, several empirical model forms with parameters to be estimated from model development data were considered. These model forms are from the general class of *mixture experiment models* [29]. Section 6.2.1 discusses mixture experiments and the two general forms of mixture experiment models used in this work. Section 6.2.2 discusses the choice between modeling unnormalized and normalized PCT releases and transformations thereof.

6.2.1 Mixture Experiment Model Forms

Linear mixture (LM) and partial quadratic mixture (PQM) model forms introduced in Section C.1.1 of Appendix C were chosen for use in modeling PCT-Boron and PCT-Sodium releases, as they were for use in modeling the VHT response. For modeling PCT-Boron and PCT-Sodium, the specific LM model form is given by

$$ln(r_B) \text{ or } ln(r_{Na}) = \sum_{i=1}^{q} b_i x_i + \varepsilon \tag{6.1}$$

while the specific PQM model form is given by

$$ln(r_B) \text{ or } ln(r_B) = \sum_{i=1}^{q} b_i x_i + \text{Selected}\left\{ \sum_{i=1}^{q} b_{ii} x_i^2 + \sum_{i<j}^{q-1} \sum^{q} b_{ij} x_i x_j \right\} + \varepsilon \ . \tag{6.2}$$

In Equations (6.1) and (6.2): $\ln(r_B)$ denotes the natural logarithm of the normalized PCT-Boron release (in g/L); $\ln(r_{Na})$ denotes the natural logarithm of the normalized PCT-Sodium release (in

g/L); the x_i (i = 1, 2, …, q) are normalized mass fractions of q glass oxide or halide components such that $\sum_{i=1}^{q} x_i = 1$; the b_i (i = 1, 2, …, q), the b_{ii} (selected), and the b_{ij} (selected) are coefficients to be estimated from data; and ε is a random error for each data point. Many statistical methods exist for the case where the ε are independent (i.e., not correlated) and normally distributed with mean 0 and standard deviation σ. In Equation (6.2), "Selected" means that only some of the terms in curly brackets are included in the model. The subset is selected using standard stepwise regression or related methods [31, 32]. PQM models are discussed in more detail and illustrated by Piepel et al. [23].

Normalization and the natural log transformation of the PCT release values are discussed further in the next section.

6.2.2 Normalization and Transformation of PCT Release Values

A transformation to "normalized" concentrations is widely employed in the data analysis and modeling of leaching data [36, 37]. The normalized PCT-Boron releases (r_B) were calculated according to the formula

$$r_B\ (\text{g/L}) = \frac{c_B\ (\text{mg/L})}{[1000\ (\text{mg/g})]\left[w_{B_2O_3}\ (\text{g } B_2O_3/\text{g glass})\right][0.3106(\text{g B/g } B_2O_3)]} \tag{6.3}$$

where c_B is the non-normalized boron release (concentration) from the 7-day PCT, and w_{B2O3} is the unnormalized mass fraction of B_2O_3 in the glass. This is calculated as

$$w_{B2O3} = W_{B2O3}/100, \tag{6.4}$$

where W_{B2O3} is the wt% of B_2O_3 in the glass. Similarly, normalized PCT-Sodium releases (r_{Na}) were calculated according to the formula

$$r_{Na}\ (\text{g/L}) = \frac{c_{Na}\ (\text{mg/L})}{[1000\ (\text{mg/g})]\left[w_{Na_2O}\ (\text{g } Na_2O/\text{g glass})\right][0.7419\ (\text{g Na/g } Na_2O)]}. \tag{6.5}$$

As seen in Equations (6.3) and (6.5), normalizing involves dividing the measured leachate concentration for a given element by the corresponding mass fraction of that element in the glass. Mechanistically, this crudely takes into account the fact that, for a given amount of glass reacted, the concentration of a specific element in the leachate should be proportional to the mass fraction of the element in the glass. This is an approximation for a number of reasons, including the fact that the mass fraction of the element in question *affects* the amount of glass reacted, and not necessarily all of the constituents in the reacted glass are released to the solution. Nevertheless,

factoring out this dependence by normalization is often empirically observed to improve model fits to leaching data and to further reduce the need for non-linear composition terms in the model.

Based on preliminary modeling work for ILAW PCT releases, Perez-Cardenas et al. [17] suggested a slight preference for models based on PCT normalized elemental releases. The fact that Contract Specification 2.2.2.17.2 specifies a limit (2 g/m^2 = 4 g/L) in terms of normalized releases was the deciding factor in the decision to model PCT normalized elemental releases in this work.

In modeling PCT elemental releases (unnormalized or normalized), it is advantageous to transform the PCT release concentrations in the leachate to the natural logarithm of the concentrations. The advantages of this transformation include:

- The PCT-Boron unnormalized releases for the subset of the Combined Matrix glasses used for modeling range from 2.853 to 64.390 ppm, while the normalized releases range from 0.152 to 2.669 g/L. The PCT-Sodium unnormalized releases range from 9.953 to 352.800 ppm, while the normalized releases range from 0.267 to 2.724 g/L. The ranges for the unnormalized releases involve more than an order-of-magnitude difference. In such cases, typically the uncertainty in making glasses, performing the PCT, and analyzing the leachate leads to smaller absolute uncertainties for smaller releases and larger absolute uncertainties for larger releases. Hence, the ULS regression assumption of equal variances for all response variable values (see Section C.2 of Appendix C) is violated. After a logarithmic transformation, variances of response values tend to be approximately equal as required for ULS regression.

- A logarithmic transformation tends to linearize the compositional dependence of leach test data and reduce the need for non-linear terms in the model form.

- A natural logarithm transformation is preferred over a common logarithm (or other base logarithm) transformation because of the approximate relationship

$$\mathrm{SD}\,[\ln(y)] \cong \mathrm{RSD}\,(y) \tag{6.6}$$

  where SD denotes standard deviation, and RSD denotes relative standard deviation (i.e., the standard deviation divided by the mean). The relationship in Equation (6.6) is very useful, in that uncertainties of the natural logarithm of the response variable y can be interpreted as RSDs of the untransformed response variable y.

For these reasons, the natural logarithmic transformation was employed for all PCT release model forms.

In summary, natural logarithmic transformations of PCT normalized releases (g/L) were used in modeling PCT-Boron and PCT-Sodium releases.

6.3 Property-Composition Model Results for PCT-Boron Release

This section discusses the results of fitting several different models using natural logarithms of ILAW PCT normalized boron release (g/L) as the response variable. Section 6.3.1 discusses the assessment of whether there is any difference (i.e., bias) in PCT-Boron data for the Existing Matrix and the Test Matrix glasses. Section 6.3.2 presents the results of modeling PCT-Boron based on compositions involving all 14 components from the ILAW design matrix. In this case, the full LM model, as well as the full LM model augmented with selected quadratic terms (i.e., PQM models), were considered. Section 6.3.3 presents the results of modeling PCT-Boron using LM and PQM models based on a reduced set of mixture components. Finally, Section 6.3.4 presents the recommended PCT-Boron models.

6.3.1 Preliminary Modeling of ILAW PCT-Boron Data to Compare Existing Matrix and Test Matrix Subsets of Data

The modeling data for ILAW PCT-Boron consist of results for the Existing Matrix and the Test Matrix, as discussed in Section 6.1.1. The glasses in these two matrices were fabricated and melted at different times, and the PCT was performed and leachates analyzed at different times. Because the modeling data were collected in two "blocks", it was prudent before performing substantial modeling work to assess whether there were any "block effects" associated with collecting the two subsets of data at different times. The results of that assessment are briefly summarized in this section.

Two variants of the LM model in Equation (6.1) were used to assess whether there were any block effects in the PCT-Boron data between the Existing Matrix and Test Matrix subsets of glasses. These two LM model variants are listed in Equations (C.6) and (C.7) of Appendix C. Both of these models were fitted to the PCT-Boron modeling data (69 glasses), and the statistical significance of the block-effect coefficients was assessed as discussed in Section C.1.2 of Appendix C. No statistically significant block effects were identified, which means it was acceptable to proceed with the ILAW PCT-Boron modeling using the data for the Combined Matrix and ignoring whether data points were from the Existing Matrix or Test Matrix.

6.3.2 Results for Full LM and PQM Models for ILAW PCT-Boron

Initially, a full LM model in the 14 components was fit to the PCT-Boron modeling data (69 glasses) with the response being the natural logarithm of PCT-Boron releases. This model form was a reasonable starting point based on the preliminary data and model assessment work by Perez-Cardenas et al. [17]. The full LM model offered marginal performance, so it was decided that a PQM model based on the full LM model should be investigated. PQM models are discussed in detail by Piepel et al. [23].

The stepwise selection routine in PROC REG of SAS [34] was used to select the quadratic terms (squared and two-component crossproduct terms) to include with the 14 linear terms in order to produce a better fitting model by including important nonlinear blending effects

of the glass components. The stepwise selection was conducted using tight limits (i.e., significance levels of 0.01 and 0.05, see Section C.4.2 of Appendix C) specified for quadratic terms to enter and remain in the PQM model. The stepwise regressions led to "full PQM" models containing linear terms for all 14 mixture components plus selected quadratic terms. The quadratic terms selected for the 0.01 stepwise significance level case were B_2O_3*MgO and Fe_2O_3*ZnO. The quadratic terms selected for the 0.05 stepwise significance level case were B_2O_3*MgO, Fe_2O_3*ZnO, B_2O_3*TiO_2, CaO*ZrO_2, and K_2O*Na_2O.

Table 6.7 contains ILAW PCT-Boron model performance summaries using both the modeling and validation data sets for the full LM model as well as the full PQM models based on stepwise significance levels of 0.01 and 0.05. The full PQM models show clear improvement over the full LM model for the modeling data. However, the full LM model performs better for the complete validation data set (the secondary validation approach described in Section 6.1.3 with all 59 validation glasses) as well as the V1 (56 glasses) and V2 (40 glasses) validation subsets. However, the full PQM models (based on 0.01 and 0.05 significance levels) perform better than the full LM model for the V3 (26 glasses) and V4 (22 glasses) validation subsets, which are the glasses closest to being within the ILAW composition region of interest.

The data-splitting validation approach (the primary validation approach described in Section 6.1.2) indicated that the full PQM models out-perform the full LM model. Summary statistics for the five splits described in Section 6.1.2 are given in Table 6.8 for both the full LM and PQM models for ILAW PCT-Boron. The columns of the table are labeled DS# to represent the five modeling/validation "data splits" of the modeling data. The splits labeled DS1, DS3, DS4, and DS5 are the 57/12 splits; the split labeled DS2 is the 56/13 split. The last column of each table shows the averages for the different statistics over the five splits. The next-to-the-last column of Table 6.2 indicates which glasses were in each of the five internal validation splits.

Section 6.3.4 assesses the full LM and PQM model results discussed in this section with the reduced LM and PQM model results in the following Section 6.3.3, and recommends two PCT-Boron models for use with LAW glasses.

6.3.3 Results for Reduced LM and PQM Models for ILAW PCT-Boron

Model reduction was the next model development approach investigated, wherein LM models for PCT-Boron involving less than the 14 components were considered. In this case, the sequential F-test model reduction approach (see Section C.4.1 of Appendix C) was used. These F-tests compare full models to reduced models obtained by excluding in turn each of the 14 terms in the full LM model discussed in the previous section. If all linear terms are significant, no model reduction occurs. Otherwise, the least significant linear term is identified. The term identified can either be: (i) normalized out (so the remaining components are renormalized) or, (ii) if it is not Others, it can be combined with Others (in which case the compositions are not renormalized). The sequence of F-tests continues until a model is obtained that does not include non-significant terms.

Reduced LM Model for ILAW PCT-Boron

For this work to reduce the PCT-Boron LM model, a significance level of 0.05 was used for the F-tests and non-significant terms were always normalized out. Another option available with the F-test approach is to force certain terms to remain in the model during the model reduction process. For PCT-Boron, Al_2O_3, B_2O_3, Li_2O, Na_2O, SiO_2, and ZrO_2 were forced into the reduced LM model. That is, they were not eligible to be dropped during model reduction. Of these components, Al_2O_3, B_2O_3, Li_2O, Na_2O, and SiO_2 were significant at each step of the model reduction process and would have been retained in the reduced LM model without being forced to remain. However, ZrO_2 would have been dropped as non-significant early in the model reduction process if it were not forced into the reduced model. Forcing ZrO_2 into the reduced linear model for PCT-Boron had very little impact on the reduced LM model performance. Table 6.9 shows the summary statistics for the ILAW PCT-Boron reduced LM models, where in turn ZrO_2 was and was not forced into the model. Ultimately, the reduced LM model with ZrO_2 was preferred because of subject matter knowledge, and the fact that quadratic terms involving ZrO_2 appear in PQM models for ILAW PCT-Boron.

The reduced LM model obtained for PCT-Boron using the F-test approach contained terms for 11 components: Al_2O_3, B_2O_3, CaO, Fe_2O_3, K_2O, Li_2O, MgO, Na_2O, SiO_2, TiO_2, and ZrO_2. Summary statistics for the reduced LM model (see Table 6.10) indicate that it performs as well or better than the full LM model (see Tables 6.7 and 6.8) for both the modeling and validation data sets.

Reduced PQM Models for ILAW PCT-Boron

Adding selected quadratic terms to the reduced LM model was also investigated, thus yielding what are referred to here as "reduced PQM models". Again, stepwise regression was used to select quadratic terms (squared and crossproduct terms) from among all possible quadratic terms formed using the terms of the reduced LM model. Different reduced PQM models were obtained depending on the value used for the stepwise significance level. Three significance levels (0.01, 0.02, and 0.05) were considered using the stepwise selection feature in the STEPWISE option of PROC REG in the SAS software package. Additionally, the MAXR selection method (coded in R [35], but like the MAXR option of PROC REG in SAS [34]) was used to identify "best" subsets of quadratic terms to include in reduced PQM models. Model development under MAXR is very similar to stepwise regression where terms can enter and leave the model, but sequential changes to the model are based on maximal increases to the model's R^2 value. MAXR tries to find the "best" model having specified numbers of terms, but it is not guaranteed to find the model with the highest R^2 value among all models having a given number of terms. Reduced PQM models generated using the MAXR selection option with up to 17 terms (the 11 linear terms from the reduced LM model plus up to 6 quadratic terms) were considered. With the STEPWISE and MAXR options, the quadratic terms available for selection into the reduced PQM models either consisted of: (i) all possible quadratic terms involving the 11 normalized components in the reduced LM model, or (ii) all quadratic terms except those involving TiO_2. In the latter case, TiO_2 was still one of the linear terms in the reduced LM model, and therefore was included as a linear term in the reduced PQM models considered. But based on glass science experience, TiO_2 was not expected to have a significant quadratic effect

and was therefore disallowed from use in quadratic terms in reduced PQM models. Performance results for all of the reduced PQM models considered, as well as the reduced LM model, applied to the ILAW PCT model development data (69 glasses) are given in Table 6.10.

The reduced LM and PQM models being considered for PCT-Boron were also applied to the five modeling/validation splits formed using the modeling data, as described previously. The averages from the data-splitting validation results are also given in Table 6.10 for the reduced models considered. Table 6.10 includes results for reduced PQM models obtained when TiO_2 was allowed in quadratic terms as well as those obtained when TiO_2 was disallowed.

Section 6.3.4 assesses the reduced LM and PQM model results discussed in this section with the full LM and PQM model results in the previous section, and recommends two PCT-Boron models for use with LAW glasses. Ultimately, the issue of whether to allow quadratic terms containing TiO_2 in PQM models was moot, as discussed in the following section.

6.3.4 Recommended ILAW PCT-Boron Models

Based on the results of the PCT-Boron model development work for:

- the modeling data
- the separate validation data set and subsets thereof
- the modeling data-splitting results

it was decided to recommend both the 11-term reduced LM model as well as the reduced PQM model for the MAXR 14-term case where TiO_2 was disallowed from quadratic terms. These ILAW PCT-Boron models are the first and last of those for which performance statistics are listed in Table 6.10. The columns for these two models in Table 6.10 are shaded. Model performance on the separate validation data set (and subsets thereof) was of particular importance when selecting the reduced PQM model to recommend.

Note the 14-term reduced PQM model when quadratic terms containing TiO_2 were allowed is the same as the 14-term model when quadratic terms containing TiO_2 were disallowed, because the former does not contain any quadratic terms involving TiO_2. Also, note from Table 6.10 that the recommended 14-term reduced PQM model has better performance statistics than the 11-term reduced LM model when considering the modeling data, the validation data set and all its subsets, and the data-splits of the modeling data. Although the 14-term PQM model seems superior by all measures, it was decided to also recommend the 11-term reduced LM model as one that might perform better than the 14-term reduced PQM model for future data sets.

Recommended Reduced LM Model for ILAW PCT-Boron

Table 6.11 gives the coefficients of the 11-term reduced LM model for ln(PCT-Boron), as well as performance statistics for the modeling data, the validation data set and its subsets, and the data-split modeling data. The performance statistics are the same as given in previous,

separate tables for this model, but are gathered into Table 6.11 for convenience. The value of R^2 = 0.7945 indicates that the reduced LM model accounts for nearly 80% of the variation in $ln(r_B)$ values in the modeling data set. While this is a reasonably large number, a larger value would be preferable. R^2_A = 0.7590 is close to R^2, indicating that the model reduction was successful in removing unneeded components. The value for R^2_P = 0.6756 is sufficiently below the R^2 and R^2_A values to indicate that there may be some influential data points in the modeling data set. In any case, R^2_P = 0.6756 provides a more conservative estimate of the fraction of variation in $ln(r_B)$ values for future data sets over the same glass composition region that might be accounted for by this reduced LM model. Over the five data splits of the modeling data, the average R^2_V was 0.6325, which is similar to the R^2_P value. The R^2 validation values for the complete validation data set, and subsets V1 and V2, range from 0.5531 to 0.5941. These fractions of variation in $ln(r_B)$ values accounted for by the reduced LM model are noticeably less than indicated by R^2_P and the average R^2_V over the data splits. However, the complete validation data set, and the V1 and V2 validation subsets, have glasses outside the LAW glass composition region of interest defined previously in Table 2.1. The validation subsets V3 and V4 contain glasses that are, respectively, mostly and completely within the composition region of interest. However, the R^2 validation values for those subsets drop to approximately zero. It is not clear whether this poor prediction performance for these subsets of the validation data set are because of something different about the validation data related to being collected at a different time, the limited composition region covered by these small subsets of validation data, or whether it is an indication of limitations of the reduced LM model for PCT-Boron.

Per Equation (6.6), the RMSE = SD[ln(r_B)] in Table 6.11 can be interpreted as the RSD in fabricating simulated LAW glasses and measuring r_B if the model does not have statistically significant LOF. Although RMSE = 0.3084 is much larger than the historical replicate RSDs (e.g., ~0.10 in Appendix F of Hrma et al. [36]) in fabricating simulated waste glasses and measuring PCT-Boron release, analysis of replicate PCT-Boron data summarized in Table 6.4 indicates a replicate RSD of ~0.21, as discussed at the end of Section 6.1.1. This suggests the model LOF may not be statistically significant. This indication is confirmed by the model LOF p-value = 0.2411 (see Section C.3 of Appendix C) in Table 6.11. However, it may be that the reduced LM model for PCT-Boron does have some LOF that was not detected by the statistical LOF test because of the relatively large uncertainty in the replicate PCT-Boron data.

Figures 6.1 through 6.4 show various regression diagnostic plots for the ln(PCT-Boron) reduced LM model applied to the 69 glasses of the modeling data set. Figures 6.1 and 6.2 generally indicate that the assumption of normally distributed errors in the PCT-Boron data is reasonable (see Section C.2 of Appendix C). Both figures show two outlying data points, one with a low PCT-Boron release compared to its predicted release (LAWM22) and one with a high PCT-Boron release compared to its predicted release (LAWM31). Figures 6.3 and 6.4 show well-distributed prediction errors for the modeling data set, although the scatter about the ideal prediction line in Figure 6.3 is larger than would be preferred. It is unclear how much of this scatter is due to model LOF and how much is due to the uncertainties inherent in the PCT-Boron data. Figure 6.4 shows two middle-layer Test Matrix glasses having large positive (LAWM31) and negative (LAWM22) standardized residuals. Although outlying, these two points did not have a major impact on the fitted model.

Figures 6.5 through 6.9 show *predicted versus measured plots* when the reduced LM model for ILAW PCT-Boron is applied to the validation data set and various subsets thereof. Also shown in these figures are 95% prediction intervals representing the model prediction uncertainty of single PCT-Boron determinations for each glass (see Sections C.5 and C.6 of Appendix C). The 95% prediction intervals are relatively wide, which is partly due to: (1) any LOF of the reduced LM model, and (2) the inherent experimental uncertainty in fabricating glasses, performing the PCT, and analyzing Boron in the PCT leachates. The consequences of model LOF and prediction uncertainties are discussed further in Section 6.6.

Recommended Reduced PQM Model for ILAW PCT-Boron

Table 6.12 gives the coefficients of the 14-term reduced PQM model for ln(PCT-Boron), as well as performance statistics for the modeling data, the validation data set and its subsets, and data-split modeling data. The modeling evaluation statistics $R^2 = 0.8799$, $R^2_A = 0.8515$, $R^2_P = 0.7653$, and RMSE = 0.2421 are substantial improvements over the corresponding statistics for the 11-term reduced LM model. The noticeable drop in values from R^2_A to R^2_P suggests that the modeling data set has some influential data points. In any case, $R^2_P = 0.7653$ provides a more conservative estimate of the fraction of variation in $ln(r_B)$ values for future data sets over the same glass composition region that might be accounted for by this reduced PQM model. Over the five data splits of the modeling data, the average R^2_V was 0.7246, which is similar to the R^2_P value. The R^2 validation values for the complete validation data set, and subsets V1 and V2, range from 0.6005 to 0.6648. These fractions of variation in $ln(r_B)$ values accounted for by the reduced PQM model are noticeably less than indicated by R^2_P and the average R^2_V over the data splits. However, the complete validation data set, and the V1 and V2 validation subsets, have glasses outside the LAW glass composition region of interest defined previously in Table 2.1. Still, the R^2 validation values for the complete set and the V1 and V2 subsets are noticeable improvements over the corresponding values for the reduced LM model. The validation subsets V3 and V4 contain glasses that are, respectively, mostly and completely within the composition region of interest. However, the R^2 validation values for those subsets are 0.1997 and 0.2236, respectively. While the values are improvements over the corresponding values for the reduced LM model, they are still quite low. It is not clear whether this poor prediction performance for these subsets of the validation data set are because of something different about the validation data related to being collected at a different time, the limited composition region covered by these small subsets of validation data, or whether it is an indication of limitations of the reduced PQM model for PCT-Boron.

Per Equation (6.6), the RMSE = SD[ln(r_B)] in Table 6.12 can be interpreted as the RSD in fabricating simulated LAW glasses and measuring r_B if the model does not have statistically significant LOF. Although RMSE = 0.2421 for the reduced PQM model is smaller than the corresponding value for the reduced LM model, it is still larger than the historical replicate RSDs (e.g., ~0.10 in Appendix F of Hrma et al. [36]) in fabricating simulated waste glasses and measuring PCT-Boron release, as discussed at the end of Section 6.1.1. However, as mentioned there, analysis of replicate PCT-Boron data summarized in Table 6.4 indicates a replicate RSD of ~0.21. This value is close to the RMSE for the reduced PQM model for PCT-Boron, and suggests this model does not have a statistically significant LOF. This indication is confirmed by the model LOF p-value = 0.4539 (see Section C.3 of Appendix C) in Table 6.12. However, it

may be that the reduced PQM model for PCT-Boron does have some LOF that was not detected by the statistical LOF test because of the relatively large uncertainty in the replicate PCT-Boron data.

Figures 6.10 through 6.14 show various regression diagnostic plots for the ln(PCT-Boron) reduced PQM model applied to the 69 glasses of the modeling data set. Figures 6.10 and 6.11 generally indicate that the assumption of normally distributed errors in the PCT-Boron data is reasonable (see Section C.2 of Appendix C). Figures 6.12 and 6.13 show some trends in the distributions of prediction errors for the modeling data set. Specifically, the outer-layer glasses tend to have PCT-Boron release under-predicted, the middle-layer glasses tend to have PCT-Boron release over-predicted. These results may be due to the nonlinear blending effects of the glass components on PCT-Boron release behavior being more complicated than can be adequately represented by a "global" reduced PQM model. Also in Figure 6.13, the Existing Matrix glasses show less scatter than for the Test Matrix glasses. This can be explained by the Existing Matrix glasses not covering the composition region as well as the Test Matrix glasses, which will tend to cause larger prediction errors for the Test Matrix glasses. Despite these trends, the scatter about the ideal prediction line in Figure 6.12 for the reduced PQM model is smaller than in Figure 6.3 for the reduced LM model. This indicates the total uncertainty of prediction is less for the reduced PQM model than for the reduced LM model. It is unclear how much of this scatter is due to any LOF of the reduced PQM model, and how much is due to the uncertainties inherent in the PCT-Boron data. No obviously outlying points are visible in Figure 6.13.

Figure 6.14 displays the *partial residual plots* for each of the 14 terms in the reduced PQM model for ln(PCT-Boron). For each data point in a modeling data set, a *partial residual plot* displays the partial residual on the y-axis, and the value of a model term on the x-axis. A partial residual is the difference between a measured and model-predicted response (ln(PCT-Boron) in this case) when one term has been left out of the model. The "best fit" line through the points in a partial residual plot for a given model term has slope equal to the coefficient for that term in the model. This type of plot is discussed in more detail by Draper and Smith [31]. A partial residual plot provides for assessing the level of support provided by the modeling data for estimating the coefficient for that model term. Although Figure 6.14 includes partial residual plots for all terms in the reduced PQM model for ln(PCT-Boron), of primary interest are the plots for the B_2O_3*MgO, Fe_2O_3*Li_2O, and Li_2O*ZrO_2 quadratic terms. All three quadratic terms are well supported by the modeling data, although two glasses (LAWM6 and LAWM8) with larger values of B_2O_3*MgO are somewhat influential for that term.

Figures 6.15 through 6.19 show predicted versus measured plots when the reduced PQM model is applied to the validation data set and various subsets thereof. Also shown in these figures are 95% prediction intervals representing the model prediction uncertainty of single PCT-Boron determinations for each glass (see Sections C.5 and C.6 of Appendix C). The 95% prediction intervals are relatively wide, which is partly due to: (1) any LOF of the reduced PQM model, and (2) the inherent experimental uncertainty in fabricating glasses, performing the PCT, and analyzing Boron in the PCT leachates. The consequences of model LOF and prediction uncertainties are discussed further in Section 6.6.

In conclusion, the recommended ILAW Phase 1 models for PCT-Boron are the 11-term reduced LM model in Table 6.11 and the 14-term reduced PQM model in Table 6.12. It is recommended that both these ILAW PCT-Boron models be applied and their performances compared during any future ILAW glass formulation and waste form qualification work.

6.4 Property-Composition Model Results for PCT-Sodium Release

This section discusses the results of fitting several different models using natural logarithms of ILAW PCT normalized sodium release (g/L) as the response variable. Section 6.4.1 discusses the assessment of whether there is any difference (i.e., bias) in PCT-Sodium data for the Existing Matrix and the Test Matrix glasses. Section 6.4.2 presents the results of modeling PCT-Sodium based on compositions involving all 14 components from the ILAW design matrix. As with the PCT-Boron modeling, the full LM model, as well as the full LM model augmented with selected quadratic terms (i.e., PQM models) were considered for PCT-Sodium modeling. Section 6.4.3 presents the results of modeling PCT-Sodium using LM and PQM models based on a reduced set of mixture components. Finally, Section 6.4.4 presents the recommended PCT-Sodium models.

6.4.1 Preliminary Modeling of ILAW PCT-Sodium Data to Compare Existing Matrix and Test Matrix Subsets of Data

The modeling data for ILAW PCT-Sodium consist of results for the Existing Matrix and the Test Matrix, as discussed in Section 6.1.1. The glasses in these two matrices were fabricated and melted at different times, and the PCT was performed and leachates analyzed at different times. Because the modeling data were collected in two "blocks", it was prudent before performing substantial modeling work to assess whether there are any "block effects" associated with collecting the two subsets of data at different times. The results of that assessment are briefly summarized in this section.

Two variants of the LM model in Equation (6.1) were used to assess whether there were any block effects in the PCT-Sodium data between the Existing Matrix and Test Matrix subsets of glasses. These two LM model variants are listed in Equations (C.6) and (C.7) of Appendix C. Both of these models were fitted to the PCT-Sodium modeling data (69 glasses), and the statistical significance of the block-effect coefficients was assessed as discussed in Section C.1.2 of Appendix C. No statistically significant (at a significance level of 0.05) block effects were identified, which means it was acceptable to proceed with the ILAW PCT-Sodium modeling using the data for the Combined Matrix and ignoring whether data points were from the Existing Matrix or Test Matrix.

6.4.2 Results for Full LM and PQM Models for ILAW PCT-Sodium

As with the ILAW PCT-Boron model development, a full LM model was the first model form considered for ILAW PCT-Sodium modeling. The full LM model included the same 14 components involved in the PCT-Boron modeling, and used the same 69 of 77 glass compositions from the ILAW Combined Matrix. The PCT-Sodium full LM model performed slightly better than the PCT-Boron full LM model for the modeling data. However, even better performance was desired. Therefore, PQM models were investigated for ILAW PCT-Sodium.

The quadratic terms for the full PQM models were generated using the stepwise regression capability in SAS [34] with 0.01 and 0.05 as stepwise significance levels (see Section C.4 of Appendix C). The quadratic terms selected for the 0.01 stepwise significance level case were Fe_2O_3*ZnO and B_2O_3*MgO. The quadratic terms selected for the 0.05 stepwise significance level case were SiO_2*Others, Li_2O*ZrO_2, Li_2O*MgO, and B_2O_3*TiO_2.

Model evaluation and validation performance results for the "full LM" model and two "full PQM" models for PCT-Sodium are listed in Table 6.13. Included in Table 6.13 are validation results for the complete validation set, as well as various validation subsets. The validation set and subsets are the same as were used for the PCT-Boron model, as discussed in Section 6.1.3.

The same five modeling/validation splits formed from the modeling data and described previously in Section 6.1.2 were used to conduct data-splitting model validation for the full LM and PQM models for PCT-Sodium being considered. The summary statistics obtained from each of the "full LM" and two "full PQM" models for PCT-Sodium models using the five modeling/validation splits are given in Table 6.14. The last column of Table 6.14 shows the averages for the different statistics over the five modeling/validation splits.

6.4.3 Results for Reduced LM and PQM Models for ILAW PCT-Sodium

As with the PCT-Boron modeling, reduced LM and PQM models for PCT-Sodium were also pursued with the goal of improving the predictive performance for validation data by dropping unnecessary terms. The iterative F-test approach (see Section C.4.1 of Appendix C) was again used to identify non-significant linear terms in the full LM model and normalize them out. Again, a significance level of 0.05 was used for the F-tests. Also, Al_2O_3, B_2O_3, Li_2O, Na_2O, SiO_2, and ZrO_2 were forced to remain in the model during model reduction. As with the PCT-Boron model reduction, ZrO_2 would have been normalized out during model reduction had it not been forced into the model. The other five components forced into the reduced LM model for PCT-Sodium were never identified as non-significant during the model reduction process, and would have remained in the model without being forced. The reduction process lead to an initial PCT-Sodium reduced LM model containing 10 terms; Al_2O_3, B_2O_3, Fe_2O_3, K_2O, Li_2O, MgO, Na_2O, SiO_2, TiO_2, and ZrO_2.

Recall that the ILAW PCT-Boron reduced LM model contained these same 10 linear terms, but also included a CaO term. Ideally, the reduced PCT-Boron and reduced PCT-Sodium

LM models would contain the same terms. Thus, summary statistics were obtained and compared for ILAW PCT-Sodium reduced LM models obtained by forcing and not forcing CaO into the reduced model. The results (presented in Table 6.15) show very little difference in model performance if CaO is forced into the reduced model. In fact, as with the PCT-Boron reduced LM model, forcing ZrO_2 into the reduced PCT-Sodium LM model has very little effect on model performance. Therefore, it was decided to retain CaO in the PCT-Sodium reduced LM model (along with Al_2O_3, B_2O_3, Li_2O, Na_2O, SiO_2, and ZrO_2 as was done for the PCT-Boron modeling) in order to have the same 11 linear terms as included in the PCT-Boron reduced LM model.

Reduced PQM models were also developed for PCT-Sodium using both the STEPWISE and MAXR selection options. The stepwise significance levels used were 0.01, 0.02, and 0.05. The quadratic terms selected were the same for the 0.01 and 0.02 stepwise significance level cases. For the MAXR selection option, reduced PQM models with up to 17 terms (the 11 linear terms from the reduced LM model for PCT-Sodium plus up to 6 quadratic terms) were considered. Again, TiO_2 was both allowed and disallowed for involvement in quadratic terms available for selection into the reduced PQM models under consideration for PCT-Sodium. Results for the reduced LM and PQM models for PCT-Sodium are presented in Table 6.16.

The reduced LM and PQM models for PCT-Sodium were applied to the five modeling/validation splits formed using the modeling data that were described previously. The averages from the data-splitting validation results are also given in Table 6.16 for the reduced PCT-Sodium models considered.

6.4.4 Recommended ILAW PCT-Sodium Models

Based on the results of the PCT-Sodium model development work for:

- the modeling data
- the separate validation data set and subsets thereof
- the modeling data-splitting results

it was decided to recommend both the 11-term reduced LM model as well as the reduced PQM model for the MAXR 16-term case where TiO_2 was disallowed from quadratic terms. The columns for these two models in Table 6.16 are shaded. Model performance on the separate validation data set (and subsets thereof) was of particular importance when selecting the reduced PQM model to recommend.

Note from Table 6.16 that the recommended 16-term reduced PQM model has better performance statistics than the 11-term reduced LM model when considering the modeling data, the validation data set and all its subsets, and the data-splits of the modeling data. Although the 16-term PQM model seems superior by all measures, it was decided to also recommend the 11-term reduced LM model as one that might perform better than the 16-term reduced PQM model for future data sets.

Recommended Reduced LM Model for ILAW PCT-Sodium

Table 6.17 gives the coefficients of the 11-term reduced LM model for ln(PCT-Sodium), as well as performance statistics for the modeling data, the validation data set and its subsets, and data-split modeling data. The performance statistics are the same as given in previous, separate tables for this model, but are gathered into Table 6.17 for convenience.

The value of $R^2 = 0.8498$ indicates that the reduced LM model accounts for roughly 85% of the variation in $ln(r_{Na})$ values in the modeling data set. While this is a reasonably large number, a larger value would be preferable. $R^2_A = 0.8239$ is close to R^2, indicating that the model reduction was successful in removing unneeded components. The value for $R^2_P = 0.7791$ is sufficiently close to the R^2 and R^2_A values to indicate that there probably are not any highly influential data points in the modeling data set. In any case, $R^2_P = 0.7791$ provides a more conservative estimate of the fraction of variation in $ln(r_{Na})$ values for future data sets over the same glass composition region that might be accounted for by this reduced LM model. Over the five data splits of the modeling data, the average R^2_V was 0.7644, which is similar to the R^2_P value. The R^2 validation values for the complete validation data set, and subsets V1 and V2, range from 0.5509 to 0.5856. These fractions of variation in $ln(r_{Na})$ values accounted for by the reduced LM model are noticeably less than indicated by R^2_P and the average R^2_V over the data splits. However, the complete validation data set, and the V1 and V2 validation subsets, have glasses outside the LAW glass composition region of interest defined previously in Table 2.1. The validation subsets V3 and V4 contain glasses that are, respectively, mostly and completely within the composition region of interest. However, the R^2 validation values for those subsets drop to 0.1824 and 0.1171, respectively. It is not clear whether this poor prediction performance for these subsets of the validation data set are because of something different about the validation data related to being collected at a different time, the limited composition region covered by these small subsets of validation data, or whether it is an indication of limitations of the reduced LM model for PCT-Sodium.

Per Equation (6.6), the RMSE = SD[ln(r_{Na})] in Table 6.17 can be interpreted as the RSD in fabricating simulated LAW glasses and measuring r_{Na} if the model does not have statistically significant LOF. The RMSE = 0.2053 is larger than the historical replicate RSDs (e.g., ~0.10 in Appendix F of Hrma et al. [36]) in fabricating simulated waste glasses and measuring PCT-Sodium, as discussed at the end of Section 6.1.1. However, as mentioned there, analysis of replicate PCT-Sodium data summarized in Table 6.4 indicates a replicate RSD of ~0.14 to 0.19. These values are close to the RMSE for the reduced LM model for PCT-Sodium, and suggest this model does not have a statistically significant LOF. This indication is confirmed by the model LOF p-value = 0.2066 (see Section C.3 of Appendix C) in Table 6.17. However, it may be that the reduced LM model for PCT-Sodium does have some LOF that was not detected by the statistical LOF test because of the relatively large uncertainty in the replicate PCT-Sodium data.

Figures 6.20 through 6.23 show various regression diagnostic plots for the ln(PCT-Sodium) reduced LM model applied to the 69 glasses of the modeling data set. Figures 6.20 and 6.21 generally indicate that the assumption of normally distributed errors in the PCT-Sodium data is reasonable (see Section C.2 of Appendix C). Figures 6.22 and 6.23 show well-distributed prediction errors for the modeling data set, except for a possible tendency to under-predict PCT-

Sodium normalized releases above about 1.8 g/L. Figure 6.23 shows four data points have somewhat extreme standardized residuals, but the number and pattern is not bothersome.

Figures 6.24 through 6.28 show *predicted versus measured plots* when the reduced LM model for ILAW PCT-Sodium is applied to the validation data set and various subsets thereof. Also shown in these figures are 95% prediction intervals representing the model prediction uncertainty of single PCT-Sodium determinations for each glass (see Sections C.5 and C.6 of Appendix C). The 95% prediction intervals are relatively wide, which is partly due to: (1) any LOF of the reduced LM model, and (2) the inherent experimental uncertainty in fabricating glasses, performing the PCT, and analyzing sodium in the PCT leachates. The consequences of model LOF and prediction uncertainties are discussed further in Section 6.6.

Recommended Reduced PQM Model for ILAW PCT-Sodium

Table 6.18 gives the coefficients of the 16-term reduced PQM model for ln(PCT-Sodium), as well as performance statistics for the modeling data, the validation data set and its subsets, and data-split modeling data. The modeling evaluation statistics $R^2 = 0.9203$, $R^2_A = 0.8977$, $R^2_P = 0.8709$, and RMSE = 0.1564 are substantial improvements over the corresponding statistics for the 11-term reduced LM model. The limited drop in values from R^2_A to R^2_P suggests that the modeling data set probably does not contain any influential data points. In any case, $R^2_P = 0.8709$ provides a more conservative estimate of the fraction of variation in $ln(r_{Na})$ values for future data sets over the same glass composition region that might be accounted for by this reduced PQM model. Over the five data splits of the modeling data, the average R^2_V was 0.8420, which is slightly less than the R^2_P value. The R^2 validation values for the complete validation data set, and subsets V1 and V2, range from 0.6643 to 0.7553. These fractions of variation in $ln(r_{Na})$ values accounted for by the reduced PQM model are noticeably less than indicated by R^2_P and the average R^2_V over the data splits. However, the complete validation data set, and the V1 and V2 validation subsets, have glasses outside the LAW glass composition region of interest defined previously in Table 2.1. Still, the R^2 validation values for the complete set and the V1 and V2 subsets are noticeable improvements over the corresponding values for the reduced LM model. The validation subsets V3 and V4 contain glasses that are, respectively, mostly and completely within the composition region of interest. The R^2 validation values for those subsets are 0.5242 and 0.5089, respectively. While these values are substantial improvements over the corresponding values for the reduced LM model, they are still lower than is desirable. It is not clear whether this poorer prediction performance for these subsets of the validation data set are because of something different about the validation data related to being collected at a different time, the limited composition region covered by these small subsets of validation data, or whether it is an indication of limitations of the reduced PQM model for PCT-Sodium.

Per Equation (6.6), the RMSE = SD[ln(r_{Na})] in Table 6.18 can be interpreted as the RSD in fabricating simulated LAW glasses and measuring r_{Na} if the model does not have statistically significant LOF. Although RMSE = 0.1564 for the reduced PQM model is smaller than the corresponding value for the reduced LM model, it is still somewhat larger than the historical replicate RSDs (e.g., ~0.10 in Appendix F of Hrma et al. [36]) in fabricating simulated waste glasses and measuring PCT-Sodium, as discussed at the end of Section 6.1.1. However, as

mentioned there, analysis of replicate PCT-Sodium data summarized in Table 6.4 indicates a replicate RSD of ~0.14 to 0.19. These values are very close to the RMSE for the reduced PQM model for PCT-Sodium, and suggest this model does not have a statistically significant LOF. This indication is confirmed by the model LOF p-value = 0.4300 (see Section C.3 of Appendix C) in Table 6.18. However, it may be that the reduced PQM model for PCT-Sodium does have some LOF that was not detected by the statistical LOF test because of the relatively large uncertainty in the replicate PCT-Sodium data.

Figures 6.29 through 6.33 show various plots for the ln(PCT-Sodium) reduced PQM model applied to the 69 glasses of the modeling data set. Figures 6.29 and 6.30 generally indicate that the assumption of normally distributed errors in the PCT-Sodium data is reasonable (see Section C.2 of Appendix C). Figures 6.31 and 6.32 show no trends in the distributions of prediction errors nor possible outliers for the modeling data set. The predicted vs. measured plot in Figure 6.31 for the reduced PQM model shows a very nice pattern, and is a clear improvement over the corresponding plot in Figure 6.22 for the reduced LM model.

Figure 6.33 displays the *partial residual plots* for each of the 16 terms in the reduced PQM model for ln(PCT-Sodium). For each data point in a modeling data set, a *partial residual plot* displays the partial residual on the y-axis, and the value of a model term on the x-axis. A partial residual is the difference between a measured and model-predicted response (ln(PCT-Sodium) in this case) when one term has been left out of the model. The "best fit" line through the points in a partial residual plot for a given model term has slope equal to the coefficient for that term in the model. This type of plot is discussed in more detail by Draper and Smith [31]. A partial residual plot provides for assessing the level of support provided by the modeling data for estimating the coefficient for that model term. Although Figure 6.33 includes partial residual plots for all terms in the reduced PQM model for ln(PCT-Sodium), of primary interest are the plots for the five quadratic terms. All five quadratic terms are well supported by the modeling data, although two glasses (LAWM6 and LAWM8) with larger values of B_2O_3*MgO are somewhat influential for that term.

Figures 6.34 through 6.38 show *predicted versus measured plots* when this model is applied to the validation data set and various subsets thereof. Also shown in these figures are 95% prediction intervals representing the model prediction uncertainty of single PCT-Sodium determinations for each glass (see Sections C.5 and C.6 of Appendix C). The 95% prediction intervals are relatively wide, which is partly due to: (1) any LOF of the reduced PQM model, and (2) the inherent experimental uncertainty in fabricating glasses, performing the PCT, and analyzing sodium in the PCT leachates. The consequences of model LOF and prediction uncertainties are discussed further in Section 6.6.

In conclusion, the recommended ILAW Phase 1 models for PCT-Sodium are the 11-term reduced LM model in Table 6.17 and the 16-term reduced PQM model in Table 6.18. Although the 16-term reduced PQM model appears to have significant advantages over the 11-term reduced LM model, it is recommended that both these ILAW PCT-Sodium models be applied and their performances compared during any future ILAW glass formulation and waste form qualification work.

6.5 Example Illustrating Model Predictions and Statistical Intervals

This section contains examples to illustrate the use of the 11-term LM model and 14-term PQM model to obtain predicted PCT-Boron releases and corresponding 90% UCIs and 95% SUCIs for a specific LAW glass composition. This section also contains examples to illustrate the use of the 11-term LM model and 16-term PQM model to obtain predicted PCT-Sodium releases and corresponding 90% UCIs for the same LAW glass composition.

As with the example in Section 5.6 illustrating the use of the ILAW VHT models, the glass composition used in this example is that of LAWA126, which is one of the glasses in the LAW Test Matrix. The composition of LAWA126 for PCT modeling is given in Table 6.1 in normalized weight percent format. In order to apply the PCT models to this composition, the weight percentages must be converted to normalized mass fractions (that sum to 1.0) for the linear components contained in the different models. Normalized mass fractions from the linear terms are then multiplied to obtain the quadratic components corresponding to the quadratic terms of the PQM models. Table 6.19 contains the composition for LAWA126 prepared for use in the different ILAW PCT models for Boron and Sodium.

For each of the different PCT models, predicted ln(PCT releases) are obtained by multiplying the composition in the format needed for the specific models by the coefficients for the different models (see Tables 6.11, 6.12, 6.17, and 6.18), then summing the results. That is, the predicted values are calculated by

$$\hat{y}(\boldsymbol{a}) = \boldsymbol{a}^T\boldsymbol{b}$$

where $\boldsymbol{a}$ is the composition of LAWA126 formatted to match the terms in a given model (from Table 6.19), T represents a matrix transpose (or vector transpose in this case), and $\boldsymbol{b}$ is the vector of model coefficients for a given model. The predicted ln(PCT release) values from each of the four ILAW PCT models are listed in the second column of Table 6.20. The predicted ln(PCT releases) in ln(g/L) units are easily converted to the usual PCT release units of g/L by exponentiation. The third column of Table 6.20 contains the predicted PCT releases in g/L units. However, as discussed in Section C.6 of Appendix C, these back-transformed PCT release predictions in g/L units should be considered estimates of the true median of the distribution of PCT releases that would result if the PCT were repeated multiple times using samples of the LAWA126 glass, not estimates of the true mean.

Equation (C.13) can be used to calculate a 90% UCI for the true mean of ln(PCT releases) from the LAWA126 glass composition for each of the ILAW PCT models. In the notation of Equation (C.13):

- $100(1-\alpha)\% = 90\%$, so that $\alpha = 0.10$.
- The vector $\boldsymbol{a}$ is the composition of LAWA126 formatted to match the terms in a given model.

- The matrix $\boldsymbol{A}$ is the design matrix of normalized linear components and selected quadratic components derived from the linear components (in the case of PQM models) formatted to match the terms in a given model.

To obtain an 90% UCI in ln(PCT release) units of ln(g/L), the quantity $t_{1-\alpha,n-p} RMSE \sqrt{\boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{a}}$ is added to the predicted PCT release $\hat{y}(\boldsymbol{a})$ described above, as indicated by Equation (C.13). The $MSE[(\boldsymbol{A}^T \boldsymbol{A})^{-1}]$ portion of this expression is the variance-covariance matrix for the estimated model coefficients, as discussed near the end of Section C.6 of Appendix C. The variance-covariance matrices for the different PCT models are listed in Appendix D. The quantity *MSE* is the mean squared error from regression, *RMSE* is the square root of *MSE*.

The 90% UCI values for the true mean ln(PCT release) in units of ln(g/L) for the LAWA126 composition based on the different ILAW PCT models are given in the fourth column of Table 6.20. Exponentiating the resulting 90% UCIs on the mean in ln(g/L) units yields 90% UCIs for the median in g/L units. For example, the 11-term LM model for PCT-Boron has 0.3991 ln(g/L) as the upper limit of the 90% UCI on the true mean ln(PCT-Boron release) for LAWA126, whereas $e^{0.3991}$ = 1.4905 g/L is the upper limit of the 90% UCI on the true median PCT-Boron release. The fifth column of Table 6.20 contains 90% UCIs for the true median PCT releases from the LAWA126 glass composition based on the different ILAW PCT models. Note that the 90% UCI values in g/L units for the different ILAW PCT models are well below the PCT release limit of 4 g/L (2 g/m^2).

As discussed in Appendix C, there are times when a SUCI may be preferred rather than an UCI. This is particularly true when the regression model (composition-property model) is to be used a large number of times for various glass compositions from a specified composition region. Equation (C.15) can be used, in much the same way as how Equation (C.13) is used to obtain UCIs, to calculate a 95% SUCI for the true mean of ln(PCT release) for glasses having a specified composition. The 95% SUCI values for the true mean ln(PCT release) in units of ln(g/L) for the LAWA126 composition based on the ILAW PCT models are given in the fifth column of Table 6.20. Exponentiating the resulting 95% SUCIs for the mean in ln(g/L) units yields 95% SUCIs for the median in g/L. The sixth column of Table 6.20 contains 95% SUCIs for the true median PCT release from the LAWA126 glass composition based on the ILAW PCT models. Note that the 95% SUCI values in g/L for the different ILAW PCT models are well below the PCT release limit of 4 g/L (2 g/m^2).

6.6 Consequences of LOFs and Prediction Uncertainties in PCT-Boron and PCT-Sodium Models

The consequences of LOFs and prediction uncertainties of PCT-Boron and PCT-Sodium models on the ability to demonstrate compliance with Contract Specification 2.2.2.17.2 will be addressed as part of work that will be documented in a separate Battelle–PNWD report. It is expected that LAW glasses to be produced in the WTP LAW vitrification plant will have PCT-

Boron and PCT-Sodium releases sufficiently below the 2 g/m^2 (= 4 g/L) limit even after accounting for composition and model uncertainties. However, this outcome is less certain than for WTP HLW glasses, where the PCT-Boron and PCT-Sodium releases have higher limiting values. Should uncertainties in the reduced LM and PQM models for PCT-Boron and PCT-Sodium releases from LAW glasses be too large to clearly demonstrate compliance with the Contract Specification 2.2.2.17.2 limit, there are two possible paths to explore.

The first path is to investigate why the PCT-Boron and PCT-Sodium normalized releases in this study appear to have larger uncertainties (from glass fabrication, PCT testing, and chemical analysis of leachate) than in similar studies in the past. Reducing the uncertainty of individual PCT-Boron and PCT-Sodium normalized releases would directly reduce the uncertainties in models developed from the data.

As a second path, it may be necessary to investigate in future modeling work the use of "local" rather than "global" modeling approaches to obtain models with smaller prediction uncertainties. One type of local modeling approach would be to develop models over smaller, local regions of LAW glass composition space. Past experience has shown that LM models may have sufficiently low uncertainty to demonstrate compliance for less expansive compositions regions. Another type of local modeling approach would be to use so-called non-parametric regression methods such as local linear (or polynomial) regression, neural networks, or others. Such modeling methods are not restricted by requiring the same global model form to apply over all subregions of the glass composition space of interest. However, the non-parametric regression methods have the disadvantage of requiring larger data sets with more evenly distributed data than does the global, parametric modeling approach.

SECTION 7
SUMMARY AND CONCLUSIONS

In the present work, data have been collected and analyzed in order to develop models that relate the VHT response and the PCT responses for boron and sodium to the composition of WTP LAW glasses. This effort constitutes Phase 1 of that model development effort. The results from this work could be used as the basis for any future ILAW model development work.

The data set was based on a Combined Matrix of glasses that was composed of 21 existing glasses (the Existing Matrix) and 56 new glasses (the Test Matrix). The compositions of the Test Matrix glasses were developed by applying statistical experimental design methods to optimally augment the set of existing glasses. The 56 Test Matrix glasses were fabricated and characterized with respect to composition and VHT and PCT responses and the data are reported herein. In addition, a set of glasses from previous work in support of the WTP Project was selected to provide an independent data set for model validation. VHT- and PCT-glass composition models were developed by regression of the Combined Matrix glasses and validated by data-splitting using the regression set as well as by independent validation using the validation set. Based on the performance of the models that were investigated, recommended models were selected.

The VHT results for the Test Matrix glasses varied from 0.11 g/m^2/day to 125 g/m^2/day, as compared to the contract requirement of < 50 g/m^2/day. The VHT results for the 21 Existing Matrix glasses ranged from less than 1 to 23 g/m^2/day. For a few of the Test Matrix glasses, the extent of VHT alteration was so high that no rate could be calculated because the entire glass coupon was altered. Five of the Test Matrix glasses were altered completely before the end of the 24-day test period. Another two glass samples had an alteration depth in excess of 700 μm (an alteration depth of ≈ 453 μm corresponds to an alteration rate of 50 g/m^2/day). These seven samples were not used in VHT modeling. During any future modeling work, efforts should be made to obtain more VHT data points near the contractual limit in order to improve predictive ability of the model in this range.

The PCT boron results varied from 0.08 g/m^2 to 17.84 g/m^2 for the Test Matrix glasses, and 0.19 g/m^2 to 0.87 g/m^2 for the Existing Matrix glasses. The 21 Existing Matrix glasses were designed to be compliant with ILAW performance requirements and, therefore, it was expected that their PCT boron results would be less than 2 g/m^2, which is the WTP contract limit. The Test Matrix glasses, however, were designed to cover a larger composition range and, accordingly, their PCT responses are expected to vary by a larger amount. Eight of the Test Matrix glasses showed PCT boron or sodium releases in excess of 2 g/m^2. These are mostly outer layer compositions, which were expected to provide a wider range of PCT values. However, these are not likely compositions to be selected for LAW processing at the WTP. Only those glasses with a PCT response of less than 2 g/m^2 were retained in the final regression set used for modeling, thereby reducing the Combined Matrix (Existing + Test Matrices) data set from 77 to 69 glasses. This is not an ideal solution, as preferably the modeling data set should have glasses with PCT

releases near and somewhat beyond the specification limit. However, the model performance was found to be degraded when additional glasses were retained because their PCT responses were much higher than for the rest of the data set.

The WTP PCT specification requires that the normalized mass losses of boron, sodium, and silicon in a seven-day PCT at 90°C be less than 2 g/m^2. However, a review of the data from the present work showed that the normalized PCT mass losses for boron and sodium were always higher than the normalized PCT mass loss for silicon. Furthermore, for every one of the 77 glasses in the Combined Matrix, the normalized PCT mass loss for silicon was below the WTP contract limit of 2 g/m^2. These results suggest that: (i) if the boron and sodium mass losses are below the WTP limit, so too will be the silicon mass loss, and (ii) the silicon mass loss does not exceed the WTP limit over the LAW glass composition region of interest. We therefore concluded that a model for silicon PCT response is not needed. Accordingly, with concurrence from WTP, only PCT boron and sodium releases were modeled.

The VHT and PCT data were fitted to linear mixture (LM) models and partial quadratic mixture (PQM) models and a variety of regression statistics were computed to assess the performance of the models. Validation of the models was performed in two ways. The primary method of validation was by data-splitting, in which a fraction of the modeling data set is left out of the model regression and the ability of the resulting model to predict the responses for the omitted data is assessed. The secondary method of validation assessed the ability of the models to predict the responses for a set of 59 glasses that composed the independent validation set (none of which were used in the model regression). The validation set was split into sub-sets based on the closeness of the glass compositions to the composition region defined by the Combined Matrix. Validation statistics were then computed for each of the subsets and the entire validation set.

For the VHT, reasonable LM and PQM models were identified (see Sections 5.3 and 5.4). However, the LM model showed significant lack-of-fit. This is likely a reflection of the complexity of the VHT process, which tends to accentuate non-linear effects of glass composition. Thus, it is reasonable that non-linear terms would be needed in the VHT model.

For PCT-Boron, an 11-term reduced LM model and a 14-term reduced PQM model were selected as the recommended ILAW Phase 1 models (see Section 6.3.4). Although the 14-term PQM model was superior by all modeling and validation measures, it was decided to also recommend the 11-term reduced LM model as one that might perform better than the 14-term reduced PQM model for future data sets. Hence, it is recommended that both these ILAW PCT-Boron models be applied and their performances compared during any future ILAW glass formulation and waste form qualification work.

For PCT-Sodium, an 11-term reduced LM model and a 16-term reduced PQM model were selected as the recommended ILAW Phase 1 models (see Section 6.4.4). Although the 16-term reduced PQM model appears to have significant advantages over the 11-term reduced LM model, it is recommended that both these ILAW PCT-Sodium models be applied and their performances compared during any future ILAW glass formulation and waste form qualification work.

SECTION 8
QUALITY ASSURANCE

The portions of this work that were performed at VSL were conducted under a quality assurance program based on NQA-1 (1989) and NQA-2a (1990) Part 2.7 that is in place at the VSL. This program is supplemented by a Quality Assurance Project Plan for WTP work [38] 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 [39]. This work was not subject to DOE/RW-0333P. This work was not subject to the requirements of WTP QAPjP [40] for environmental regulatory data.

Five of the existing glasses (LAWA44, LAWA54, LAWA56, LAWA88, and LAWA102) were prepared and characterized at VSL during Part B1 of the contract under BNFL. The remaining glasses were prepared and characterized during the Bechtel contract. An NQA-1 based QA program was in place during all of the work. Compositions of archived samples of Part B1 glasses were reanalyzed at the VSL as part of the present work and the results are presented in this report.

The QA requirements for the PNWD work were met through the Quality Assurance Project Plan [41] for the PNWD Waste Treatment Plant Support Project (WTPSP). The WTPSP implementing procedures [42] comply with the requirements of NQA-1 and NQA-2a Part 2.7.

SECTION 9
REFERENCES

[1] Swanberg, D.J., "LAW Glass Property Composition Modeling," BNI Test Specification, 24590-LAW-TSP-RT-01-013, Rev. 1, River Protection Project, Waste Treatment Plant, Richland, WA, November 27, 2001.

[2] Swanberg, D.J., "Statistics for HLW & LAW Glass Property-Composition Modeling," BNI Test Specification, 24590-WTP-TSP-RT-02-001, Rev. 0, River Protection Project, Waste Treatment Plant, Richland, WA, May 20, 2002.

[3] Gan, H., and Pegg, I.L., "LAW Glass Property-Composition Modeling," Test Plan, VSL-02T4800-1, Rev. 1, Vitreous State Laboratory, The Catholic University of America, Washington, DC, April 2002.

[4] Piepel, G.F., and Cooley, S.K., "Statistics for IHLW and ILAW Property-Composition Modeling," Test Plan, TP-RPP-WTP-179, Rev. 1, Battelle, Pacific Northwest Division, Richland, WA, July 2002.

[5] Rielley, E., Muller, I. S., and Pegg, I. L., "Preparation and Testing of LAW Matrix Glasses to Support WTP Property-Composition Model Development," VSL-04R4480-1, Rev. 0, Vitreous State Laboratory, The Catholic University of America, Washington, DC, April 21, 2004.

[6] Feng, Z, Perez-Cardenas, F., Gan, H., and Pegg, I. L., "Summary and Recommendations on Viscosity and Electrical Conductivity Model Forms to Support LAW Vitrification," VSL-03L4480-2, Rev. 1, Vitreous State Laboratory, The Catholic University of America, Washington, DC, October 22, 2004.

[7] Kot, W., Klatt, K., Muller, I.S., Will C.N., and Pegg, I.L., "Regulatory Spike Testing for RPP-WTP LAW and HLW Glasses," VSL-03R3760-1, Rev. 1, Vitreous State Laboratory, The Catholic University of America, Washington, DC, August 1, 2003.

[8] Cooley, S.K., Piepel, G.F., Gan, H., Muller, I.S., and Pegg, I.L., "Test Matrix to Support Property-Composition Model Development for RPP-WTP LAW Glasses", VSL-02S4600-3, Rev. 1, Vitreous State Laboratory, The Catholic University of America, Washington, DC, November 26, 2003.

[9] Kirkbride, R.A., et. al., "Tank Farm Contractor Operations and Utilization Plan," HNF-SD-WM-SP-012, Rev. 3A, CH2M Hill Hanford Group, Richland, WA, December 2001.

[10] Kirkbride, R.A., et. al., "Tank Farm Contractor Operations and Utilization Plan," HNF-SD-WM-SP-012, Rev. 2, CH2M Hill Hanford Group, Richland, WA, April 2000.

[11] Morrey, E.V., "LAW Pilot Melter and DM100 Sub-Envelope Changeover Testing," RPP-WTP Test Specification, 24590-LAW-TSP-RT-02-012, Rev 0, River Protection Project, Waste Treatment Plant, Richland, WA, August 13, 2002.

[12] Muller, I.S., Buechele, A.C., and Pegg, I.L., "Glass Formulation And Testing With RPP-WTP LAW Simulants," Final Report, VSL-01R3560-2, Rev. 0, Vitreous State Laboratory, The Catholic University of America, Washington, DC, February 23, 2001.

[13] Muller, I.S., Gan, H., and Pegg, I.L., "Physical and Rheological Properties of Waste Simulants and Melter Feeds for RPP-WTP LAW Vitrification," VSL-01R3520-1, Rev. 0, Vitreous State Laboratory, The Catholic University of America, Washington, DC, January 16, 2001.

[14] Muller, I.S. and Pegg, I.L., "Baseline LAW Glass Formulation Testing," VSL-03R3460-1, Rev. 0, Vitreous State Laboratory, The Catholic University of America, Washington, DC, August 5, 2003.

[15] Muller I.S. and Pegg, I.L., "Glass Formulations to Support Melter Testing", VSL-03R3460-2, Rev.0, Vitreous State Laboratory, The Catholic University of America, Washington, DC, February 5, 2004.

[16] Perez-Cardenas, F., Gan, H., and Pegg, I.L., Summary and Recommendations on VHT Model Form to Support LAW Vitrification, Letter Report VSL-03L3780-3, Rev. 0, Vitreous State Laboratory, The Catholic University of America, Washington, DC, September 15, 2003.

[17] Perez-Cardenas, F., Gan, H., and Pegg, I.L., Summary and Recommendations on PCT Model Form to Support LAW Vitrification, Letter Report VSL-03L4480-1, Rev. 0, Vitreous State Laboratory, The Catholic University of America, Washington, DC, November 10, 2003.

[18] Musick, C.A., "Updated Instructions for ILAW Regulatory Spike Testing," CCN 049799, River Protection Project, Waste Treatment Plant, Richland, WA, January 9, 2003.

[19] Piepel, G.F., Anderson, C.M., and Redgate, P.E., "Response Surface Designs for Irregularly-Shaped Regions" (Parts 1, 2, and 3), 1993 Proceedings of the Section on Physical and Engineering Sciences, pp. 205-227, American Statistical Association, Alexandria, VA, 1993.

[20] "Design, Construction, and Commissioning of the Hanford Tank Waste Treatment and Immobilization Plant", Contract Number: DE-AC27-01RV14136, Modification A029, U. S. Department of Energy, Office of River Protection, Richland WA, 2001, as amended.

[21] Pegg, I.L., Gan, H., Muller, I.S., McKeown, D.A., and Matlack, K.S., "Summary of Preliminary Results on Enhanced Sulfate Incorporation During Vitrification of LAW Feeds", VSL-00R3630-1, Rev. 1, Vitreous State Laboratory, The Catholic University of America, Washington, DC, April 5, 2000.

[22] Gan, H. and Pegg, I.L., Development of Property-Composition Models for RPP-WTP LAW Glasses, VSL-01R6600-1, Rev. 0, Vitreous State Laboratory, The Catholic University of America, Washington, D.C., August 6, 2001.

[23] Piepel, G.F., Szychowski, J.M. and Loeppky, J.L., "Augmenting Scheffé Linear Mixture Models with Squared and/or Crossproduct Terms", *Journal of Quality Technology*, 34, 297-314, 2002.

[24] Muller, I.S., and Pegg, I.L., "LAW Glass Formulation to Support AZ-102 Actual Waste Testing," Final Report, VSL-03R3470-1, Rev. 0, The Catholic University of America, Washington, DC, August 15, 2003.

[25] Muller, I.S., and Pegg, I.L., "LAW Glass Formulation to Support AP-101 Actual Waste Testing," Final Report, VSL-03R3470-2, Rev. 0, The Catholic University of America, Washington, DC, August 13, 2003.

[26] Muller, I.S., and Pegg, I.L., "LAW Glass Formulation to Support AZ-101 Actual Waste Testing," Final Report, VSL-03R3470-3, Rev. 0, The Catholic University of America, Washington, DC, September 17, 2003.

[27] Matlack, K.S., Morgan, S. and Pegg, I.L., "Melter Tests with LAW Envelope A and C Simulants to Support Enhanced Sulfate Incorporation", Report VSL-01R3501-2, Rev.0, January 26, 2001.

[28] "Products and Secondary Wastes Plan (PSWP)," RPP-WTP Project, PL-W375-TE00001, Rev. 0, April 12, 2000.

[29] Cornell, J.A., *Experiments with Mixtures*, Third Edition, John Wiley and Sons, NY, 2002.

[30] Vienna, J.D., Jorgensen, B.M., Jiricka, A., Smith, D.E., McGrail, B.P., Allen, B.R., Marra, J.C., Brown, K.G., Peeler, D.K., Reamer, I.A., Ebert, W.L., "Hanford Immobilized LAW Product Acceptance: Initial Tanks Focus Area Testing Data Package," PNNL-13101, Pacific Northwest National Laboratory, Richland, WA, February, 2000.

[31] Draper, N.R. and Smith, H., *Applied Regression Analysis*, Third Edition, John Wiley and Sons, Inc., New York, NY, 1998.

[32] Montgomery, D.C., Peck, E.A., and Vining, G.G., *Introduction to Linear Regression Analysis*, Third Edition, John Wiley and Sons, New York, NY, 2001.

[33] Piepel, G.F., "A Component Slope Linear Model for Mixture Experiments", PNWD-SA-6313, Rev. 1, Battelle–Pacific Northwest Division, Richland, WA, 2004.

[34] SAS (2001). *SAS Release 8.2*, SAS Institute, Inc., Cary. NC.

[35] Ihaka, R. and Gentleman, R., "R: A Language for Data Analysis and Graphics", *Journal of Computational and Graphical Statistics*, 5, 299-314, 1996.

[36] Hrma, P.R., Piepel, G.F., Schweiger, M.J., Smith, D.E., Kim, D.S., Redgate, P.E., Vienna, J.D., LoPresti, C.A., Simpson, D.B., Peeler, D.K., and Langowski, M.H. (1994), *Property/ Composition Relationships for Hanford High-Level Waste Glasses Melting at 1150℃*, PNL-10359, Volumes 1 and 2, Pacific Northwest Laboratory, Richland, WA, December 1994.

[37] Gan, H. and Pegg, I.L., Development of Property-Composition Models for RPP-WTP HLW Glasses, VSL-01R3600-1, Rev. 0, Vitreous State Laboratory, The Catholic University of America, Washington, D.C., July 30, 2001.

[38] "Quality Assurance Project Plan for RPP-WTP Support Activities Conducted by VSL," Vitreous State Laboratory, The Catholic University of America, Washington, DC, QAPP Rev. 6, 11/12/03.

[39] "Master List of Controlled VSL Manuals and Standard Operating Procedures in Use," QA-MLCP, Rev. 3, Vitreous State Laboratory, The Catholic University of America, Washington, DC, February 16, 2004.

[40] Blumenkranz, D., "Quality Assurance Project Plan for Testing Programs Generating Environmental Regulatory Data," PL-24590-QA00001, Rev. 0 (RPP-WTP-QAPjP), River Protection Project, Waste Treatment Plant, Richland, WA, June 7, 2001.

[41] PNWD, "River Protection Program-Waste Treatment Plant Support Project-Quality Assurance Project Plan," Rev. 2, Battelle–Pacific Northwest Division, Richland, WA, April, 2004.

[42] PNWD, "Waste Treatment Plant Support Project─Quality Assurance Requirements and Description," Rev. 2, Battelle–Pacific Northwest Division, Richland, WA, September 2004.

Table 2.1. Component Constraints [(a)] for ILAW Test Matrix.

Component	Inner Layer		Middle Layer		Outer Layer	
	Lower Bound (wt%)	**Upper Bound (wt%)**	**Lower Bound (wt%)**	**Upper Bound (wt%)**	**Lower Bound (wt%)**	**Upper Bound (wt%)**
Al_2O_3	6	7	5	8	3.5	9
B_2O_3	8	11	7	12	6	13
CaO	5	7	2	8	0	10
Fe_2O_3	3	5	2	6.5	0	8
K_2O	0.1	0.3	0.1	2	0	4
Li_2O	1	2.5	0.5	3	0	4.5
MgO	1.5	2.5	1	3.5	0	5
Na_2O	12 (Envelope C, Upper)	14 (Envelope A, Lower)	10 (Envelope C, Lower)	17 (Envelope A, Middle)	5 (Envelope B, Lower)	22 (Envelope A, Upper)
SiO_2	45	48	42	50	40	52
SO_3	0.1[(b)]	1[(b)]	0.1[(b)]	1[(b)]	0.1[(b)]	1
TiO_2	1	2	0.5	2.5	0	3
ZnO	3.5	4.6	2	5	1	5
ZrO_2	2	3	1	3.5	0	4
Others	0.05	2	0.05	2	0.05	2
Runs	14 plus the center-point of the inner layer		20		15 outer layer runs in addition to 21 existing LAW glasses.	
Cumulative number of glasses	15		35		71 (including the 21 existing glasses, but excluding the 6 replicates)	

(a) The wt% values of the components Al_2O_3 to Others are constrained to sum to 100% for every glass.
(b) The achieved range of SO_3 is 0.346 – 0.425 wt% for the inner layer, 0.236 – 0.560 wt% for the middle layer, and 0.160 – 1.0 wt% for the outer layer.

Table 2.2. Property Constraints for ILAW Test Matrix.

Property	Lower Limit	Upper Limit
Viscosity at 1150°C (η_{1150})	10 poise	100 poise
Electrical Conductivity at 1150°C (σ_{1150})	0.2 S/cm (inner, middle layers) 0.1 S/cm (outer layer)	0.6 S/cm (inner, middle layers) 0.7 S/cm (outer layer)
7-Day B PCT (r_B^{PCT})	(a)	2 g/l (inner, middle layers) 4 g/l (outer layer)
7-Day Na PCT (r_{Na}^{PCT})	(a)	2 g/l (inner, middle layers) 4 g/l (outer layer)
7-Day Si PCT (r_{Si}^{PCT})	(a)	2 g/l (inner, middle layers) 4 g/l (outer layer)
Sulfur Incorporation		
Wt% SO_3 for Inner Layer	-0.02959 Na_2O + 0.76	-0.02959 Na_2O + 0.78
Wt% SO_3 for Middle Layer	-0.023529 Na_2O + 0.635294	-0.032922 Na_2O + 0.888888
Wt% SO_3 for Outer Layer	-0.014118 Na_2O + 0.470588	-0.0453 Na_2O + 1.52

(a) No lower bound constraint imposed.

Table 2.3. Model-Based[(a)] Glass Property Constraints for ILAW Test Matrix.

Property		Viscosity	Electrical Conductivity	PCT-B	PCT-Na	PCT-Si
Modeled Response		$\ln(\eta_{1150})$	$\ln(\sigma_{1150})$	$\ln(r_B^{PCT})$	$\ln(r_{Na}^{PCT})$	$\ln(r_{Si}^{PCT})$
Units		ln(poise)	ln(S/cm)	ln(g/l)	ln(g/l)	ln(g/l)
Components (wt%)		**Constraint Coefficients, Lower and Upper Bounds**				
Al_2O_3		-0.18657	-0.01728	-0.118843	-0.136346	-0.07013
B_2O_3		-0.02217	+0.023548	+0.086761	-0.039907	-0.01172
CaO		-0.0361966	-0.02433	-0.042865	-0.032381	-0.0286
Fe_2O_3		+0.0390715	-0.01971	-0.012574	-0.085602	-0.00444
K_2O		-0.0282883	-0.03656	+0.084951	+0.071036	+0.05056
Li_2O		-0.290011	+0.206174	+0.333015	+0.234093	+0.20773
MgO		+0.0117262	-0.09654	+0.257082	+0.217455	+0.123
Na_2O		-0.044155	+0.114266	+0.132831	+0.079692	+0.08841
SiO_2		+0.1485	-0.01638	-0.070351	-0.10662	-0.01381
SO_3		(b)	(b)	+0.105346	+0.006431	+0.09766
TiO_2		-0.022756	(b)	+0.013925	-0.01047	+0.05648
ZnO		+0.05186	-0.01459	-0.15096	-0.264853	-0.09995
ZrO_2		+0.09522	-0.07185	-0.218869	-0.259572	-0.13203
Others		+0.016989	(b)	-0.0624969	-0.065025	-0.102079
Lower Bound	Outer Layer	5.30295 (e),(f)	-0.577345	(c)	(c)	(c)
	Inner & Middle Layers		0.115802			
Upper Bound	Outer Layer	7.60553	1.36857	-0.267129	-4.635913	2.555237 (d)
	Inner & Middle Layers		1.21441 (f)	-0.426018 (f)	-5.32906 (f)	1.86209 (e),(f)

(a) Intercepts in the original property-composition models of the form $\ln(\text{property}) = A_0 + \Sigma A_i x_i$ are incorporated into the lower and upper bounds of the constraint expressions so that $LB \leq \Sigma A_i x_i \leq UB$.
(b) A blank cell indicates the component has a minor effect on the property and is not included in the model used to form the constraint. The coefficients for these components were set to zero (i.e., they were simply not included in the regression).
(c) No lower bounds were imposed for these properties.
(d) Constraint unnecessary (i.e., unachievable) for the outer layer.
(e) Constraint unnecessary (i.e., unachievable) for the middle layer.
(f) Constraint unnecessary (i.e., unachievable) for the inner layer

Table 2.4. Target Compositions of Test Matrix Glasses (wt%).

Glass ID	Run [(a)] Order	Layer	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SiO_2	SO_3	TiO_2	ZnO	ZrO_2	Others [(b)]	Sum
LAWM1	36	Outer	9.00	6.00	10.00	8.00	4.00	4.50	0.00	5.00	44.45	1.00	3.00	5.00	0.00	0.05	100
LAWM2	41	Outer	3.50	6.00	10.00	8.00	0.00	4.50	5.00	5.00	47.00	1.00	3.00	5.00	0.00	2.00	100
LAWM3	29	Outer	9.00	6.00	10.00	8.00	0.00	4.47	5.00	11.48	40.00	1.00	0.00	1.00	4.00	0.05	100
LAWM4	24	Outer	3.50	13.00	10.00	5.54	4.00	4.50	0.00	5.00	41.41	1.00	3.00	5.00	4.00	0.05	100
LAWM5	31	Outer	9.00	6.00	5.77	8.00	4.00	4.50	0.00	5.00	48.68	1.00	3.00	1.00	4.00	0.05	100
LAWM6	55	Outer	9.00	10.61	10.00	8.00	4.00	0.00	5.00	9.00	40.00	0.34	3.00	1.00	0.00	0.05	100
LAWM7	45	Outer	5.43	6.94	10.00	8.00	0.00	2.58	5.00	5.00	52.00	1.00	3.00	1.00	0.00	0.05	100
LAWM8	38	Outer	9.00	13.00	6.43	0.00	0.00	2.08	5.00	5.00	44.49	1.00	3.00	5.00	4.00	2.00	100
LAWM9	15	Outer	3.50	6.00	10.00	8.00	4.00	2.39	0.00	5.00	49.71	0.40	0.00	5.00	4.00	2.00	100
LAWM10	5	Outer	9.00	13.00	10.00	0.00	0.00	4.50	0.00	13.07	40.15	0.28	3.00	1.00	4.00	2.00	100
LAWM11	56	Outer	3.50	13.00	9.40	5.31	4.00	4.50	0.00	11.48	46.76	1.00	0.00	1.00	0.00	0.05	100
LAWM12	22	Outer	3.50	13.00	0.00	2.31	4.00	4.50	1.97	14.25	42.20	0.27	3.00	5.00	4.00	2.00	100
LAWM13	28	Outer	3.50	6.00	10.00	8.00	3.79	0.00	0.00	22.00	40.00	0.52	3.00	2.16	0.00	1.03	100
LAWM14	35	Outer	3.50	6.00	2.05	0.00	0.00	0.88	5.00	22.00	52.00	0.52	3.00	5.00	0.00	0.05	100
LAWM15	16	Outer	9.00	9.36	0.00	6.28	0.00	0.00	3.72	22.00	43.48	0.16	3.00	1.00	0.00	2.00	100
LAWM16	8	Middle	8.00	12.00	8.00	6.50	0.10	3.00	1.00	10.00	42.45	0.40	2.50	5.00	1.00	0.05	100
LAWM17	19	Middle	5.00	12.00	2.21	6.50	2.00	0.50	3.50	17.00	42.00	0.24	0.50	5.00	3.50	0.05	100
LAWM18	46	Middle	8.00	12.00	8.00	6.50	0.10	3.00	1.00	10.00	42.00	0.40	2.50	2.00	2.50	2.00	100
LAWM19	43	Middle	8.00	12.00	8.00	2.00	2.00	0.50	1.00	13.17	42.00	0.33	0.50	5.00	3.50	2.00	100
LAWM20	6	Middle	5.00	7.00	8.00	2.00	2.00	2.26	3.50	17.00	42.00	0.24	0.50	5.00	3.50	2.00	100
LAWM21	32	Middle	5.00	10.89	8.00	6.50	2.00	3.00	1.00	10.00	42.00	0.56	2.50	5.00	3.50	0.05	100
LAWM22	40	Middle	8.00	7.00	2.00	6.50	2.00	0.50	3.50	17.00	42.00	0.33	0.67	5.00	3.50	2.00	100
LAWM23	7	Middle	5.00	7.00	8.00	2.00	2.00	3.00	1.00	10.00	48.44	0.56	2.50	5.00	3.50	2.00	100
LAWM24	42	Middle	8.00	12.00	2.00	6.50	2.00	0.64	1.00	17.00	47.07	0.24	0.50	2.00	1.00	0.05	100
LAWM25	30	Middle	8.00	12.00	2.00	3.68	2.00	3.00	3.50	10.00	49.92	0.40	0.50	2.00	1.00	2.00	100
LAWM26	39	Middle	8.00	12.00	4.97	2.00	0.10	3.00	1.00	10.00	49.87	0.56	0.50	5.00	1.00	2.00	100
LAWM27	26	Middle	8.00	7.00	8.00	6.50	2.00	0.50	3.50	13.37	42.00	0.32	2.50	3.31	1.00	2.00	100
LAWM28	49	Middle	5.00	12.00	8.00	6.50	0.70	0.69	1.00	10.00	50.00	0.56	2.50	2.00	1.00	0.05	100
LAWM29	34	Middle	7.56	7.00	2.00	6.50	2.00	3.00	3.50	10.00	46.85	0.40	2.50	5.00	3.50	0.19	100
LAWM30	48	Middle	8.00	12.00	2.00	6.50	0.10	2.02	1.00	17.00	42.00	0.24	0.59	5.00	3.50	0.05	100

(a) Random order in which glasses were batched and melted.
(b) The composition of the "Others" component is given in Table 2.5.

Table 2.4. Target Compositions of Test Matrix Glasses (wt%)(continued).

Glass ID	Run [(a)] Order	Layer	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SiO_2	SO_3	TiO_2	ZnO	ZrO_2	Others [(b)]	Sum
LAWM31	14	Middle	5.00	7.00	8.00	6.50	0.10	3.00	1.00	16.75	42.31	0.34	2.50	2.00	3.50	2.00	100
LAWM32	11	Middle	5.14	7.00	2.00	2.00	2.00	3.00	3.50	16.51	50.00	0.35	0.50	5.00	1.00	2.00	100
LAWM33	10	Middle	5.00	12.00	8.00	6.50	1.72	0.90	1.00	17.00	42.00	0.33	2.50	2.00	1.00	0.05	100
LAWM34	13	Middle	5.00	8.35	8.00	6.29	2.00	3.00	1.00	17.00	42.00	0.33	1.48	2.00	3.50	0.05	100
LAWM35	1	Middle	5.00	12.00	6.18	4.41	0.10	0.50	3.50	17.00	42.00	0.24	2.50	2.00	2.57	2.00	100
LAWM36	12	Inner	7.00	11.00	7.00	5.00	0.30	2.50	1.50	12.00	45.00	0.40	2.00	3.50	2.00	0.80	100
LAWM37	21	Inner	6.75	11.00	7.00	5.00	0.30	2.50	2.50	12.00	45.00	0.40	1.00	3.50	3.00	0.05	100
LAWM38	54	Inner	7.00	8.00	7.00	3.00	0.15	2.50	1.50	14.00	48.00	0.35	1.00	3.50	2.00	2.00	100
LAWM39	2	Inner	7.00	9.05	5.00	3.00	0.10	2.50	2.50	14.00	48.00	0.35	1.00	3.50	2.00	2.00	100
LAWM40	50	Inner	6.00	11.00	5.00	5.00	0.10	1.00	1.50	14.00	48.00	0.37	1.00	3.50	3.00	0.53	100
LAWM41	37	Inner	7.00	8.00	7.00	5.00	0.30	1.00	2.50	14.00	45.00	0.37	1.00	4.60	2.23	2.00	100
LAWM42	18	Inner	6.00	8.00	5.00	4.03	0.10	2.50	1.50	14.00	48.00	0.37	2.00	3.50	3.00	2.00	100
LAWM43	47	Inner	7.00	8.68	5.00	5.00	0.30	2.50	2.50	12.00	45.00	0.42	2.00	4.60	3.00	2.00	100
LAWM44	44	Inner	6.32	10.03	7.00	5.00	0.10	1.00	1.50	12.00	48.00	0.40	2.00	4.60	2.00	0.05	100
LAWM45	20	Inner	7.00	8.00	5.78	5.00	0.30	1.42	1.50	14.00	48.00	0.35	2.00	4.60	2.00	0.05	100
LAWM46	4	Inner	6.00	11.00	6.51	5.00	0.10	1.00	2.50	12.00	47.94	0.40	1.00	3.50	3.00	0.05	100
LAWM47	17	Inner	6.20	8.00	7.00	5.00	0.10	1.00	2.50	14.00	48.00	0.34	1.31	3.50	3.00	0.05	100
LAWM48	9	Inner	6.23	11.00	5.27	5.00	0.10	1.00	1.50	12.00	48.00	0.40	2.00	3.50	2.00	2.00	100
LAWM49	53	Inner	7.00	10.90	5.00	3.00	0.10	1.00	1.50	14.00	47.53	0.37	1.00	4.60	2.00	2.00	100
LAWM50	52	Center	6.52	9.69	6.10	4.11	0.20	1.67	2.03	13.08	46.94	0.38	1.53	4.10	2.53	1.12	100
Replicates		**Replicate Of**															
LAWM51	25	LAWM50	6.52	9.69	6.10	4.11	0.20	1.67	2.03	13.08	46.94	0.38	1.53	4.10	2.53	1.12	100
LAWM52	23	LAWA88	6.08	9.70	1.99	5.53	2.58	0.00	1.47	20.00	43.99	0.21	1.99	2.95	2.99	0.52	100
LAWM53	3	LAWM1	9.00	6.00	10.00	8.00	4.00	4.50	0.00	5.00	44.45	1.00	3.00	5.00	0.00	0.05	100
LAWM54	33	LAWM9	3.50	6.00	10.00	8.00	4.00	2.39	0.00	5.00	49.71	0.40	0.00	5.00	4.00	2.00	100
LAWM55	27	LAWM12	3.50	13.00	0.00	2.31	4.00	4.50	1.97	14.25	42.20	0.27	3.00	5.00	4.00	2.00	100
LAWM56	51	LAWM35	5.00	12.00	6.18	4.41	0.10	0.50	3.50	17.00	42.00	0.24	2.50	2.00	2.57	2.00	100

(a) Random order in which glasses were batched and melted.
(b) The composition of the "Others" component is given in Table 2.5.

Table 2.5. Composition of the Grouped Component "Others" for ILAW 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 2.6. Target Glass Compositions of Existing Matrix Glasses (wt%).

Glass ID	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SiO_2	SO_3	TiO_2	ZnO	ZrO_2	Cl	Cr_2O_3	Cs_2O	F	NiO	P_2O_5	Re_2O_7	Sum
LAWA44R10	6.20	8.90	1.99	6.98	0.50	0.00	1.99	20.00	44.55	0.10	1.99	2.96	2.99	0.65	0.02	0.00	0.01	0.00	0.03	0.10	100
LAWA53	6.09	6.11	7.77	7.40	0.49	0.00	1.46	19.72	41.66	1.48[(a)]	1.09	2.95	2.95	0.64	0.02	0.00	0.01	0.00	0.03	0.10	100
LAWA56	6.09	11.93	1.95	7.40	0.49	0.00	1.46	19.72	41.66	1.48[(a)]	1.09	2.95	2.95	0.64	0.02	0.00	0.01	0.00	0.03	0.10	100
LAWA88R1	6.08	9.70	1.99	5.53	2.58	0.00	1.47	20.00	43.99	0.21	1.99	2.95	2.99	0.33	0.01	0.00	0.00	0.00	0.07	0.10	100
LAWA102R1	6.06	10.00	5.07	5.41	0.26	2.50	1.50	14.49	46.60	2.50[(a)]	1.14	3.06	3.02	0.33	0.02	0.00	0.03	0.00	0.13	0.10	102[*]
LAWA126	5.64	9.82	1.99	5.54	3.88	0.00	1.48	18.46	44.12	0.35	2.00	2.96	2.99	0.20	0.02	0.16	0.30	0.00	0.08	0.10	100
LAWA128	6.03	7.07	2.08	5.79	3.88	0.00	1.18	18.46	46.09	0.35	2.09	3.09	3.13	0.20	0.02	0.16	0.30	0.00	0.08	0.10	100
LAWA130	6.03	8.95	2.08	2.86	3.88	0.00	1.18	18.46	46.09	0.35	2.09	4.14	3.13	0.20	0.02	0.16	0.30	0.00	0.08	0.10	100
LAWB65	6.17	9.91	6.67	5.28	0.26	4.29	2.96	5.46	48.35	1.28[(a)]	1.39	4.65	3.15	0.00	0.10	0.00	0.07	0.00	0.01	0.10	100
LAWB66	6.17	9.91	8.17	5.28	0.26	4.29	2.96	5.46	48.35	1.28[(a)]	1.39	3.15	3.15	0.00	0.10	0.00	0.07	0.00	0.01	0.10	100
LAWB68	6.17	8.41	8.17	5.28	0.26	4.29	2.96	5.46	48.35	1.28[(a)]	1.39	4.65	3.15	0.00	0.10	0.00	0.07	0.00	0.01	0.10	100
LAWB78	6.15	12.33	7.12	3.25	0.23	3.05	2.97	9.78	47.00	0.78	0.00	4.00	3.15	0.01	0.05	0.00	0.08	0.00	0.05	0.10	100
LAWB79	6.15	12.33	7.12	3.25	0.23	3.51	2.97	8.62	47.70	0.78	0.00	4.00	3.15	0.01	0.05	0.00	0.08	0.00	0.05	0.10	100
LAWB80	6.15	12.33	7.12	3.25	1.99	3.51	2.97	6.62	47.95	0.78	0.00	4.00	3.15	0.01	0.05	0.00	0.08	0.00	0.05	0.10	100
LAWB83	6.18	10.03	6.78	5.29	0.19	4.31	2.97	5.47	48.60	0.65	1.39	4.84	3.16	0.01	0.04	0.00	0.06	0.00	0.04	0.10	100
LAWB84	6.18	10.03	6.68	5.29	0.19	4.40	2.97	5.47	48.60	0.65	1.39	4.84	3.16	0.01	0.04	0.00	0.06	0.00	0.04	0.10	100
LAWB85	6.18	11.52	5.28	5.29	0.19	4.31	2.97	5.47	48.60	0.65	1.39	4.84	3.16	0.01	0.04	0.00	0.06	0.00	0.04	0.10	100
LAWB86	6.18	12.41	5.73	5.29	0.19	4.35	2.97	5.47	48.60	0.65	0.00	4.84	3.16	0.01	0.04	0.00	0.06	0.00	0.04	0.10	100
C100-G-136B	6.12	10.08	6.40	6.47	0.15	2.73	1.51	11.86	46.67	0.63	1.12	3.01	3.02	0.12	0.02	0.00	0.06	0.02	0.12	0.0	100
LAWC27	6.12	12.19	8.55	0.01	0.14	2.73	1.50	11.96	48.88	0.48	1.12	3.02	3.02	0.11	0.02	0.00	0.05	0.00	0.11	0.10	100
LAWC32	6.49	10.05	9.04	2.42	0.14	2.73	1.50	11.96	46.74	0.48	1.12	4.02	3.02	0.11	0.02	0.00	0.05	0.00	0.11	0.10	100

(a) Excess SO_3 was added to test saturation sulfate solubility in the glass. For property-composition modeling, the SO_3 value as measured by XRF was used.

Table 4.1. VHT Results for Test Matrix Glasses.

Glass Name	Alteration Depth (μm)	Days	Measured Density (g/cc)	Rate ($g/m^2/d$) Calculated for Measured Density	Comparison to Limit of 50 $g/m^2/d$
Contract limit	**-[(a)]**	**>7**	**-**	**50**	**-**
LAWM1	82	24	2.74	9.42	19%
LAWM2	75	24	2.76	8.61	17%
LAWM3	34	24	2.65	3.75	8%
LAWM4	5	24	2.72	0.57	1%
LAWM5	7	24	2.80	0.82	2%
LAWM6	19	24	2.66	2.11	4%
LAWM7	26	24	2.66	2.88	6%
LAWM8	13	24	2.85	1.54	3%
LAWM9	1	24	2.66	0.11	0%
LAWM10	114	24	2.65	12.57	25%
LAWM11	700	24	2.62	76.52	153%
LAWM12	> 1100	24	2.68	> 122	> 246%
LAWM13	> 1100	24	2.61	> 119	> 239%
LAWM14	> 1000	24	2.62	> 120	> 241%
LAWM15	856	24	2.67	95.05	190%
LAWM16	71	24	2.65	7.84	16%
LAWM17	3	24	2.65	0.33	1%
LAWM18	15	24	2.57	1.61	3%
LAWM19	1	24	2.58	0.11	0%
LAWM20	116	24	2.83	13.69	27%
LAWM21	9	24	2.77	1.04	2%
LAWM22	2	24	2.70	0.22	0%
LAWM23	9	24	2.70	1.01	2%
LAWM24	123	24	2.67	13.71	27%
LAWM25R1	41	24	2.48	4.24	8%
LAWM26	31	24	2.62	3.38	7%
LAWM27	45	24	2.70	5.07	10%
LAWM28	6	24	2.58	0.65	1%

(a) A dash (-) indicates an empty data field.

Table 4.1. VHT Results for Test Matrix Glasses (continued).

Glass Name	Alteration Depth (μm)	Days	Measured Density (g/cc)	Rate ($g/m^2/d$) Calculated for Measured Density	Comparison to Limit of 50 $g/m^2/d$
Contract limit	**-[a]**	**>7**	**-**	**50**	**-**
LAWM29	9	24	2.67	1.00	2%
LAWM30	181[b]	24	2.72	21.29	43%
LAWM31	48	24	2.73	5.46	11%
LAWM32	> 1100	24	2.63	> 120	> 241%
LAWM33R1	34	24	2.67	3.78	8%
LAWM34	420	24	2.78	48.71	97%
LAWM35	4[b]	24	2.53	0.95	2%
LAWM36	107	24	2.54	11.34	23%
LAWM37	10	24	2.58	1.07	2%
LAWM38	171	24	2.76	19.68	39%
LAWM39	112	24	2.65	12.36	25%
LAWM40	3	24	2.49	0.31	1%
LAWM41	43	24	2.65	4.75	9%
LAWM42	7	24	2.65	0.77	2%
LAWM43	9	24	2.66	1.00	2%
LAWM44	20[b]	24	2.55	2.23	4%
LAWM45	44	24	2.70	4.95	10%
LAWM46	3	24	2.66	0.33	1%
LAWM47	25	24	2.77	2.88	6%
LAWM48	5	24	2.85	0.59	1%
LAWM49	23	24	2.57	2.47	5%
LAWM50	4	24	2.66	0.44	1%
LAWM51	5	24	2.59	0.54	1%
LAWM52	28	24	2.65	3.09	6%
LAWM53	90	24	2.73	10.24	20%
LAWM54R1	3	24	2.52	0.31	1%
LAWM55	> 1100	24	2.73	> 125	> 250%
LAWM56	6	24	2.73	0.68	1%

(a) A dash (-) indicates an empty data field.
(b) Values reflect averaging correction made after the electronic data set was submitted to WTP.

Table 4.2. VHT Results for Existing Matrix Glasses.

Glass Name[(a)]	Alteration Depth (μm)	Days	Measured Density (g/cc)	Rate ($g/m^2/d$) [(b)]	Compared to Limit of 50 $g/m^2/d$
LAWA44R10	9	24	2.67	1.0	2.00%
LAWA53*	7.4	23.5	-[(c)]	0.8	1.67%
LAWA56*	15	23.5	-	1.7	3.39%
LAWA88R1	13	24	2.67	1.4	2.89%
LAWA102R1**	34	24	2.61	3.7	7.40%
LAWA126**	22	24	2.687	2.5	4.93%
LAWA128	8	24	-	0.9	1.77%
LAWA130**	6	24	-	0.7	1.33%
LAWB65**	10.4	24	-	1.1	2.30%
LAWB66**	17	24	-	1.9	3.76%
LAWB68**	18	24	-	2.0	3.98%
LAWB78**	23	24	-	2.5	5.09%
LAWB79**	11	24	-	1.2	2.43%
LAWB80**	10	24	-	1.1	2.21%
LAWB83**	16	24	2.75	1.8	3.67%
LAWB84**	15	24	-	1.7	3.32%
LAWB85**	11	24	-	1.2	2.43%
LAWB86**	15	24	-	1.7	3.32%
C100G136B*	23	24	2.65	2.5	5.08%
LAWC27**	177	24	-	19.5	39.09%
LAWC32**	206	24	-	22.7	45.49%

(a) A * denotes the data were reported in [12]. A ** denotes the data were reported in [14].
(b) Rate calculated with measured density if available or with an average density of 2.65 g/cc.
(c) A dash (-) indicates an empty data field.

Table 4.3. Target Compositions of Test Matrix Glasses (mol %).

Oxide	LAWM1	LAWM2	LAWM3	LAWM4	LAWM5	LAWM6	LAWM7	LAWM8	LAWM9
Al_2O_3	5.77	2.09	5.57	2.23	5.86	5.88	3.32	5.53	2.25
B_2O_3	5.64	5.24	5.43	12.11	5.72	10.15	6.23	11.70	5.65
BaO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CaO	11.66	10.83	11.24	11.56	6.82	11.87	11.14	7.18	11.68
CdO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01
Cl	0.04	1.37	0.04	0.04	0.04	0.04	0.04	1.41	1.48
Cr_2O_3	0.00	0.13	0.00	0.00	0.00	0.00	0.00	0.13	0.14
F	0.03	0.96	0.02	0.03	0.03	0.03	0.02	0.99	1.03
Fe_2O_3	3.28	3.04	3.16	2.25	3.32	3.34	3.13	0.00	3.28
K_2O	2.78	0.00	0.00	2.75	2.82	2.83	0.00	0.00	2.78
Li_2O	9.85	9.15	9.44	9.77	9.99	0.00	5.39	4.36	5.24
MgO	0.00	7.54	7.82	0.00	0.00	8.26	7.75	7.77	0.00
Na_2O	5.28	4.90	11.68	5.23	5.35	9.67	5.04	5.05	5.29
NiO	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.03	0.03
P_2O_5	0.01	0.43	0.01	0.01	0.01	0.01	0.01	0.44	0.46
PbO	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.01
SiO_2	48.38	47.52	41.97	44.69	53.75	44.33	54.04	46.38	54.20
SO_3	0.82	0.76	0.79	0.81	0.83	0.29	0.78	0.78	0.33
TiO_2	2.46	2.28	0.00	2.43	2.49	2.50	2.34	2.35	0.00
ZnO	4.02	3.73	0.77	3.98	0.82	0.82	0.77	3.85	4.02
ZrO_2	0.00	0.00	2.05	2.10	2.15	0.00	0.00	2.03	2.13
Sum	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00

Table 4.3. Target Compositions of Test Matrix Glasses (mol %) (continued).

Oxide	LAWM10	LAWM11	LAWM12	LAWM13	LAWM14	LAWM15	LAWM16	LAWM17	LAWM18	LAWM19	LAWM20	LAWM21	LAWM22	LAWM23	LAWM24
Al_2O_3	5.46	2.14	2.16	2.28	2.10	5.76	5.11	3.27	5.06	5.13	3.05	3.22	5.22	3.07	5.25
B_2O_3	11.55	11.64	11.72	5.73	5.26	8.77	11.23	11.49	11.12	11.28	6.25	10.26	6.69	6.30	11.53
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	11.03	10.45	0.00	11.85	2.23	0.00	9.29	2.63	9.20	9.33	8.87	9.36	2.37	8.94	2.38
CdO	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.00
Cl	1.40	0.04	1.42	0.77	0.03	1.47	0.04	0.04	1.46	1.48	1.40	0.04	1.50	1.42	0.04
Cr_2O_3	0.13	0.00	0.13	0.07	0.00	0.14	0.00	0.00	0.14	0.14	0.13	0.00	0.14	0.13	0.00
F	0.97	0.02	0.99	0.54	0.02	1.03	0.03	0.03	1.02	1.03	0.98	0.03	1.05	0.99	0.03
Fe_2O_3	0.00	2.07	0.91	3.33	0.00	2.57	2.65	2.71	2.63	0.82	0.78	2.67	2.71	0.79	2.72
K_2O	0.00	2.65	2.67	2.67	0.00	0.00	0.07	1.42	0.07	1.39	1.32	1.39	1.41	1.33	1.42
Li_2O	9.31	9.39	9.46	0.00	1.80	0.00	6.54	1.12	6.48	1.09	4.71	6.58	1.11	6.29	1.43
MgO	0.00	0.00	3.07	0.00	7.58	6.03	1.62	5.79	1.60	1.62	5.40	1.63	5.77	1.56	1.66
Na_2O	13.04	11.54	14.44	23.58	21.68	23.16	10.51	18.29	10.41	13.91	17.05	10.58	18.24	10.12	18.34
NiO	0.02	0.00	0.03	0.01	0.00	0.03	0.00	0.00	0.03	0.03	0.02	0.00	0.03	0.03	0.00
P_2O_5	0.43	0.01	0.44	0.24	0.01	0.46	0.01	0.01	0.45	0.46	0.44	0.01	0.47	0.44	0.01
PbO	0.01	0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.00
SiO_2	41.32	48.50	44.09	44.23	52.84	47.20	46.01	46.60	45.09	45.72	43.44	45.84	46.48	50.54	52.38
SO_3	0.22	0.78	0.21	0.43	0.40	0.13	0.33	0.20	0.32	0.27	0.18	0.46	0.27	0.44	0.20
TiO_2	2.32	0.00	2.36	2.49	2.29	2.45	2.04	0.42	2.02	0.41	0.39	2.05	0.56	1.96	0.42
ZnO	0.76	0.77	3.86	1.77	3.75	0.80	4.00	4.10	1.59	4.02	3.82	4.03	4.08	3.85	1.64
ZrO_2	2.01	0.00	2.04	0.00	0.00	0.00	0.53	1.89	1.31	1.86	1.77	1.86	1.89	1.78	0.54
Sum	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00

Table 4.3. Target Compositions of Test Matrix Glasses (mol %) (continued).

Oxide	LAWM25	LAWM26	LAWM27	LAWM28	LAWM29	LAWM30	LAWM31	LAWM32	LAWM33	LAWM34	LAWM35	LAWM36	LAWM37	LAWM38	LAWM39	LAWM40
Al_2O_3	4.90	4.90	5.11	3.21	4.84	5.25	3.12	3.09	3.23	3.17	3.13	4.41	4.25	4.29	4.28	3.84
B_2O_3	10.76	10.77	6.55	11.30	6.57	11.53	6.40	6.15	11.34	7.75	11.01	10.14	10.14	7.19	8.12	10.32
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	0.00
CaO	2.23	5.53	9.30	9.35	2.33	2.38	9.08	2.18	9.38	9.22	7.04	8.01	8.01	7.81	5.56	5.82
CdO	0.00	0.00	0.01	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
Cl	1.41	1.41	1.47	0.04	0.14	0.04	1.44	1.38	0.04	0.04	1.44	0.58	0.04	1.41	1.41	0.39
Cr_2O_3	0.13	0.13	0.14	0.00	0.01	0.00	0.13	0.13	0.00	0.00	0.14	0.05	0.00	0.13	0.13	0.04
F	0.98	0.98	1.03	0.03	0.10	0.03	1.00	0.96	0.03	0.03	1.01	0.40	0.03	0.99	0.98	0.27
Fe_2O_3	1.44	0.78	2.65	2.67	2.66	2.72	2.59	0.77	2.68	2.55	1.76	2.01	2.01	1.18	1.17	2.04
K_2O	1.33	0.07	1.38	0.49	1.39	0.07	0.07	1.30	1.20	1.37	0.07	0.20	0.20	0.10	0.07	0.07
Li_2O	6.27	6.27	1.09	1.51	6.56	4.53	6.39	6.14	1.98	6.49	1.07	5.37	5.37	5.23	5.22	2.19
MgO	5.42	1.55	5.66	1.63	5.67	1.66	1.58	5.31	1.63	1.60	5.55	2.39	3.98	2.33	3.87	2.43
Na_2O	10.07	10.08	14.06	10.58	10.54	18.34	17.21	16.30	18.04	17.72	17.53	12.43	12.43	14.13	14.10	14.75
NiO	0.03	0.03	0.03	0.00	0.00	0.00	0.03	0.02	0.00	0.00	0.03	0.01	0.00	0.03	0.03	0.01
P_2O_5	0.44	0.44	0.46	0.01	0.04	0.01	0.45	0.43	0.01	0.01	0.45	0.18	0.01	0.44	0.44	0.12
PbO	0.01	0.01	0.01	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.00	0.00	0.01	0.01	0.00
SiO_2	51.85	51.86	45.56	54.54	50.92	46.74	44.84	50.91	45.97	45.17	44.66	48.07	48.07	49.97	49.85	52.17
SO_3	0.31	0.44	0.26	0.46	0.33	0.20	0.27	0.26	0.27	0.27	0.19	0.32	0.32	0.27	0.27	0.30
TiO_2	0.39	0.39	2.04	2.05	2.04	0.50	1.99	0.38	2.06	1.19	2.00	1.61	0.80	0.78	0.78	0.82
ZnO	1.53	3.84	2.65	1.61	4.01	4.11	1.56	3.76	1.62	1.59	1.57	2.76	2.76	2.69	2.68	2.81
ZrO_2	0.51	0.51	0.53	0.53	1.85	1.90	1.81	0.50	0.53	1.84	1.34	1.04	1.56	1.02	1.01	1.59
Sum	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00

Table 4.3. Target Compositions of Test Matrix Glasses (mol %) (continued).

Oxide	LAWM41	LAWM42	LAWM43	LAWM44	LAWM45	LAWM46	LAWM47	LAWM48	LAWM49	LAWM50	LAWM51	LAWM52	LAWM53	LAWM54	LAWM55	LAWM56
Al_2O_3	4.42	3.72	4.39	4.05	4.48	3.83	3.94	3.95	4.40	4.10	4.10	4.01	5.77	2.25	2.16	3.13
B_2O_3	7.40	7.27	7.96	9.41	7.49	10.27	7.45	10.22	10.04	8.92	8.92	9.37	5.64	5.65	11.72	11.01
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	0.00
CaO	8.04	5.64	5.70	8.16	6.72	7.55	8.09	6.08	5.72	6.98	6.98	2.39	11.66	11.68	0.00	7.04
CdO	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00
Cl	1.45	1.43	1.44	0.04	0.04	0.04	0.04	1.46	1.45	0.81	0.81	0.62	0.04	1.48	1.42	1.44
Cr_2O_3	0.14	0.13	0.14	0.00	0.00	0.00	0.00	0.14	0.14	0.08	0.08	0.00	0.00	0.14	0.13	0.14
F	1.01	1.00	1.01	0.03	0.03	0.03	0.03	1.02	1.01	0.56	0.56	0.00	0.03	1.03	0.99	1.01
Fe_2O_3	2.02	1.60	2.00	2.05	2.04	2.04	2.03	2.03	1.20	1.65	1.65	2.33	3.28	3.28	0.91	1.76
K_2O	0.21	0.07	0.20	0.07	0.21	0.07	0.07	0.07	0.07	0.14	0.14	1.84	2.78	2.78	2.67	0.07
Li_2O	2.15	5.30	5.35	2.19	3.10	2.18	2.17	2.16	2.15	3.57	3.57	0.00	9.85	5.24	9.46	1.07
MgO	3.99	2.36	3.97	2.43	2.43	4.03	4.02	2.41	2.39	3.23	3.23	2.46	0.00	0.00	3.07	5.55
Na_2O	14.54	14.30	12.38	12.65	14.73	12.59	14.65	12.52	14.48	13.53	13.53	21.71	5.28	5.29	14.44	17.53
NiO	0.03	0.03	0.03	0.00	0.00	0.00	0.00	0.03	0.03	0.01	0.01	0.00	0.00	0.03	0.03	0.03
P_2O_5	0.45	0.45	0.45	0.01	0.01	0.01	0.01	0.45	0.45	0.25	0.25	0.07	0.01	0.46	0.44	0.45
PbO	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00	0.00	0.01	0.01	0.01
SiO_2	48.22	50.56	47.87	52.20	52.07	51.86	51.79	51.67	50.71	50.08	50.08	49.26	48.38	54.20	44.09	44.66
SO_3	0.29	0.29	0.34	0.33	0.28	0.33	0.28	0.33	0.29	0.31	0.31	0.18	0.82	0.33	0.21	0.19
TiO_2	0.81	1.58	1.60	1.64	1.63	0.81	1.06	1.62	0.80	1.23	1.23	1.68	2.46	0.00	2.36	2.00
ZnO	3.64	2.72	3.61	3.69	3.68	2.80	2.79	2.78	3.62	3.23	3.23	2.44	4.02	4.02	3.86	1.57
ZrO_2	1.17	1.54	1.56	1.06	1.06	1.58	1.58	1.05	1.04	1.32	1.32	1.63	0.00	2.13	2.04	1.34
Sum	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00

Table 4.4. Target Compositions of Existing Matrix Glasses (mol %).

Oxide	LAWA44R10	LAWA53	LAWA56	LAWA88R1	LAWA102R1	LAWA126	LAWA128	LAWA130	LAWB65	LAWB66	LAWB68	LAWB78	LAWB79	LAWB80	LAWB83
Al_2O_3	4.07	3.99	4.05	4.01	3.82	3.72	3.98	3.92	3.81	3.79	3.80	3.79	3.77	3.79	3.81
B_2O_3	8.56	5.86	11.61	9.37	9.24	9.48	6.84	8.53	8.96	8.92	7.58	11.12	11.06	11.13	9.05
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	2.38	9.26	2.35	2.39	5.81	2.38	2.50	2.46	7.49	9.13	9.14	7.98	7.93	7.98	7.60
CdO	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
Cl	1.23	1.21	1.22	0.63	0.61	0.39	0.39	0.38	0.00	0.00	0.00	0.01	0.01	0.01	0.01
Cr_2O_3	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.04	0.04	0.04	0.02	0.02	0.02	0.02
F	0.03	0.04	0.04	0.00	0.09	1.06	1.06	1.05	0.24	0.23	0.23	0.26	0.26	0.26	0.21
Fe_2O_3	2.93	3.10	3.14	2.33	2.18	2.33	2.44	1.19	2.08	2.07	2.08	1.28	1.27	1.28	2.08
K_2O	0.36	0.35	0.35	1.84	0.18	2.77	2.77	2.73	0.17	0.17	0.17	0.16	0.16	1.33	0.13
Li_2O	0.00	0.00	0.00	0.00	5.38	0.00	0.00	0.00	9.04	8.99	9.01	6.41	7.33	7.38	9.06
MgO	3.31	2.42	2.45	2.46	2.38	2.46	1.97	1.94	4.63	4.61	4.62	4.62	4.60	4.63	4.63
Na_2O	21.61	21.26	21.55	21.71	15.11	20.00	20.05	19.76	5.55	5.52	5.53	9.91	8.69	6.71	5.55
NiO	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
P_2O_5	0.03	0.03	0.03	0.07	0.12	0.07	0.07	0.07	0.01	0.01	0.01	0.04	0.04	0.04	0.03
PbO	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
SiO_2	49.65	46.32	46.95	49.26	49.81	49.30	51.62	50.88	50.67	50.41	50.50	49.11	49.58	50.14	50.85
SO_3	0.08	1.24	1.25	0.18	0.36	0.29	0.29	0.29	1.01	1.00	1.00	0.61	0.61	0.61	0.51
TiO_2	1.67	0.91	0.92	1.68	0.92	1.68	1.76	1.73	1.10	1.09	1.09	0.00	0.00	0.00	1.10
ZnO	2.44	2.42	2.45	2.44	2.42	2.44	2.55	3.38	3.60	2.42	3.59	3.09	3.07	3.09	3.74
ZrO_2	1.63	1.60	1.62	1.63	1.58	1.63	1.71	1.68	1.61	1.60	1.60	1.61	1.60	1.61	1.61
Sum	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00

Table 4.4. Target Compositions of Existing Matrix Glasses (mol %) (continued).

Oxide	LAWB84	LAWB85	LAWB86	C100-G-136B	LAWC27	LAWC32
Al_2O_3	3.81	3.83	3.81	3.87	3.72	4.01
B_2O_3	9.05	10.44	11.21	9.35	10.85	9.09
BaO	0.00	0.00	0.00	0.00	0.00	0.00
CaO	7.49	5.94	6.43	7.37	9.45	10.16
CdO	0.00	0.00	0.00	0.00	0.00	0.00
Cl	0.01	0.01	0.01	0.22	0.19	0.20
Cr_2O_3	0.02	0.02	0.02	0.01	0.01	0.01
F	0.21	0.21	0.21	0.20	0.18	0.18
Fe_2O_3	2.08	2.09	2.08	2.62	0.00	0.96
K_2O	0.13	0.13	0.13	0.10	0.09	0.09
Li_2O	9.25	9.09	9.16	5.90	5.67	5.77
MgO	4.63	4.65	4.64	2.41	2.31	2.35
Na_2O	5.55	5.57	5.55	12.36	11.96	12.16
NiO	0.00	0.00	0.00	0.02	0.00	0.00
P_2O_5	0.03	0.03	0.03	0.11	0.09	0.09
PbO	0.00	0.00	0.00	0.00	0.00	0.00
SiO_2	50.80	51.02	50.86	50.15	50.42	49.02
SO_3	0.51	0.51	0.51	0.43	0.37	0.38
TiO_2	1.09	1.10	0.00	0.90	0.87	0.88
ZnO	3.73	3.75	3.74	2.39	2.30	3.11
ZrO_2	1.61	1.62	1.61	1.58	1.52	1.54
Sum	100.00	100.00	100.00	100.00	100.00	100.00

Table 4.5. PCT Results for Test Matrix Glasses.

-[(a)]	LAWM1	LAWM2	LAWM3	LAWM4	LAWM5[(b)]	LAWM6	LAWM7	LAWM8	LAWM9	LAWM10
7-Day PCT, Stainless Steel Vessel; S/V=2000m^{-1} Concentration in ppm										
B	2.85	12.57	14.86	18.59	4.59	18.04	5.39	13.00	3.92	9.78
Na	10.81	31.74	98.87	22.32	10.40	47.66	15.97	10.30	19.07	42.94
Si	27.31	67.17	47.31	36.68	36.38	36.07	52.08	29.21	31.50	26.25
7-Day PCT Normalized Concentrations (in g/L)										
B	0.15	0.67	0.80	0.46	0.25	0.55	0.25	0.32	0.21	0.24
Na	0.29	0.86	1.16	0.60	0.28	0.71	0.43	0.28	0.51	0.44
Si	0.13	0.31	0.25	0.19	0.16	0.19	0.21	0.14	0.14	0.14
pH	10.84	11.03	11.68	10.67	10.53	10.55	10.13	9.46	10.46	11.06
7-Day PCT Normalized Mass Loss (in g/m^2)										
B	0.08	0.34	0.40	0.23	0.12	0.27	0.12	0.16	0.11	0.12
Na	0.15	0.43	0.58	0.30	0.14	0.36	0.22	0.14	0.26	0.22
Si	0.07	0.15	0.13	0.09	0.08	0.10	0.11	0.07	0.07	0.07
7-Day PCT Normalized Loss Rate (in g/d/m^2)										
B	0.01	0.05	0.06	0.03	0.02	0.04	0.02	0.02	0.02	0.02
Na	0.02	0.06	0.08	0.04	0.02	0.05	0.03	0.02	0.04	0.03
Si	0.01	0.02	0.02	0.01	0.01	0.01	0.02	0.01	0.01	0.01

(a) A dash (-) indicates an empty data field.
(b) These data differ from the electronic data set sent earlier. During the initial analysis, after dilution of the leachate, the concentrations were below the detection limit of the DCP. The analysis was subsequently repeated without dilution of the leachate, and the data are reported here.

Table 4.5. PCT Results for Test Matrix Glasses (continued).

-[(a)]	LAWM11	LAWM12	LAWM13	LAWM14	LAWM15	LAWM16	LAWM17	LAWM18	LAWM19	LAWM20
7-Day PCT, Stainless Steel Vessel; S/V=2000m^{-1} Concentration in ppm										
B	46.93	1199.00	46.12	37.17	63.09	10.62	467.00	16.12	18.80	58.05
Na	120.40	1701.00	804.90	352.80	251.30	30.79	1006.00	37.77	54.12	343.60
Si	120.30	468.10	223.00	276.30	101.20	31.34	179.00	37.39	36.13	147.50
7-Day PCT Normalized Concentrations (in g/L)										
B	1.16	29.70	2.48	2.00	2.17	0.29	12.53	0.43	0.50	2.67
Na	1.41	16.09	4.93	2.16	1.54	0.42	7.98	0.51	0.55	2.72
Si	0.55	2.37	1.19	1.14	0.50	0.16	0.91	0.19	0.18	0.75
pH	11.54	11.92	12.34	11.72	11.37	10.58	11.55	10.53	10.48	11.91
7-Day PCT Normalized Mass Loss (in g/m^2)										
B	0.58	14.85	1.24	1.00	1.09	0.14	6.27	0.22	0.25	1.34
Na	0.71	8.04	2.47	1.08	0.77	0.21	3.99	0.25	0.28	1.36
Si	0.28	1.19	0.60	0.57	0.25	0.08	0.46	0.10	0.09	0.38
7-Day PCT Normalized Loss Rate (in g/d/m^2)										
B	0.08	2.12	0.18	0.14	0.16	0.02	0.90	0.03	0.04	0.19
Na	0.10	1.15	0.35	0.15	0.11	0.03	0.57	0.04	0.04	0.19
Si	0.04	0.17	0.09	0.08	0.04	0.01	0.07	0.01	0.01	0.05

(a) A dash (-) indicates an empty data field.

Table 4.5. PCT Results for Test Matrix Glasses (continued).

-[(a)]	LAWM21	LAWM22	LAWM23	LAWM24	LAWM25R1	LAWM26	LAWM27	LAWM28	LAWM29	LAWM30
7-Day PCT, Stainless Steel Vessel; S/V=2000m^{-1} Concentration in ppm										
B	30.16	8.53	6.06	39.26	30.37	15.77	15.00	13.77	10.96	43.96
Na	70.94	78.57	37.94	103.80	42.73	26.37	84.37	39.23	36.31	129.00
Si	61.49	56.35	45.74	62.85	61.98	48.99	49.29	49.44	60.93	60.51
7-Day PCT Normalized Concentrations (in g/L)										
B	0.89	0.39	0.28	1.05	0.82	0.42	0.69	0.37	0.50	1.18
Na	0.96	0.62	0.51	0.82	0.58	0.36	0.85	0.53	0.49	1.02
Si	0.31	0.29	0.20	0.29	0.27	0.21	0.25	0.21	0.28	0.31
pH	10.97	11.04	10.84	10.57	10.03	10.18	11.06	9.97	10.55	10.86
7-Day PCT Normalized Mass Loss (in g/m^2)										
B	0.45	0.20	0.14	0.53	0.41	0.21	0.35	0.18	0.25	0.59
Na	0.48	0.31	0.26	0.41	0.29	0.18	0.43	0.26	0.24	0.51
Si	0.16	0.14	0.10	0.14	0.13	0.11	0.13	0.11	0.14	0.15
7-Day PCT Normalized Loss Rate (in $g/d/m^2$)										
B	0.06	0.03	0.02	0.08	0.06	0.03	0.05	0.03	0.04	0.08
Na	0.07	0.04	0.04	0.06	0.04	0.03	0.06	0.04	0.03	0.07
Si	0.02	0.02	0.01	0.02	0.02	0.02	0.02	0.02	0.02	0.02

(a) A dash (-) indicates an empty data field.

Table 4.5. PCT Results for Test Matrix Glasses (continued).

-[(a)]	LAWM31	LAWM32	LAWM33R1	LAWM34	LAWM35	LAWM36	LAWM37	LAWM38	LAWM39	LAWM40
7-Day PCT, Stainless Steel Vessel; S/V=2000m^{-1} Concentration in ppm										
B	49.43	43.46	159.50	135.50	392.50	16.70	42.29	9.50	15.11	26.25
Na	272.20	225.00	518.70	538.00	836.00	54.06	87.79	71.16	48.09	75.38
Si	146.40	202.30	179.50	234.40	168.90	49.52	65.99	58.99	47.67	65.45
7-Day PCT Normalized Concentrations (in g/L)										
B	2.27	2.00	4.28	5.22	10.53	0.49	1.24	0.38	0.54	0.77
Na	2.19	1.84	4.11	4.27	6.63	0.61	0.99	0.69	0.46	0.73
Si	0.74	0.87	0.91	1.19	0.86	0.24	0.31	0.26	0.21	0.29
pH	11.85	11.43	11.66	12.14	11.35	10.64	10.93	11.24	10.75	10.37
7-Day PCT Normalized Mass Loss (in g/m^2)										
B	1.14	1.00	2.14	2.61	5.27	0.24	0.62	0.19	0.27	0.38
Na	1.10	0.92	2.06	2.13	3.31	0.30	0.49	0.34	0.23	0.36
Si	0.37	0.43	0.46	0.60	0.43	0.12	0.16	0.13	0.11	0.15
7-Day PCT Normalized Loss Rate (in $g/d/m^2$)										
B	0.16	0.14	0.31	0.37	0.75	0.03	0.09	0.03	0.04	0.05
Na	0.16	0.13	0.29	0.30	0.47	0.04	0.07	0.05	0.03	0.05
Si	0.05	0.06	0.07	0.09	0.06	0.02	0.02	0.02	0.02	0.02

(a) A dash (-) indicates an empty data field.

Table 4.5. PCT Results for Test Matrix Glasses (continued).

-[(a)]	LAWM41	LAWM42	LAWM43	LAWM44	LAWM45	LAWM46	LAWM47	LAWM48	LAWM49	LAWM50
7-Day PCT, Stainless Steel Vessel; S/V=2000m^{-1} Concentration in ppm										
B	8.95	13.23	17.73	15.50	10.60	16.35	12.96	16.01	18.16	19.49
Na	60.85	60.31	58.03	50.46	60.82	41.60	75.99	50.77	52.35	61.17
Si	49.26	60.31	58.02	52.35	51.51	40.86	60.47	51.75	47.81	55.67
7-Day PCT Normalized Concentrations (in g/L)										
B	0.36	0.53	0.66	0.50	0.43	0.48	0.52	0.47	0.54	0.65
Na	0.59	0.58	0.65	0.57	0.59	0.47	0.73	0.57	0.50	0.63
Si	0.23	0.27	0.28	0.23	0.23	0.18	0.27	0.23	0.22	0.25
pH	10.74	10.78	11.65	10.33	10.88	10.17	10.86	10.23	10.51	10.53
7-Day PCT Normalized Mass Loss (in g/m^2)										
B	0.18	0.27	0.33	0.25	0.21	0.24	0.26	0.23	0.27	0.32
Na	0.29	0.29	0.33	0.28	0.29	0.23	0.37	0.29	0.25	0.32
Si	0.12	0.13	0.14	0.12	0.11	0.09	0.13	0.12	0.11	0.13
7-Day PCT Normalized Loss Rate (in g/d/m^2)										
B	0.03	0.04	0.05	0.04	0.03	0.03	0.04	0.03	0.04	0.05
Na	0.04	0.04	0.05	0.04	0.04	0.03	0.05	0.04	0.04	0.05
Si	0.02	0.02	0.02	0.02	0.02	0.01	0.02	0.02	0.02	0.02

(a) A dash (-) indicates an empty data field.

Table 4.5. PCT Results for Test Matrix Glasses (continued).

-[(a)]	LAWM51	LAWM52	LAWM53	LAWM54R1	LAWM55	LAWM56
7-Day PCT, Stainless Steel Vessel; S/V=2000m^{-1} Concentration in ppm						
B	20.84	43.56	3.34	6.94	1440.00	543.10
Na	69.67	172.50	9.95	13.64	2426.00	1233.00
Si	57.32	84.73	23.67	32.05	441.80	209.50
7-Day PCT Normalized Concentrations (in g/L)						
B	0.69	1.45	0.18	0.37	35.67	14.58
Na	0.72	1.16	0.27	0.37	22.94	9.78
Si	0.26	0.41	0.11	0.14	2.24	1.07
pH	10.54	11.37	10.74	10.35	12.05	11.38
7-Day PCT Normalized Mass Loss (in g/m^2)						
B	0.35	0.72	0.09	0.19	17.84	7.29
Na	0.36	0.58	0.13	0.18	11.47	4.89
Si	0.13	0.21	0.06	0.07	1.12	0.53
7-Day PCT Normalized Loss Rate (in $g/d/m^2$)						
B	0.05	0.10	0.01	0.03	2.55	1.04
Na	0.05	0.08	0.02	0.03	1.64	0.70
Si	0.02	0.03	0.01	0.01	0.16	0.08

(a) A dash (-) indicates an empty data field.

Table 4.6. PCT Results for Existing Matrix Glasses.

-[(a)]	LAWA44R10	LAWA53	LAWA56	LAWA88R1	LAWA102R1	LAWA126	LAWA128	LAWA130[(c)]	LAWB65[(c)]	LAWB66[(c)]	LAWB68[(c)]
7-Day PCT, Stainless Steel Vessel; S/V=2000m^{-1} Concentration in ppm											
B	29.81	15.40	64.39	49.18	26.74	36.47	13.80	25.59	17.14	18.11	13.18
Na	139.90	156.30	172.30	192.20	78.61	143.50	118.90	126.50	19.39	22.20	19.27
Si	90.30	68.32	64.02	93.01	78.43	68.28	75.55	76.74	46.73	48.55	44.78
7-Day PCT Normalized Concentrations (in g/L)											
B	1.08	0.81	1.74	1.63	0.86	1.20	0.63	0.92	0.56	0.59	0.50
Na	0.94	1.07	1.18	1.30	0.73	1.05	0.87	0.92	0.48	0.55	0.48
Si	0.43	0.35	0.33	0.45	0.36	0.33	0.35	0.36	0.21	0.21	0.20
pH	10.27	11.52	10.65	10.92	9.92	10.74	11.03	10.65	10.82	10.17	10.34
7-Day PCT Normalized Mass Loss (in g/m^2)											
B	0.54	0.41	0.87	0.82	0.43	0.60	0.31	0.46	0.28	0.29	0.25
Na	0.47	0.53	0.59	0.65	0.36	0.52	0.43	0.46	0.24	0.27	0.24
Si	0.22	0.18	0.16	0.23	0.18	0.17	0.18	0.18	0.10	0.11	0.10
7-Day PCT Normalized Loss Rate (in $g/d/m^2$)											
B	0.08	0.06	0.12	0.12	0.06	0.09	0.04	0.07	0.04	0.04	0.04
Na	0.07	0.08	0.08	0.09	0.05	0.07	0.06	0.07	0.03	0.04	0.03
Si	0.03	0.03	0.02	0.03	0.03	0.02	0.03	0.03	0.01	0.02	0.01

(a) A dash (-) indicates an empty data field.
(b) The data were reported in [12].
(c) The data were reported in [14].

Table 4.6. PCT Results for Existing Matrix Glasses (continued).

-[a]	LAWB78[c]	LAWB79[c]	LAWB80[c]	LAWB83[c]	LAWB84[c]	LAWB85[c]	LAWB86[c]	C100G136B[b]	LAWC27[c]	LAWC32[c]
7-Day PCT, Stainless Steel Vessel; S/V=2000m^{-1} Concentration in ppm										
B	46.94	41.78	33.76	19.06	21.02	23.29	48.31	23.01	14.27	13.05
Na	80.68	62.59	35.79	21.38	22.72	20.30	41.00	61.38	39.02	49.04
Si	70.59	67.28	56.41	52.35	55.73	55.69	75.22	58.30	41.86	45.34
7-Day PCT Normalized Concentrations (in g/L)										
B	1.23	1.09	0.88	0.61	0.68	0.65	1.25	0.74	0.38	0.42
Na	1.11	0.98	0.73	0.53	0.56	0.50	1.01	0.70	0.44	0.55
Si	0.32	0.30	0.25	0.23	0.25	0.25	0.33	0.27	0.18	0.21
pH	10.58	10.35	10.25	10.16	10.16	10.11	10.14	10.11	10.82	10.58
7-Day PCT Normalized Mass Loss (in g/m^2)										
B	0.61	0.55	0.44	0.31	0.34	0.33	0.63	0.37	0.19	0.21
Na	0.56	0.49	0.36	0.26	0.28	0.25	0.50	0.35	0.22	0.28
Si	0.16	0.15	0.13	0.12	0.12	0.12	0.17	0.13	0.09	0.10
7-Day PCT Normalized Loss Rate (in g/d/m^2)										
B	0.09	0.08	0.06	0.04	0.05	0.05	0.09	0.05	0.03	0.03
Na	0.08	0.07	0.05	0.04	0.04	0.04	0.07	0.05	0.03	0.04
Si	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.01	0.01

(a) A dash (-) indicates an empty data field.
(b) The data were reported in [12].
(c) The data were reported in [14].

Table 5.1. Normalized[(a)] Compositions (wt%) for ILAW VHT Modeling Data.

Glass	Layer[(b)]	Replicate[(c)]	Retained[(d)]	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SO_3	SiO_2	TiO_2	ZnO	ZrO_2	Others	Sum
LAWM1	Outer	LAWM53	YES	9.000	6.000	10.000	8.000	4.000	4.500	0.000	5.000	1.000	44.450	3.000	5.000	0.000	0.050	100
LAWM2	Outer	NO	YES	3.500	6.000	10.000	8.000	0.000	4.500	5.000	5.000	1.000	47.000	3.000	5.000	0.000	2.000	100
LAWM3	Outer	NO	YES	9.000	6.000	10.000	8.000	0.000	4.471	5.000	11.479	1.000	40.000	0.000	1.000	4.000	0.050	100
LAWM4	Outer	NO	YES	3.500	13.000	10.000	5.535	4.000	4.500	0.000	5.000	1.000	41.415	3.000	5.000	4.000	0.050	100
LAWM5	Outer	NO	YES	9.000	6.000	5.768	8.000	4.000	4.500	0.000	5.000	1.000	48.682	3.000	1.000	4.000	0.050	100
LAWM6	Outer	NO	YES	9.000	10.609	10.000	8.000	4.000	0.000	5.000	8.997	0.344	40.000	3.000	1.000	0.000	0.050	100
LAWM7	Outer	NO	YES	5.426	6.946	10.000	8.000	0.000	2.578	5.000	5.000	1.000	52.000	3.000	1.000	0.000	0.050	100
LAWM8	Outer	NO	YES	9.000	13.000	6.429	0.000	0.000	2.080	5.000	5.000	1.000	44.491	3.000	5.000	4.000	2.000	100
LAWM9	Outer	LAWM54R1	YES	3.500	6.000	10.000	8.000	4.000	2.388	0.000	5.000	0.400	49.712	0.000	5.000	4.000	2.000	100
LAWM10	Outer	NO	YES	9.000	13.000	10.000	0.000	0.000	4.500	0.000	13.067	0.286	40.147	3.000	1.000	4.000	2.000	100
LAWM11	Outer	NO	NO	3.500	13.000	9.403	5.311	4.000	4.500	0.000	11.479	1.000	46.757	0.000	1.000	0.000	0.050	100
LAWM12	Outer	LAWM55	NO	3.500	13.000	0.000	2.309	4.000	4.500	1.970	14.253	0.269	42.199	3.000	5.000	4.000	2.000	100
LAWM13	Outer	NO	NO	3.500	6.000	10.000	8.000	3.784	0.000	0.000	22.000	0.523	40.000	3.000	2.163	0.000	1.029	100
LAWM14	Outer	NO	NO	3.500	6.000	2.045	0.000	0.000	0.881	5.000	22.000	0.523	52.000	3.000	5.000	0.000	0.050	100
LAWM15	Outer	NO	NO	9.000	9.357	0.000	6.283	0.000	0.000	3.724	22.000	0.160	43.475	3.000	1.000	0.000	2.000	100
LAWM16	Middle	NO	YES	8.000	12.000	8.000	6.500	0.100	3.000	1.000	10.000	0.400	42.450	2.500	5.000	1.000	0.050	100
LAWM17	Middle	NO	YES	5.000	12.000	2.214	6.500	2.000	0.500	3.500	17.000	0.236	42.000	0.500	5.000	3.500	0.050	100
LAWM18	Middle	NO	YES	8.000	12.000	8.000	6.500	0.100	3.000	1.000	10.000	0.400	42.000	2.500	2.000	2.500	2.000	100
LAWM19	Middle	NO	YES	8.000	12.000	8.000	2.000	2.000	0.500	1.000	13.174	0.326	42.000	0.500	5.000	3.500	2.000	100
LAWM20	Middle	NO	YES	5.000	7.000	8.000	2.000	2.000	2.264	3.500	17.000	0.236	42.000	0.500	5.000	3.500	2.000	100
LAWM21	Middle	NO	YES	5.000	10.890	8.000	6.500	2.000	3.000	1.000	10.000	0.560	42.000	2.500	5.000	3.500	0.050	100
LAWM22	Middle	NO	YES	8.000	7.000	2.000	6.500	2.000	0.500	3.500	17.000	0.330	42.000	0.670	5.000	3.500	2.000	100
LAWM23	Middle	NO	YES	5.000	7.000	8.000	2.000	2.000	3.000	1.000	10.000	0.560	48.440	2.500	5.000	3.500	2.000	100
LAWM24	Middle	NO	YES	8.000	12.000	2.000	6.500	2.000	0.641	1.000	17.000	0.236	47.073	0.500	2.000	1.000	0.050	100
LAWM25R1	Middle	NO	YES	8.000	12.000	2.000	3.679	2.000	3.000	3.500	10.000	0.400	49.921	0.500	2.000	1.000	2.000	100
LAWM26	Middle	NO	YES	8.000	12.000	4.967	2.000	0.100	3.000	1.000	10.000	0.560	49.874	0.500	5.000	1.000	2.000	100
LAWM27	Middle	NO	YES	8.000	7.000	8.000	6.500	2.000	0.500	3.500	13.372	0.321	42.000	2.500	3.307	1.000	2.000	100
LAWM28	Middle	NO	YES	5.000	12.000	8.000	6.500	0.702	0.688	1.000	10.000	0.560	50.000	2.500	2.000	1.000	0.050	100
LAWM29	Middle	NO	YES	7.558	7.000	2.000	6.500	2.000	3.000	3.500	10.000	0.400	46.850	2.500	5.000	3.500	0.192	100
LAWM30	Middle	NO	YES	8.000	12.000	2.000	6.500	0.100	2.022	1.000	17.000	0.236	42.000	0.592	5.000	3.500	0.050	100
LAWM31	Middle	NO	YES	5.000	7.000	8.000	6.500	0.100	3.000	1.000	16.751	0.338	42.311	2.500	2.000	3.500	2.000	100
LAWM32	Middle	NO	NO	5.144	7.000	2.000	2.000	2.000	3.000	3.500	16.510	0.346	50.000	0.500	5.000	1.000	2.000	100
LAWM33R1	Middle	NO	YES	5.000	12.000	8.000	6.500	1.721	0.899	1.000	17.000	0.330	42.000	2.500	2.000	1.000	0.050	100
LAWM34	Middle	NO	YES	5.000	8.354	8.000	6.293	2.000	3.000	1.000	17.000	0.330	42.000	1.474	2.000	3.500	0.050	100
LAWM35	Middle	LAWM56	YES	5.000	12.000	6.178	4.411	0.100	0.500	3.500	17.000	0.236	42.000	2.500	2.000	2.575	2.000	100
LAWM36	Inner	NO	YES	7.000	11.000	7.000	5.000	0.300	2.500	1.500	12.000	0.405	45.000	2.000	3.500	2.000	0.795	100
LAWM37	Inner	NO	YES	6.745	11.000	7.000	5.000	0.300	2.500	2.500	12.000	0.405	45.000	1.000	3.500	3.000	0.050	100
LAWM38	Inner	NO	YES	7.000	8.000	7.000	3.000	0.154	2.500	1.500	14.000	0.346	48.000	1.000	3.500	2.000	2.000	100
LAWM39	Inner	NO	YES	7.000	9.054	5.000	3.000	0.100	2.500	2.500	14.000	0.346	48.000	1.000	3.500	2.000	2.000	100
LAWM40	Inner	NO	YES	6.000	11.000	5.000	5.000	0.100	1.000	1.500	14.000	0.366	48.000	1.000	3.500	3.000	0.534	100

Table 5.1. Normalized[(a)] Compositions (wt%) for ILAW VHT Modeling Data (continued).

Glass	Layer[(b)]	Replicate[(c)]	Retained[(d)]	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SO_3	SiO_2	TiO_2	ZnO	ZrO_2	Others	Sum
LAWM41	Inner	NO	YES	7.000	8.000	7.000	5.000	0.300	1.000	2.500	14.000	0.366	45.000	1.000	4.600	2.234	2.000	100
LAWM42	Inner	NO	YES	6.000	8.000	5.000	4.034	0.100	2.500	1.500	14.000	0.366	48.000	2.000	3.500	3.000	2.000	100
LAWM43	Inner	NO	YES	7.000	8.675	5.000	5.000	0.300	2.500	2.500	12.000	0.425	45.000	2.000	4.600	3.000	2.000	100
LAWM44	Inner	NO	YES	6.317	10.028	7.000	5.000	0.100	1.000	1.500	12.000	0.405	48.000	2.000	4.600	2.000	0.050	100
LAWM45	Inner	NO	YES	7.000	8.000	5.782	5.000	0.300	1.422	1.500	14.000	0.346	48.000	2.000	4.600	2.000	0.050	100
LAWM46	Inner	NO	YES	6.000	11.000	6.510	5.000	0.100	1.000	2.500	12.000	0.405	47.935	1.000	3.500	3.000	0.050	100
LAWM47	Inner	NO	YES	6.198	8.000	7.000	5.000	0.100	1.000	2.500	14.000	0.346	48.000	1.307	3.500	3.000	0.050	100
LAWM48	Inner	NO	YES	6.225	11.000	5.270	5.000	0.100	1.000	1.500	12.000	0.405	48.000	2.000	3.500	2.000	2.000	100
LAWM49	Inner	NO	YES	7.000	10.904	5.000	3.000	0.100	1.000	1.500	14.000	0.366	47.530	1.000	4.600	2.000	2.000	100
LAWM50	Center	LAWM51	YES	6.524	9.691	6.104	4.107	0.204	1.666	2.030	13.083	0.383	46.938	1.527	4.100	2.531	1.114	100
LAWM51	Center	LAWM50	YES	6.524	9.691	6.104	4.107	0.204	1.666	2.030	13.083	0.383	46.938	1.527	4.100	2.531	1.114	100
LAWM52	Existing	LAWA88	YES	6.080	9.698	1.991	5.531	2.583	0.000	1.475	20.000	0.214	43.991	1.991	2.950	2.987	0.509	100
LAWM53	Outer	LAWM01	YES	9.000	6.000	10.000	8.000	4.000	4.500	0.000	5.000	1.000	44.450	3.000	5.000	0.000	0.050	100
LAWM54R1	Outer	LAWM09	YES	3.500	6.000	10.000	8.000	4.000	2.388	0.000	5.000	0.400	49.712	0.000	5.000	4.000	2.000	100
LAWM55	Outer	LAWM12	NO	3.500	13.000	0.000	2.309	4.000	4.500	1.970	14.253	0.269	42.199	3.000	5.000	4.000	2.000	100
LAWM56	Middle	LAWM35	YES	5.000	12.000	6.178	4.411	0.100	0.500	3.500	17.000	0.236	42.000	2.500	2.000	2.575	2.000	100
LAWA44	Existing	NO	YES	6.200	8.900	1.990	6.980	0.500	0.000	1.990	20.000	0.550	44.550	1.990	2.960	2.990	0.400	100
LAWA53	Existing	NO	YES	6.090	6.110	7.770	7.400	0.490	0.000	1.460	19.720	0.590	41.660	1.090	2.950	2.950	1.720	100
LAWA56	Existing	NO	YES	6.090	11.930	1.950	7.400	0.490	0.000	1.460	19.720	0.620	41.660	1.090	2.950	2.950	1.690	100
LAWA88	Existing	LAWM52	YES	6.080	9.700	1.990	5.530	2.580	0.000	1.470	20.000	0.210	43.990	1.990	2.950	2.990	0.520	100
LAWA102R1	Existing	NO	YES	6.060	10.000	5.070	5.410	0.260	2.500	1.500	14.490	0.720	46.600	1.140	3.060	3.020	0.170	100
LAWA126	Existing	NO	YES	5.640	9.820	1.990	5.540	3.880	0.000	1.480	18.460	0.310	44.120	2.000	2.960	2.990	0.810	100
LAWA128	Existing	NO	YES	6.030	7.070	2.080	5.790	3.880	0.000	1.180	18.460	0.300	46.090	2.090	3.090	3.130	0.810	100
LAWA130	Existing	NO	YES	6.030	8.950	2.080	2.860	3.880	0.000	1.180	18.460	0.330	46.090	2.090	4.140	3.130	0.780	100
LAWB65	Existing	NO	YES	6.170	9.910	6.670	5.280	0.260	4.290	2.960	5.460	0.890	48.350	1.390	4.650	3.150	0.570	100
LAWB66	Existing	NO	YES	6.170	9.910	8.170	5.280	0.260	4.290	2.960	5.460	0.650	48.350	1.390	3.150	3.150	0.810	100
LAWB68	Existing	NO	YES	6.170	8.410	8.170	5.280	0.260	4.290	2.960	5.460	0.830	48.350	1.390	4.650	3.150	0.630	100
LAWB78	Existing	NO	YES	6.150	12.330	7.120	3.250	0.230	3.050	2.970	9.780	0.510	47.000	0.000	4.000	3.150	0.460	100
LAWB79	Existing	NO	YES	6.150	12.330	7.120	3.250	0.230	3.510	2.970	8.620	0.580	47.700	0.000	4.000	3.150	0.390	100
LAWB80	Existing	NO	YES	6.150	12.330	7.120	3.250	1.990	3.510	2.970	6.620	0.580	47.950	0.000	4.000	3.150	0.380	100
LAWB83	Existing	NO	YES	6.180	10.030	6.780	5.290	0.190	4.310	2.970	5.470	0.490	48.600	1.390	4.840	3.160	0.300	100
LAWB84	Existing	NO	YES	6.180	10.030	6.680	5.290	0.190	4.400	2.970	5.470	0.440	48.600	1.390	4.840	3.160	0.360	100
LAWB85	Existing	NO	YES	6.180	11.520	5.280	5.290	0.190	4.310	2.970	5.470	0.480	48.600	1.390	4.840	3.160	0.320	100
LAWB86	Existing	NO	YES	6.180	12.410	5.730	5.290	0.190	4.350	2.970	5.470	0.430	48.600	0.000	4.840	3.160	0.380	100
C100G136B	Existing	NO	YES	6.120	10.080	6.400	6.470	0.150	2.730	1.510	11.860	0.630	46.670	1.120	3.010	3.020	0.230	100
LAWC27	Existing	NO	YES	6.120	12.190	8.550	0.010	0.140	2.730	1.500	11.960	0.410	48.880	1.120	3.020	3.020	0.350	100
LAWC32	Existing	NO	YES	6.490	10.050	9.040	2.420	0.140	2.730	1.500	11.960	0.380	46.740	1.120	4.020	3.020	0.390	100

(a) The compositions listed in this table are normalized versions of target compositions of the glasses, including the target values of SO_3.
(b) Layer of the Combined Matrix: Existing = Existing Matrix, Outer = outer layer of Test Matrix, Middle = middle layer of Test Matrix, Inner = inner layer of Test Matrix, and Center = a center point.
(c) If a given glass has a replicate, the glass ID is listed. If not, NO is listed.
(d) YES means the data point was used in developing VHT models, NO means it was not used.

Table 5.2. VHT Alteration Depths and Data Splitting Validation Sets for ILAW VHT Modeling Data.

Glass	Layer[(a)]	Replicate[(b)]	Retained[(c)]	VHT Alteration Depth (μ)	VHT Data Splitting Validation Set[(d)]
LAWM1	Outer	LAWM53	YES	82.0	NA
LAWM2	Outer	NO	YES	75.0	1
LAWM3	Outer	NO	YES	34.0	3
LAWM4	Outer	NO	YES	5.0	2
LAWM5	Outer	NO	YES	7.0	2
LAWM6	Outer	NO	YES	19.0	3
LAWM7	Outer	NO	YES	26.0	5
LAWM8	Outer	NO	YES	13.0	5
LAWM9	Outer	LAWM54R1	YES	1.0	NA
LAWM10	Outer	NO	YES	114.0	4
LAWM11	Outer	NO	NO	700.0	NA
LAWM12	Outer	LAWM55	NO	1100.0	NA
LAWM13	Outer	NO	NO	1100.0	NA
LAWM14	Outer	NO	NO	1100.0	NA
LAWM15	Outer	NO	NO	856.0	NA
LAWM16	Middle	NO	YES	71.0	5
LAWM17	Middle	NO	YES	3.0	4
LAWM18	Middle	NO	YES	15.0	4
LAWM19	Middle	NO	YES	1.0	2
LAWM20	Middle	NO	YES	116.0	5
LAWM21	Middle	NO	YES	9.0	1
LAWM22	Middle	NO	YES	2.0	3
LAWM23	Middle	NO	YES	9.0	2
LAWM24	Middle	NO	YES	123.0	1
LAWM25R1	Middle	NO	YES	41.0	5
LAWM26	Middle	NO	YES	31.0	1
LAWM27	Middle	NO	YES	45.0	3
LAWM28	Middle	NO	YES	6.0	1
LAWM29	Middle	NO	YES	9.0	3
LAWM30	Middle	NO	YES	181.0	4
LAWM31	Middle	NO	YES	48.0	4
LAWM32	Middle	NO	NO	1100.0	NA
LAWM33R1	Middle	NO	YES	34.0	4
LAWM34	Middle	NO	YES	420.0	1
LAWM35	Middle	LAWM56	YES	4.0	NA
LAWM36	Inner	NO	YES	107.0	2
LAWM37	Inner	NO	YES	10.0	1
LAWM38	Inner	NO	YES	171.0	2
LAWM39	Inner	NO	YES	112.0	3
LAWM40	Inner	NO	YES	3.0	5
LAWM41	Inner	NO	YES	43.0	1
LAWM42	Inner	NO	YES	7.0	3
LAWM43	Inner	NO	YES	9.0	4
LAWM44	Inner	NO	YES	20.0	4
LAWM45	Inner	NO	YES	44.0	2
LAWM46	Inner	NO	YES	3.0	1
LAWM47	Inner	NO	YES	25.0	4
LAWM48	Inner	NO	YES	5.0	3
LAWM49	Inner	NO	YES	23.0	3
LAWM50	Center	LAWM51	YES	4.0	NA
LAWM51	Center	LAWM50	YES	5.0	NA
LAWM52	Existing	LAWA88	YES	28.0	NA
LAWM53	Outer	LAWM01	YES	90.0	NA

Table 5.2. VHT Alteration Depths and Data Splitting Validation Sets for ILAW VHT Modeling Data (continued).

Glass	Layer[(a)]	Replicate[(b)]	Retained[(c)]	VHT Alteration Depth (μ)	VHT Data Splitting Validation Set[(d)]
LAWM54R1	Outer	LAWM09	YES	3.0	NA
LAWM55	Outer	LAWM12	NO	1100.0	NA
LAWM56	Middle	LAWM35	YES	6.0	NA
LAWA44	Existing	NO	YES	9.0	5
LAWA53	Existing	NO	YES	7.4	4
LAWA56	Existing	NO	YES	15.0	1
LAWA88	Existing	LAWM52	YES	12.0	NA
LAWA102R1	Existing	NO	YES	34.0	2
LAWA126	Existing	NO	YES	22.0	5
LAWA128	Existing	NO	YES	6.0	4
LAWA130	Existing	NO	YES	6.0	5
LAWB65	Existing	NO	YES	10.4	2
LAWB66	Existing	NO	YES	17.0	1
LAWB68	Existing	NO	YES	18.0	2
LAWB78	Existing	NO	YES	23.0	2
LAWB79	Existing	NO	YES	11.0	3
LAWB80	Existing	NO	YES	10.0	5
LAWB83	Existing	NO	YES	16.0	5
LAWB84	Existing	NO	YES	15.0	2
LAWB85	Existing	NO	YES	11.0	4
LAWB86	Existing	NO	YES	15.0	3
C100G136B	Existing	NO	YES	23.0	1
LAWC27	Existing	NO	YES	177.0	3
LAWC32	Existing	NO	YES	206.0	5

(a) Layer of the Combined Matrix: Existing = Existing Matrix, Outer = outer layer of Test Matrix, Middle = middle layer of Test Matrix, Inner = inner layer of Test Matrix, and Center = a center point.
(b) If a given glass has a replicate, the glass ID is listed. If not, NO is listed.
(c) YES means the data point was used in developing VHT models, NO means it was not used.
(d) NA denotes glasses not included in the modeling dataset. Numbers from 1 to 5 denote the five split validation subsets.

Table 5.3. Variation in VHT Responses for Replicate Pairs.

Glass IDs of Replicate Pairs	Included in VHT Modeling Data?	VHT Alteration Depth	
		μ	ln(μ)
LAWM01	Yes	82	4.4067
LAWM53	Yes	90	4.4998
		%RSD [(a)] = 6.58	**SD = 0.0658**
LAWM09	Yes	1	0.0000
LAWM54R1	Yes	3	1.0986
		%RSD = 70.71	**SD = 0.7768**
LAWM12	No	>1100	>7.0030
LAWM55	No	>1100	>7.0030
		%RSD = NA	**SD =NA**
LAWM35	Yes	4	1.3863
LAWM56	Yes	6	1.7916
		%RSD = 28.28	**SD = 0.2867**
LAWM50	Yes	4	1.3863
LAWM51	Yes	5	1.6094
		%RSD = 15.71	**SD = 0.1578**
LAWM52	Yes	28	3.3322
LAWA88R1	Yes	12	2.4849
		%RSD = 56.57	**SD = 0.5991**
Pooled Over All 5 Replicate Pairs Used for Modeling		**%RSD = 43.10**	**SD = 0.4634**
Pooled Over 4 Replicate Pairs (excluding LAWM52/LAWA88R1 pair)[(b)]		**%RSD = 39.02**	**SD = 0.4228**

(a) %RSD = 100*(Standard Deviation / Mean)

(b) This pair is a "near replicate" pair rather than an "exact replicate" pair. The compositions are close enough to treat as replicates, but were not identified as such by statistical software that automatically finds replicates and performs model LOF tests.

Table 5.4. Normalized[(a)] Compositions (wt%) for ILAW VHT Validation Data.

Glass	Ag2O	Al2O3	B2O3	BaO	Cl	CaO	Cr2O3	Cs2O	F	Fe2O3	K2O	Li2O	MgO	MnO	Na2O	NiO	P2O5	PbO	Re2O7	SO3	SiO2	TiO2	ZnO	ZrO2	Sum
A1C1-1	0.000	6.069	9.213	0.000	0.903	2.765	0.015	0.000	0.086	6.566	0.344	0.626	1.868	0.008	18.628	0.006	0.033	0.000	0.000	0.219	44.909	1.777	2.979	2.985	100
A1C1-2	0.000	6.068	9.484	0.000	0.647	3.542	0.013	0.000	0.168	6.183	0.252	1.252	1.749	0.017	17.235	0.012	0.065	0.000	0.000	0.263	45.479	1.567	3.006	2.996	100
A1C1-3	0.000	6.066	9.756	0.000	0.391	4.319	0.011	0.000	0.251	5.801	0.160	1.878	1.629	0.025	15.843	0.019	0.098	0.000	0.000	0.307	46.049	1.357	3.034	3.008	100
A2-AP101	0.000	5.617	9.821	0.000	0.424	1.987	0.021	0.149	0.350	5.531	3.812	0.000	1.476	0.000	18.462	0.000	0.077	0.000	0.000	0.401	43.988	1.986	2.938	2.961	100
A2B1-1	0.000	5.754	9.867	0.000	0.322	3.180	0.024	0.150	0.283	5.467	2.904	1.074	1.851	0.000	15.214	0.000	0.068	0.000	0.000	0.462	45.117	1.838	3.413	3.011	100
A2B1-2	0.000	5.892	9.914	0.000	0.220	4.374	0.027	0.150	0.215	5.402	1.996	2.148	2.226	0.000	11.967	0.000	0.059	0.000	0.000	0.524	46.247	1.690	3.887	3.061	100
A3-AN104	0.000	6.052	9.919	0.000	0.787	5.028	0.021	0.149	0.006	5.366	0.328	2.478	1.480	0.000	14.641	0.000	0.112	0.000	0.000	0.369	46.088	1.134	3.041	3.001	100
A88AP101R1	0.000	6.099	9.828	2.000	0.130	0.000	0.020	0.000	0.230	5.549	2.140	0.000	1.480	0.000	19.996	0.000	0.070	0.000	0.100	0.280	44.121	2.000	2.959	2.999	100
A88Si+15	0.000	6.139	9.479	1.930	0.140	0.000	0.020	0.000	0.250	5.349	2.370	0.000	1.430	0.000	22.178	0.000	0.080	0.000	0.110	0.310	42.546	1.930	2.850	2.890	100
A88Si-15	0.000	6.052	10.213	2.071	0.110	0.000	0.010	0.000	0.200	5.762	1.881	0.000	1.540	0.000	17.665	0.000	0.060	0.000	0.090	0.250	45.844	2.071	3.071	3.111	100
B1-AZ101	0.000	6.168	10.007	0.000	0.017	6.761	0.034	0.151	0.080	5.272	0.180	4.296	2.976	0.000	5.472	0.000	0.041	0.000	0.000	0.646	48.507	1.395	4.835	3.162	100
C1-AN107	0.000	6.064	10.027	0.000	0.135	5.097	0.009	0.000	0.333	5.418	0.068	2.505	1.510	0.034	14.450	0.025	0.131	0.000	0.000	0.351	46.618	1.147	3.061	3.019	100
C22AN107	0.000	6.099	10.068	0.000	0.080	5.109	0.020	0.000	0.150	5.589	0.090	2.509	1.510	0.000	14.417	0.030	0.120	0.020	0.100	0.310	46.561	1.140	3.059	3.019	100
C22Si+15	0.000	6.045	9.838	0.000	0.090	5.004	0.020	0.000	0.160	5.484	0.100	2.452	1.471	0.000	16.203	0.000	0.130	0.000	0.100	0.340	45.506	1.111	2.992	2.952	100
C22Si-15	0.000	6.171	10.321	0.000	0.070	5.231	0.020	0.000	0.130	5.701	0.070	2.570	1.550	0.000	12.561	0.000	0.100	0.000	0.100	0.270	47.725	1.170	3.140	3.100	100
C2-AN102C35	0.000	6.069	9.416	0.000	0.389	7.350	0.012	0.150	0.114	3.596	0.091	3.251	1.490	0.000	11.975	0.000	0.159	0.000	0.000	0.631	47.245	1.078	3.989	2.997	100
LAWA104	0.001	6.612	8.592	0.000	0.717	1.920	0.022	0.001	0.010	6.732	0.550	0.000	1.920	0.000	22.006	0.000	0.037	0.002	0.100	0.105	43.001	1.925	2.861	2.887	100
LAWA105	0.001	7.028	8.283	0.000	0.780	1.851	0.022	0.001	0.010	6.492	0.600	0.000	1.851	0.000	24.008	0.000	0.040	0.002	0.100	0.110	41.433	1.851	2.757	2.781	100
LAWA133	0.000	6.203	8.899	0.000	0.559	5.483	0.020	0.000	0.040	3.486	0.429	0.000	1.998	0.000	19.976	0.000	0.100	0.000	0.100	0.220	44.527	1.998	2.966	2.996	100
LAWA134	0.000	5.644	9.959	0.000	0.200	2.018	0.020	0.000	0.290	5.624	3.726	0.000	1.498	0.000	17.721	0.000	0.080	0.000	0.100	0.330	44.731	2.028	2.997	3.037	100
LAWA135	0.000	5.653	10.087	0.000	0.190	2.047	0.020	0.000	0.280	5.693	3.575	0.000	1.518	0.000	17.008	0.000	0.070	0.000	0.100	0.320	45.281	2.047	3.036	3.076	100
LAWA136	0.000	5.653	10.087	0.000	0.190	3.046	0.020	0.000	0.280	5.693	3.575	0.000	1.518	0.000	17.008	0.000	0.070	0.000	0.100	0.320	44.282	2.047	3.036	3.076	100
LAWA33	0.000	11.974	8.853	0.000	0.580	0.000	0.020	0.000	0.040	5.772	3.101	0.000	1.991	0.000	20.006	0.000	0.080	0.010	0.000	0.100	38.221	2.491	4.271	2.491	100
LAWA49	0.001	6.201	8.902	0.000	0.650	0.000	0.020	0.001	0.010	9.982	0.500	0.000	1.480	0.000	20.004	0.000	0.030	0.001	0.100	0.095	44.560	1.990	2.481	2.991	100
LAWA51	0.001	6.203	11.972	0.000	0.586	0.000	0.018	0.001	0.010	6.998	0.451	0.000	1.484	0.000	18.004	0.000	0.030	0.001	0.100	0.086	46.580	1.996	2.488	2.989	100
LAWA52	0.001	6.181	6.191	0.000	0.650	7.882	0.020	0.001	0.010	7.512	0.500	0.000	1.480	0.000	20.005	0.000	0.030	0.000	0.100	0.095	42.260	1.100	2.991	2.991	100
LAWA60	0.001	8.531	11.232	0.000	0.650	4.321	0.020	0.001	0.010	0.000	0.500	0.000	1.990	0.000	20.003	0.000	0.034	0.000	0.100	0.095	44.560	1.994	2.965	2.992	100
LAWB60	0.000	6.145	12.317	0.000	0.008	11.861	0.047	0.000	0.078	0.001	0.234	4.608	2.965	0.000	6.614	0.000	0.045	0.000	0.100	0.781	47.901	0.000	3.148	3.148	100
LAWB62	0.000	6.163	9.899	0.000	0.000	11.937	0.100	0.000	0.070	0.000	0.260	5.784	2.957	0.000	5.464	0.000	0.010	0.000	0.100	1.279	48.297	1.388	3.147	3.147	100
LAWB63	0.000	6.543	9.899	0.000	0.000	9.300	0.100	0.000	0.070	0.000	0.260	5.024	2.957	0.000	5.464	0.000	0.010	0.000	0.100	1.279	48.676	1.388	5.784	3.147	100
LAWB64	0.000	6.163	9.899	0.000	0.000	6.663	0.100	0.000	0.070	3.276	0.260	5.784	2.957	0.000	5.464	0.000	0.010	0.000	0.100	1.279	48.297	1.388	5.144	3.147	100
LAWB67	0.000	6.163	9.899	0.000	0.000	5.164	0.100	0.000	0.070	5.274	0.260	4.285	2.957	0.000	5.464	0.000	3.007	0.000	0.100	1.279	48.297	1.388	3.147	3.147	100
LAWB69	0.000	6.143	12.316	0.000	0.010	10.449	0.050	0.000	0.080	0.000	0.230	4.605	2.967	0.000	6.613	0.000	0.050	0.000	0.100	0.779	47.897	0.000	4.565	3.147	100
LAWB70	0.000	6.144	12.318	0.000	0.010	6.613	0.050	0.000	0.080	3.247	0.230	4.605	2.967	0.000	6.613	0.000	0.050	0.000	0.100	0.779	47.902	0.000	5.145	3.147	100
LAWB71	0.000	6.144	10.769	0.000	0.010	6.613	0.050	0.000	0.080	3.247	0.230	4.605	2.967	0.000	6.613	0.000	0.050	0.000	0.100	0.779	47.902	1.548	5.145	3.147	100
LAWB72	0.000	6.144	12.318	0.000	0.010	7.113	0.050	0.000	0.080	3.247	0.230	4.106	2.967	0.000	6.613	0.000	0.050	0.000	0.100	0.779	47.902	0.000	5.145	3.147	100
LAWB73	0.000	6.163	9.899	0.000	0.000	9.300	0.100	0.000	0.070	1.898	0.260	5.024	2.957	0.000	5.464	0.000	0.010	0.000	0.100	1.279	48.297	1.388	4.645	3.147	100
LAWB74	0.000	6.163	10.289	0.000	0.000	8.650	0.100	0.000	0.070	1.898	0.260	5.284	2.957	0.000	5.464	0.000	0.010	0.000	0.100	1.279	48.297	1.388	4.645	3.147	100
LAWB75	0.000	6.163	11.747	0.000	0.000	8.650	0.100	0.000	0.070	1.898	0.260	5.284	1.498	0.000	5.464	0.000	0.010	0.000	0.100	1.279	48.297	1.388	4.645	3.147	100
LAWB76	0.000	6.163	11.747	0.000	0.000	8.650	0.100	0.000	0.070	1.898	0.260	5.784	1.498	0.000	5.464	0.000	0.010	0.000	0.100	1.279	49.186	0.000	4.645	3.147	100

Table 5.4. Normalized[(a)] Compositions (wt%) for ILAW VHT Validation Data (continued).

Glass	Ag2O	Al2O3	B2O3	BaO	Cl	CaO	Cr2O3	Cs2O	F	Fe2O3	K2O	Li2O	MgO	MnO	Na2O	NiO	P2O5	PbO	Re2O7	SO3	SiO2	TiO2	ZnO	ZrO2	Sum
LAWB77	0.000	6.144	12.318	0.000	0.010	6.613	0.050	0.000	0.080	2.198	0.230	4.106	2.967	0.000	6.613	0.000	0.050	0.000	0.100	0.779	47.902	1.548	5.145	3.147	100
LAWB81	0.000	6.144	12.318	0.000	0.010	7.113	0.050	0.000	0.080	3.247	0.230	4.256	2.967	0.000	6.613	0.000	0.050	0.000	0.100	0.779	47.902	0.000	4.995	3.147	100
LAWB82	0.000	6.144	10.070	0.000	0.010	7.113	0.050	0.000	0.080	9.491	0.230	4.256	1.479	0.000	6.613	0.000	0.050	0.000	0.100	0.779	45.395	0.000	4.995	3.147	100
LAWB89	0.000	6.173	10.019	0.000	0.010	6.773	0.040	0.000	0.060	5.284	0.190	4.995	2.967	0.000	4.076	0.000	0.040	0.000	0.100	0.649	49.246	1.388	4.835	3.157	100
LAWB90	0.000	6.173	10.019	0.000	0.010	6.773	0.040	0.000	0.060	5.284	0.190	3.606	2.967	0.000	6.862	0.000	0.040	0.000	0.100	0.649	47.847	1.388	4.835	3.157	100
LAWB91	0.000	6.173	10.019	0.000	0.010	6.773	0.040	0.000	0.060	5.284	0.190	2.917	2.967	0.000	8.710	0.000	0.040	0.000	0.100	0.649	46.689	1.388	4.835	3.157	100
LAWB92	0.000	6.173	10.019	0.000	0.010	6.773	0.040	0.000	0.060	5.284	0.190	2.218	2.967	0.000	10.099	0.000	0.040	0.000	0.100	0.649	45.999	1.388	4.835	3.157	100
LAWB93	0.000	6.173	10.019	0.000	0.010	6.773	0.040	0.000	0.060	5.284	0.190	4.655	2.967	0.000	4.775	0.000	0.040	0.000	0.100	0.649	48.886	1.388	4.835	3.157	100
LAWB94	0.000	6.173	10.019	0.000	0.010	6.773	0.040	0.000	0.060	5.284	0.190	5.354	2.967	0.000	3.376	0.000	0.040	0.000	0.100	0.649	49.585	1.388	4.835	3.157	100
LAWB95	0.000	6.172	10.017	0.000	0.010	6.771	0.040	0.000	0.060	5.283	0.190	5.763	2.966	0.000	2.457	0.000	0.040	0.000	0.100	0.649	50.105	1.388	4.834	3.156	100
LAWC15	0.000	6.231	8.952	0.000	0.078	2.010	0.003	0.002	0.470	7.021	0.142	0.000	2.010	0.000	20.004	0.035	0.015	0.004	0.100	0.127	44.788	2.000	2.997	3.011	100
LAWC25	0.000	5.789	9.538	0.000	0.120	6.059	0.019	0.000	0.060	6.119	8.089	0.000	1.430	0.004	11.218	0.000	0.110	0.000	0.094	0.410	44.172	1.060	2.850	2.860	100
LAWC26	0.000	6.113	13.245	0.000	0.110	6.403	0.020	0.000	0.050	0.010	0.140	2.727	1.498	0.000	11.947	0.000	0.110	0.000	0.100	0.479	49.895	1.119	3.017	3.017	100
LAWC28	0.000	6.114	10.040	0.000	0.110	12.807	0.020	0.000	0.050	0.010	0.140	2.727	1.499	0.000	11.948	0.000	0.110	0.000	0.100	0.480	46.693	1.119	3.017	3.017	100
LAWC29	0.000	6.543	10.039	0.000	0.110	9.609	0.020	0.000	0.050	0.010	0.140	2.727	1.498	0.000	11.947	0.000	0.110	0.000	0.100	0.479	47.128	1.119	5.354	3.017	100
LAWC30	0.000	6.113	10.039	0.000	0.110	6.403	0.020	0.000	0.050	4.095	0.140	2.727	1.498	0.000	11.947	0.000	0.110	0.000	0.100	0.479	46.689	1.119	5.344	3.017	100
LAWC31	0.000	6.113	10.039	0.000	0.110	7.402	0.020	0.000	0.050	4.425	0.140	2.727	1.498	0.000	11.947	0.000	0.110	0.000	0.100	0.479	46.689	1.119	4.016	3.017	100
LAWC33	0.000	6.139	10.089	0.000	0.110	6.939	0.020	0.000	0.050	4.440	0.140	2.750	1.510	0.000	11.999	0.000	0.110	0.000	0.100	0.480	46.925	1.130	4.040	3.030	100
TFA-BASE	0.000	7.001	10.001	0.000	0.280	0.000	0.000	0.000	0.010	5.501	0.410	0.000	1.500	0.000	20.002	0.000	0.060	0.000	0.090	0.070	49.075	3.000	1.500	1.500	100

[(a)] The compositions listed in this table are normalized versions of target compositions of the glasses, including the target values of SO_3.

Table 5.5. VHT Alteration Depths and Subsets of ILAW Validation Data.

Glass ID	VHT Alteration Depth (μ)	V1[(a)]	V2[(a)]
A1C1-1	6	YES	YES
A1C1-2	31	YES	YES
A1C1-3	6	YES	YES
A2-AP101	7	YES	YES
A2B1-1	5	YES	YES
A2B1-2	6	YES	YES
A3-AN104	6	YES	YES
A88AP101R1	13	NO	NO
A88Si+15	290	NO	NO
A88Si-15	4	NO	NO
B1-AZ101	14	YES	YES
C1-AN107	80	YES	YES
C22AN107	9	YES	YES
C22Si+15	23	YES	YES
C22Si-15	29	YES	YES
C2-AN102C35	154	YES	YES
LAWA104	59	YES	NO
LAWA105	359	YES	NO
LAWA133	5	YES	YES
LAWA134	2	YES	YES
LAWA135	3	YES	YES
LAWA136	3	YES	YES
LAWA33	541	NO	NO
LAWA49	30	NO	NO
LAWA51	5	NO	NO
LAWA52	67	YES	NO
LAWA60	56	YES	NO
LAWB60	68	NO	NO
LAWB62	36.7	NO	NO
LAWB63	71.5	NO	NO
LAWB64	15	NO	NO
LAWB67	15	NO	NO
LAWB69	128	YES	NO
LAWB70	31	YES	NO
LAWB71	12	YES	NO
LAWB72	23	YES	NO
LAWB73	31	NO	NO
LAWB74	52	NO	NO
LAWB75	59	NO	NO
LAWB76	78	NO	NO
LAWB77	17	YES	NO

Table 5.5. VHT Alteration Depths and Subsets of ILAW Validation Data (continued).

Glass ID	VHT Alteration Depth (μ)	V1[(a)]	V2[(a)]
LAWB81	24	YES	YES
LAWB82	32	NO	NO
LAWB89	16	NO	NO
LAWB90	14	YES	YES
LAWB91	12	YES	YES
LAWB92	10	YES	YES
LAWB93	15	YES	NO
LAWB94	14	NO	NO
LAWB95	11	NO	NO
LAWC15	4.9	YES	YES
LAWC25	69.5	NO	NO
LAWC26	22	YES	NO
LAWC28	92	NO	NO
LAWC29	106	YES	NO
LAWC30	60	YES	NO
LAWC31	110	YES	YES
LAWC33	17	YES	YES
TFA-BASE	86	NO	NO

(a) YES indicates the data point is in the validation subset, NO indicates it is not.

Table 5.6. ILAW VHT LM Model and Performance Summary.

ln(VHT Alt. Depth) LM Model Term	Coefficient Estimate	Coefficient Stand. Dev.		Statistic from Modeling Data[(a)]	Value
Al2O3	11.7128	7.8287		R^2	0.6408
B2O3	-5.9130	5.1941		R^2 Adjusted (R^2_A)	0.5574
CaO	10.0563	5.0032		R^2 Predicted (R^2_P)	0.2982
Fe2O3	-15.7556	6.4253		RMSE	0.8741
K2O	1.5082	9.0956		Model LOF p-value	0.0744
Li2O	82.1995	12.2134		N (no. of data pts.)	70
MgO	3.9119	8.7910			
Na2O	25.8835	3.6384			
SO3	-58.7608	67.3358			
SiO2	0.6115	2.1901		**Statistic from Validation Data[(b)]**	**Value**
TiO2	-4.6026	12.9250			
ZnO	-1.0438	9.1868		R^2 All (59)	0.2337
ZrO2	-64.7178	11.2727		R^2 V1 (37)	0.5105
Others	-32.8570	14.1826		R^2 V2 (24)	0.3779

Statistic from Data Splitting[(c)]	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.7227	0.6364	0.7088	0.7299	0.7539	0.7103
R^2 Adjusted (R^2_A)	0.6167	0.4973	0.5975	0.6266	0.6598	0.5996
R^2 Predicted (R^2_P)	0.1342	0.0306	0.1386	0.1256	0.4303	0.1718
RMSE	0.7701	0.8810	0.8071	0.7877	0.7468	0.7986
SSE	20.1630	26.3924	22.1500	21.0963	18.9646	21.7533
R^2 Validation (R^2_V)	0.4070	0.7373	0.1801	-0.2986	-0.4387	0.1174

(a) The evaluation statistics are defined in Section C.2 of Appendix C.
(b) R^2 validation is defined in Section S.4 of Appendix S. The descriptions of the complete validation set (All) and the two validation subsets (V1 and V2) are described in Section 5.1.3.
(c) The evaluation and validation statistics calculated for data-splits are defined the same as for separate modeling and validation sets. Section 5.1.2 describes how the data-splitting was accomplished.

Table 5.7. ILAW VHT PQM Model and Performance Summary.

ln(VHT Alt. Depth) PQM Model Term	Coefficient Estimate	Coefficient Stand. Dev.
Al2O3	49.8620	10.6690
B2O3	8.5808	10.8948
CaO	-21.4725	66.7783
Fe2O3	18.3252	14.3877
K2O	137.6727	37.8461
Li2O	113.4367	12.9342
MgO	-31.3959	16.6632
Na2O	35.2036	6.3984
SO3	-707.4950	179.2587
SiO2	-15.5899	5.2535
TiO2	-20.1469	20.2361
ZnO	1.8503	9.9902
ZrO2	-73.6987	10.6568
Others	-83.5317	19.7374
MgO*TiO2	1430.2732	652.5926
Al2O3*K2O	-1206.9348	441.0861
CaO*Fe2O3	-486.3382	223.0160
K2O*ZnO	-1288.2916	466.7119
B2O3*CaO	-731.6002	184.1978
B2O3*SO3	6505.9075	1796.2424
MgO*Others	1733.1272	732.3378
CaO*SiO2	304.4759	134.0449

Statistic from Modeling Data[(a)]	Value
R^2	0.8727
R^2 Adjusted (R^2_A)	0.8170
R^2 Predicted (R^2_P)	0.7496
RMSE	0.5620
Model LOF p-value	0.2960
N (no. of data pts.)	70

Statistic from Validation Data[(b)]	Value
R^2 All (59)	0.0307
R^2 V1 (37)	0.5542
R^2 V2 (24)	0.3553

Statistic from Data Splitting[(c)]	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.8841	0.8685	0.9006	0.8663	0.8705	0.8780
R^2 Adjusted (R^2_A)	0.8165	0.7917	0.8426	0.7884	0.7949	0.8068
R^2 Predicted (R^2_P)	0.7416	0.7068	0.7585	0.6031	0.6844	0.6989
RMSE	0.5582	0.5981	0.5284	0.6182	0.6043	0.5814
SSE	11.2177	12.8789	10.0521	13.7565	13.1476	12.2106
R^2 Validation (R^2_V)	0.7190	0.6660	0.5411	0.8792	0.7854	0.7181

(a) The evaluation statistics are defined in Section C.2 of Appendix C.
(b) R^2 validation is defined in Section S.4 of Appendix S. The descriptions of the complete validation set (All) and the two validation subsets (V1 and V2) are described in Section 5.1.3.
(c) The evaluation and validation statistics calculated for data-splits are defined the same as for separate modeling and validation sets. Section 5.1.2 describes how the data-splitting was accomplished.

Table 5.8. LAWA126 Composition in Formats Needed for Use in ILAW VHT Models

Component	LAWA126 Composition (wt%)	LAWA126 Composition (mass fractions) For Use In VHT LM Model	LAWA126 Composition (mass fractions) For Use In VHT PQM Model
Al2O3	5.640	0.056	0.056
B2O3	9.820	0.098	0.098
CaO	1.990	0.020	0.020
Fe2O3	5.540	0.055	0.055
K2O	3.880	0.039	0.039
Li2O	0.000	0.000	0.000
MgO	1.480	0.015	0.015
Na2O	18.460	0.185	0.185
SO3	0.309	0.003	0.003
SiO2	44.120	0.441	0.441
TiO2	2.000	0.020	0.020
ZnO	2.960	0.030	0.030
ZrO2	2.990	0.030	0.030
Others	0.810	0.008	0.008
MgO*TiO2	NA	NA	0.000
Al2O3*K2O	NA	NA	0.002
CaO*Fe2O3	NA	NA	0.001
K2O*ZnO	NA	NA	0.001
B2O3*CaO	NA	NA	0.002
B2O3*SO3	NA	NA	0.000
MgO*Others	NA	NA	0.000
CaO*SiO2	NA	NA	0.009

Table 5.9. Predicted VHT Alteration Depths and Corresponding 90% UCIs and 95% SUCIs for LAWA126Composition Used in ILAW VHT Models

Model	Predicted ln(VHT) in ln(microns)	Predicted VHT in microns	90% UCI on Mean ln(VHT) in ln(microns)	90% UCI on Median VHT in microns	95% SUCI on Mean ln(VHT) in ln(microns)	95% SUCI on Median VHT in microns
14-Term VHT LM Model	2.0652	7.8868	2.4845	11.9952	3.6086	36.9156
22-Term VHT PQM Model	2.5168	12.3895	2.8532	17.3439	4.0320	56.3761

Table 6.1. Normalized[a] Compositions (wt%) for ILAW PCT Modeling Data.

Glass ID	Layer[b]	Replicate[c]	Retained[d]	Al2O3	B2O3	CaO	Fe2O3	K2O	Li2O	MgO	Na2O	SO3 .XRF[e]	SiO2	TiO2	ZnO	ZrO2	Others	Sum
LAWM1	Outer	LAWM53	YES	9.044	6.029	10.049	8.039	4.019	4.522	0.000	5.024	0.518	44.666	3.015	5.024	0.000	0.050	100
LAWM2	Outer	NO	YES	3.512	6.020	10.033	8.027	0.000	4.515	5.017	5.017	0.669	47.157	3.010	5.017	0.000	2.007	100
LAWM3	Outer	NO	YES	9.033	6.022	10.036	8.029	0.000	4.487	5.018	11.521	0.639	40.146	0.000	1.004	4.015	0.050	100
LAWM4	Outer	NO	YES	3.516	13.058	10.044	5.560	4.018	4.520	0.000	5.022	0.561	41.598	3.013	5.022	4.018	0.050	100
LAWM5	Outer	NO	YES	9.041	6.028	5.794	8.037	4.018	4.521	0.000	5.023	0.545	48.906	3.014	1.005	4.018	0.050	100
LAWM6	Outer	NO	YES	9.002	10.612	10.002	8.002	4.001	0.000	5.001	8.999	0.319	40.010	3.001	1.000	0.000	0.050	100
LAWM7	Outer	NO	YES	5.441	6.966	10.028	8.023	0.000	2.585	5.014	5.014	0.719	52.148	3.009	1.003	0.000	0.050	100
LAWM8	Outer	NO	YES	9.028	13.040	6.448	0.000	0.000	2.087	5.015	5.015	0.696	44.628	3.009	5.015	4.012	2.006	100
LAWM9	Outer	LAWM54R1	YES	3.505	6.009	10.016	8.013	4.006	2.392	0.000	5.008	0.244	49.790	0.000	5.008	4.006	2.003	100
LAWM10	Outer	NO	YES	9.005	13.007	10.006	0.000	0.000	4.503	0.000	13.074	0.229	40.170	3.002	1.001	4.002	2.001	100
LAWM11	Outer	NO	YES	3.503	13.013	9.412	5.317	4.004	4.504	0.000	11.490	0.904	46.802	0.000	1.001	0.000	0.050	100
LAWM12	Outer	LAWM55	NO	3.501	13.005	0.000	2.310	4.002	4.502	1.971	14.259	0.228	42.216	3.001	5.002	4.002	2.001	100
LAWM13	Outer	NO	NO	3.501	6.001	10.002	8.002	3.785	0.000	0.000	22.005	0.503	40.008	3.001	2.164	0.000	1.030	100
LAWM14	Outer	NO	YES	3.500	5.999	2.045	0.000	0.000	0.881	5.000	21.998	0.532	51.996	3.000	5.000	0.000	0.050	100
LAWM15	Outer	NO	YES	8.999	9.356	0.000	6.283	0.000	0.000	3.724	21.997	0.173	43.470	3.000	1.000	0.000	2.000	100
LAWM16	Middle	NO	YES	8.006	12.008	8.006	6.505	0.100	3.002	1.001	10.007	0.331	42.479	2.502	5.003	1.001	0.050	100
LAWM17	Middle	NO	NO	5.002	12.005	2.215	6.503	2.001	0.500	3.501	17.007	0.197	42.016	0.500	5.002	3.501	0.050	100
LAWM18	Middle	NO	YES	8.005	12.007	8.005	6.504	0.100	3.002	1.001	10.006	0.340	42.025	2.502	2.001	2.501	2.001	100
LAWM19	Middle	NO	YES	7.997	11.996	7.997	1.999	1.999	0.500	1.000	13.169	0.363	41.984	0.500	4.998	3.499	1.999	100
LAWM20	Middle	NO	YES	5.001	7.002	8.002	2.001	2.001	2.265	3.501	17.005	0.206	42.013	0.500	5.001	3.501	2.001	100
LAWM21	Middle	NO	YES	5.005	10.901	8.008	6.507	2.002	3.003	1.001	10.010	0.460	42.042	2.503	5.005	3.504	0.050	100
LAWM22	Middle	NO	YES	7.990	6.991	1.998	6.492	1.998	0.499	3.496	16.979	0.451	41.949	0.670	4.994	3.496	1.998	100
LAWM23	Middle	NO	YES	5.011	7.016	8.018	2.004	2.004	3.007	1.002	10.022	0.337	48.549	2.506	5.011	3.508	2.004	100
LAWM24	Middle	NO	YES	8.000	12.000	2.000	6.500	2.000	0.641	1.000	17.000	0.233	47.075	0.500	2.000	1.000	0.050	100
LAWM25R1	Middle	NO	YES	8.011	12.017	2.003	3.684	2.003	3.004	3.505	10.014	0.263	49.990	0.501	2.003	1.001	2.003	100
LAWM26	Middle	NO	YES	8.005	12.008	4.970	2.001	0.100	3.002	1.001	10.007	0.493	49.907	0.500	5.003	1.001	2.001	100
LAWM27	Middle	NO	YES	8.006	7.005	8.006	6.505	2.001	0.500	3.503	13.382	0.247	42.031	2.502	3.310	1.001	2.002	100
LAWM28	Middle	NO	YES	5.010	12.024	8.016	6.513	0.703	0.690	1.002	10.020	0.358	50.102	2.505	2.004	1.002	0.050	100
LAWM29	Middle	NO	YES	7.565	7.006	2.002	6.506	2.002	3.003	3.503	10.009	0.312	46.892	2.502	5.004	3.503	0.192	100
LAWM30	Middle	NO	YES	8.003	12.004	2.001	6.502	0.100	2.023	1.000	17.006	0.201	42.015	0.592	5.002	3.501	0.050	100
LAWM31	Middle	NO	YES	5.002	7.002	8.003	6.502	0.100	3.001	1.000	16.757	0.304	42.325	2.501	2.001	3.501	2.001	100
LAWM32	Middle	NO	YES	5.146	7.002	2.001	2.001	2.001	3.001	3.501	16.515	0.314	50.016	0.500	5.002	1.000	2.001	100
LAWM33R1	Middle	NO	NO	5.002	12.005	8.003	6.503	1.722	0.899	1.000	17.007	0.291	42.016	2.501	2.001	1.000	0.050	100
LAWM34	Middle	NO	NO	5.002	8.356	8.003	6.295	2.001	3.001	1.000	17.006	0.296	42.014	1.475	2.001	3.501	0.050	100
LAWM35	Middle	LAWM56	NO	5.003	12.006	6.182	4.413	0.100	0.500	3.502	17.009	0.183	42.022	2.501	2.001	2.576	2.001	100
LAWM36	Inner	NO	YES	7.003	11.004	7.003	5.002	0.300	2.501	1.501	12.005	0.367	45.017	2.001	3.501	2.001	0.795	100
LAWM37	Inner	NO	YES	6.751	11.009	7.006	5.004	0.300	2.502	2.502	12.010	0.322	45.037	1.001	3.503	3.002	0.050	100
LAWM38	Inner	NO	YES	6.998	7.998	6.998	2.999	0.154	2.499	1.500	13.996	0.371	47.988	1.000	3.499	1.999	1.999	100
LAWM39	Inner	NO	YES	7.007	9.063	5.005	3.003	0.100	2.502	2.502	14.013	0.253	48.045	1.001	3.503	2.002	2.002	100
LAWM40	Inner	NO	YES	6.003	11.006	5.003	5.003	0.100	1.001	1.501	14.008	0.309	48.027	1.001	3.502	3.002	0.535	100
LAWM41	Inner	NO	YES	7.002	8.002	7.002	5.001	0.300	1.000	2.501	14.003	0.344	45.010	1.000	4.601	2.235	2.000	100

Table 6.1. Normalized[(a)] Compositions (wt%) for ILAW PCT Modeling Data (continued).

Glass ID	Layer[(b)]	Replicate[(c)]	Retained[(d)]	Al2O3	B2O3	CaO	Fe2O3	K2O	Li2O	MgO	Na2O	SO3 .XRF[(e)]	SiO2	TiO2	ZnO	ZrO2	Others	Sum
LAWM42	Inner	NO	YES	6.004	8.005	5.003	4.037	0.100	2.502	1.501	14.009	0.299	48.032	2.001	3.502	3.002	2.001	100
LAWM43	Inner	NO	YES	7.003	8.678	5.002	5.002	0.300	2.501	2.501	12.004	0.388	45.017	2.001	4.602	3.001	2.001	100
LAWM44	Inner	NO	YES	6.325	10.039	7.008	5.006	0.100	1.001	1.502	12.014	0.290	48.055	2.002	4.605	2.002	0.050	100
LAWM45	Inner	NO	YES	7.003	8.003	5.784	5.002	0.300	1.423	1.501	14.005	0.308	48.018	2.001	4.602	2.001	0.050	100
LAWM46	Inner	NO	YES	6.012	11.023	6.523	5.010	0.100	1.002	2.505	12.025	0.199	48.034	1.002	3.507	3.006	0.050	100
LAWM47	Inner	NO	YES	6.200	8.003	7.003	5.002	0.100	1.000	2.501	14.006	0.305	48.020	1.307	3.501	3.001	0.050	100
LAWM48	Inner	NO	YES	6.235	11.017	5.278	5.008	0.100	1.002	1.502	12.018	0.255	48.072	2.003	3.505	2.003	2.003	100
LAWM49	Inner	NO	YES	7.001	10.905	5.001	3.000	0.100	1.000	1.500	14.002	0.353	47.536	1.000	4.601	2.000	2.000	100
LAWM50	Center	LAWM51	YES	6.530	9.700	6.109	4.111	0.204	1.668	2.032	13.095	0.290	46.982	1.528	4.104	2.533	1.115	100
LAWM51	Center	LAWM50	YES	6.528	9.697	6.108	4.110	0.204	1.667	2.031	13.092	0.315	46.970	1.528	4.103	2.533	1.115	100
LAWM52	Existing	LAWA88	YES	6.083	9.701	1.992	5.533	2.584	0.000	1.476	20.007	0.177	44.007	1.992	2.951	2.988	0.509	100
LAWM53	Outer	LAWM01	YES	9.031	6.021	10.035	8.028	4.014	4.516	0.000	5.017	0.657	44.604	3.010	5.017	0.000	0.050	100
LAWM54R1	Outer	LAWM09	YES	3.505	6.009	10.014	8.011	4.006	2.392	0.000	5.007	0.257	49.783	0.000	5.007	4.006	2.003	100
LAWM55	Outer	LAWM12	NO	3.501	13.004	0.000	2.310	4.001	4.502	1.971	14.258	0.236	42.213	3.001	5.002	4.001	2.001	100
LAWM56	Middle	LAWM35	NO	4.990	11.975	6.166	4.402	0.100	0.499	3.493	16.965	0.440	41.914	2.495	1.996	2.570	1.996	100
LAWA44R10	Existing	NO	YES	6.229	8.941	1.999	7.012	0.502	0.000	1.999	20.093	0.090	44.756	1.999	2.974	3.004	0.402	100
LAWA53	Existing	NO	YES	6.088	6.108	7.768	7.398	0.490	0.000	1.460	19.715	0.615	41.650	1.090	2.949	2.949	1.720	100
LAWA56	Existing	NO	YES	6.096	11.942	1.952	7.407	0.490	0.000	1.461	19.739	0.524	41.700	1.091	2.953	2.953	1.692	100
LAWA88R1	Existing	LAWM52	YES	6.081	9.702	1.990	5.531	2.581	0.000	1.470	20.004	0.190	43.999	1.990	2.951	2.991	0.520	100
LAWA102R1	Existing	NO	YES	6.063	10.005	5.072	5.413	0.260	2.501	1.501	14.497	0.674	46.622	1.141	3.061	3.021	0.170	100
LAWA126	Existing	NO	YES	5.640	9.820	1.990	5.540	3.880	0.000	1.480	18.460	0.309	44.120	2.000	2.960	2.990	0.810	100
LAWA128	Existing	NO	YES	6.030	7.070	2.080	5.790	3.880	0.000	1.180	18.461	0.296	46.092	2.090	3.090	3.130	0.810	100
LAWA130	Existing	NO	YES	6.030	8.950	2.080	2.860	3.880	0.000	1.180	18.460	0.329	46.090	2.090	4.140	3.130	0.780	100
LAWB65	Existing	NO	YES	6.170	9.910	6.670	5.280	0.260	4.290	2.960	5.460	0.892	48.349	1.390	4.650	3.150	0.570	100
LAWB66	Existing	NO	YES	6.170	9.910	8.170	5.280	0.260	4.290	2.960	5.460	0.650	48.350	1.390	3.150	3.150	0.810	100
LAWB68	Existing	NO	YES	6.170	8.410	8.170	5.280	0.260	4.290	2.960	5.460	0.831	48.350	1.390	4.650	3.150	0.630	100
LAWB78	Existing	NO	YES	6.150	12.330	7.120	3.250	0.230	3.050	2.970	9.780	0.507	47.001	0.000	4.000	3.150	0.460	100
LAWB79	Existing	NO	YES	6.150	12.330	7.120	3.250	0.230	3.510	2.970	8.620	0.580	47.700	0.000	4.000	3.150	0.390	100
LAWB80	Existing	NO	YES	6.150	12.330	7.120	3.250	1.990	3.510	2.970	6.620	0.582	47.949	0.000	4.000	3.150	0.380	100
LAWB83	Existing	NO	YES	6.180	10.030	6.780	5.290	0.190	4.310	2.970	5.470	0.494	48.598	1.390	4.840	3.160	0.300	100
LAWB84	Existing	NO	YES	6.180	10.030	6.680	5.290	0.190	4.400	2.970	5.470	0.440	48.600	1.390	4.840	3.160	0.360	100
LAWB85	Existing	NO	YES	6.180	11.519	5.280	5.290	0.190	4.310	2.970	5.470	0.485	48.598	1.390	4.840	3.160	0.320	100
LAWB86	Existing	NO	YES	6.180	12.410	5.730	5.290	0.190	4.350	2.970	5.470	0.432	48.599	0.000	4.840	3.160	0.380	100
C100G136B	Existing	NO	YES	6.134	10.103	6.415	6.485	0.150	2.736	1.513	11.887	0.400	46.778	1.123	3.017	3.027	0.231	100
LAWC27	Existing	NO	YES	6.120	12.191	8.550	0.010	0.140	2.730	1.500	11.961	0.405	48.882	1.120	3.020	3.020	0.350	100
LAWC32	Existing	NO	YES	6.490	10.050	9.040	2.420	0.140	2.730	1.500	11.960	0.380	46.740	1.120	4.020	3.020	0.390	100

(a) The compositions listed in this table are normalized versions of target compositions of the glasses, after replacing the target values of SO_3 by XRF analyzed values. That is, after replacing the target SO_3 values by analyzed values, the component wt% values were summed for each glass, and the wt% value for each component divided by the sum for that glass and multiplied by 100. The result is normalized wt% values summing to 100 wt%.

(b) Layer of the Combined Matrix: Existing = Existing Matrix, Outer = outer layer of Test Matrix, Middle = middle layer of Test Matrix, Inner = inner layer of Test Matrix, and Center = a center point.

(c) If a given glass has a replicate, the glass ID is listed. If not, NO is listed. (d) YES means the data point was used in developing PCT models, NO means it was not used.

(d) SO_3.XRF indicates that the SO_3 composition is based on chemical analysis by XRF.

Table 6.2. PCT Releases and Data Splitting Validation Sets for ILAW PCT Modeling Data.

Glass ID	Layer[a]	Replicate[b]	Retained[c]	B (ppm)	Na (ppm)	Si (ppm)	B (g/L)	Na (g/L)	Si (g/L)	B Data Splitting Validation Set	Na Data Splitting Validation Set
LAWM1	Outer	LAWM53	YES	2.8530	10.8100	27.3100	0.1524	0.2900	0.1308	NA	NA
LAWM2	Outer	NO	YES	12.5700	31.7400	67.1700	0.6723	0.8528	0.3047	1	3
LAWM3	Outer	NO	YES	14.8600	98.8700	47.3100	0.7946	1.1568	0.2521	1	5
LAWM4	Outer	NO	YES	18.5900	22.3200	36.6800	0.4584	0.5991	0.1886	2	5
LAWM5	Outer	NO	YES	4.5900	10.4000	36.3800	0.2452	0.2791	0.1591	3	3
LAWM6	Outer	NO	YES	18.0400	47.6600	36.0700	0.5474	0.7139	0.1929	4	1
LAWM7	Outer	NO	YES	5.3870	15.9700	52.0800	0.2490	0.4293	0.2137	4	1
LAWM8	Outer	NO	YES	13.0000	10.3000	29.2100	0.3210	0.2768	0.1400	2	2
LAWM9	Outer	LAWM54R1	YES	3.9230	19.0700	31.5000	0.2102	0.5133	0.1353	NA	NA
LAWM10	Outer	NO	YES	9.7800	42.9400	26.2500	0.2421	0.4427	0.1398	2	3
LAWM11	Outer	NO	YES	46.9300	120.4000	120.3000	1.1613	1.4125	0.5499	1	2
LAWM12	Outer	LAWM55	NO	1199.0000	1701.0000	468.1000	29.6859	16.0806	2.3722	NA	NA
LAWM13	Outer	NO	NO	46.1200	804.9000	223.0000	2.4746	4.9308	1.1924	NA	NA
LAWM14	Outer	NO	YES	37.1700	352.8000	276.3000	1.9950	2.1619	1.1368	3	5
LAWM15	Outer	NO	YES	63.0900	251.3000	101.2000	2.1713	1.5400	0.4981	5	3
LAWM16	Middle	NO	YES	10.6200	30.7900	31.3400	0.2848	0.4148	0.1578	1	5
LAWM17	Middle	NO	NO	467.0000	1006.0000	179.0000	12.5263	7.9738	0.9114	NA	NA
LAWM18	Middle	NO	YES	16.1200	37.7700	37.3900	0.4323	0.5088	0.1903	1	1
LAWM19	Middle	NO	YES	18.8000	54.1200	36.1300	0.5047	0.5540	0.1841	3	2
LAWM20	Middle	NO	YES	58.0500	343.6000	147.5000	2.6695	2.7237	0.7511	2	2
LAWM21	Middle	NO	YES	30.1600	70.9400	61.4900	0.8909	0.9553	0.3129	1	2
LAWM22	Middle	NO	YES	8.5270	78.5700	56.3500	0.3927	0.6238	0.2874	2	2
LAWM23	Middle	NO	YES	6.0570	37.9400	45.7400	0.2780	0.5103	0.2016	5	2
LAWM24	Middle	NO	YES	39.2600	103.8000	62.8500	1.0534	0.8230	0.2856	3	1
LAWM25R1	Middle	NO	YES	30.3700	42.7300	61.9800	0.8138	0.5752	0.2652	3	1
LAWM26	Middle	NO	YES	15.7700	26.3700	48.9900	0.4229	0.3552	0.2100	4	4
LAWM27	Middle	NO	YES	15.0000	84.3700	49.2900	0.6895	0.8499	0.2509	3	2
LAWM28	Middle	NO	YES	13.7700	39.2300	49.4400	0.3687	0.5277	0.2111	4	4
LAWM29	Middle	NO	YES	10.9600	36.3100	60.9300	0.5037	0.4890	0.2780	2	3
LAWM30	Middle	NO	YES	43.9600	129.0000	60.5100	1.1792	1.0225	0.3081	2	1
LAWM31	Middle	NO	YES	49.4300	272.2000	146.4000	2.2730	2.1896	0.7400	1	1
LAWM32	Middle	NO	YES	43.4600	225.0000	202.3000	1.9985	1.8365	0.8653	4	4
LAWM33R1	Middle	NO	NO	159.5000	518.7000	179.5000	4.2782	4.1113	0.9140	NA	NA
LAWM34	Middle	NO	NO	135.5000	538.0000	234.4000	5.2212	4.2645	1.1936	NA	NA
LAWM35	Middle	LAWM56	NO	392.5000	836.0000	168.9000	10.5265	6.6254	0.8599	NA	NA
LAWM36	Inner	NO	YES	16.7000	54.0600	49.5200	0.4887	0.6070	0.2353	5	1
LAWM37	Inner	NO	YES	42.2900	87.7900	65.9900	1.2369	0.9853	0.3135	5	4
LAWM38	Inner	NO	YES	9.5030	71.1600	58.9900	0.3826	0.6853	0.2630	1	4
LAWM39	Inner	NO	YES	15.1100	48.0900	47.6700	0.5369	0.4626	0.2123	3	4
LAWM40	Inner	NO	YES	26.2500	75.3800	65.4500	0.7680	0.7254	0.2915	5	2
LAWM41	Inner	NO	YES	8.9500	60.8500	49.2600	0.3602	0.5858	0.2341	3	4
LAWM42	Inner	NO	YES	13.2300	60.3100	60.3100	0.5321	0.5803	0.2686	1	2
LAWM43	Inner	NO	YES	17.7300	58.0300	58.0200	0.6579	0.6516	0.2757	5	3
LAWM44	Inner	NO	YES	15.5000	50.4600	52.3500	0.4971	0.5662	0.2331	1	4
LAWM45	Inner	NO	YES	10.6000	60.8200	51.5100	0.4265	0.5854	0.2295	5	3
LAWM46	Inner	NO	YES	16.3500	41.6000	40.8600	0.4776	0.4663	0.1820	4	5
LAWM47	Inner	NO	YES	12.9600	75.9900	60.4700	0.5214	0.7314	0.2694	5	5
LAWM48	Inner	NO	YES	16.0100	50.7700	51.7500	0.4680	0.5695	0.2303	3	5
LAWM49	Inner	NO	YES	18.1600	52.3500	47.8100	0.5362	0.5040	0.2152	2	5
LAWM50	Center	LAWM51	YES	19.4900	61.1700	55.6700	0.6470	0.6297	0.2535	NA	NA
LAWM51	Center	LAWM50	YES	20.8400	69.6700	57.3200	0.6920	0.7174	0.2611	NA	NA
LAWM52	Existing	LAWA88	YES	43.5600	172.5000	84.7300	1.4458	1.1622	0.4119	NA	NA

Table 6.2. PCT Releases and Data Splitting Validation Sets for ILAW PCT Modeling Data (continued).

Glass ID	Layer[(a)]	Replicate[(b)]	Retained[(c)]	B (ppm)	Na (ppm)	Si (ppm)	B (g/L)	Na (g/L)	Si (g/L)	B Data Splitting Validation Set[(d)]	Na Data Splitting Validation Set[(d)]
LAWM53	Outer	LAWM01	YES	3.3370	9.9530	23.6700	0.1785	0.2674	0.1135	NA	NA
LAWM54R1	Outer	LAWM09	YES	6.9400	13.6400	32.0500	0.3719	0.3672	0.1377	NA	NA
LAWM55	Outer	LAWM12	NO	1440.0000	2426.0000	441.8000	35.6556	22.9363	2.2391	NA	NA
LAWM56	Middle	LAWM35	NO	543.1000	1233.0000	209.5000	14.6030	9.7969	1.0693	NA	NA
LAWA44R10	Existing	NO	YES	29.8100	139.9000	90.3000	1.0736	0.9386	0.4316	4	1
LAWA53	Existing	NO	YES	15.4000	156.3000	68.3200	0.8118	1.0687	0.3509	2	3
LAWA56	Existing	NO	YES	64.3900	172.3000	64.0200	1.7363	1.1766	0.3284	2	1
LAWA88R1	Existing	LAWM52	YES	49.1800	192.2000	93.0100	1.6322	1.2952	0.4522	NA	NA
LAWA102R1	Existing	NO	YES	26.7400	78.6100	78.4300	0.8606	0.7310	0.3599	4	4
LAWA126	Existing	NO	YES	36.4700	143.5000	68.2800	1.1958	1.0479	0.3311	3	2
LAWA128	Existing	NO	YES	13.8000	118.9000	75.5500	0.6285	0.8682	0.3507	3	4
LAWA130	Existing	NO	YES	25.5900	126.5000	76.7400	0.9207	0.9237	0.3562	2	5
LAWB65	Existing	NO	YES	17.1400	19.3900	46.7300	0.5569	0.4787	0.2068	5	2
LAWB66	Existing	NO	YES	18.1100	22.2007	48.5530	0.5884	0.5481	0.2148	1	5
LAWB68	Existing	NO	YES	13.1837	19.2747	44.7807	0.5048	0.4759	0.1981	4	1
LAWB78	Existing	NO	YES	46.9400	80.6800	70.5900	1.2258	1.1120	0.3213	4	4
LAWB79	Existing	NO	YES	41.7800	62.5900	67.2800	1.0911	0.9788	0.3018	5	3
LAWB80	Existing	NO	YES	33.7600	35.7900	56.4100	0.8817	0.7288	0.2517	5	3
LAWB83	Existing	NO	YES	19.0600	21.3800	52.3500	0.6119	0.5269	0.2305	2	3
LAWB84	Existing	NO	YES	21.0200	22.7200	55.7300	0.6748	0.5599	0.2453	2	3
LAWB85	Existing	NO	YES	23.2900	20.3000	55.6900	0.6510	0.5003	0.2452	4	4
LAWB86	Existing	NO	YES	48.3100	41.0000	75.2200	1.2535	1.0104	0.3311	1	5
C100G136B	Existing	NO	YES	23.0100	61.3800	58.3000	0.7333	0.6960	0.2666	4	5
LAWC27	Existing	NO	YES	14.2700	39.0200	41.8600	0.3769	0.4398	0.1832	5	2
LAWC32	Existing	NO	YES	13.0460	49.0380	45.3380	0.4180	0.5527	0.2075	3	1

(a) Layer of the Combined Matrix: Existing = Existing Matrix, Outer = outer layer of Test Matrix, Middle = middle layer of Test Matrix, Inner = inner layer of Test Matrix, and Center = a center point.
(b) If a given glass has a replicate, the glass ID is listed. If not, NO is listed.
(c) YES means the data point was used in developing PCT models, NO means it was not used.
(d) NA denotes glasses not included in the modeling dataset. Numbers from 1 to 5 denote the five split validation subsets.

Table 6.3. Performance Results Investigating Number of Glasses to Drop for ILAW PCT Models.

PCT-Boron Models[a]	**Linear Mixture Model**							**Partial Quadratic Mixture Model with 0.01[b]**							**Partial Quadratic Mixture Model with 0.05[b]**					
Number Dropped[c]	0	2	3	5	7	8		0	2	3	5	7	8		0	2	3	5	7	8
R^2	0.8236	0.7688	0.7812	0.7758	0.7928	0.7978		0.9364	0.9502	0.9329	0.8833	0.8781	0.8699		0.9756	0.9659	0.9710	0.9376	0.9300	0.9073
R^2 Adjusted (R^2_A)	0.7872	0.7196	0.7338	0.7256	0.7447	0.7500		0.9181	0.9317	0.9110	0.8493	0.8442	0.8331		0.9636	0.9495	0.9567	0.9114	0.9014	0.8739
R^2 Predicted (R^2_P)	0.6799	0.5726	0.5893	0.5670	0.5959	0.6148		0.8792	0.8903	0.8667	0.7791	0.7632	0.7406		0.9303	0.9143	0.9248	0.8643	0.8452	0.8011
RMSE	0.4960	0.4791	0.4346	0.3747	0.3256	0.3142		0.3077	0.2364	0.2513	0.2777	0.2544	0.2567		0.2052	0.2033	0.1752	0.2129	0.2024	0.2232
R^2 Validation Statistics[d]																				
R^2 All (59)	0.0909	0.1876	0.2838	0.4498	0.5431	0.5798		-0.1476	-0.3031	-0.0130	-0.1760	0.3638	0.3685		-0.3092	0.0032	0.4134	0.3640	0.3984	0.4545
R^2 V1: Trimmed (56)	0.1014	0.2046	0.2957	0.4667	0.5580	0.5928		-0.0311	0.0460	0.1267	-0.0845	0.4083	0.4124		0.0537	0.4336	0.4550	0.4053	0.4150	0.4656
R^2 V2: SCC +/- 10% (40)	-0.0917	0.0760	0.2006	0.4057	0.4978	0.5516		0.0000	0.3114	0.0818	0.0483	0.3776	0.3833		0.2206	0.4013	0.2428	0.3413	0.2749	0.4232
R^2 V3: SCC (26)	-1.8295	-1.2491	-0.8984	-0.3001	-0.0770	0.0206		-1.5261	-0.5426	-0.9445	-0.2900	-0.0173	-0.0106		-0.6972	-0.2962	-0.2104	-0.1873	0.1680	0.2559
R^2 V4: SCC & MCC (22)	-2.1377	-1.4629	-1.0616	-0.4146	-0.1773	-0.0672		-1.1766	-0.8531	-1.0684	-0.4695	-0.1668	-0.1585		-0.3537	-0.5042	-0.3067	-0.2513	0.0557	0.1968

PCT-Sodium Models[a]	**Linear Mixture Model**							**Partial Quadratic Mixture Model with 0.01[b]**							**Partial Quadratic Mixture Model with 0.05[b]**					
Number Dropped[c]	0	2	3	5	7	8		0	2	3	5	7	8		0	2	3	5	7	8
R^2	0.8341	0.8042	0.8241	0.8455	0.8287	0.8555		0.9235	0.9245	0.9174	0.9002	0.8755	0.8951		0.9776	0.9645	0.9619	0.9528	0.9472	0.9332
R^2 Adjusted (R^2_A)	0.7998	0.7625	0.7860	0.8109	0.7889	0.8213		0.9030	0.9002	0.8924	0.8734	0.8409	0.8654		0.9667	0.9463	0.9433	0.9330	0.9256	0.9073
R^2 Predicted (R^2_P)	0.7065	0.6529	0.6840	0.7196	0.7004	0.7535		0.8499	0.8404	0.8263	0.8206	0.7670	0.8049		0.9464	0.9139	0.9026	0.9039	0.8890	0.8722
RMSE	0.4041	0.3696	0.3263	0.2642	0.2437	0.2067		0.2812	0.2395	0.2314	0.2162	0.2115	0.1794		0.1649	0.1757	0.1680	0.1573	0.1446	0.1489
R^2 Validation Statistics[d]																				
R^2 All (59)	0.1498	0.3007	0.3851	0.5011	0.5525	0.5781		0.4467	0.4344	0.4988	0.3499	0.4093	0.4596		0.2516	0.1602	-0.3448	-0.0079	0.4402	0.3717
R^2 V1: Trimmed (56)	0.1218	0.2759	0.3493	0.4793	0.5374	0.5716		0.5072	0.5101	0.5541	0.3332	0.3957	0.4517		0.4214	0.3039	0.0743	0.6339	0.5479	0.3393
R^2 V2: SCC +/- 10% (40)	-0.2254	0.0417	0.1632	0.4103	0.5058	0.5706		0.2175	0.2494	0.3057	0.2929	0.3755	0.4686		0.1690	0.1323	0.3128	0.6292	0.4823	0.4469
R^2 V3: SCC (26)	-1.8395	-1.0510	-0.7205	-0.1005	0.0423	0.1809		-0.8397	-0.7764	-0.5907	0.0584	0.1291	0.2460		-0.0343	-0.2560	-0.2348	0.1497	0.1358	0.4003
R^2 V4: SCC & MCC (22)	-2.1701	-1.2550	-0.8760	-0.1942	-0.0249	0.1234		-0.9866	-0.8559	-0.7328	-0.0648	0.0231	0.1586		-0.1512	-0.3548	-0.3376	0.1406	0.1020	0.3424

(a) The evaluation statistics are defined in Section C.2 of Appendix C.
(b) Partial quadratic mixture models were developed using significance levels of 0.01 and 0.05 to decide when to stop adding quadratic terms. See the discussion in Section C.3.2 of Appendix C.
(c) The number of data points with the highest PCT releases that were dropped from the modeling dataset.
(d) R^2 validation is defined in Section C.4 of Appendix C. The descriptions of the complete validation set (All) and the various validation subsets (V1 to V4) are described in Section 6.1.3. A negative R^2 validation value means that the sum of squares of model prediction errors is larger than if the mean response value over the validation data were used as the predicted value for each glass. In other words, the model predicts worse for the validation data than the mean response value does.

Table 6.4. Variation in PCT-Boron and PCT-Sodium Responses for Replicate Pairs.

Glass IDs of Replicate Pairs	Included in PCT Modeling Data?	PCT-Boron		PCT-Sodium	
		g/L	ln(g/L)	g/L	ln(g/L)
LAWM01	Yes	0.1524	-1.88125	0.2900	-1.23787
LAWM53	Yes	0.1785	-1.72317	0.2674	-1.31901
		%RSD [(a)] = 11.15	**SD = 0.1118**	**%RSD = 5.73**	**SD = 0.0574**
LAWM09	Yes	0.2102	-1.55970	0.5133	-0.66689
LAWM54R1	Yes	0.3719	-0.98913	0.3672	-1.00185
		%RSD = 39.29	**SD = 0.4035**	**%RSD = 23.47**	**SD = 0.2368**
LAWM12	No	29.6859	3.39067	16.0806	2.77761
LAWM55	No	35.6556	3.57391	22.9363	3.13272
		%RSD = 12.92	**SD = 0.1296**	**%RSD = 24.85**	**SD = 0.2511**
LAWM35	No	10.5265	2.35390	6.6254	1.89091
LAWM56	No	14.6030	2.68123	9.7969	2.28207
		%RSD = 22.94	**SD = 0.2315**	**%RSD = 27.31**	**SD = 0.2766**
LAWM50	Yes	0.6470	-0.43541	0.6297	-0.46251
LAWM51	Yes	0.6920	-0.36817	0.7174	-0.33212
		%RSD = 4.75	**SD = 0.0475**	**%RSD = 9.21**	**SD = 0.0922**
LAWM52	Yes	1.4458	0.36866	1.1622	0.15031
LAWA88R1	Yes	1.6322	0.48993	1.2952	0.25867
		%RSD = 8.56	**SD = 0.0857**	**%RSD = 7.65**	**SD = 0.0766**
Pooled Over All 6 Replicate Pairs		**%RSD = 20.24**	**SD = 0.2063**	**%RSD = 18.66**	**SD = 0.1886**
Pooled Over 4 Replicate Pairs Used for Modeling		**%RSD = 21.00**	**SD = 0.2150**	**%RSD = 13.48**	**SD = 0.1358**

(a) %RSD = 100*(Standard Deviation / Mean)

Table 6.5. Normalized[(a)] Compositions (wt%) for ILAW PCT Validation Data.

Glass ID	Ag2O	Al2O3	B2O3	Cl	CaO	Cr2O3	Cs2O	F	Fe2O3	K2O	Li2O	MgO	MnO	Na2O	NiO	P2O5	PbO	Re2O7	SO3 .XRF	SiO2	TiO2	ZnO	ZrO2	Sum
LAWA104	0.001	6.612	8.592	0.717	1.921	0.022	0.001	0.010	6.732	0.550	0.000	1.921	0.000	22.006	0.000	0.037	0.002	0.100	0.103	43.002	1.925	2.861	2.887	100
LAWA105	0.001	7.029	8.284	0.780	1.851	0.022	0.001	0.010	6.493	0.600	0.000	1.851	0.000	24.012	0.000	0.040	0.002	0.100	0.093	41.440	1.851	2.757	2.781	100
LAWA33	0.000	11.974	8.853	0.580	0.000	0.020	0.000	0.040	5.772	3.101	0.000	1.991	0.000	20.007	0.000	0.080	0.010	0.000	0.095	38.223	2.491	4.271	2.491	100
LAWA49	0.001	6.203	8.904	0.650	0.000	0.020	0.001	0.010	9.984	0.500	0.000	1.481	0.000	20.009	0.000	0.030	0.001	0.100	0.073	44.570	1.991	2.481	2.991	100
LAWA51	0.001	6.204	11.974	0.586	0.000	0.018	0.001	0.010	6.999	0.451	0.000	1.484	0.000	18.006	0.000	0.030	0.001	0.100	0.073	46.586	1.997	2.489	2.989	100
LAWA52	0.001	6.181	6.191	0.650	7.882	0.020	0.001	0.010	7.512	0.500	0.000	1.480	0.000	20.005	0.000	0.030	0.000	0.100	0.095	42.260	1.100	2.991	2.991	100
LAWA60	0.001	8.531	11.231	0.650	4.320	0.020	0.001	0.010	0.000	0.500	0.000	1.990	0.000	20.001	0.000	0.034	0.000	0.100	0.104	44.556	1.994	2.965	2.992	100
LAWC15	0.000	6.225	8.942	0.078	2.008	0.003	0.002	0.470	7.014	0.142	0.000	2.008	0.000	19.983	0.035	0.015	0.004	0.100	0.230	44.742	1.998	2.993	3.007	100
LAWC25	0.000	5.782	9.527	0.120	6.052	0.019	0.000	0.060	6.112	8.079	0.000	1.428	0.003	11.205	0.000	0.110	0.000	0.094	0.530	44.120	1.059	2.846	2.856	100
TFA-BASE	0.000	7.000	10.001	0.280	0.000	0.000	0.000	0.010	5.500	0.410	0.000	1.500	0.000	20.001	0.000	0.060	0.000	0.090	0.075	49.072	3.000	1.500	1.500	100
LAWA133	0.000	6.204	8.901	0.559	5.484	0.020	0.000	0.040	3.486	0.430	0.000	1.998	0.000	19.979	0.000	0.100	0.000	0.100	0.204	44.534	1.998	2.967	2.997	100
LAWA134	0.000	5.647	9.964	0.200	2.019	0.020	0.000	0.290	5.627	3.728	0.000	1.499	0.000	17.730	0.000	0.080	0.000	0.100	0.276	44.755	2.029	2.998	3.038	100
LAWA135	0.000	5.655	10.092	0.190	2.048	0.020	0.000	0.280	5.695	3.577	0.000	1.519	0.000	17.016	0.000	0.070	0.000	0.100	0.271	45.303	2.048	3.038	3.078	100
LAWA136	0.000	5.656	10.092	0.190	3.048	0.020	0.000	0.280	5.696	3.577	0.000	1.519	0.000	17.017	0.000	0.070	0.000	0.100	0.267	44.306	2.048	3.038	3.078	100
LAWB60	0.000	6.154	12.335	0.008	11.878	0.047	0.000	0.078	0.001	0.234	4.614	2.969	0.000	6.623	0.000	0.045	0.000	0.100	0.642	47.968	0.000	3.152	3.152	100
LAWB62	0.000	6.188	9.939	0.000	11.986	0.100	0.000	0.070	0.000	0.261	5.807	2.969	0.000	5.476	0.000	0.010	0.000	0.100	0.886	48.494	1.394	3.159	3.159	100
LAWB63	0.000	6.572	9.944	0.000	9.342	0.100	0.000	0.070	0.000	0.261	5.047	2.970	0.000	5.479	0.000	0.010	0.000	0.100	0.844	48.896	1.395	5.810	3.161	100
LAWB64	0.000	6.201	9.960	0.000	6.704	0.101	0.000	0.070	3.297	0.261	5.819	2.975	0.000	5.488	0.000	0.010	0.000	0.101	0.681	48.594	1.397	5.176	3.166	100
LAWB67	0.000	6.183	9.931	0.000	5.181	0.100	0.000	0.070	5.291	0.261	4.299	2.966	0.000	5.472	0.000	3.016	0.000	0.100	0.971	48.452	1.393	3.157	3.157	100
LAWB69	0.000	6.151	12.333	0.010	10.462	0.050	0.000	0.080	0.000	0.230	4.611	2.971	0.000	6.621	0.000	0.050	0.000	0.100	0.649	47.960	0.000	4.571	3.151	100
LAWB70	0.000	6.159	12.347	0.010	6.629	0.050	0.000	0.080	3.255	0.230	4.616	2.974	0.000	6.629	0.000	0.050	0.000	0.100	0.541	48.017	0.000	5.157	3.154	100
LAWB71	0.000	6.162	10.802	0.010	6.633	0.050	0.000	0.080	3.257	0.230	4.619	2.976	0.000	6.633	0.000	0.050	0.000	0.100	0.480	48.047	1.553	5.160	3.156	100
LAWB72	0.000	6.155	12.339	0.010	7.125	0.050	0.000	0.080	3.252	0.230	4.113	2.972	0.000	6.625	0.000	0.050	0.000	0.100	0.607	47.985	0.000	5.154	3.152	100
LAWB73	0.000	6.187	9.937	0.000	9.336	0.100	0.000	0.070	1.905	0.261	5.044	2.968	0.000	5.485	0.000	0.010	0.000	0.100	0.897	48.484	1.394	4.663	3.159	100
LAWB74	0.000	6.195	10.342	0.000	8.695	0.099	0.000	0.070	1.908	0.261	5.311	2.972	0.000	5.492	0.000	0.010	0.000	0.100	0.771	48.546	1.396	4.669	3.163	100
LAWB75	0.000	6.181	11.780	0.000	8.675	0.100	0.000	0.070	1.903	0.260	5.299	1.503	0.000	5.480	0.000	0.010	0.000	0.100	0.998	48.434	1.392	4.658	3.155	100
LAWB76	0.000	6.180	11.778	0.000	8.673	0.100	0.000	0.070	1.903	0.260	5.799	1.502	0.000	5.478	0.000	0.010	0.000	0.100	1.017	49.316	0.000	4.657	3.155	100
LAWB77	0.000	6.160	12.349	0.010	6.630	0.050	0.000	0.080	2.203	0.230	4.116	2.975	0.000	6.630	0.000	0.050	0.000	0.100	0.524	48.025	1.552	5.158	3.155	100
LAWB81	0.000	6.155	12.340	0.010	7.126	0.050	0.000	0.080	3.253	0.230	4.263	2.972	0.000	6.625	0.000	0.050	0.000	0.100	0.599	47.989	0.000	5.004	3.153	100
LAWB82	0.000	6.163	10.101	0.010	7.134	0.050	0.000	0.080	9.519	0.230	4.269	1.483	0.000	6.633	0.000	0.050	0.000	0.100	0.478	45.532	0.000	5.010	3.156	100
LAWB89	0.000	6.186	10.040	0.010	6.787	0.040	0.000	0.060	5.295	0.190	5.005	2.973	0.000	4.084	0.000	0.040	0.000	0.100	0.443	49.348	1.391	4.845	3.163	100
LAWB90	0.000	6.193	10.050	0.010	6.794	0.040	0.000	0.060	5.301	0.190	3.617	2.976	0.000	6.884	0.000	0.040	0.000	0.100	0.338	47.997	1.393	4.850	3.166	100
LAWB91	0.000	6.191	10.047	0.010	6.792	0.040	0.000	0.060	5.299	0.190	2.925	2.975	0.000	8.735	0.000	0.040	0.000	0.100	0.367	46.821	1.392	4.848	3.165	100
LAWB92	0.000	6.187	10.041	0.010	6.788	0.040	0.000	0.060	5.296	0.190	2.222	2.973	0.000	10.121	0.000	0.040	0.000	0.100	0.429	46.101	1.392	4.845	3.164	100
LAWB93	0.000	6.185	10.039	0.010	6.786	0.040	0.000	0.060	5.295	0.190	4.664	2.973	0.000	4.784	0.000	0.040	0.000	0.100	0.453	48.983	1.391	4.844	3.163	100
LAWB94	0.000	6.183	10.034	0.010	6.783	0.040	0.000	0.060	5.292	0.190	5.362	2.971	0.000	3.381	0.000	0.040	0.000	0.100	0.497	49.661	1.391	4.842	3.161	100
LAWB95	0.000	6.185	10.038	0.010	6.785	0.040	0.000	0.060	5.294	0.190	5.764	2.972	0.000	2.452	0.000	0.040	0.000	0.100	0.463	50.209	1.391	4.844	3.162	100
C22AN107	0.000	6.102	10.074	0.080	5.112	0.020	0.000	0.140	5.582	0.090	2.511	1.511	0.000	14.425	0.030	0.120	0.020	0.100	0.272	46.588	1.140	3.061	3.021	100
LAWC26	0.000	6.121	13.263	0.110	6.411	0.020	0.000	0.050	0.010	0.140	2.731	1.500	0.000	11.963	0.000	0.110	0.000	0.100	0.347	49.962	1.120	3.021	3.021	100
LAWC28	0.000	6.117	10.045	0.110	12.814	0.020	0.000	0.050	0.010	0.140	2.729	1.499	0.000	11.954	0.000	0.110	0.000	0.100	0.430	46.717	1.119	3.018	3.018	100

Table 6.5. Normalized[(a)] Compositions (wt%) for ILAW PCT Validation Data (continued).

Glass ID	Ag2O	Al2O3	B2O3	Cl	CaO	Cr2O3	Cs2O	F	Fe2O3	K2O	Li2O	MgO	MnO	Na2O	NiO	P2O5	PbO	Re2O7	SO3 .XRF	SiO2	TiO2	ZnO	ZrO2	Sum
LAWC29	0.000	6.550	10.050	0.110	9.620	0.020	0.000	0.050	0.010	0.140	2.730	1.500	0.000	11.960	0.000	0.110	0.000	0.100	0.371	47.180	1.120	5.360	3.020	100
LAWC30	0.000	6.122	10.053	0.110	6.412	0.020	0.000	0.050	4.101	0.140	2.731	1.500	0.000	11.964	0.000	0.110	0.000	0.100	0.340	46.754	1.120	5.352	3.021	100
LAWC31	0.000	6.119	10.048	0.110	7.408	0.020	0.000	0.050	4.429	0.140	2.729	1.500	0.000	11.957	0.000	0.110	0.000	0.100	0.392	46.730	1.120	4.019	3.019	100
LAWC33	0.000	6.146	10.100	0.110	6.947	0.020	0.000	0.050	4.444	0.140	2.753	1.511	0.000	12.012	0.000	0.110	0.000	0.100	0.373	46.976	1.131	4.044	3.033	100
A88AP101R1	0.000	6.099	9.828	0.130	2.000	0.020	0.000	0.230	5.549	2.140	0.000	1.480	0.000	19.996	0.000	0.070	0.000	0.100	0.281	44.121	2.000	2.959	2.999	100
A88Si+15	0.000	6.141	9.481	0.140	1.930	0.020	0.000	0.250	5.351	2.370	0.000	1.430	0.000	22.182	0.000	0.080	0.000	0.110	0.290	42.554	1.930	2.850	2.890	100
A88Si-15	0.000	6.055	10.219	0.110	2.072	0.010	0.000	0.200	5.765	1.882	0.000	1.541	0.000	17.676	0.000	0.060	0.000	0.090	0.191	45.871	2.072	3.073	3.113	100
C22Si+15	0.000	6.032	9.817	0.090	4.993	0.020	0.180	0.160	5.473	0.100	2.447	1.468	0.000	16.168	0.030	0.130	0.020	0.110	0.313	45.409	1.109	2.986	2.946	100
C22Si-15	0.000	6.173	10.325	0.070	5.233	0.020	0.000	0.130	5.703	0.070	2.571	1.551	0.000	12.566	0.000	0.100	0.000	0.100	0.231	47.743	1.171	3.142	3.102	100
A1C1-1	0.000	6.091	9.122	0.910	2.741	0.015	0.150	0.086	6.501	0.350	0.620	1.850	0.000	19.164	0.006	0.033	0.000	0.000	0.212	44.478	1.760	2.951	2.961	100
A1C1-2	0.000	6.075	9.418	0.651	3.523	0.000	0.150	0.170	6.135	0.250	1.251	1.732	0.000	17.676	0.010	0.070	0.000	0.000	0.231	45.150	1.551	2.983	2.973	100
A1C1-3	0.000	6.053	9.705	0.400	4.302	0.000	0.150	0.251	5.763	0.160	1.871	1.621	0.000	16.169	0.019	0.098	0.000	0.000	0.287	45.786	1.351	3.022	2.992	100
C1-AN107	0.000	6.066	10.029	0.060	5.095	0.010	0.150	0.280	5.415	0.070	2.502	1.511	0.030	14.463	0.030	0.130	0.000	0.000	0.288	46.633	1.151	3.063	3.023	100
A2-AP101	0.000	5.620	9.826	0.424	1.988	0.021	0.150	0.350	5.534	3.814	0.000	1.477	0.000	18.472	0.000	0.077	0.000	0.000	0.346	44.012	1.987	2.940	2.962	100
A2B1-1	0.000	5.761	9.879	0.322	3.184	0.024	0.150	0.283	5.473	2.907	1.075	1.853	0.000	15.232	0.000	0.068	0.000	0.000	0.346	45.170	1.840	3.417	3.014	100
A2B1-2	0.000	5.898	9.924	0.221	4.378	0.027	0.150	0.215	5.407	1.998	2.150	2.228	0.000	11.979	0.000	0.059	0.000	0.000	0.423	46.294	1.692	3.891	3.064	100
B1-AZ101	0.000	6.178	10.023	0.017	6.772	0.034	0.151	0.080	5.281	0.181	4.303	2.980	0.000	5.481	0.000	0.041	0.000	0.000	0.485	48.586	1.397	4.843	3.167	100
C2AN102C35	0.000	6.074	9.424	0.389	7.356	0.012	0.150	0.114	3.599	0.091	3.254	1.491	0.000	11.985	0.000	0.159	0.010	0.000	0.537	47.285	1.079	3.992	3.000	100
A3-AN104	0.000	6.054	9.921	0.787	5.029	0.021	0.149	0.006	5.367	0.328	2.478	1.480	0.000	14.644	0.000	0.112	0.000	0.000	0.351	46.096	1.135	3.041	3.001	100

(a) The compositions listed in this table are normalized versions of target compositions of the glasses, after replacing the target values of SO_3 by XRF analyzed values. That is, after replacing the target SO_3 values by analyzed values, the component wt% values were summed for each glass, and the wt% values divided by the sums and multiplied by 100. The result is normalized wt% values summing to 100 wt%.

Table 6.6. PCT Releases and Subsets of ILAW Validation Data.

Glass ID	B (ppm)	Na (ppm)	Si (ppm)	B (g/L)	Na (g/L)	Si (g/L)	V1[(a)]	V2[(a)]	V3[(a)]	V4[(a)]
LAWA104	30.9900	171.5000	84.5900	1.1616	1.0505	0.4205	YES	YES	NO	NO
LAWA105	49.2700	282.3000	108.4000	1.9155	1.5848	0.5592	YES	YES	NO	NO
LAWA33	31.3400	132.6000	60.0000	1.1401	0.8934	0.3356	NO	NO	NO	NO
LAWA49	17.1800	86.7100	63.3800	0.6214	0.5842	0.3040	YES	NO	NO	NO
LAWA51	26.2400	69.3200	52.5000	0.7058	0.5189	0.2409	YES	NO	NO	NO
LAWA52	16.3600	163.6000	67.8200	0.8510	1.1024	0.3431	YES	YES	NO	NO
LAWA60	20.1100	92.5000	47.7200	0.5767	0.6234	0.2290	YES	YES	YES	NO
LAWC15	18.2900	99.4900	67.5900	0.6587	0.6711	0.3229	YES	YES	YES	YES
LAWC25	18.9300	64.0600	45.1200	0.6399	0.7707	0.2186	NO	NO	NO	NO
TFA-BASE	24.3900	96.5600	73.5200	0.7855	0.6508	0.3203	YES	NO	NO	NO
LAWA133	29.8900	168.3000	92.7200	1.0815	1.1355	0.4451	YES	YES	YES	YES
LAWA134	28.3900	102.5000	63.0600	0.9176	0.7793	0.3012	YES	YES	YES	YES
LAWA135	27.2000	93.7800	62.6800	0.8680	0.7429	0.2958	YES	YES	YES	YES
LAWA136	23.8500	89.4400	61.1500	0.7611	0.7085	0.2951	YES	YES	YES	YES
LAWB60	16.9500	21.8300	42.8300	0.4426	0.4443	0.1909	YES	NO	NO	NO
LAWB62	10.0200	14.4700	37.8100	0.3247	0.3562	0.1667	YES	NO	NO	NO
LAWB63	11.1500	14.1200	37.7000	0.3611	0.3474	0.1648	YES	NO	NO	NO
LAWB64	17.2500	19.8900	47.7900	0.5578	0.4886	0.2102	YES	NO	NO	NO
LAWB67	14.9750	11.5110	50.9060	0.4856	0.2836	0.2246	NO	NO	NO	NO
LAWB69	18.8200	23.4400	44.2500	0.4915	0.4772	0.1972	YES	YES	NO	NO
LAWB70	42.8100	46.0000	69.0100	1.1166	0.9354	0.3072	YES	YES	NO	NO
LAWB71	21.5000	27.1900	52.4400	0.6410	0.5525	0.2333	YES	YES	NO	NO
LAWB72	33.6500	37.7800	58.1400	0.8783	0.7687	0.2590	YES	YES	NO	NO
LAWB73	12.7400	15.4700	39.5100	0.4129	0.3802	0.1742	YES	NO	NO	NO
LAWB74	14.5000	16.3400	41.8800	0.4516	0.4010	0.1844	YES	NO	NO	NO
LAWB75	12.5700	11.7300	36.1000	0.3436	0.2886	0.1593	YES	NO	NO	NO
LAWB76	15.3700	14.6400	42.6900	0.4203	0.3602	0.1851	YES	NO	NO	NO
LAWB77	27.7300	29.5300	52.0300	0.7232	0.6004	0.2316	YES	YES	NO	NO
LAWB81	34.4600	38.5900	59.1500	0.8994	0.7851	0.2635	YES	YES	NO	NO
LAWB82	15.5800	22.4300	39.8500	0.4968	0.4558	0.1871	YES	NO	NO	NO
LAWB89	18.6000	14.0800	58.4700	0.5967	0.4647	0.2533	YES	NO	NO	NO
LAWB90	19.4100	27.7800	57.2600	0.6220	0.5440	0.2550	YES	YES	YES	NO
LAWB91	24.6500	44.9200	62.7900	0.7901	0.6932	0.2867	YES	YES	YES	YES
LAWB92	28.4300	59.6300	64.6600	0.9119	0.7942	0.2998	YES	YES	YES	YES
LAWB93	26.6900	17.5500	52.0000	0.8563	0.4945	0.2269	YES	YES	NO	NO
LAWB94	22.1200	11.7500	52.8700	0.7100	0.4684	0.2276	YES	NO	NO	NO
LAWB95	20.8500	8.0200	51.4900	0.6690	0.4409	0.2192	YES	NO	NO	NO
C22AN107	35.5000	119.1000	89.7500	1.1349	1.1129	0.4118	YES	YES	YES	YES
LAWC26	28.1600	58.9500	50.0700	0.6838	0.6643	0.2142	YES	YES	NO	NO
LAWC28	8.9200	38.9100	35.7200	0.2860	0.4388	0.1635	YES	NO	NO	NO
LAWC29	9.4570	36.7300	36.2300	0.3031	0.4140	0.1642	YES	YES	NO	NO
LAWC30	18.6400	58.2600	56.6400	0.5972	0.6564	0.2590	YES	YES	NO	NO
LAWC31	17.1370	55.5680	52.2450	0.5493	0.6264	0.2390	YES	YES	YES	YES
LAWC33	21.9700	67.9000	66.0500	0.7006	0.7620	0.3006	YES	YES	YES	YES
A88AP101R1	41.9000	173.5000	84.9700	1.3731	1.1696	0.4117	YES	YES	YES	YES
A88Si+15	73.0300	329.4000	113.8000	2.4808	2.0017	0.5717	YES	YES	NO	NO
A88Si-15	20.5800	85.6200	65.5600	0.6486	0.6529	0.3055	YES	YES	YES	NO
C22Si+15	40.8000	154.6000	103.5000	1.3385	1.2889	0.4873	YES	YES	YES	YES
C22Si-15	28.2700	83.4100	75.6200	0.8818	0.8947	0.3386	YES	YES	YES	NO
A1C1-1	24.8900	119.6000	80.5700	0.8788	0.8413	0.3872	YES	YES	YES	YES

Table 6.6. PCT Releases and Subsets of ILAW Validation Data (continued).

Glass ID	B (ppm)	Na (ppm)	Si (ppm)	B (g/L)	Na (g/L)	Si (g/L)	V1[(a)]	V2[(a)]	V3[(a)]	V4[(a)]
A1C1-2	24.2200	113.8000	78.1900	0.8282	0.8679	0.3702	YES	YES	YES	YES
A1C1-3	27.5200	98.3300	78.7300	0.9132	0.8198	0.3676	YES	YES	YES	YES
C1-AN107	32.0100	113.8000	89.6400	1.0279	1.0606	0.4109	YES	YES	YES	YES
A2-AP101	47.4600	152.9000	81.6500	1.5556	1.1158	0.3966	YES	YES	YES	YES
A2B1-1	21.8900	73.1100	68.7900	0.7136	0.6470	0.3256	YES	YES	YES	YES
A2B1-2	21.0300	53.6800	65.2900	0.6825	0.6041	0.3015	YES	YES	YES	YES
B1-AZ101	24.3000	21.5200	58.0400	0.7808	0.5293	0.2554	YES	YES	YES	YES
C2-AN102C35	19.8200	66.8600	64.1900	0.6773	0.7520	0.2902	YES	YES	YES	YES
A3-AN104	33.3200	115.1000	84.5000	1.0817	1.0595	0.3919	YES	YES	YES	YES

(a) YES indicates the data point is in the validation subset, NO indicates it is not.

Table 6.7. Performance Summary of Full LM and PQM Models for ILAW PCT-Boron.

Statistic For Modeling Data[(a)]	Full LM	Full PQM with 0.01[(b)]	Full PQM with 0.05[(b)]
R^2	0.7978	0.8699	0.9073
R^2 Adjusted (R^2_A)	0.7500	0.8331	0.8739
R^2 Predicted (R^2_P)	0.6148	0.7406	0.8011
RMSE	0.3142	0.2567	0.2232
R^2 For Validation Data[(c)]			
All (59)	0.5798	0.3685	0.4545
V1 (56)	0.5928	0.4124	0.4656
V2 (40)	0.5516	0.3833	0.4232
V3 (26)	0.0206	-0.0106	0.2559
V4 (22)	-0.0672	-0.1585	0.1968

(a) The evaluation statistics are defined in Section C.2 of Appendix C.
(b) Partial quadratic mixture models were developed using significance levels of 0.01 and 0.05 to decide when to stop adding quadratic terms. See the discussion in Section C.3.2 of Appendix C.
(c) R^2 validation is defined in Section C.4 of Appendix C. The descriptions of the complete validation set (All) and the various validation subsets (V1 to V4) are described in Section 5.1.3. A negative R^2 validation value means that the sum of squares of model prediction errors is larger than if the mean response value over the validation data were used as the predicted value for each glass. In other words, the model predicts worse for the validation data than the mean response value does.

Table 6.8. Data-Splitting Results for Full LM and PQM Models for ILAW PCT-Boron.

Full LM	**DS1**	**DS2**	**DS3**	**DS4**	**DS5**	**Average**
R^2 [(a)]	0.8360	0.8529	0.8072	0.8004	0.7981	0.8189
R^2 Adjusted (R^2_A)	0.7864	0.8074	0.7489	0.7400	0.7370	0.7640
R^2 Predicted (R^2_P)	0.6073	0.6671	0.5634	0.5476	0.5572	0.5885
RMSE	0.2966	0.2735	0.3228	0.3283	0.3302	0.3103
SSE	3.7836	3.1418	4.4795	4.6348	4.6874	4.1454
R^2 Validation (R^2_V) [(b)]	0.4398	0.4203	0.6395	0.4953	0.7375	0.5465
Full PQM with 0.01	**DS1**	**DS2**	**DS3**	**DS4**	**DS5**	**Average**
R^2 [(a)]	0.8890	0.8861	0.9002	0.8861	0.8767	0.8876
R^2 Adjusted (R^2_A)	0.8483	0.8434	0.8637	0.8444	0.8315	0.8463
R^2 Predicted (R^2_P)	0.7373	0.7071	0.7666	0.6545	0.7236	0.7178
RMSE	0.2500	0.2466	0.2378	0.2540	0.2643	0.2505
SSE	2.5619	2.4332	2.3176	2.6441	2.8631	2.5640
R^2 Validation (R^2_V) [(b)]	0.6357	0.5914	0.5414	0.3861	0.7674	0.5844
Full PQM with 0.05	**DS1**	**DS2**	**DS3**	**DS4**	**DS5**	**Average**
R^2 [(a)]	0.9110	0.9152	0.9213	0.9230	0.9231	0.9187
R^2 Adjusted (R^2_A)	0.8688	0.8739	0.8840	0.8866	0.8867	0.8800
R^2 Predicted (R^2_P)	0.7127	0.7564	0.7647	0.7860	0.7906	0.7621
RMSE	0.2325	0.2213	0.2193	0.2168	0.2167	0.2213
SSE	2.0544	1.8125	1.8282	1.7867	1.7838	1.8531
R^2 Validation (R^2_V) [(b)]	0.7850	0.7372	0.7356	0.5007	0.7359	0.6989

(a) The evaluation statistics are defined in Section C.2 of Appendix C.
(b) R^2 validation is defined in Section C.4 of Appendix C.

Table 6.9. Performance Summary Comparison of Reduced LM Models for ILAW PCT-Boron Where ZrO_2 is Dropped or Forced Into Model.

Statistic For Modeling Data	**ZrO_2 Forced In**	**ZrO_2 Dropped**
R^2 [(a)]	0.7945	0.7942
R^2 Adjusted (R^2_A)	0.7590	0.7628
R^2 Predicted (R^2_P)	0.6756	0.6893
RMSE	0.3084	0.3060

(a) The evaluation statistics are defined in Section C.2 of Appendix C.

Table 6.10. Performance Summary of Reduced LM and PQM Models for ILAW PCT-Boron.

Selection Method[a]	**Stepwise**							**MAXR**							
Reduced Models	**LM**	**PQM 0.05**	**PQM 0.02**	**PQM 0.01**	**PQM 0.05, No TiO_2 Quad.**	**PQM 0.02, No TiO_2 Quad.**	**PQM 0.01, No TiO_2 Quad.**	**17 Terms**	**16 Terms**	**15 Terms**	**14 Terms**	**17 Terms, No TiO_2 Quad.**	**16 Terms, No TiO_2 Quad.**	**15 Terms, No TiO_2 Quad.**	**14 Terms, No TiO_2 Quad.**
R^2 [b]	0.7945	0.9237	0.9099	0.8407	0.9197	0.9047	0.8407	0.9173	0.9099	0.8988	0.8799	0.9130	0.9047	0.8932	0.8799
R^2 Adjusted (R^2_A)	0.7590	0.8983	0.8844	0.8099	0.8929	0.8777	0.8099	0.8918	0.8844	0.8726	0.8515	0.8863	0.8777	0.8656	0.8515
R^2 Predicted (R^2_P)	0.6756	0.8446	0.8198	0.7355	0.8362	0.8071	0.7355	0.8386	0.8198	0.8082	0.7653	0.8333	0.8071	0.7961	0.7653
RMSE	0.3084	0.2004	0.2136	0.2739	0.2056	0.2197	0.2739	0.2067	0.2136	0.2243	0.2421	0.2119	0.2197	0.2304	0.2421
Reduced Linear Terms in Model	Al_2O_3, B_2O_3, CaO, Fe_2O_3, K_2O, Li_2O, MgO, Na_2O, SiO_2, TiO_2, ZrO_2														
Selected Quadratic Terms in Model (Elements rather than oxides shown for space reasons)	N/A	BMg, LiZr, FeLi, FeTi, BCa, AlTi, KK	BMg, LiZr, FeLi, FeTi, BCa	BMg	BMg, LiZr, FeLi, KK, CaMg, NaSi, CaSi	BMg, LiZr, FeLi, KK, CaMg	BMg	AlTi, BCa, BMg, FeLi, FeTi, LiZr	BCa, BMg, FeLi, FeTi, LiZr	BMg, FeLi, FeTi, LiZr	BMg, FeLi, LiZr	BMg, FeLi, LiZr, KK, CaMg, NaSi	BMg, FeLi, LiZr, KK, CaMg	BMg, FeLi, LiZr, KK	BMg, FeLi, LiZr
# Model Terms	11	17	16	12	18	16	12	17	16	15	14	17	16	15	14
R^2 For Validation Data[c]															
All (59)	0.5755	0.1638	0.5894	0.5090	0.0155	-0.0534	0.5090	0.5755	0.5894	0.5841	0.6005	0.0315	-0.0534	-0.0507	0.6005
V1 (56)	0.5941	0.6018	0.6565	0.5473	0.5803	0.6328	0.5473	0.6243	0.6565	0.6506	0.6618	0.6376	0.6328	0.6118	0.6618
V2 (40)	0.5531	0.5335	0.5847	0.5327	0.5234	0.6085	0.5327	0.5494	0.5847	0.6011	0.6468	0.5536	0.6085	0.6052	0.6468
V3 (26)	0.0334	-0.1588	0.0783	0.0105	-0.1946	0.0396	0.0105	-0.0437	0.0783	0.1784	0.1997	-0.1089	0.0396	0.0672	0.1997
V4 (22)	-0.0606	0.1332	0.1494	-0.1129	0.1974	0.1626	-0.1129	0.1381	0.1494	0.1734	0.2236	0.2286	0.1626	0.1724	0.2236
Statistic Averages Over 5 Data-Splitting Sets															
R^2 [b]	0.8128	0.9310	0.9187	0.8556	0.9277	0.9158	0.8556	0.9249	0.9187	0.9078	0.8918	0.9222	0.9158	0.9041	0.8918
R^2 Adjusted (R^2_A)	0.7720	0.9008	0.8889	0.8201	0.8959	0.8848	0.8201	0.8947	0.8889	0.8769	0.8590	0.8908	0.8848	0.8720	0.8590
R^2 Predicted (R^2_P)	0.6638	0.8132	0.7983	0.7179	0.8054	0.7898	0.7179	0.8065	0.7983	0.7838	0.7377	0.8091	0.7898	0.7709	0.7377
RMSE	0.3048	0.2011	0.2129	0.2708	0.2058	0.2167	0.2708	0.2072	0.2129	0.2241	0.2397	0.2109	0.2167	0.2285	0.2397
R^2 Validation (R^2_V) [d]	0.6325	0.8088	0.7757	0.6886	0.7960	0.7342	0.6886	0.8004	0.7757	0.7759	0.7246	0.7781	0.7342	0.7520	0.7246

(a) The stepwise and MAXR methods for selecting quadratic terms for PQM models are discussed in Section C.3.2 of Appendix C.
(b) The evaluation statistics are defined in Section C.2 of Appendix C.
(c) R^2 validation is defined in Section C.4 of Appendix C. The descriptions of the complete validation set (All) and the various validation subsets (V1 to V4) are described in Section 6.1.3. A negative R^2 validation value means that the sum of squares of model prediction errors is larger than if the mean response value over the validation data were used as the predicted value for each glass. In other words, the model predicts worse for the validation data than the mean response value does.
(d) R^2 validation is defined in Section C.4 of Appendix C.

Table 6.11. ILAW PCT-Boron 11-Term Reduced LM Model and Performance Summary.

ln(PCT-Boron) Reduced LM Model Term	Coefficient Estimate	Coefficient Stand. Dev.
Al2O3	-16.9174	2.4406
B2O3	7.8091	1.6773
CaO	-5.5738	1.6069
Fe2O3	4.5734	1.7869
K2O	4.4046	2.8000
Li2O	17.6434	3.5153
MgO	19.1577	2.9273
Na2O	9.4051	1.0525
SiO2	-3.7673	0.6411
TiO2	-10.8549	3.9055
ZrO2	-0.8260	3.0184

Statistic from Modeling Data[a]	Value
R^2	0.7945
R^2 Adjusted (R^2_A)	0.7590
R^2 Predicted (R^2_P)	0.6756
RMSE	0.3084
Model LOF p-value	0.2411
N (no. of data pts.)	69

Statistic from Validation Data[b]	Value
R^2 All (59)	0.5755
R^2 V1 (56)	0.5941
R^2 V2 (40)	0.5531
R^2 V3 (26)	0.0334
R^2 V4 (22)	-0.0606

Statistic from Data Splitting[c]	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.8327	0.8527	0.7990	0.7847	0.7949	0.8128
R^2 Adjusted (R^2_A)	0.7963	0.8200	0.7553	0.7379	0.7504	0.7720
R^2 Predicted (R^2_P)	0.6942	0.7265	0.6297	0.6258	0.6427	0.6638
RMSE	0.2897	0.2645	0.3186	0.3296	0.3217	0.3048
SSE	3.8604	3.1471	4.6704	4.9977	4.7598	4.2871
R^2 Validation (R^2_V)	0.4715	0.4298	0.7155	0.8071	0.7383	0.6325

(a) The evaluation statistics are defined in Section C.2 of Appendix C.
(b) R^2 validation is defined in Section C.4 of Appendix C. The descriptions of the complete validation set (All) and the various validation subsets (V1 to V4) are described in Section 5.1.3. A negative R^2 validation value means that the sum of squares of model prediction errors is larger than if the mean response value over the validation data were used as the predicted value for each glass. In other words, the model predicts worse for the validation data than the mean response value does.
(c) The evaluation and validation statistics calculated for data-splits are defined the same as for separate modeling and validation sets. Section 5.1.2 describes how the data-splitting was accomplished.

Table 6.12. ILAW PCT-Boron 14-Term Reduced PQM Model and Performance Summary.

ln(PCT-Boron) Reduced PQM Model Term	Coefficient Estimate	Coefficient Stand. Dev.		Statistic from Modeling Data[(a)]	Value
Al2O3	-19.9158	2.0396		R^2	0.8799
B2O3	1.6716	1.9860		R^2 Adjusted (R^2_A)	0.8515
CaO	-1.5471	1.4203		R^2 Predicted (R^2_P)	0.7653
Fe2O3	-0.8289	2.7877		RMSE	0.2421
K2O	4.9225	2.2219		Model LOF p-value	0.4539
Li2O	-6.9721	8.2401		N (no. of data pts.)	69
MgO	-25.7905	8.5379			
Na2O	15.2327	1.2571		**Statistic from Validation Data[(b)]**	**Value**
SiO2	-3.1991	0.5297			
TiO2	-11.0586	3.1441		R^2 All (59)	0.6005
ZrO2	-18.0011	4.8676		R^2 V1 (56)	0.6618
B2O3*MgO	493.3071	92.1397		R^2 V2 (40)	0.6468
Fe2O3*Li2O	349.7992	107.8955		R^2 V3 (26)	0.1997
Li2O*ZrO2	541.9078	149.1598		R^2 V4 (22)	0.2236

Statistic from Data Splitting[(c)]	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.8944	0.8900	0.9125	0.8894	0.8729	0.8918
R^2 Adjusted (R^2_A)	0.8624	0.8559	0.8861	0.8560	0.8344	0.8590
R^2 Predicted (R^2_P)	0.7643	0.7247	0.8132	0.6768	0.7093	0.7377
RMSE	0.2381	0.2366	0.2174	0.2443	0.2620	0.2397
SSE	2.4370	2.3508	2.0326	2.5668	2.9511	2.4677
R^2 Validation (R^2_V)	0.7170	0.7739	0.5060	0.7111	0.9150	0.7246

(a) The evaluation statistics are defined in Section C.2 of Appendix C.
(b) R^2 validation is defined in Section C.4 of Appendix C. The descriptions of the complete validation set (All) and the various validation subsets (V1 to V4) are described in Section C.1.3.
(c) The evaluation and validation statistics calculated for data-splits are defined the same as for separate modeling and validation sets. Section 6.1.2 describes how the data-splitting was accomplished.

Table 6.13. Performance Summary of Full LM and PQM Models for ILAW PCT-Sodium.

Statistic For Modeling Data[(a)]	Full LM	Full PQM 0.01[(b)]	Full PQM 0.05[(b)]
R^2	0.8555	0.8951	0.9332
R^2 Adjusted (R^2_A)	0.8213	0.8654	0.9073
R^2 Predicted (R^2_P)	0.7535	0.8049	0.8722
RMSE	0.2067	0.1794	0.1489
R^2 For Validation Data[(c)]			
All (59)	0.5781	0.4596	0.3717
V1 (56)	0.5716	0.4517	0.3393
V2 (40)	0.5706	0.4686	0.4469
V3 (26)	0.1809	0.2460	0.4003
V4 (22)	0.1234	0.1586	0.3424

(a) The evaluation statistics are defined in Section C.2 of Appendix C.
(b) Partial quadratic mixture models were developed using significance levels of 0.01 and 0.05 to decide when to stop adding quadratic terms. See the discussion in Section C.3.2 of Appendix C.
(c) R^2 validation is defined in Section C.4 of Appendix C. The descriptions of the complete validation set (All) and the various validation subsets (V1 to V4) are described in Section 6.1.3.

Table 6.14. Data Splitting Results for Full LM and PQM Models for ILAW PCT-Sodium.

Full LM	**DS1**	**DS2**	**DS3**	**DS4**	**DS5**	**Average**
R^2 [(a)]	0.8687	0.8554	0.8656	0.8703	0.8725	0.8665
R^2 Adjusted (R^2_A)	0.8290	0.8106	0.8250	0.8311	0.8340	0.8259
R^2 Predicted (R^2_P)	0.7537	0.7026	0.7484	0.7362	0.7336	0.7349
RMSE	0.2053	0.2049	0.2090	0.2059	0.2025	0.2055
SSE	1.8121	1.7628	1.8781	1.8228	1.7635	1.8078
R^2 Validation (R^2_V) [(b)]	0.6291	0.8020	0.6967	0.7369	0.7032	0.7136
Full PQM with 0.01[(c)]	**DS1**	**DS2**	**DS3**	**DS4**	**DS5**	**Average**
R^2 [(a)]	0.9002	0.8975	0.8948	0.9143	0.9169	0.9047
R^2 Adjusted (R^2_A)	0.8636	0.8591	0.8563	0.8830	0.8864	0.8697
R^2 Predicted (R^2_P)	0.7272	0.7921	0.7860	0.8084	0.8239	0.7875
RMSE	0.1833	0.1767	0.1894	0.1714	0.1675	0.1777
SSE	1.3778	1.2486	1.4703	1.2043	1.1503	1.2903
R^2 Validation (R^2_V) [(b)]	0.7574	0.8390	0.7344	0.7267	0.6899	0.7495
Full PQM with 0.05[(c)]	**DS1**	**DS2**	**DS3**	**DS4**	**DS5**	**Average**
R^2 [(a)]	0.9316	0.9304	0.9331	0.9507	0.9447	0.9381
R^2 Adjusted (R^2_A)	0.8965	0.8937	0.8988	0.9254	0.9163	0.9061
R^2 Predicted (R^2_P)	0.8075	0.8272	0.8566	0.8840	0.8566	0.8464
RMSE	0.1597	0.1535	0.1589	0.1369	0.1438	0.1506
SSE	0.9432	0.8480	0.9347	0.6931	0.7653	0.8369
R^2 Validation (R^2_V) [(b)]	0.9037	0.9006	0.6483	0.8078	0.8161	0.8153

(a) The evaluation statistics are defined in Section C.2 of Appendix C.
(b) R^2 validation is defined in Section C.4 of Appendix C.
(c) Partial quadratic mixture models were developed using significance levels of 0.01 and 0.05 to decide when to stop adding quadratic terms. See the discussion in Section C.3.2 of Appendix C.

Table 6.15. Performance Summary Comparison of Reduced LM Models for ILAW PCT-Sodium Where ZrO_2 and CaO are Dropped or Forced Into Model.

Statistic For Modeling Data[(a)]	**Both ZrO_2 and CaO Dropped**	**ZrO_2 Forced In, CaO Dropped**	**Both ZrO_2 and CaO Forced In**
R^2	0.8453	0.8472	0.8498
R^2 Adjusted (R^2_A)	0.8247	0.8239	0.8239
R^2 Predicted (R^2_P)	0.7897	0.7861	0.7791
RMSE	0.2048	0.2052	0.2053

(a) The evaluation statistics are defined in Section C.2 of Appendix C.

Table 6.16. Performance Summary of Reduced LM and PQM Models for ILAW PCT-Sodium.

Selection Method[a]		**Stepwise**						**MAXR**							
Reduced Models	**LM**	**PQM 0.05**	**PQM 0.02**	**PQM 0.01**	**PQM 0.05, No TiO_2 Quad.**	**PQM 0.02, No TiO_2 Quad.**	**PQM 0.01, No TiO_2 Quad.**	**17 Terms**	**16 Terms**	**15 Terms**	**14 Terms**	**17 Terms, No TiO_2 Quad.**	**16 Terms, No TiO_2 Quad.**	**15 Terms, No TiO_2 Quad.**	**14 Terms, No TiO_2 Quad.**
R^2 [b]	0.8498	0.9458	0.8987	0.8987	0.9186	0.9109	0.8886	0.9231	0.9159	0.9087	0.8995	0.9240	0.9203	0.9109	0.9004
R^2 Adjusted (R^2_A)	0.8239	0.9263	0.8748	0.8748	0.8955	0.8878	0.8647	0.8994	0.8921	0.8851	0.8757	0.9006	0.8977	0.8878	0.8768
R^2 Predicted (R^2_P)	0.7791	0.8942	0.8174	0.8174	0.8625	0.8466	0.8238	0.8408	0.8446	0.8346	0.8097	0.8758	0.8709	0.8466	0.8390
RMSE	0.2053	0.1328	0.1731	0.1731	0.1581	0.1638	0.1799	0.1551	0.1606	0.1658	0.1724	0.1542	0.1564	0.1638	0.1717
Reduced Linear Terms in Model	Al_2O_3, B_2O_3, CaO, Fe_2O_3, K_2O, Li_2O, MgO, Na_2O, SiO_2, TiO_2, ZrO_2														
Selected Quadratic Terms in Model (Elements rather than oxides shown for space reasons)	N/A	LiTi, AlK, CaZr, TiTi, FeFe, AlB, NaTi, BK	LiTi, AlK, CaZr	LiTi, AlK, CaZr	BMg, LiZr, FeK, AlMg, FeLi	BMg, LiZr, FeK, AlMg	BMg, LiZr	AlMg, BLi, BMg, CaNa, CaZr, LiTi	AlMg, BMg, CaNa, CaZr, LiTi	BTi, BMg, CaZr, LiTi	BTi, CaZr, LiTi	KK, BK, BMg, FeK, FeLi, LiZr	BK, BMg, FeK, FeLi, LiZr	AlMg, BMg, FeK, LiZr	BMg, FeK, LiZr
# Model Terms	11	19	14	14	16	15	13	17	16	15	14	17	16	15	14
R^2 For Validation Data[c]															
All (59)	0.5509	0.5387	0.3317	0.3317	0.6325	0.4839	0.4823	0.4804	0.4648	0.4041	0.4097	0.5134	0.6643	0.4839	0.4974
V1 (56)	0.5619	0.5492	0.3135	0.3135	0.6692	0.5047	0.5028	0.4900	0.4704	0.3900	0.3910	0.7209	0.7177	0.5047	0.5228
V2 (40)	0.5856	0.5824	0.5600	0.5600	0.6921	0.6170	0.6257	0.4847	0.4904	0.5236	0.5319	0.7481	0.7553	0.6170	0.6432
V3 (26)	0.1824	0.3642	0.2432	0.2432	0.4271	0.3587	0.3563	-0.0845	0.0084	0.2356	0.2108	0.4844	0.5242	0.3587	0.3974
V4 (22)	0.1171	0.4494	0.1863	0.1863	0.3855	0.2857	0.2846	-0.1767	-0.0868	0.1739	0.1537	0.5008	0.5089	0.2857	0.3259
Statistic Averages Over 5 Data-Splitting Sets															
R^2 [b]	0.8583	0.9504	0.9067	0.9067	0.9248	0.9175	0.8957	0.9294	0.9223	0.9155	0.9077	0.9286	0.9254	0.9175	0.9078
R^2 Adjusted (R^2_A)	0.8274	0.9267	0.8783	0.8783	0.8971	0.8899	0.8672	0.9011	0.8937	0.8872	0.8796	0.8998	0.8979	0.8899	0.8797
R^2 Predicted (R^2_P)	0.7652	0.8833	0.8065	0.8065	0.8485	0.8360	0.8099	0.8220	0.8266	0.8137	0.7921	0.8633	0.8602	0.8360	0.8283
RMSE	0.2047	0.1332	0.1718	0.1718	0.1575	0.1633	0.1795	0.1547	0.1605	0.1653	0.1708	0.1554	0.1568	0.1633	0.1707
R^2 Validation (R^2_V)[d]	0.7644	0.8673	0.8016	0.8016	0.8111	0.8097	0.8001	0.8087	0.8213	0.8211	0.7970	0.8506	0.8420	0.8097	0.7927

(a) The stepwise and MAXR methods for selecting quadratic terms for PQM models are discussed in Section C.3.2 of Appendix C.

(b) The evaluation statistics are defined in Section C.2 of Appendix C.

(c) R^2 validation is defined in Section C.4 of Appendix C. The descriptions of the complete validation set (All) and the various validation subsets (V1 to V4) are described in Section 6.1.3. A negative R^2 validation value means that the sum of squares of model prediction errors is larger than if the mean response value over the validation data were used as the predicted value for each glass. In other words, the model predicts worse for the validation data than the mean response value does.

(d) R^2 validation is defined in Section C.4 of Appendix C**.**

Table 6.17. ILAW PCT-Sodium 11-Term Reduced LM Model and Performance Summary.

ln(PCT-Sodium) Reduced LM Model Term	Coefficient Estimate	Coefficient Stand. Dev.
Al2O3	-14.6100	1.6244
B2O3	3.0941	1.1163
CaO	0.9491	1.0695
Fe2O3	2.9655	1.1893
K2O	5.2771	1.8636
Li2O	14.2009	2.3396
MgO	14.9188	1.9483
Na2O	9.7066	0.7005
SiO2	-3.4193	0.4267
TiO2	-7.7765	2.5993
ZrO2	-2.2774	2.0089

Statistic from Modeling Data[(a)]	Value
R^2	0.8498
R^2 Adjusted (R^2_A)	0.8239
R^2 Predicted (R^2_P)	0.7791
RMSE	0.2053
Model LOF p-value	0.2066
N (no. of data pts.)	69

Statistic from Validation Data[(b)]	Value
R^2 All (59)	0.5509
R^2 V1 (56)	0.5619
R^2 V2 (40)	0.5856
R^2 V3 (26)	0.1824
R^2 V4 (22)	0.1171

Statistic from Data Splitting[(c)]	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.8597	0.8512	0.8543	0.8644	0.8620	0.8583
R^2 Adjusted (R^2_A)	0.8292	0.8181	0.8227	0.8349	0.8320	0.8274
R^2 Predicted (R^2_P)	0.7787	0.7457	0.7605	0.7767	0.7646	0.7652
RMSE	0.2052	0.2008	0.2104	0.2036	0.2037	0.2047
SSE	1.9364	1.8139	2.0357	1.9066	1.9093	1.9204
R^2 Validation (R^2_V)	0.7202	0.8326	0.7803	0.7447	0.7442	0.7644

(a) The evaluation statistics are defined in Section C.2 of Appendix C.
(b) R^2 validation is defined in Section C.4 of Appendix C. The descriptions of the complete validation set (All) and the various validation subsets (V1 to V4) are described in Section 6.1.3. A negative R^2 validation value means that the sum of squares of model prediction errors is larger than if the mean response value over the validation data were used as the predicted value for each glass. In other words, the model predicts worse for the validation data than the mean response value does.
(c) The evaluation and validation statistics calculated for data-splits are defined the same as for separate modeling and validation sets. Section 6.1.2 describes how the data-splitting was accomplished.

Table 6.18. ILAW PCT-Sodium 16-Term Reduced PQM Model and Performance Summary.

ln(PCT-Sodium) Reduced PQM Model Term	Coefficient Estimate	Coefficient Stand. Dev.		Statistic from Modeling Data[(a)]	Value
Al2O3	-17.2629	1.5291		R^2	0.9203
B2O3	2.2622	2.1167		R^2 Adjusted (R^2_A)	0.8977
CaO	3.9240	0.9382		R^2 Predicted (R^2_P)	0.8709
Fe2O3	2.1598	1.9638		RMSE	0.1564
K2O	41.2770	10.3718		Model LOF p-value	0.4300
Li2O	-5.4762	5.4220		N (no. of data pts.)	69
MgO	-9.9926	6.2247			
Na2O	12.9487	0.8199			
SiO2	-3.4173	0.4208			
TiO2	-8.1687	2.0342		**Statistic from Validation Data[(b)]**	**Value**
ZrO2	-19.8097	3.4285			
B2O3*K2O	-199.2665	77.2015		R^2 All (59)	0.6643
B2O3*MgO	267.6811	63.8820		R^2 V1 (56)	0.7177
Fe2O3*K2O	-266.2859	79.4419		R^2 V2 (40)	0.7553
Fe2O3*Li2O	201.4967	70.4097		R^2 V3 (26)	0.5242
Li2O*ZrO2	526.3173	101.6048		R^2 V4 (22)	0.5089

Statistic from Data Splitting[(c)]	DS1	DS2	DS3	DS4	DS5	Average
R^2	0.9177	0.9126	0.9174	0.9386	0.9404	0.9254
R^2 Adjusted (R^2_A)	0.8876	0.8799	0.8872	0.9161	0.9186	0.8979
R^2 Predicted (R^2_P)	0.8530	0.8420	0.8496	0.8622	0.8943	0.8602
RMSE	0.1664	0.1631	0.1677	0.1451	0.1418	0.1568
SSE	1.1356	1.0646	1.1537	0.8632	0.8247	1.0084
R^2 Validation (R^2_V)	0.8891	0.9166	0.8785	0.7886	0.7375	0.8420

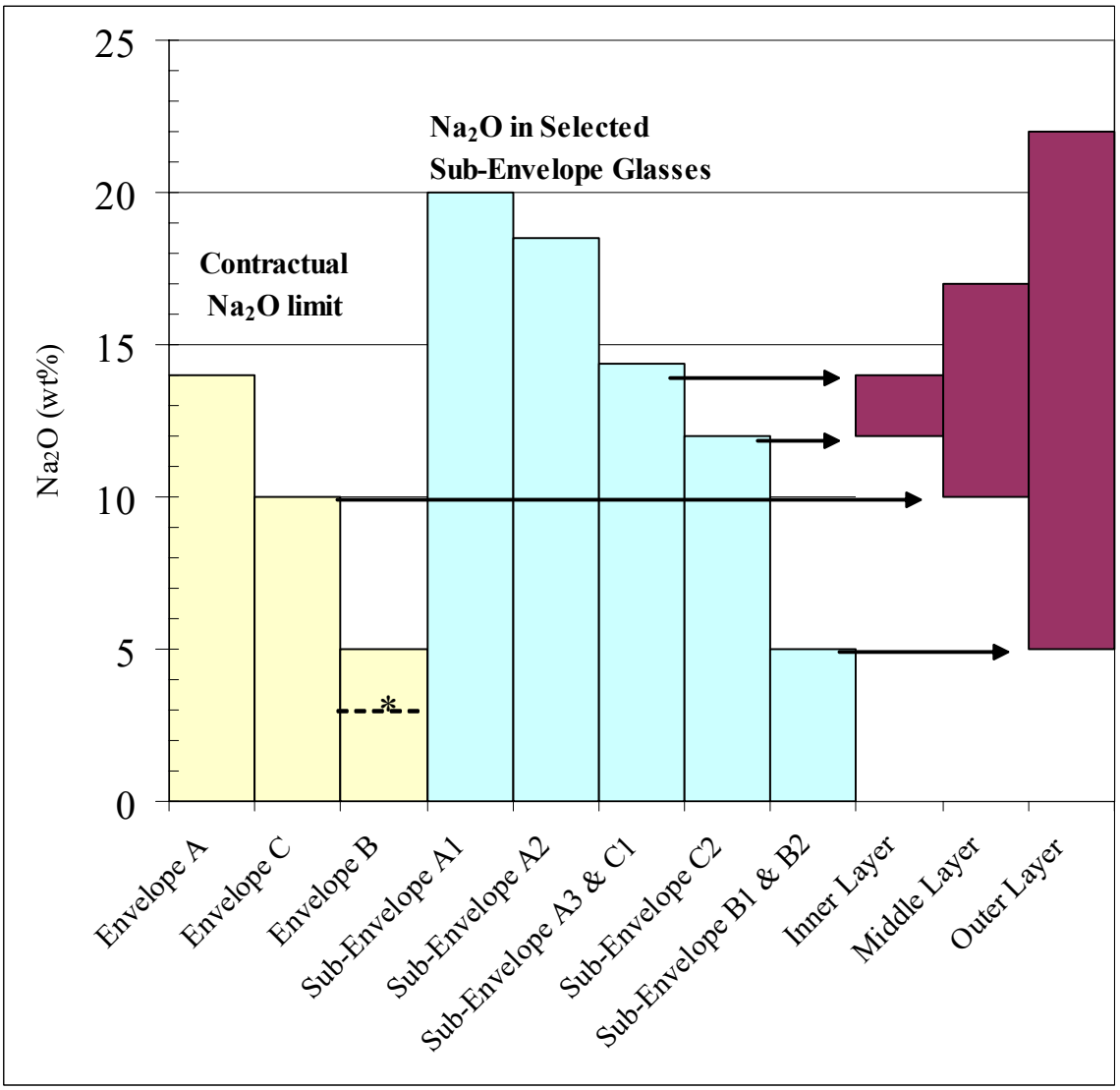
(a) The evaluation statistics are defined in Section C.2 of Appendix C.
(b) R^2 validation is defined in Section C.4 of Appendix C. The descriptions of the complete validation set (All) and the various validation subsets (V1 to V4) are described in Section 6.1.3.
(c) The evaluation and validation statistics calculated for data-splits are defined the same as for separate modeling and validation sets. Section 6.1.2 describes how the data-splitting was accomplished.

Table 6.19. LAWA126 Composition in Formats Needed for Use in ILAW PCT Models.

Component	LAWA126 Composition (wt%)	LAWA126 Composition (mass fractions) For Use In PCT-B LM Model	LAWA126 Composition (mass fractions) For Use In PCT-B PQM Model	LAWA126 Composition (mass fractions) For Use In PCT-Na LM Model	LAWA126 Composition (mass fractions) For Use In PCT-Na PQM Model
Al2O3	5.640	0.059	0.059	0.059	0.059
B2O3	9.820	0.102	0.102	0.102	0.102
CaO	1.990	0.021	0.021	0.021	0.021
Fe2O3	5.540	0.058	0.058	0.058	0.058
K2O	3.880	0.040	0.040	0.040	0.040
Li2O	0.000	0.000	0.000	0.000	0.000
MgO	1.480	0.015	0.015	0.015	0.015
Na2O	18.460	0.192	0.192	0.192	0.192
SO3.XRF	0.309	NA	NA	NA	NA
SiO2	44.120	0.460	0.460	0.460	0.460
TiO2	2.000	0.021	0.021	0.021	0.021
ZnO	2.960	NA	NA	NA	NA
ZrO2	2.990	0.031	0.031	0.031	0.031
Others	0.810	NA	NA	NA	NA
B2O3*MgO	NA	NA	0.002	NA	0.002
Fe2O3*Li2O	NA	NA	0.000	NA	0.000
Li2O*ZrO2	NA	NA	0.000	NA	0.000
B2O3*K2O	NA	NA	NA	NA	0.004
Fe2O3*K2O	NA	NA	NA	NA	0.002

Table 6.20. Predicted PCT Releases and Corresponding 90% UCIs and 95% SUCIs for LAWA126 Composition Used in ILAW PCT Models.

Model	Predicted ln(PCT) in ln(g/L)	Predicted PCT in g/L	90% UCI on Mean ln(PCT) in ln(g/L)	90% UCI on Median PCT in g/L	95% SUCI on Mean ln(PCT) in ln(g/L)	95% SUCI on Median PCT in g/L
11-Term PCT-B LM Model	0.2522	1.2868	0.3991	1.4905	0.7400	2.0960
14-Term PCT-B PQM Model	0.1689	1.1841	0.2879	1.3336	0.6069	1.8347
11-Term PCT-Na LM Model	0.1545	1.1670	0.2523	1.2869	0.4792	1.6147
16-Term PCT-Na PQM Model	0.0461	1.0471	0.1247	1.1328	0.3530	1.4234



* For LAW AZ-102 the requirement of 5 wt% Na_2O was changed to "reduced waste loading as necessary to avoid excessive K-3 corrosion and other negative effects caused by the high sulfate to sodium ratio" via WTP Test Exception 24590-LAW-TEF-RT-02-002 dated 10/21/02. The WTP contract limit was subsequently revised to 3 wt% Na_2O.

Figure 2.1. Na_2O Concentrations Used as the Basis for ILAW Test Matrix Development.

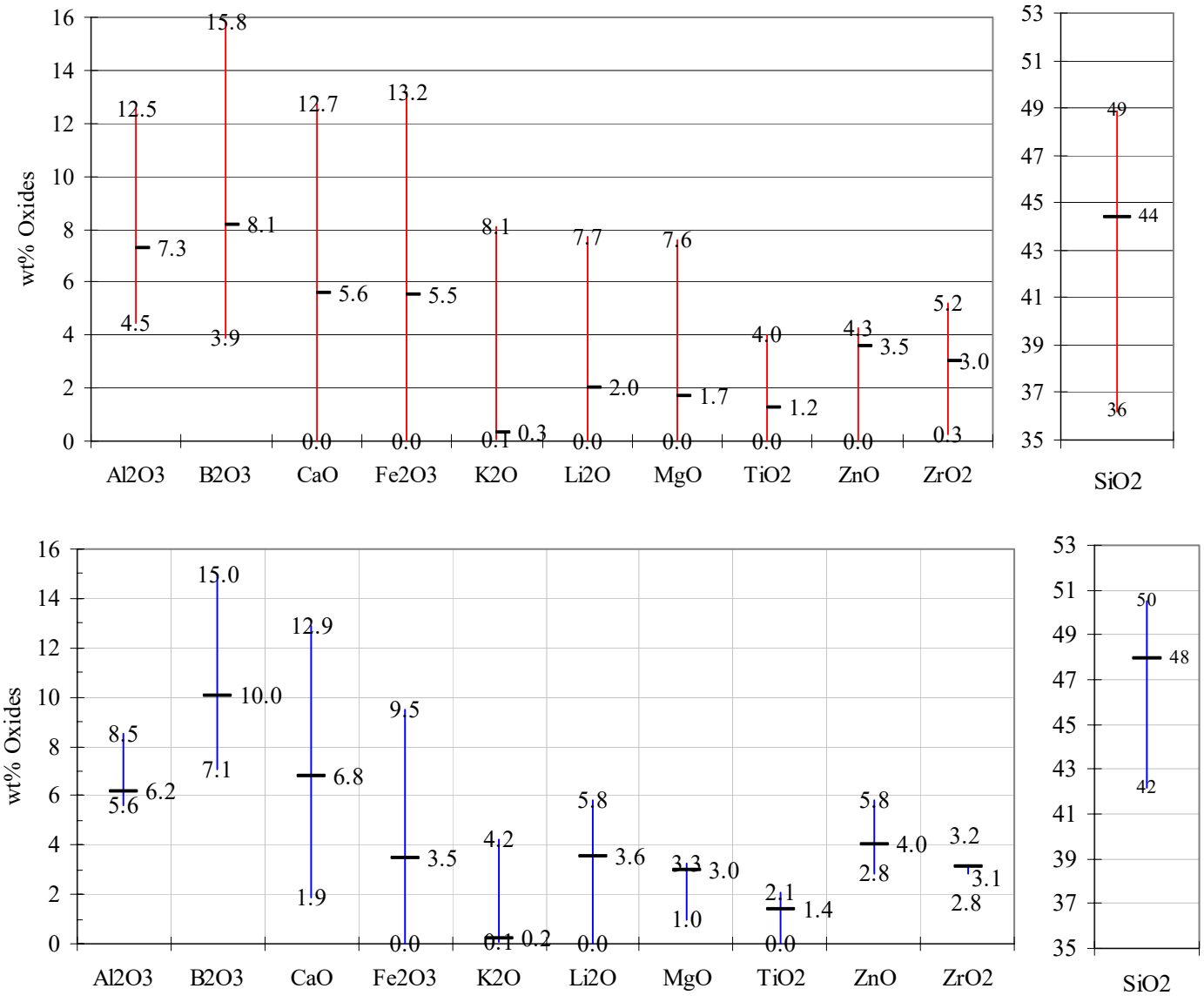


Figure 2.2. Concentration Ranges and Mean of LAW Glass Components Tested at VSL During Part A and B1 (top) and Part B2 (bottom).

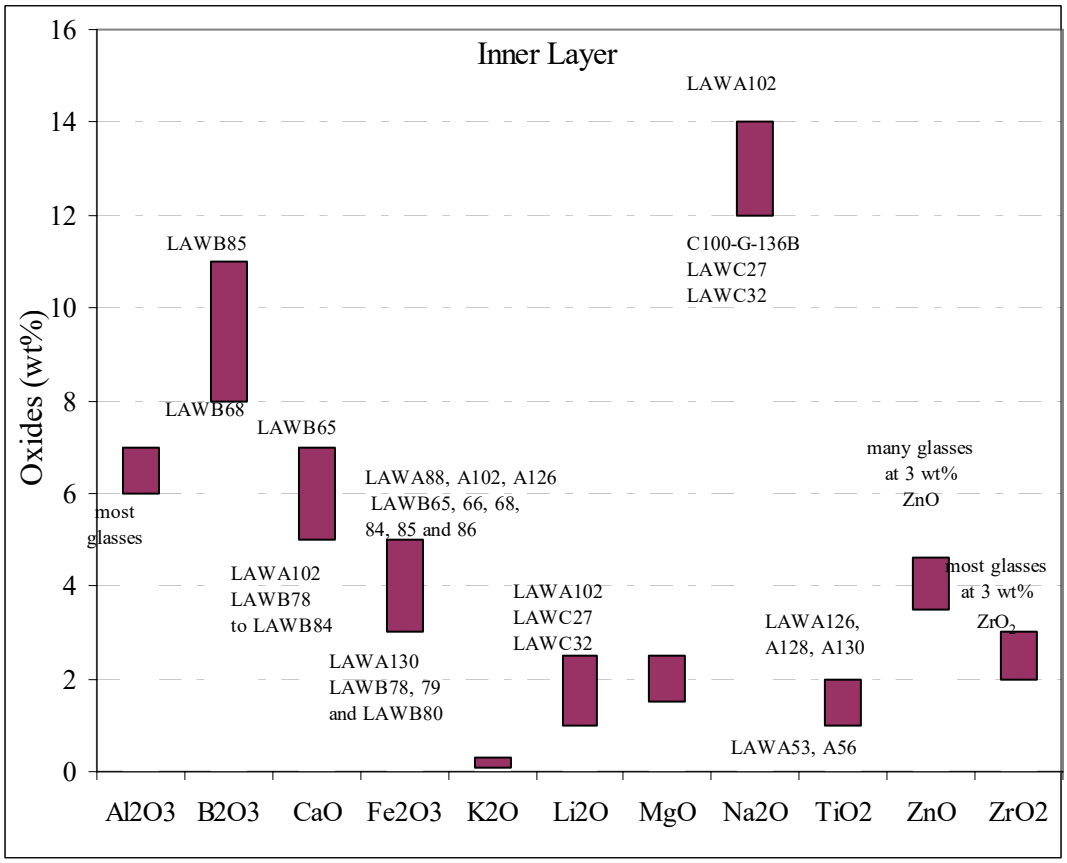


Figure 2.3. Compositions of the 21 Existing Matrix Glasses as They Relate to the Inner Layer.

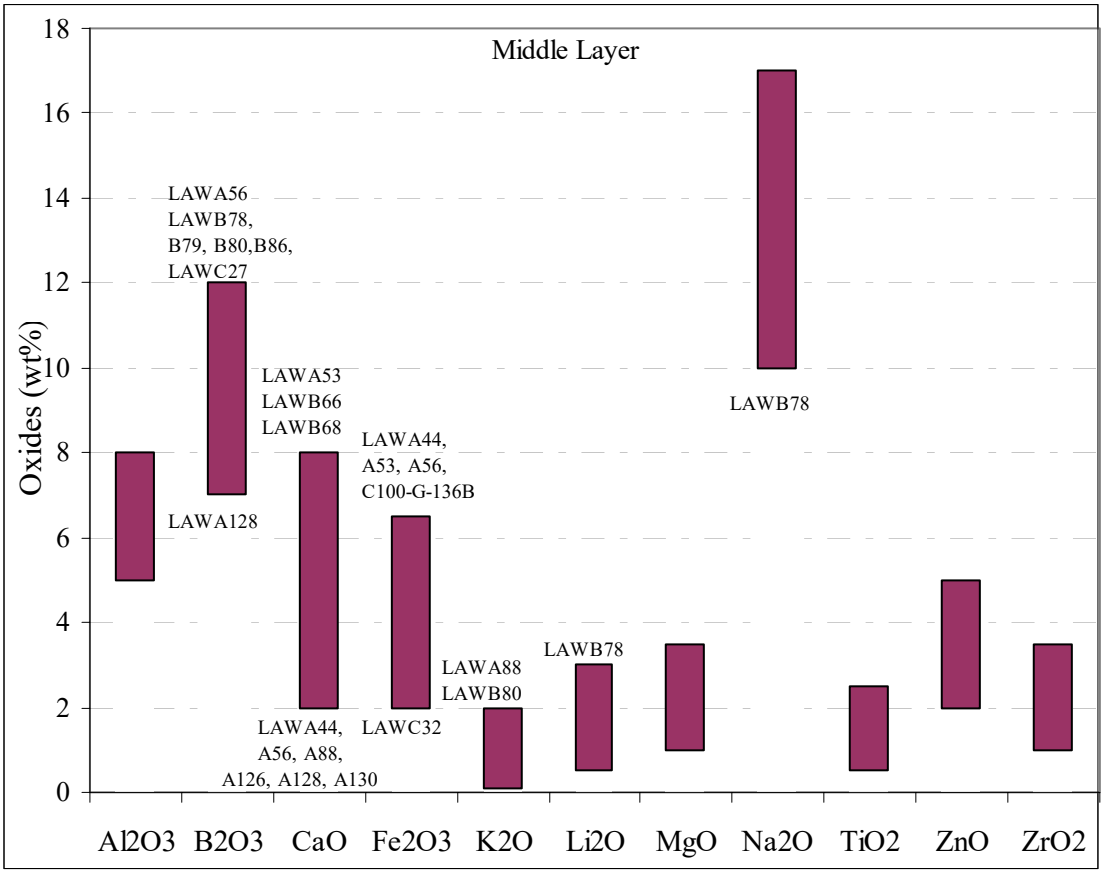


Figure 2.4. Compositions of the 21 Existing Matrix Glasses as They Relate to the Middle Layer.

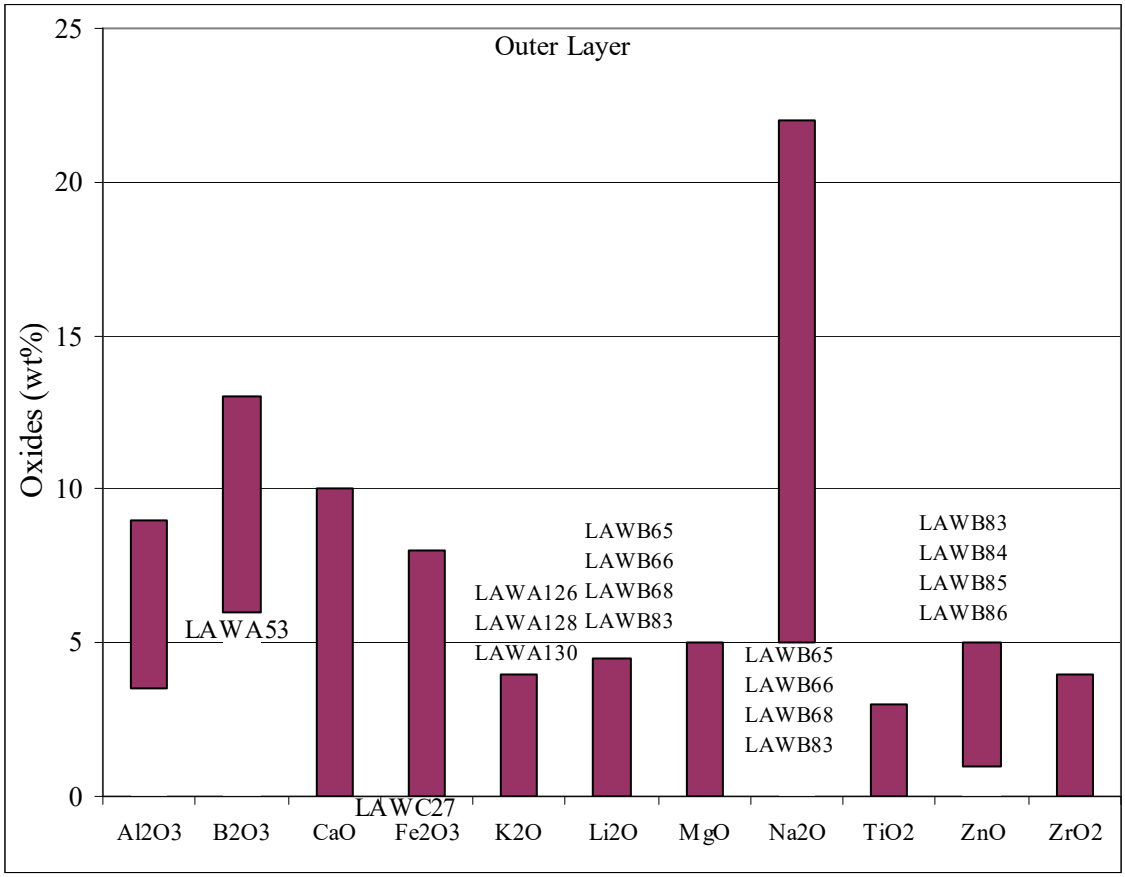


Figure 2.5. Compositions of the 21 Existing Matrix Glasses as They Relate to the Outer Layer.

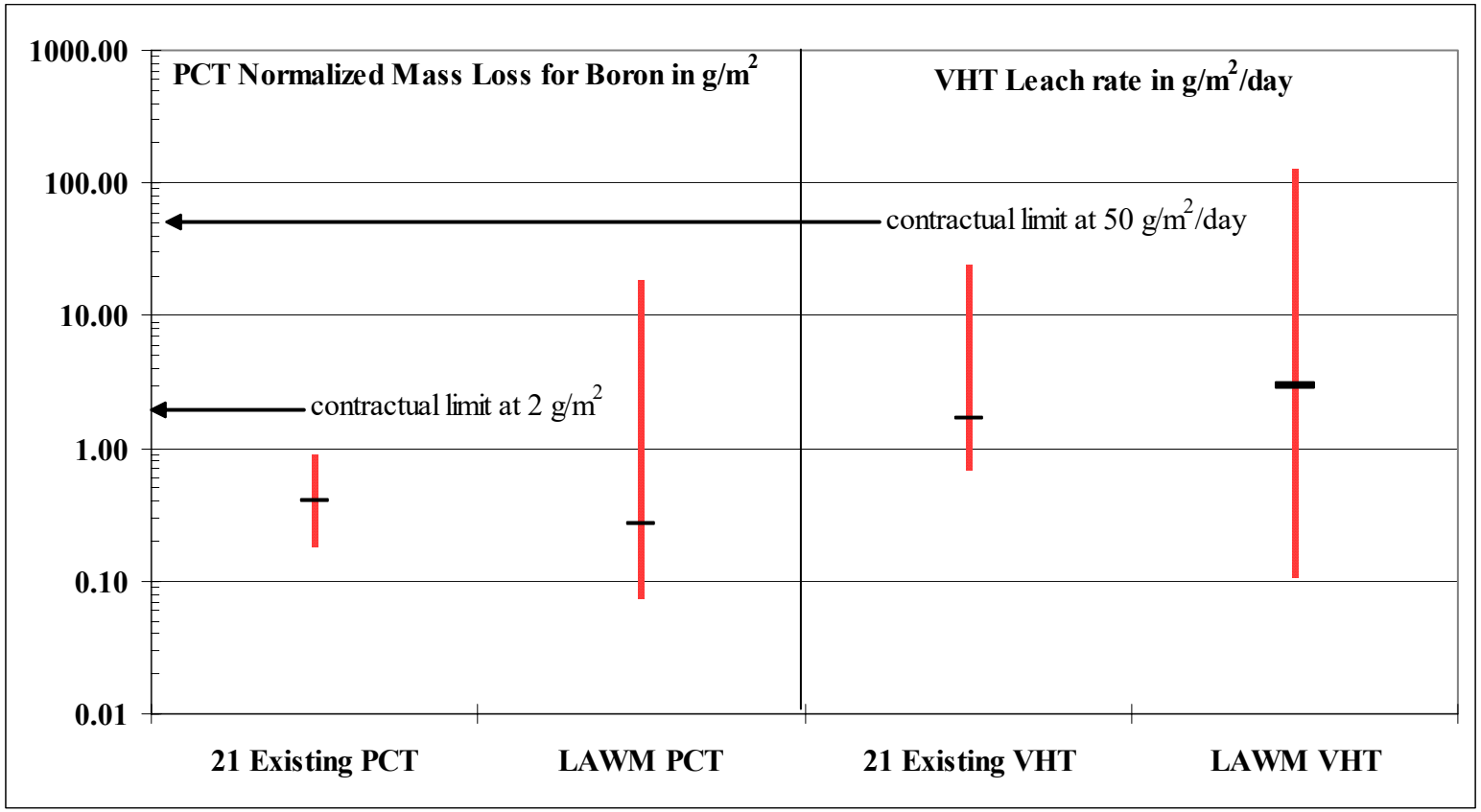


Figure 2.6. Ranges of VHT and PCT Responses for the 21 Existing Matrix Glasses and the 56 Test Matrix Glasses.

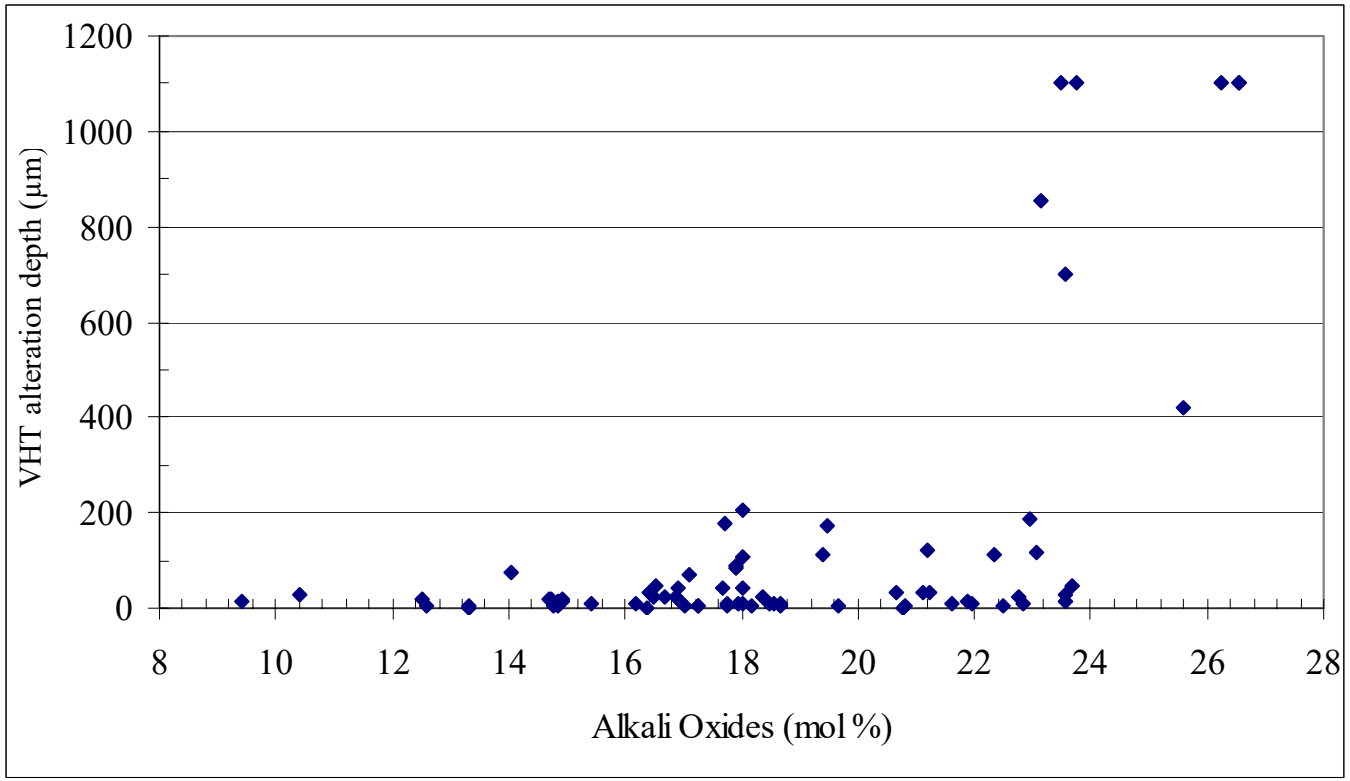


Figure 4.1. VHT Alteration Depth (in µm) as a Function of the Sum of Alkali Oxides ($Li_2O+Na_2O+K_2O$) in mol % for Existing and Test Matrix Glasses.

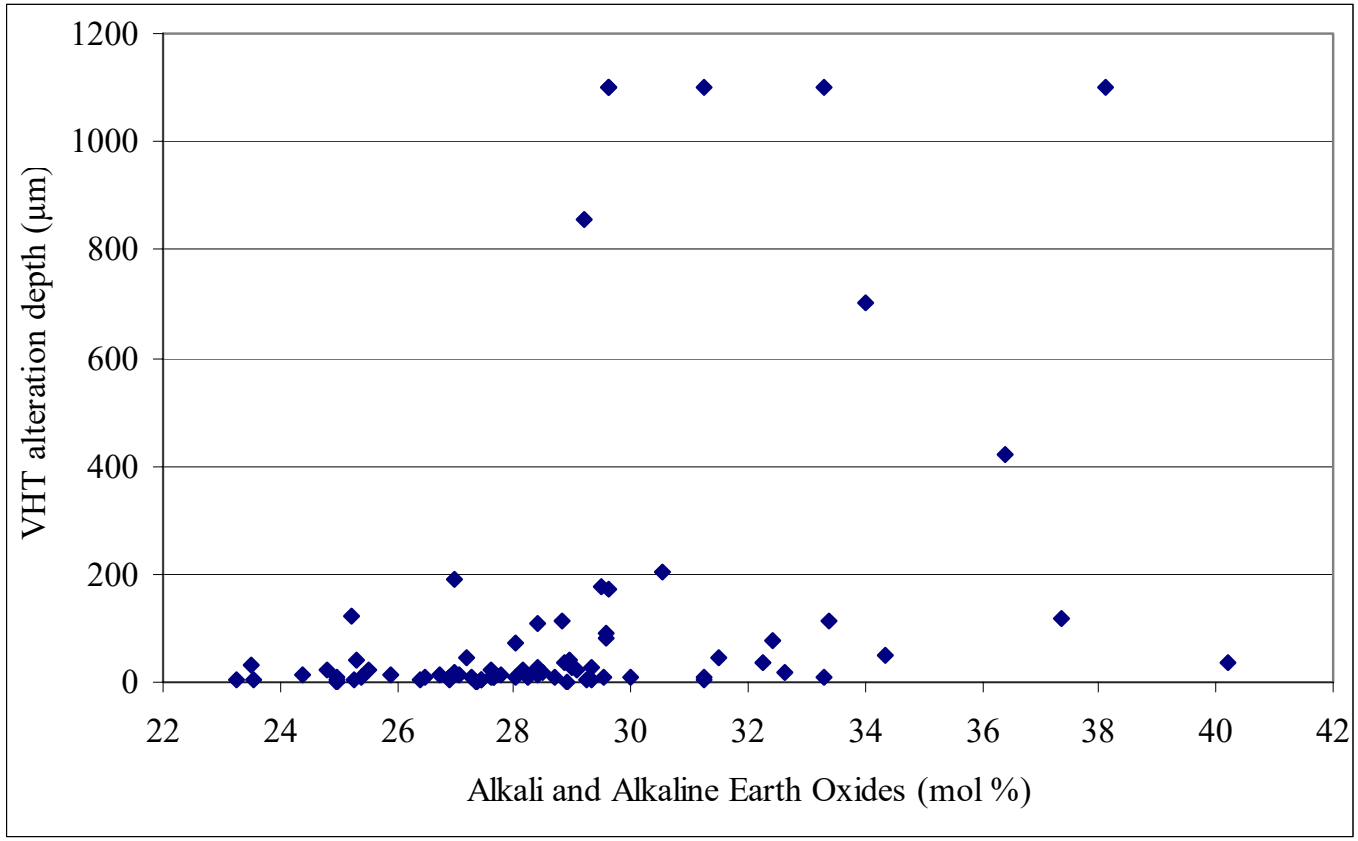


Figure 4.2. VHT Alteration Depth (in µm) as a Function of the Sum of Alkali and Alkaline Earth Oxides ($Li_2O+Na_2O+K_2O+CaO+MgO$) in mol % for Existing and Test Matrix Glasses.

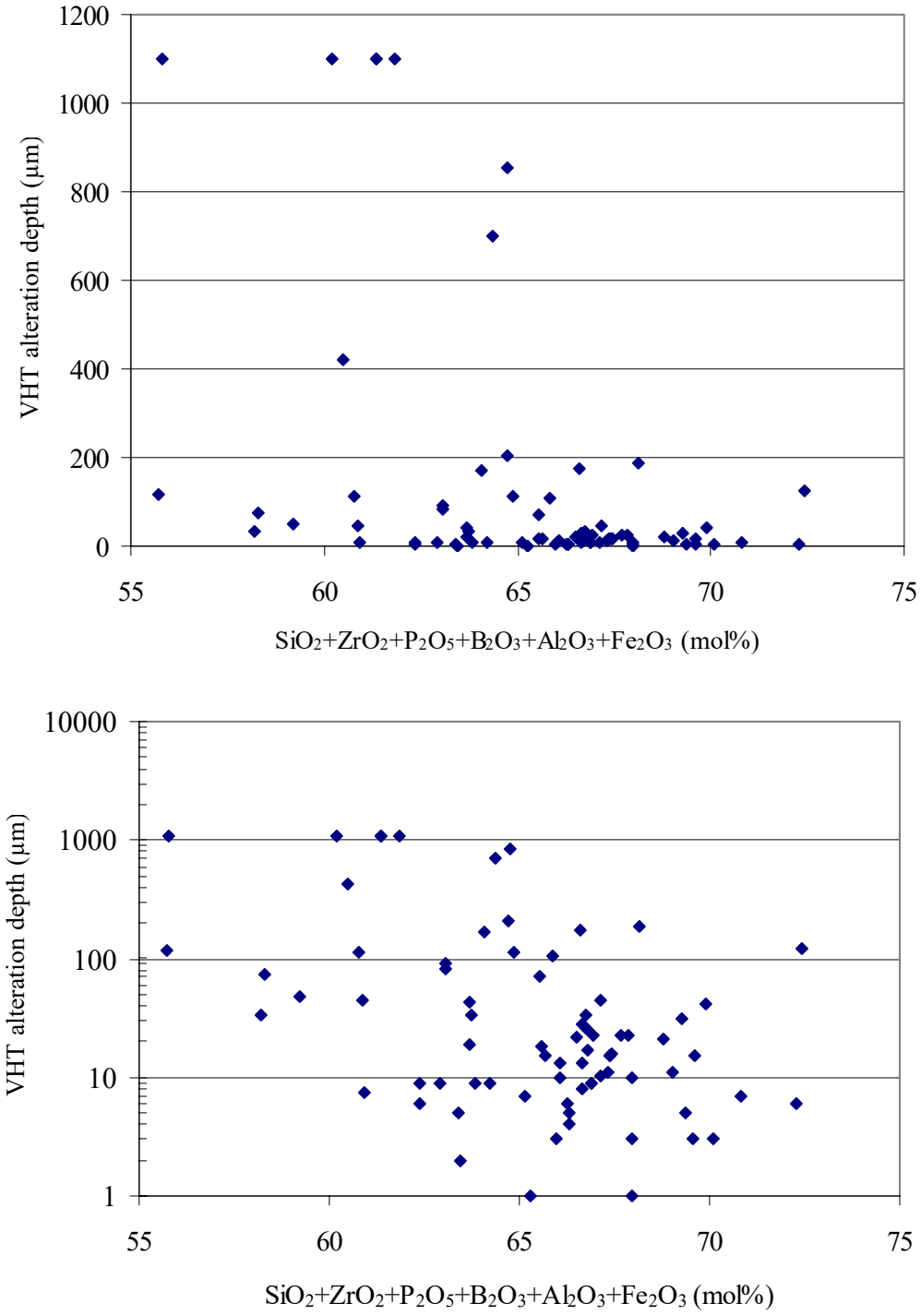


Figure 4.3. VHT Alteration Depth (in µm) as a Function of the Sum of Valence III, IV, and V Components (SiO_2+ZrO_2+P_2O_5+B_2O_3+ Al_2O_3+Fe_2O_3) in mol % for Existing and Test Matrix Glasses; linear scale (top) and log scale (bottom).

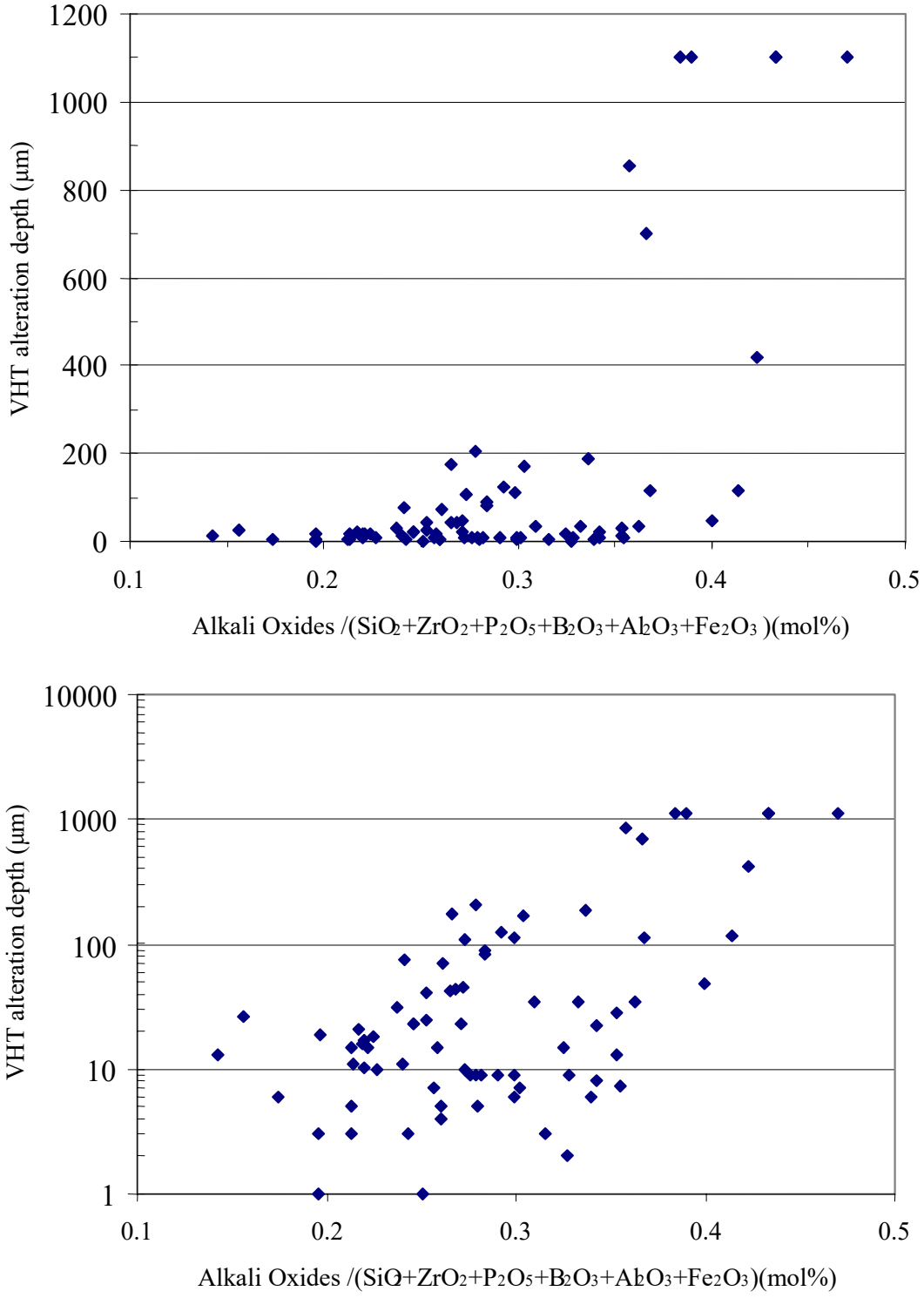


Figure 4.4. VHT alteration Depth (in µm) as a Function of the Ratio of Alkali Oxides ($Li_2O+Na_2O+K_2O$) to Glass Formers ($SiO_2+ZrO_2+P_2O_5+B_2O_3+ Al_2O_3+Fe_2O_3$) in mol % for Existing and Test Matrix Glasses; linear scale(top) and log scale (bottom).

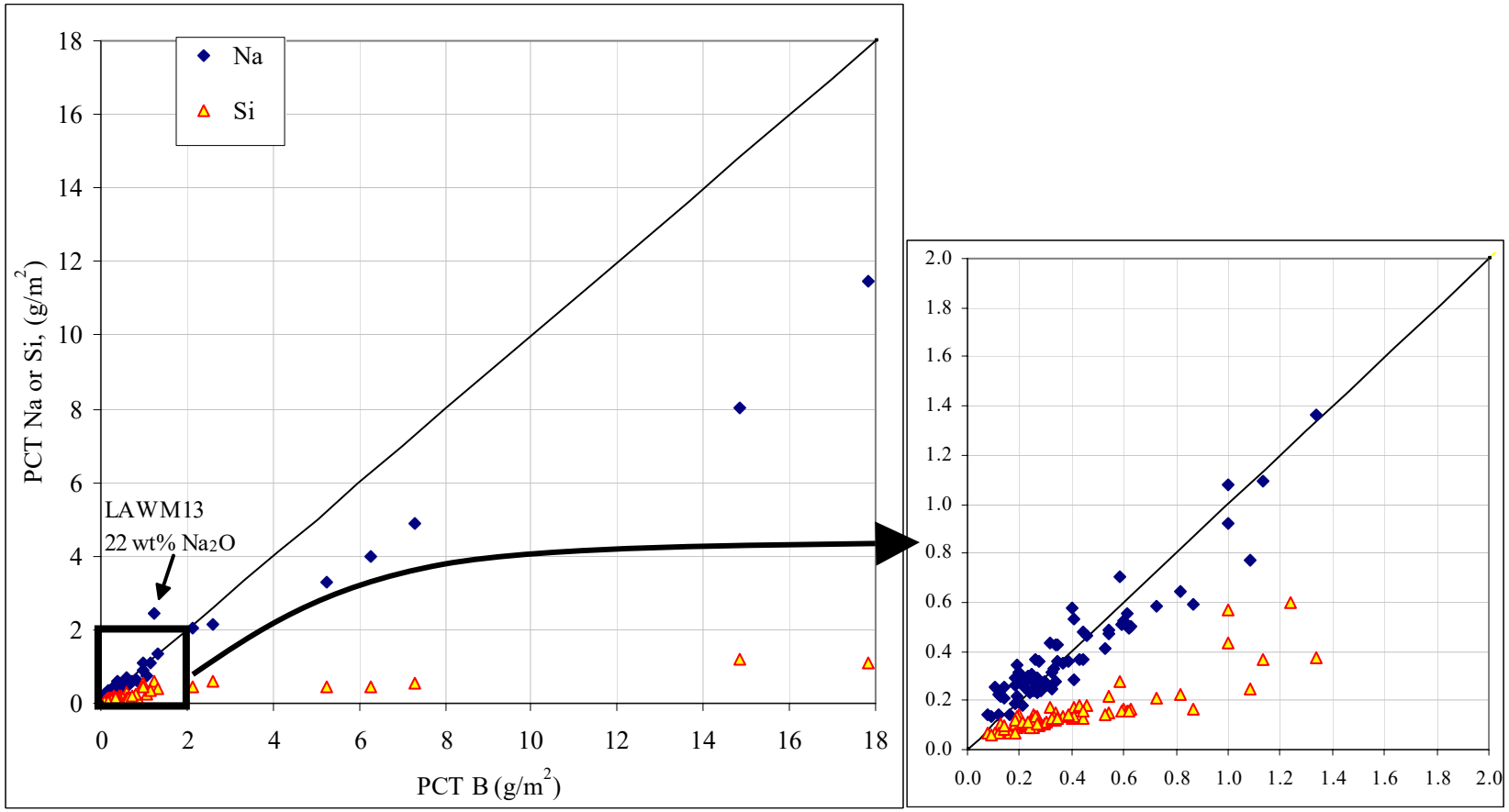


Figure 4.5. PCT Sodium and Silicon Releases as a Function of PCT Boron Release for the Existing Matrix and Test Matrix Glasses.
(Na and B leach approximately congruently in glasses with low leach rates; see figure on right)

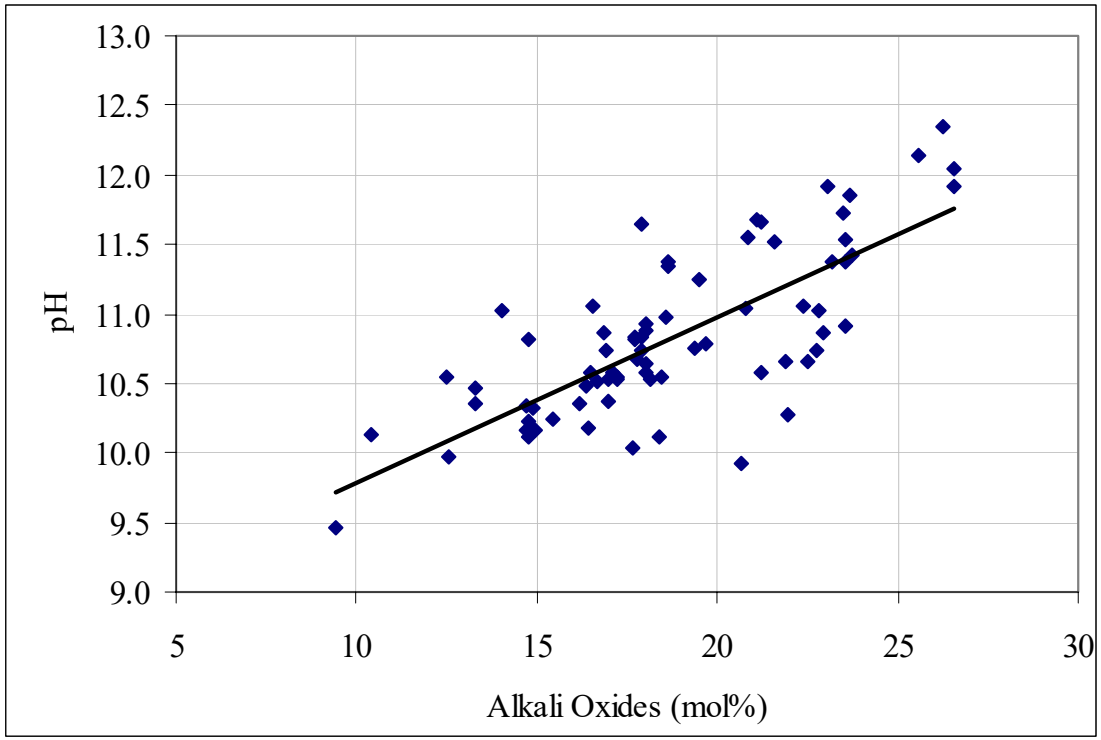


Figure 4.6. Measured pH at 20°C in the 7-day PCT Leachate as a Function of the Sum of Alkali Oxides ($Li_2O+Na_2O+K_2O$) in mol % for Existing and Test Matrix Glasses.

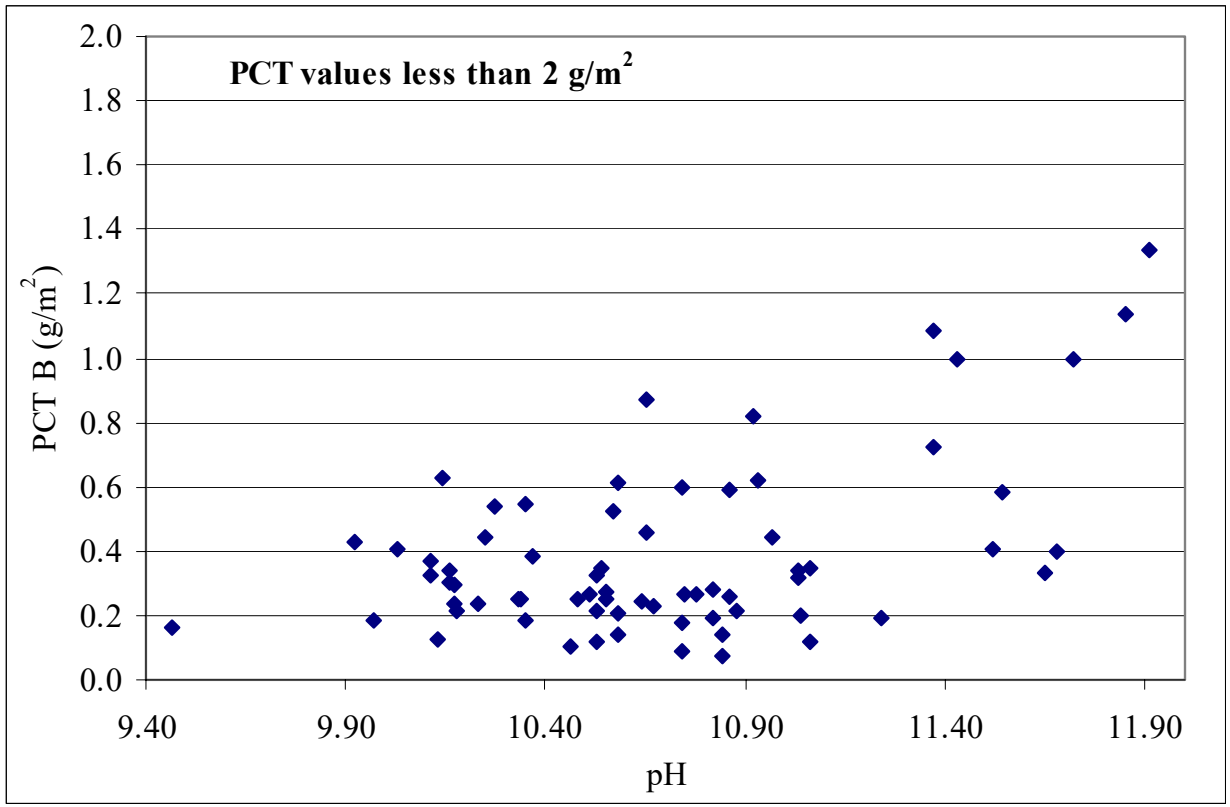


Figure 4.7. Plot of the PCT Boron Release as a Function of the pH Measured at 20°C in the 7-day PCT Leachate.

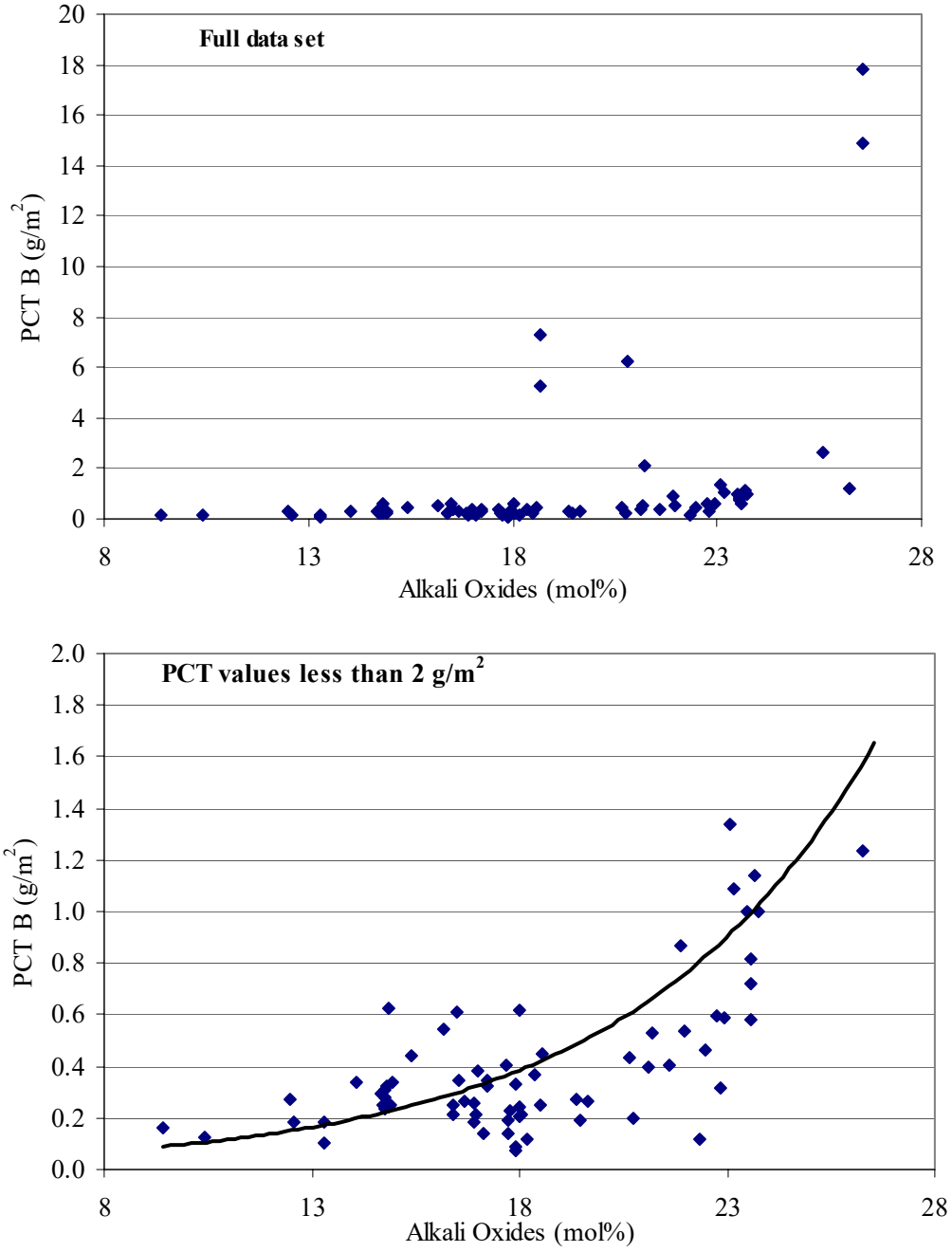


Figure 4.8. PCT Boron Release as a Function of the Sum of Alkali Oxides ($Li_2O+Na_2O+K_2O$) in mol % for Existing and Test Matrix Glasses.

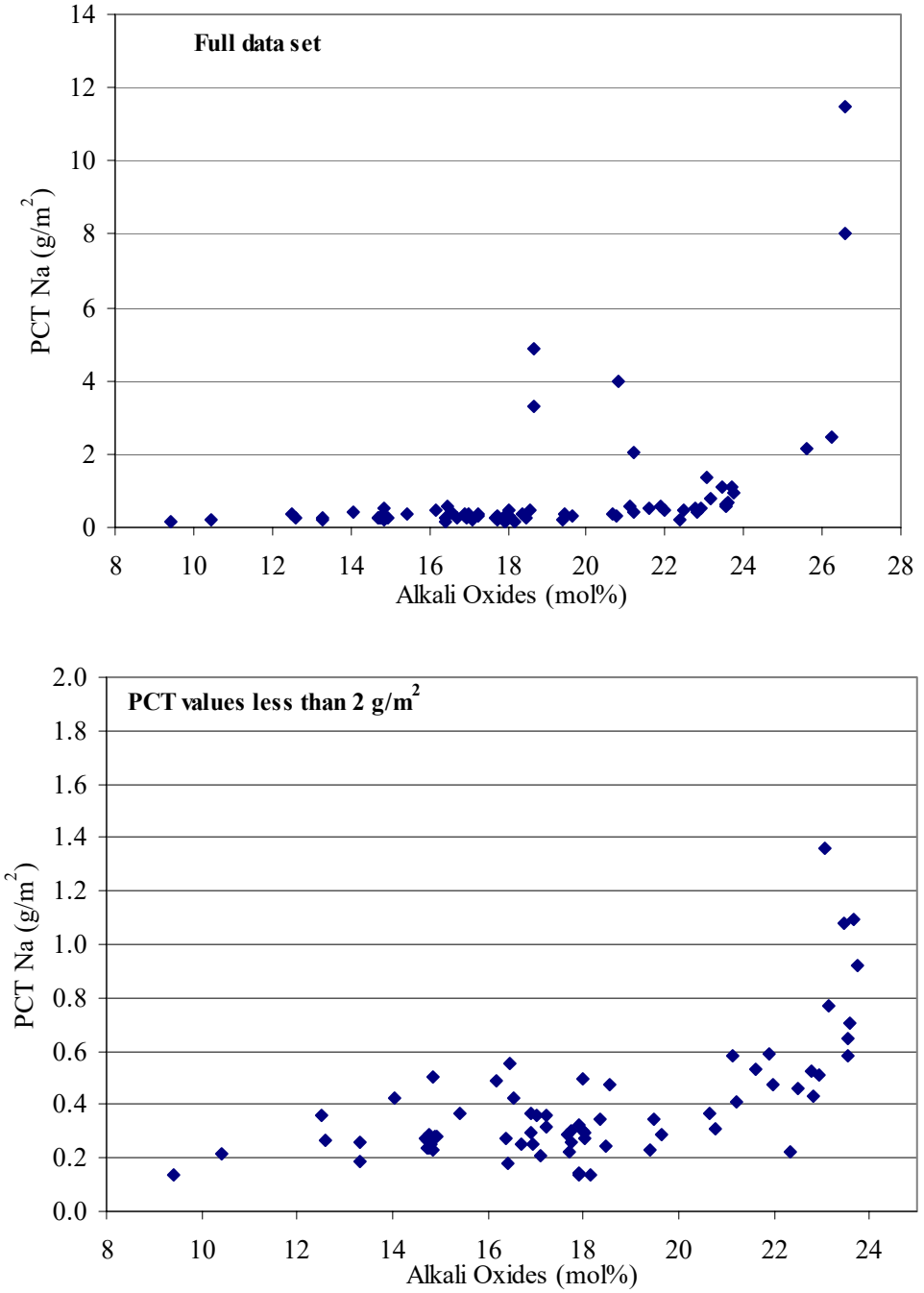


Figure 4.9. PCT Sodium Release as a Function of the Sum of Alkali Oxides ($Li_2O+Na_2O+K_2O$) in mol % for Existing and Test Matrix Glasses.

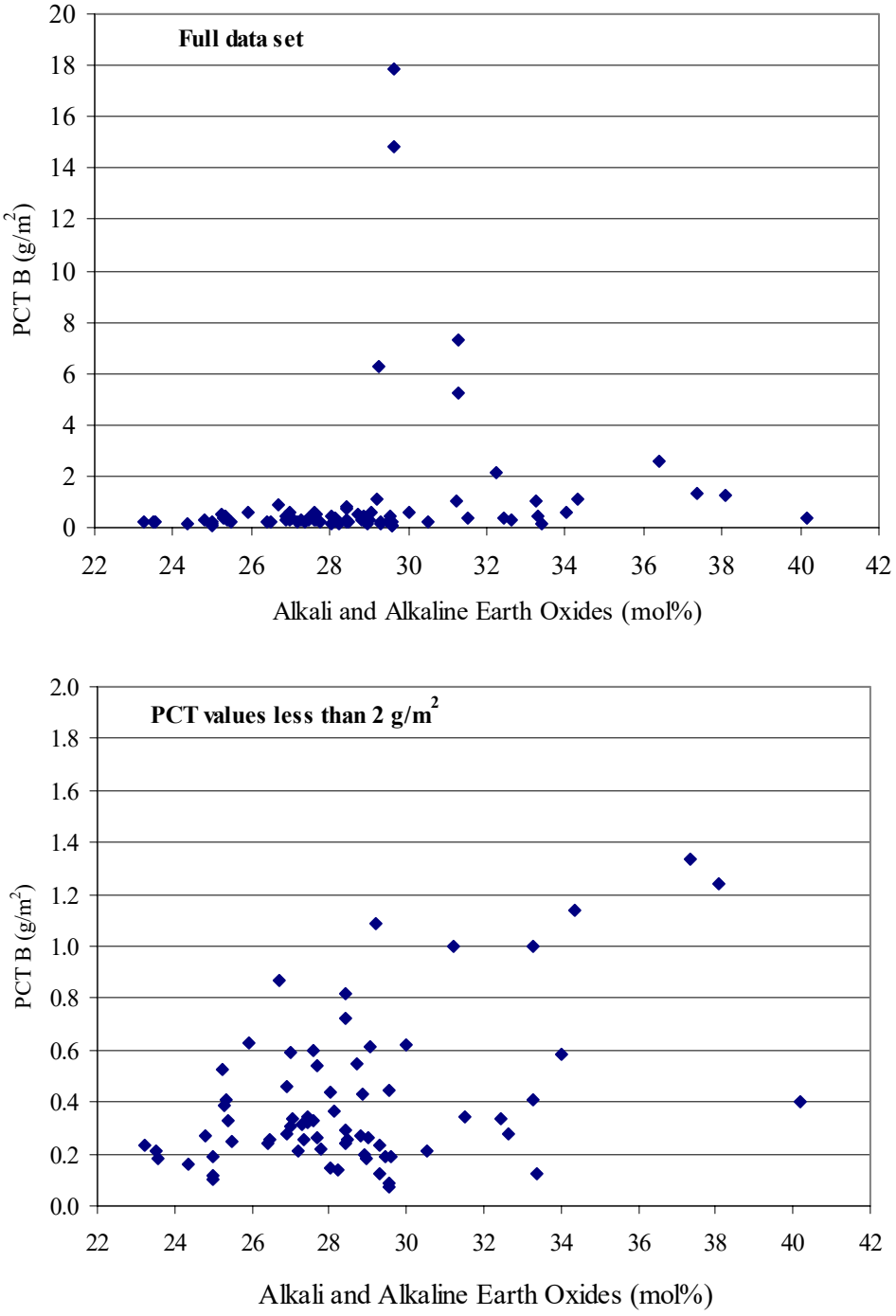


Figure 4.10. PCT Boron Release as a Function of the Sum of Alkali and Alkaline Earth Oxides ($Li_2O+Na_2O+K_2O+CaO+MgO$) in mol % for Existing and Test Matrix Glasses.

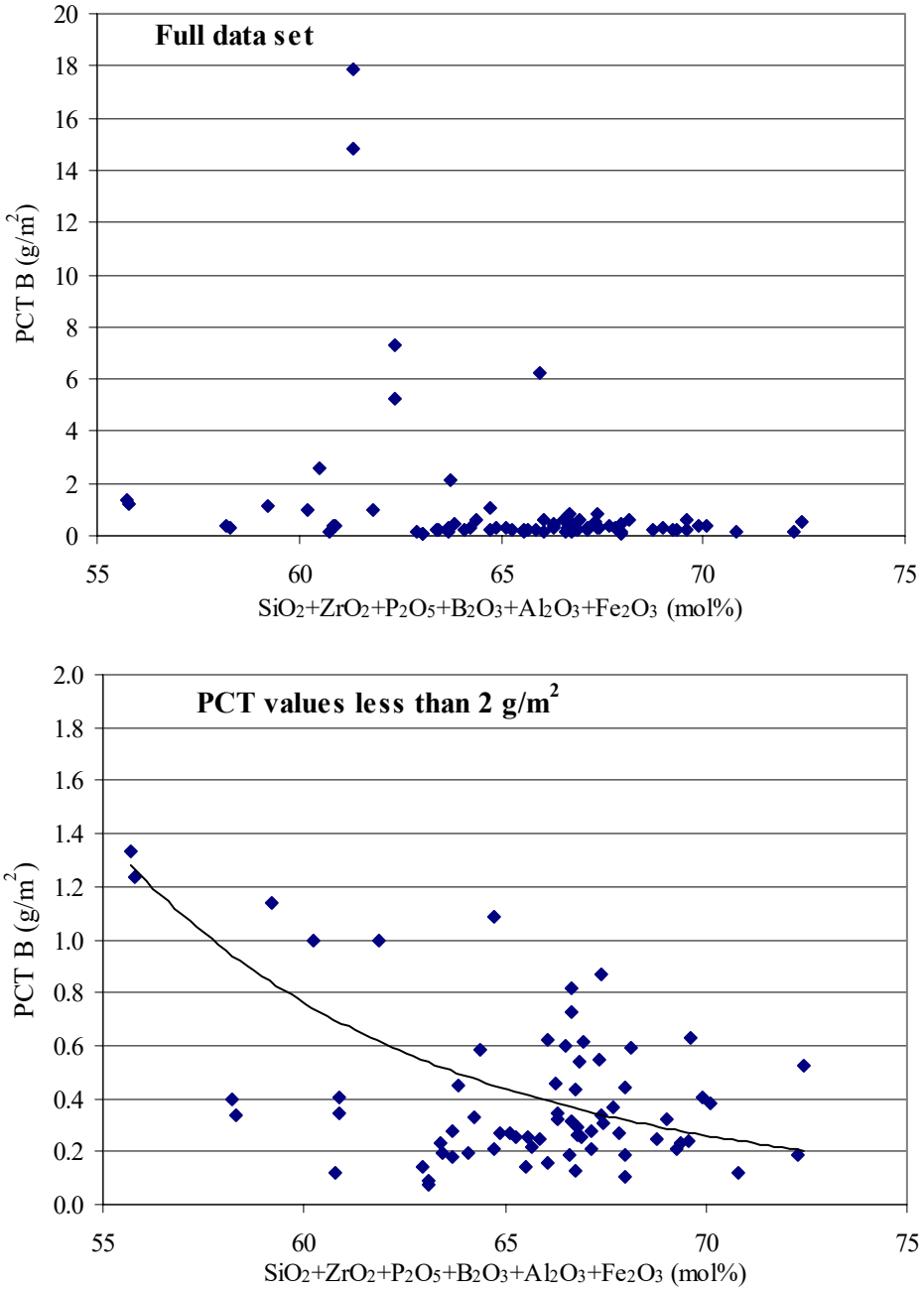


Figure 4.11. PCT Boron Release as a Function of the Sum of Valence III, IV, and V Components (SiO_2+ZrO_2+P_2O_5+B_2O_3+ Al_2O_3+Fe_2O_3) in mol % for Existing and Test Matrix Glasses.

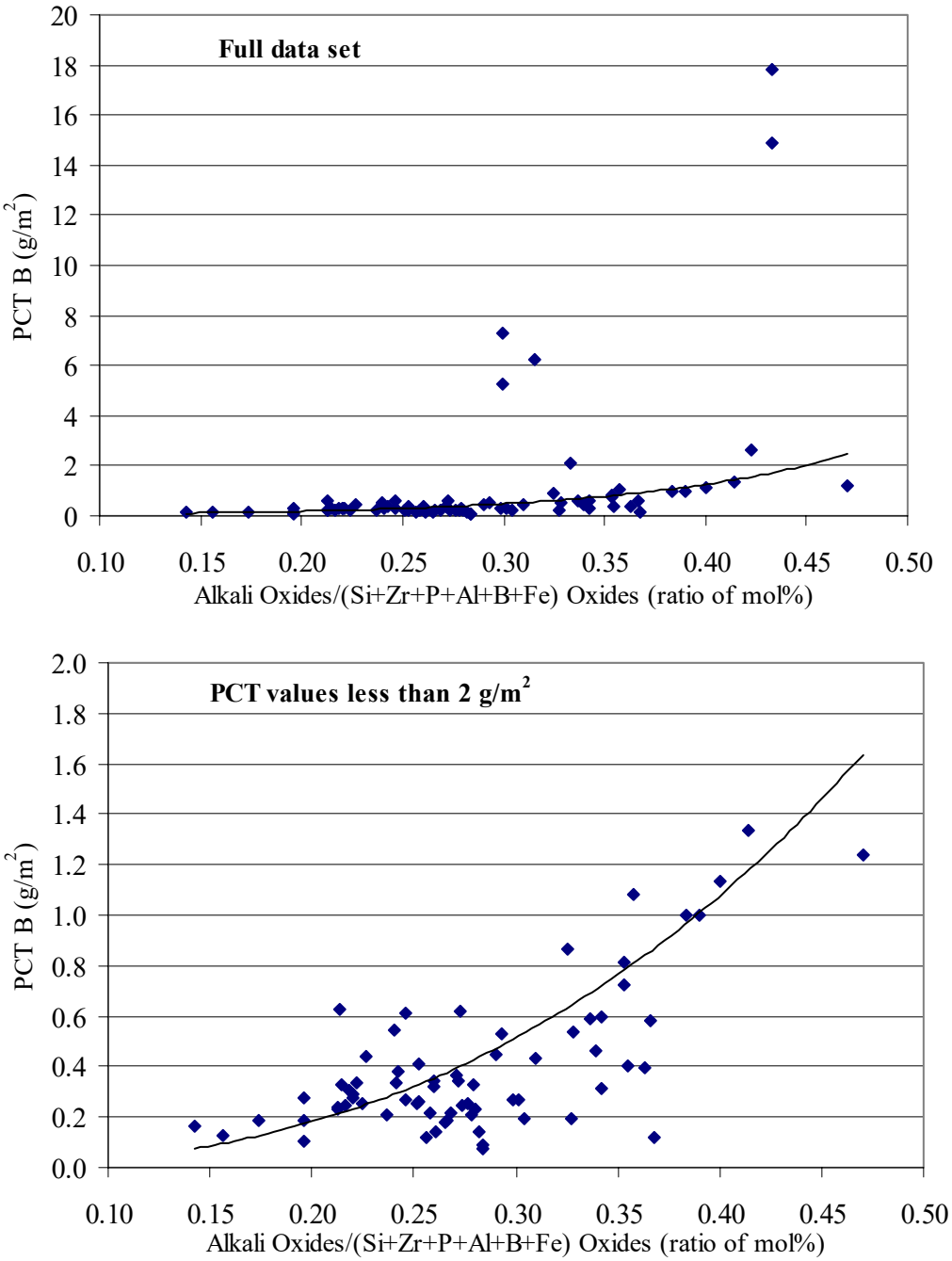


Figure 4.12. PCT Boron Release as a Function of the Ratio of Alkali Oxides ($Li_2O+Na_2O+K_2O$) to Glass Formers ($SiO_2+ZrO_2+P_2O_5+B_2O_3+Al_2O_3+Fe_2O_3$) in mol % for Existing and Test Matrix Glasses.

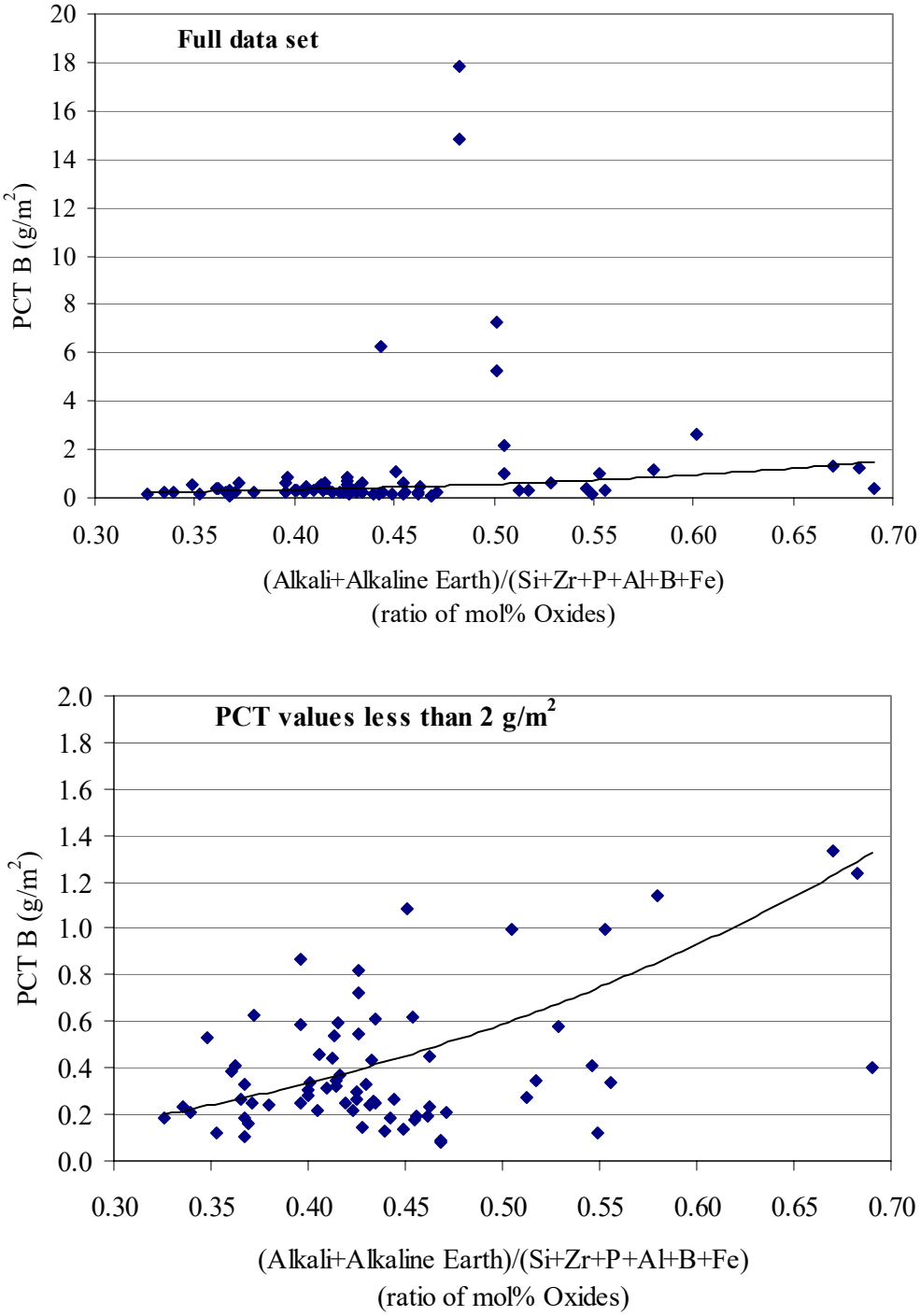


Figure 4.13. PCT Boron Release as a Function of the Ratio of Alkali and Alkali Earth Oxides ($Li_2O+Na_2O+K_2O+CaO+MgO$) to Glass Formers ($SiO_2+ZrO_2+P_2O_5+B_2O_3+ Al_2O_3+Fe_2O_3$) in mol % for Existing and Test Matrix Glasses.

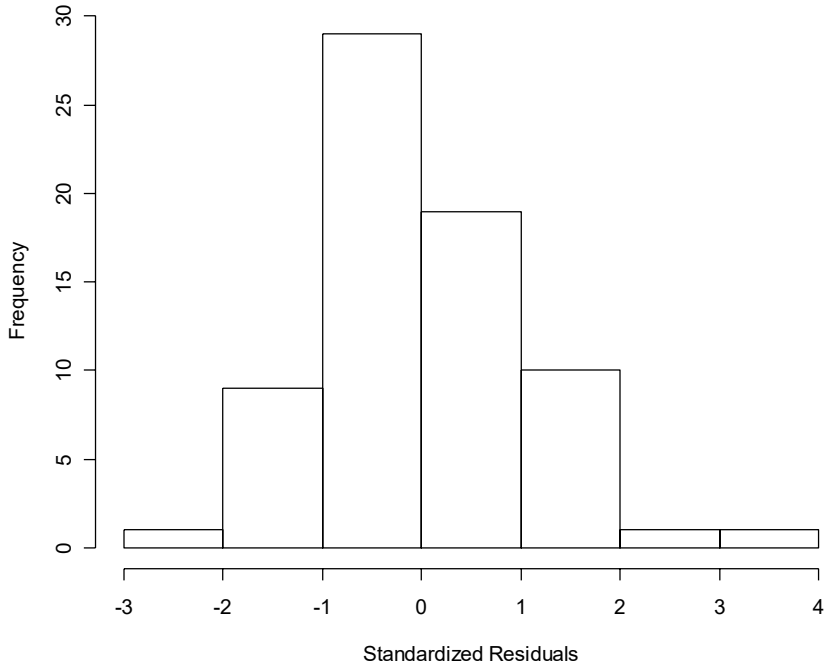


Figure 5.1. Histogram of Standardized Residuals for ILAW VHT LM Model.

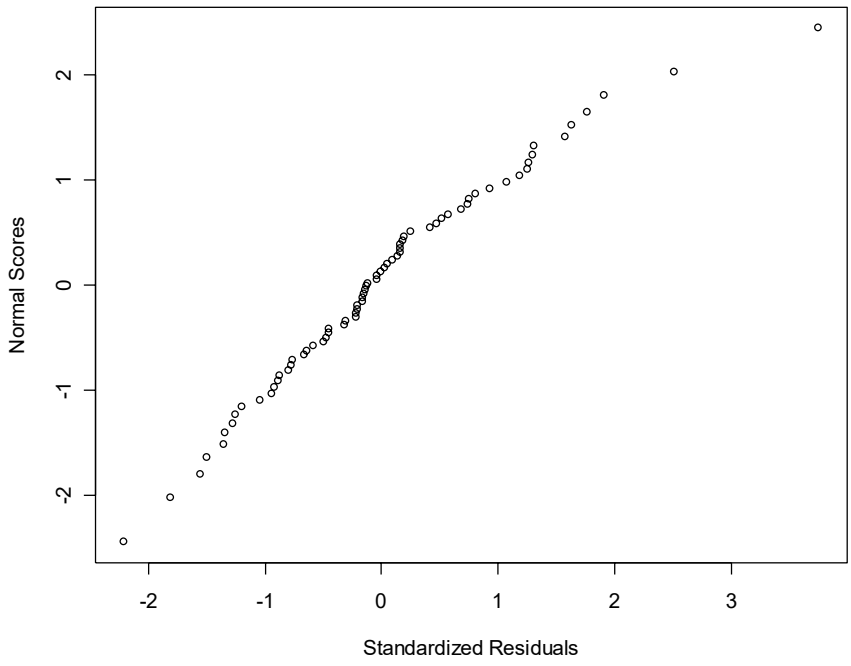


Figure 5.2. Normality Plot Associated with ILAW VHT LM Model.

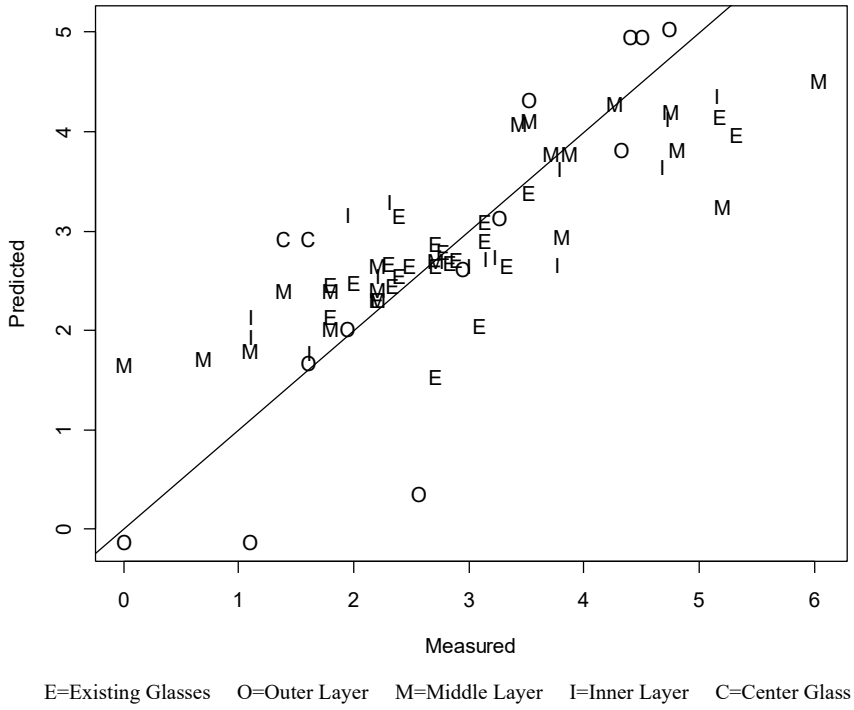


Figure 5.3. Predicted Versus Measured Plot for ILAW VHT LM Model.

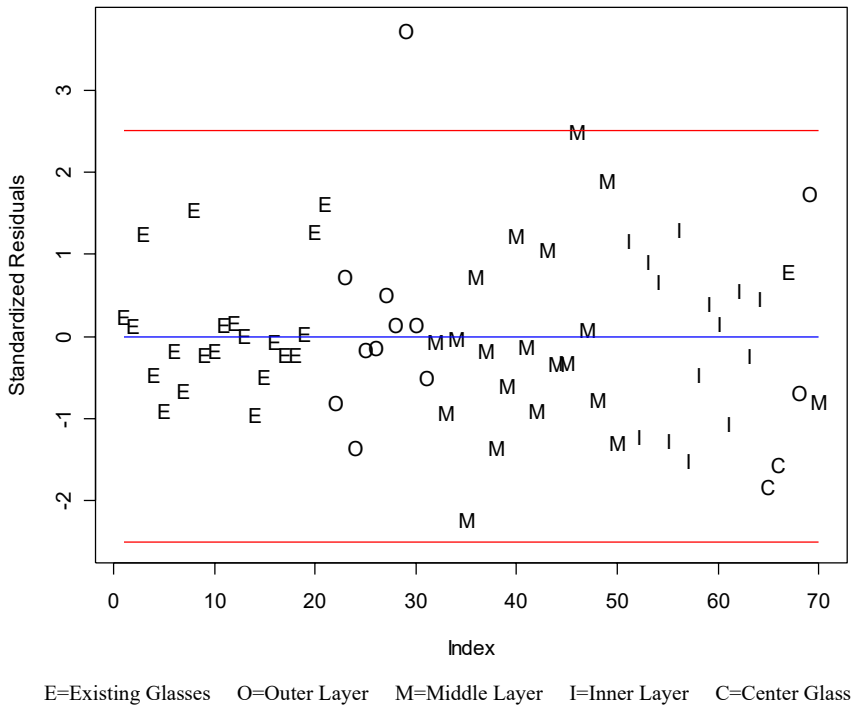


Figure 5.4. Standardized Residuals Plot for ILAW VHT LM Model.

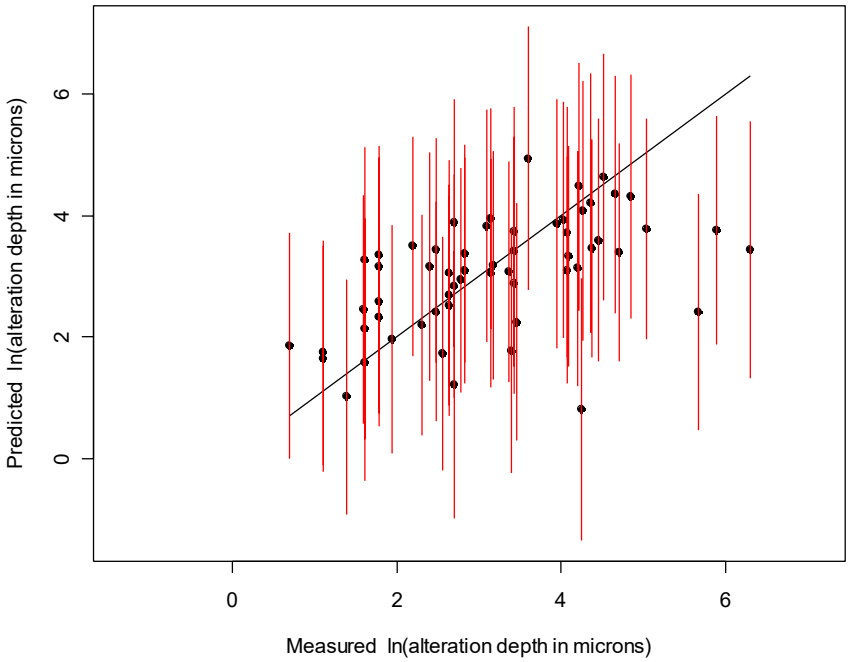


Figure 5.5. Predicted Versus Measured Plot for ILAW VHT LM Model Applied to All 59 Validation Glasses.

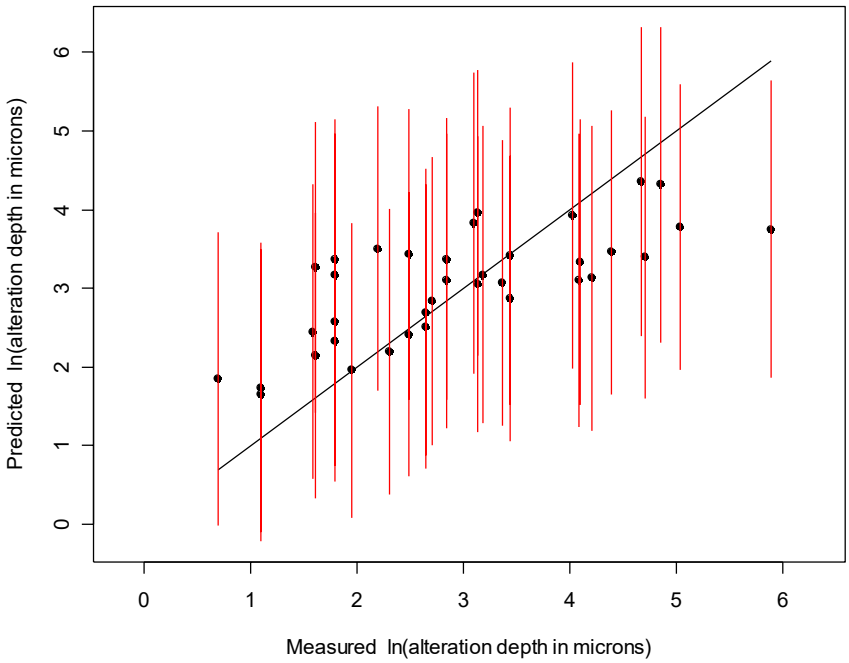


Figure 5.6. Predicted Versus Measured Plot for ILAW VHT LM Model. Applied to the 37 Subset V1 Validation Glasses

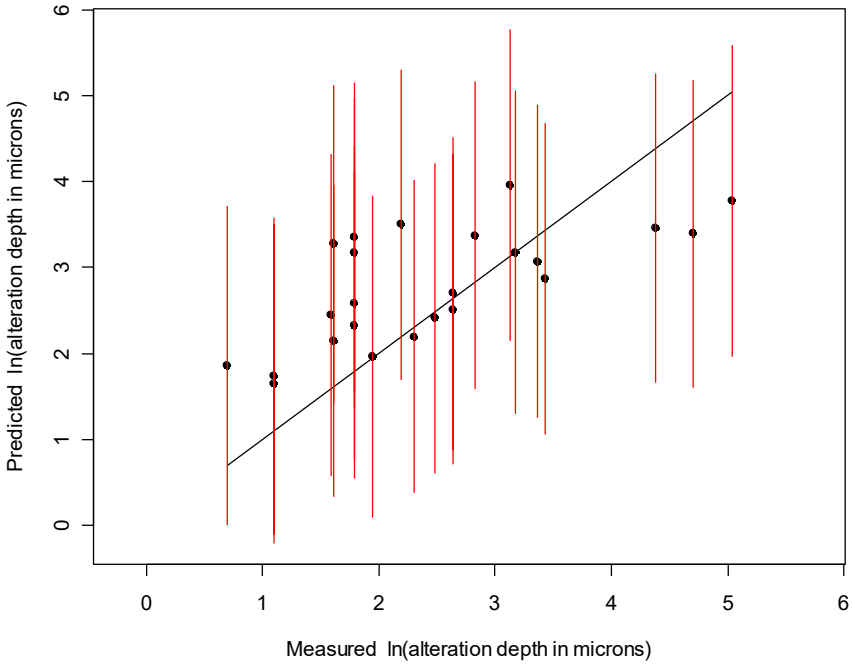


Figure 5.7. Predicted Versus Measured Plot for ILAW VHT LM Model Applied to the 24 Subset V2 Validation Glasses.

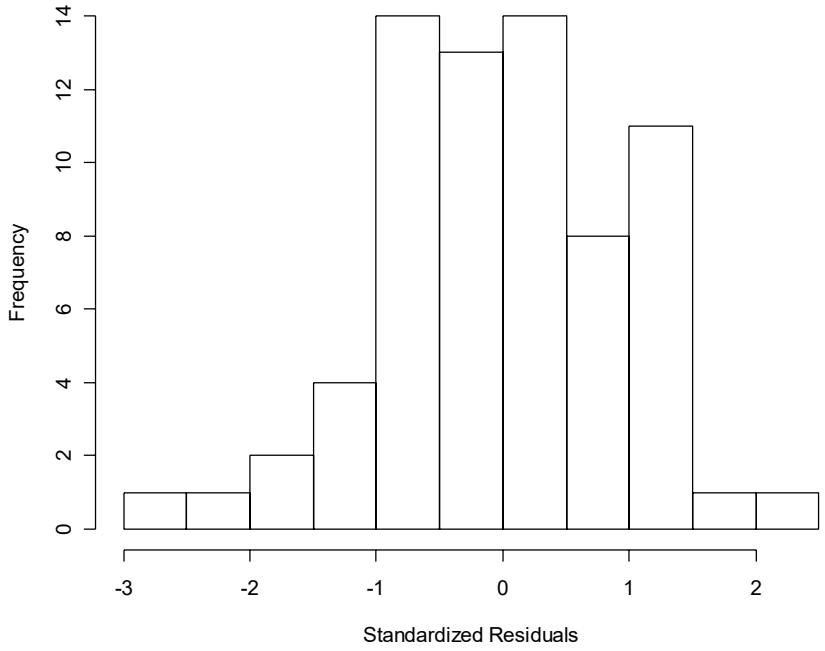


Figure 5.8. Histogram of Standardized Residuals for ILAW VHT PQM Model.

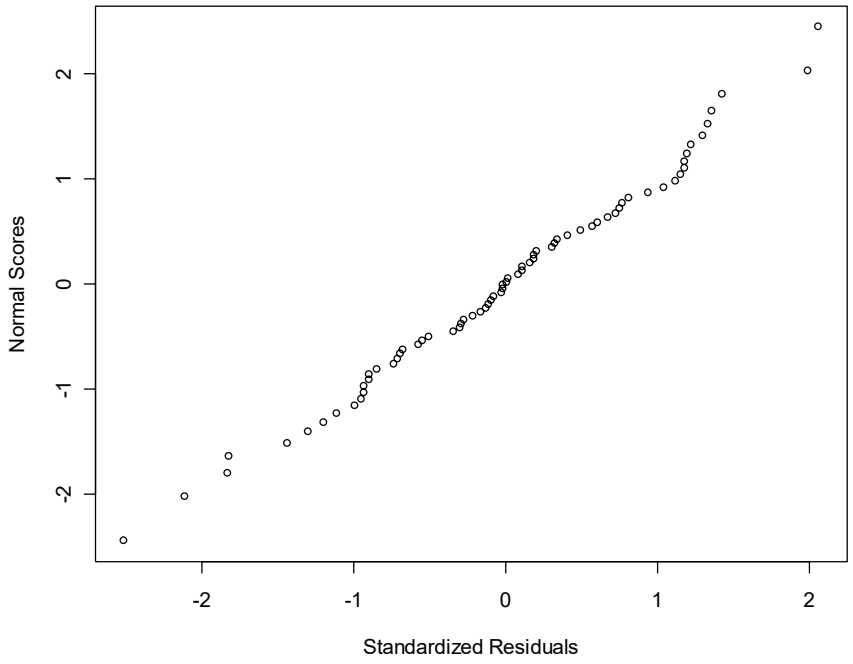


Figure 5.9. Normality Plot Associated with ILAW VHT PQM Model.

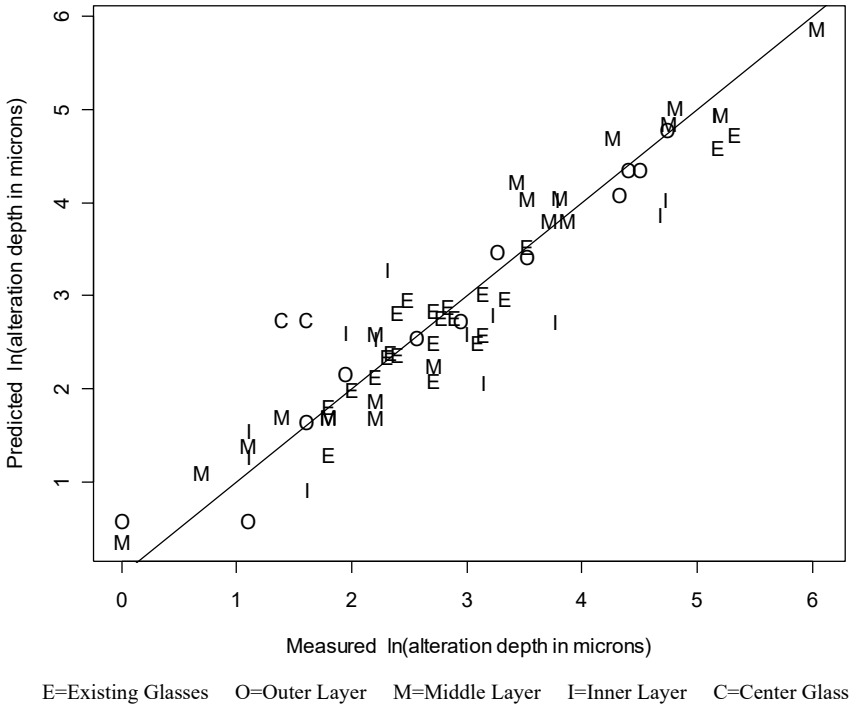


Figure 5.10. Predicted Versus Measured Plot for ILAW VHT PQM Model.

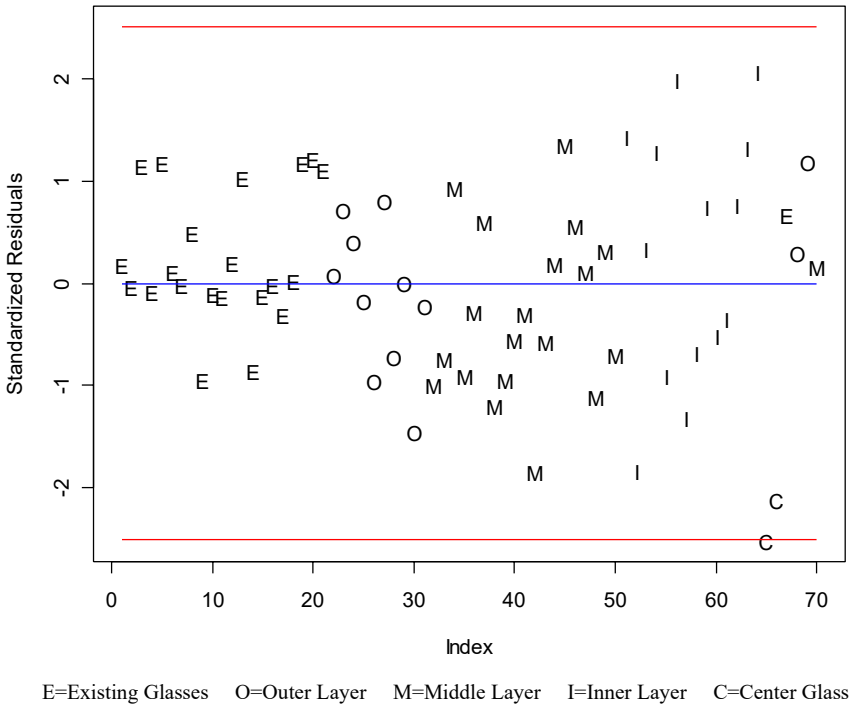


Figure 5.11. Standardized Residuals Plot for ILAW VHT PQM Model.

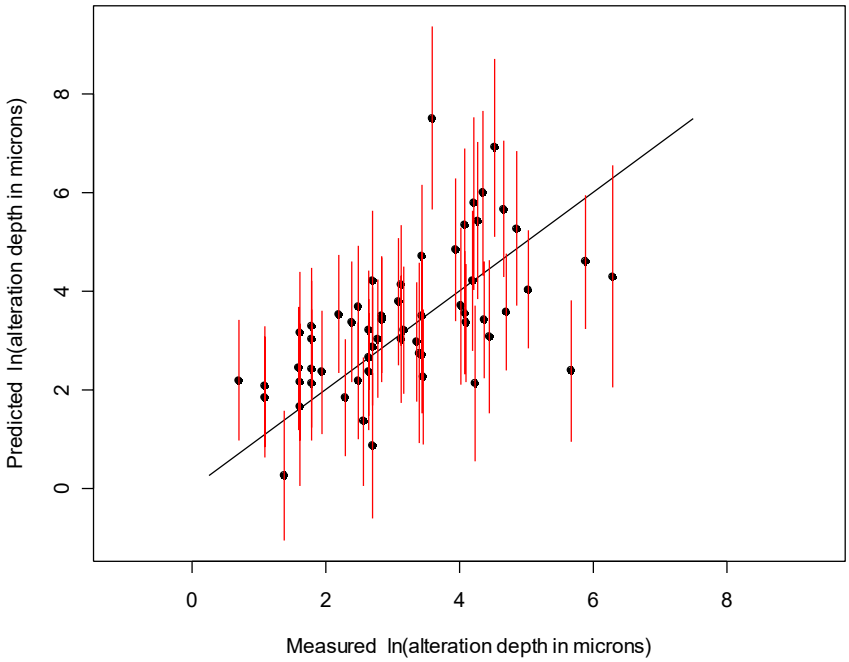


Figure 5.12. Predicted Versus Measured Plot for ILAW VHT PQM Model Applied to All 59 Validation Glasses.

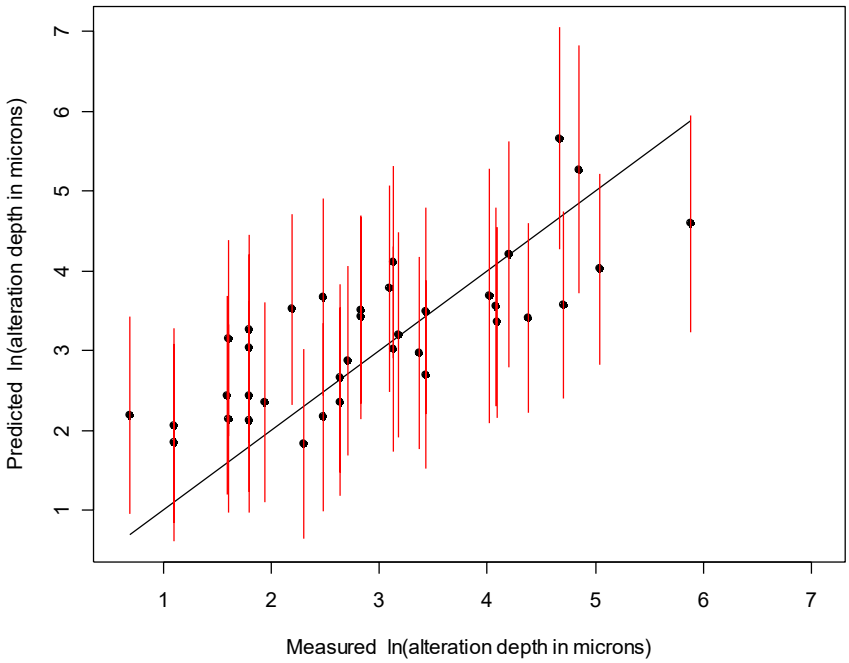


Figure 5.13. Predicted Versus Measured Plot for ILAW VHT PQM Model Applied to the 37 Subset V1 Validation Glasses.

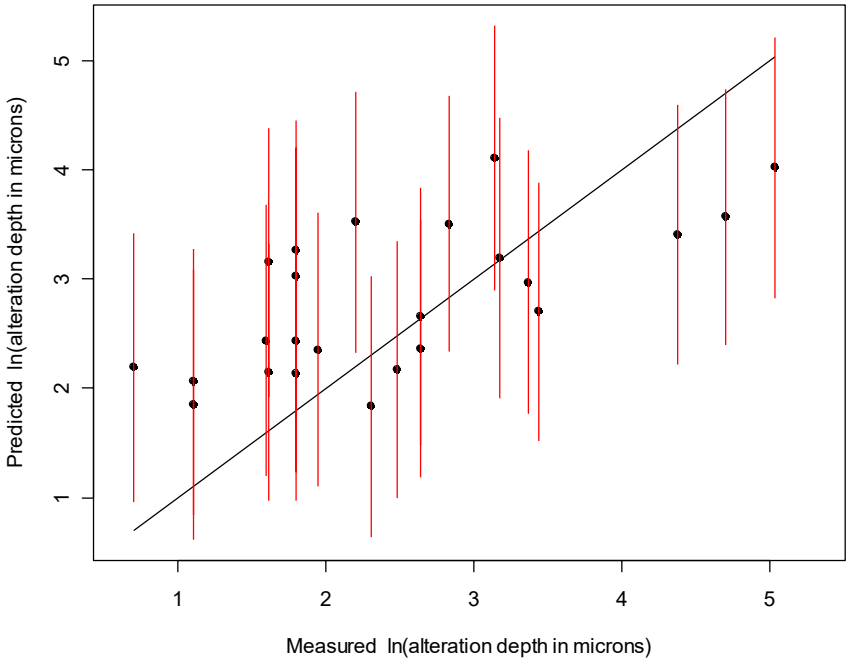


Figure 5.14. Predicted Versus Measured Plot for ILAW VHT PQM Model Applied to the 24 Subset V2 Validation Glasses.

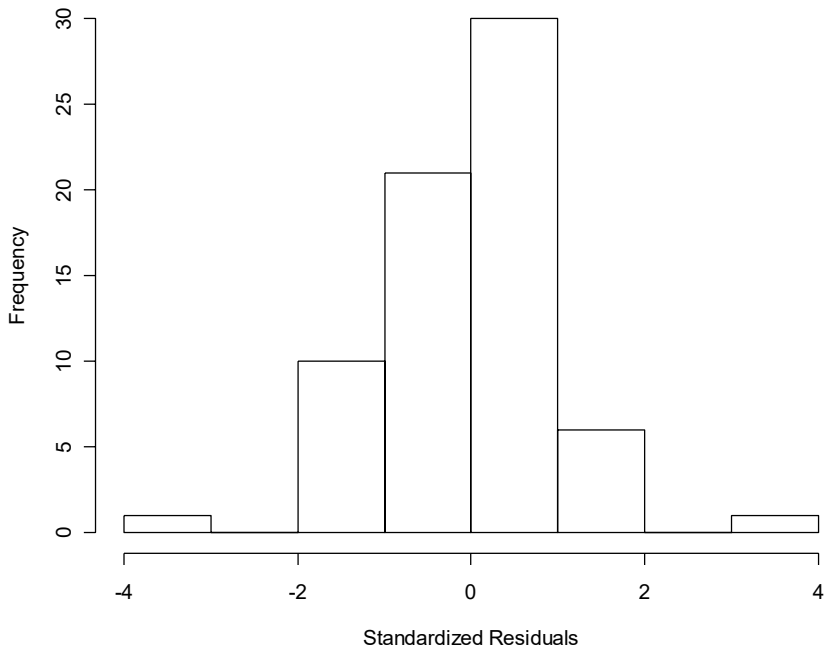


Figure 6.1. Histogram of Standardized Residuals for ILAW PCT-Boron Reduced LM Model.

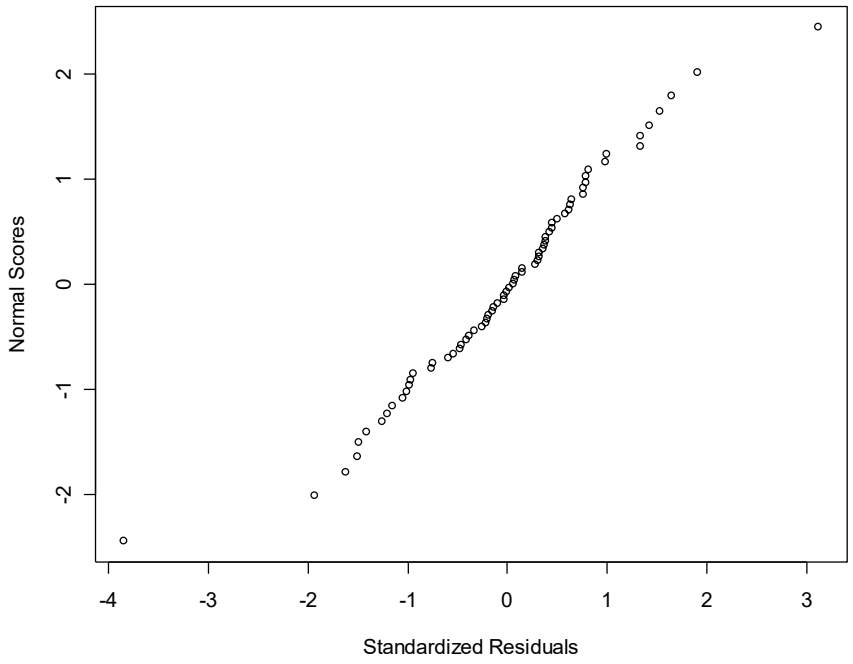


Figure 6.2. Normality Plot Associated with ILAW PCT-Boron Reduced LM Model.

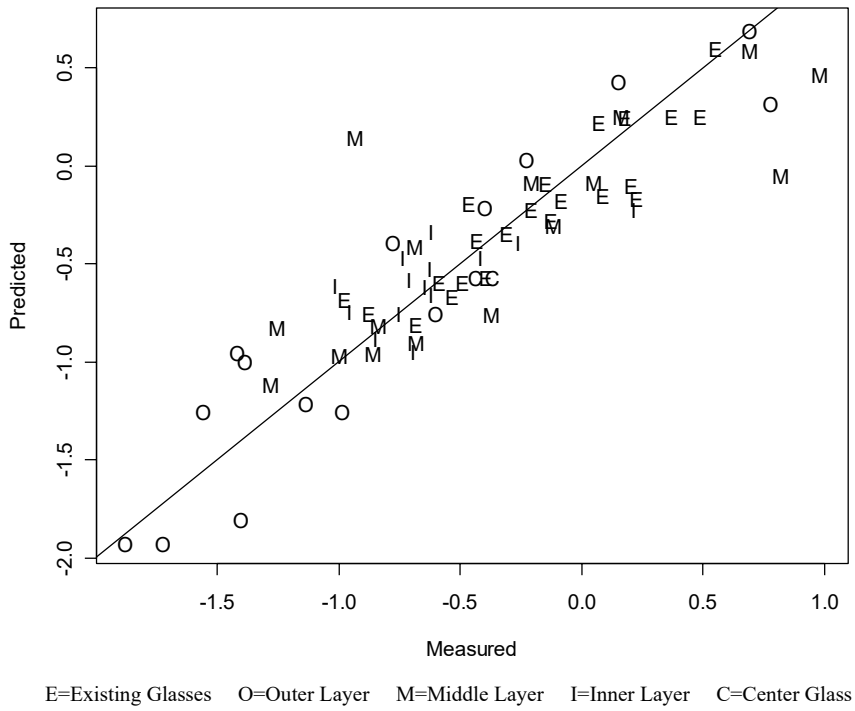


Figure 6.3. Predicted Versus Measured Plot for ILAW PCT-Boron Reduced LM Model.

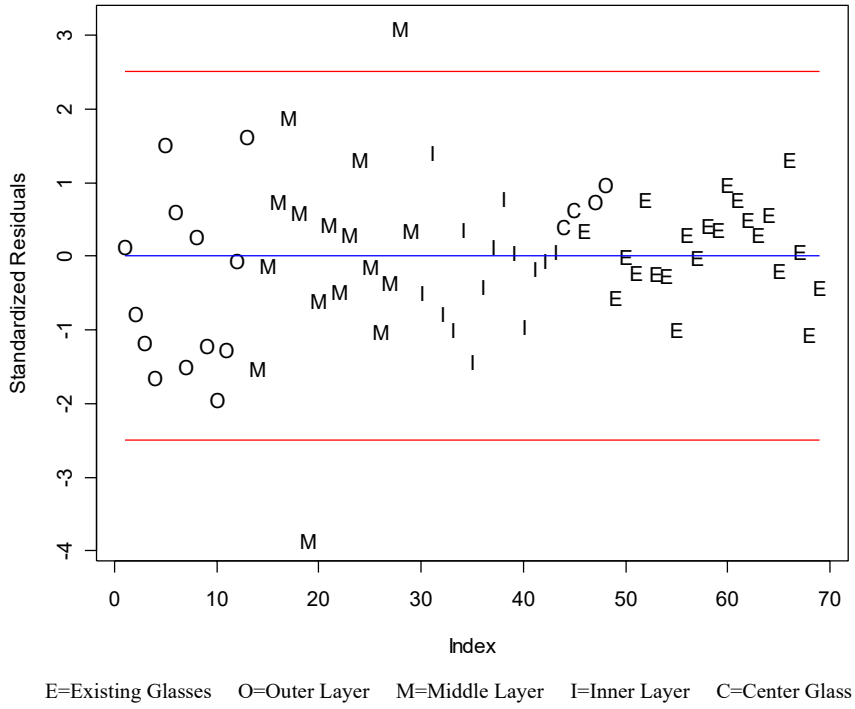


Figure 6.4. Standardized Residuals Plot for ILAW PCT-Boron Reduced LM Model.

.

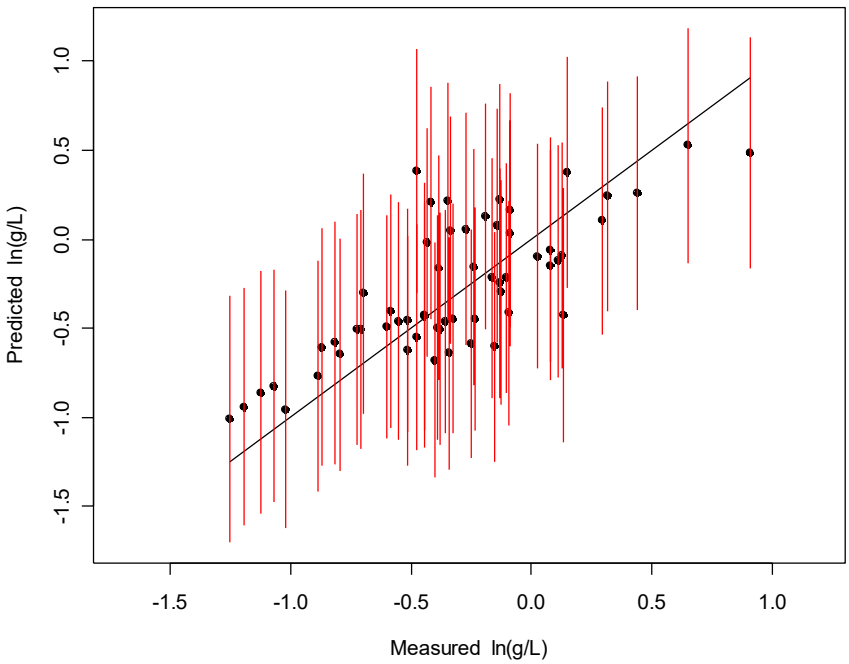


Figure 6.5. Predicted Versus Measured Plot for ILAW PCT-Boron Reduced LM Model Applied to All 59 Validation Glasses.

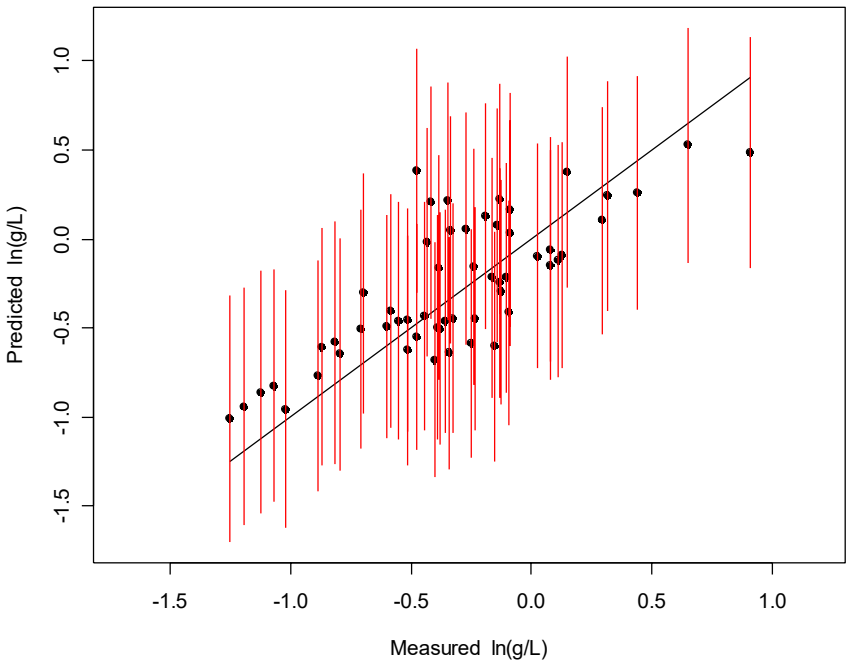


Figure 6.6. Predicted Versus Measured Plot for ILAW PCT-Boron Reduced LM Model Applied to the 56 Subset V1 Validation Glasses.

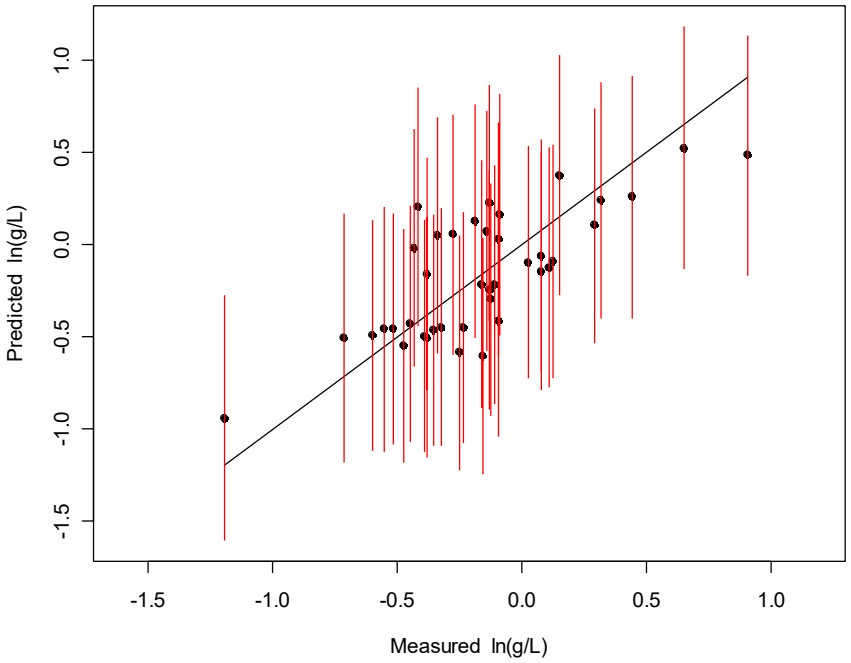


Figure 6.7. Predicted Versus Measured Plot for ILAW PCT-Boron Reduced LM Model Applied to the 40 Subset V2 Validation Glasses

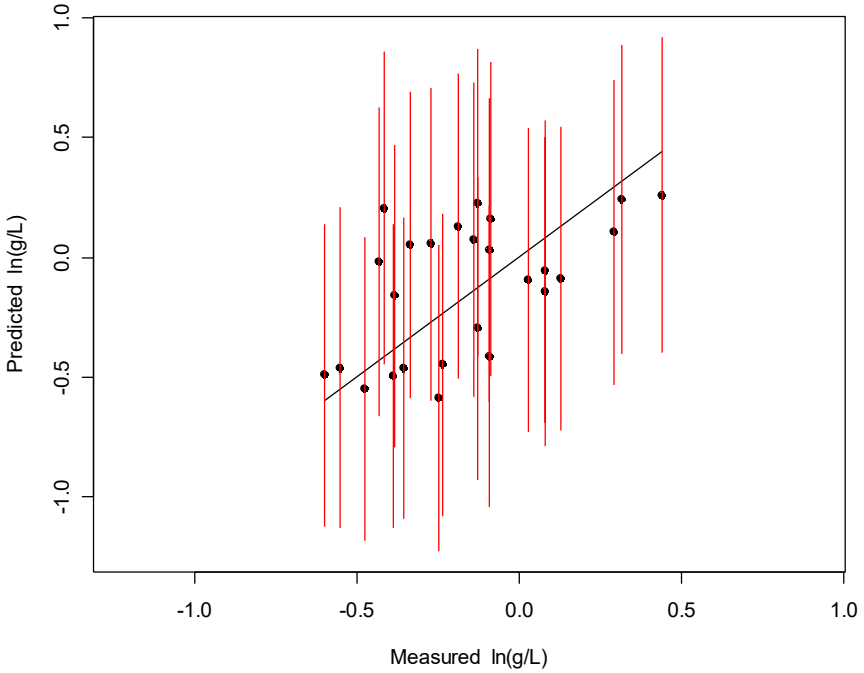


Figure 6.8. Predicted Versus Measured Plot for ILAW PCT-Boron Reduced LM Model Applied to the 26 V3 Validation Glasses.

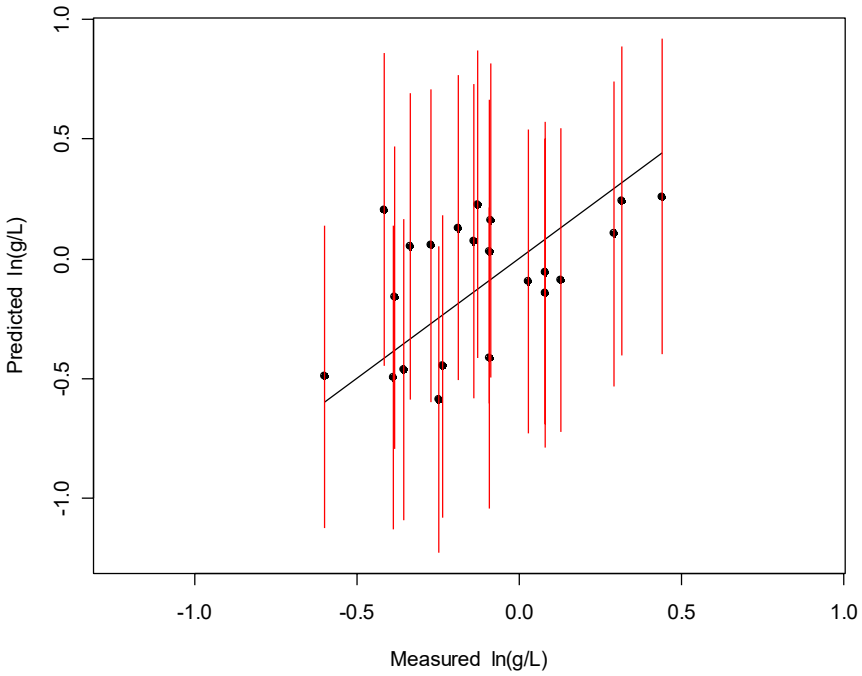


Figure 6.9. Predicted Versus Measured Plot for ILAW PCT-Boron Reduced LM Model Applied to the 22 Subset V4 Validation Glasses.

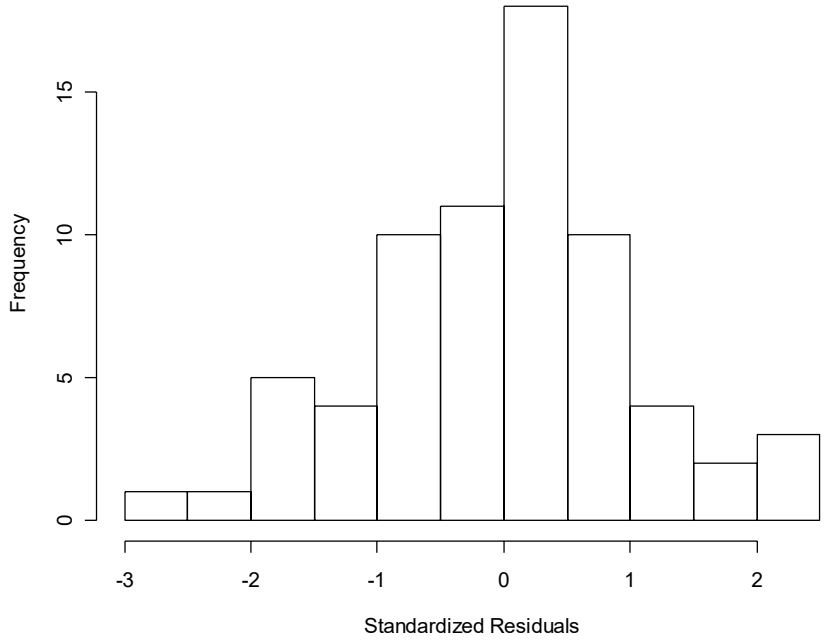


Figure 6.10. Histogram of Standardized Residuals for ILAW PCT-Boron Reduced PQM Model.

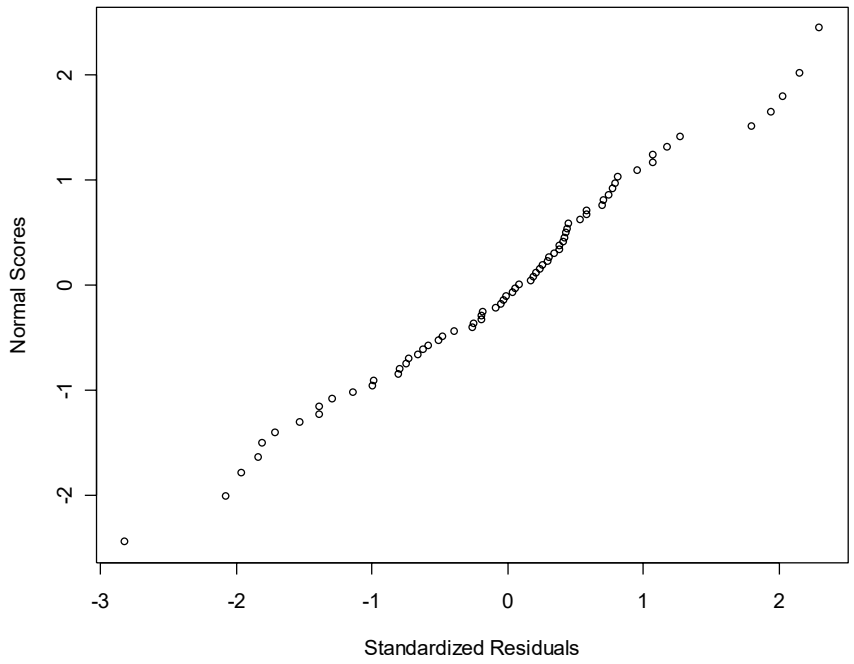


Figure 6.11. Normality Plot Associated with ILAW PCT-Boron Reduced PQM Model.

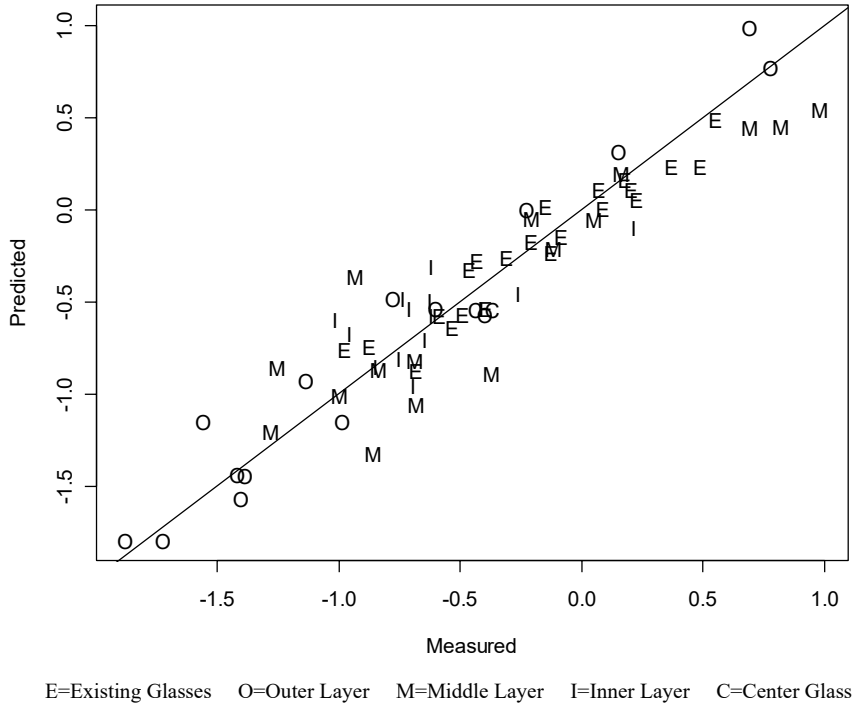


Figure 6.12. Predicted Versus Measured Plot for ILAW PCT-Boron Reduced PQM Model.

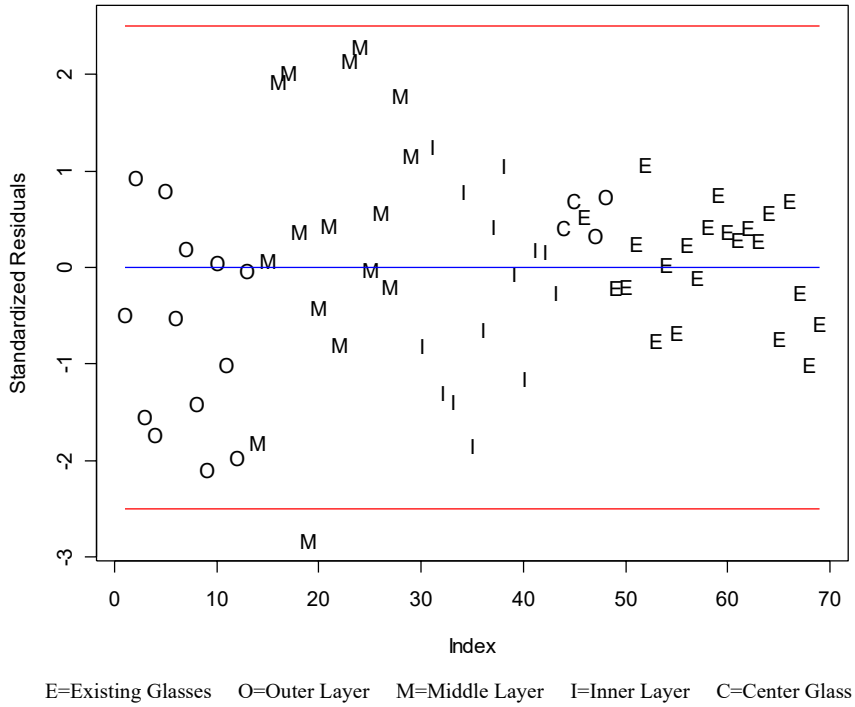


Figure 6.13. Standardized Residuals Plot for ILAW PCT-Boron Reduced PQM Model.

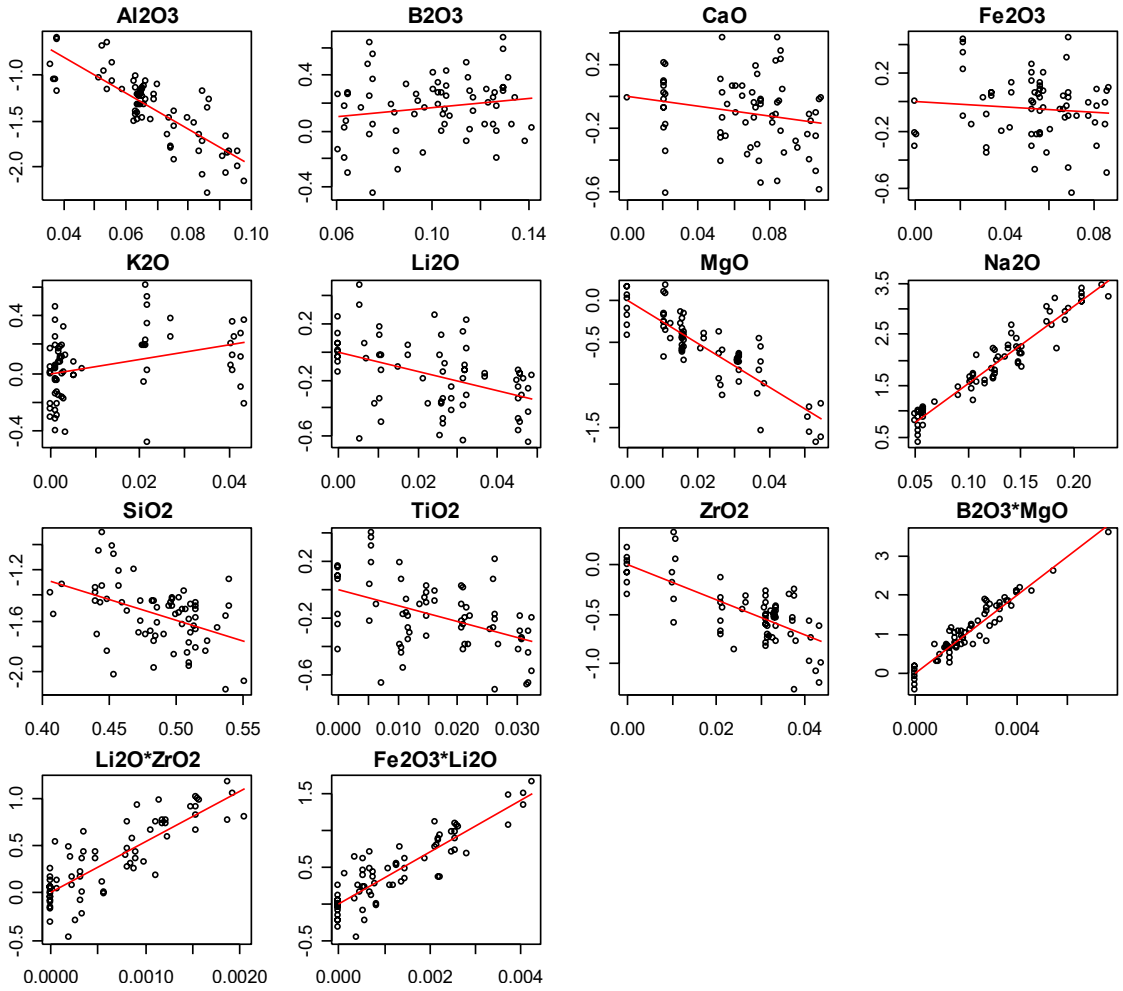


Figure 6.14. Partial Residual Plots for ILAW PCT-Boron Reduced PQM Model.

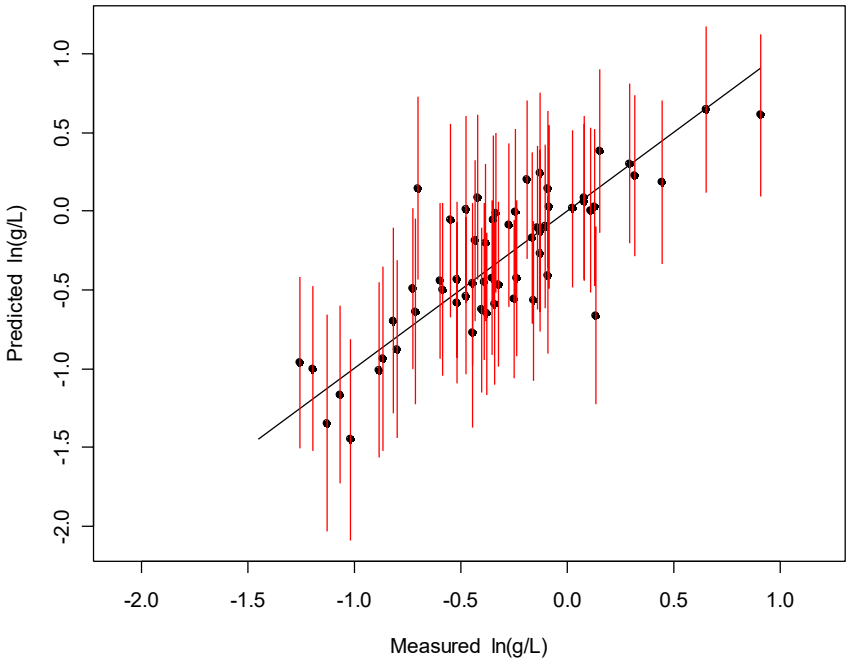


Figure 6.15. Predicted Versus Measured Plot for ILAW PCT-Boron Reduced PQM Model Applied to All 59 Validation Glasses.

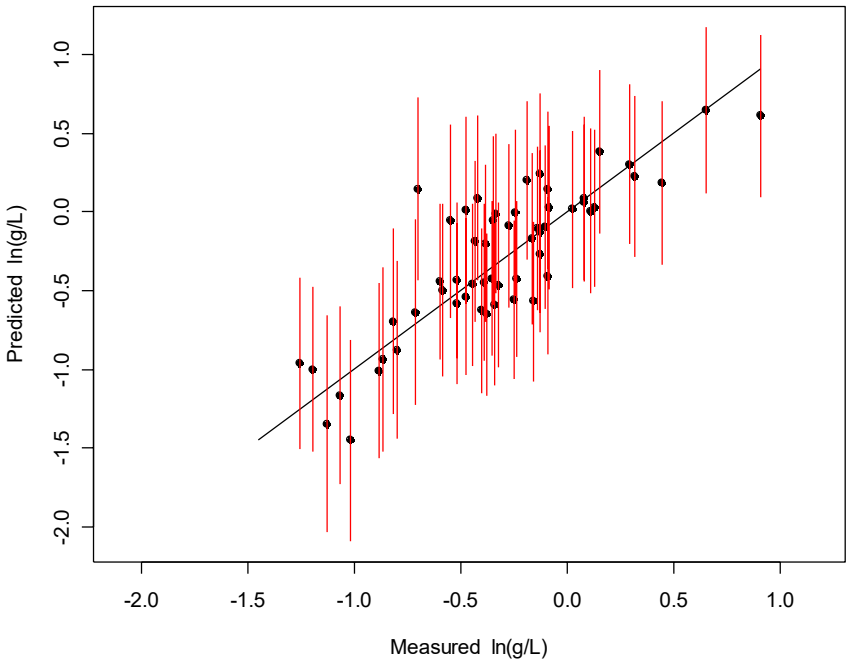


Figure 6.16. Predicted Versus Measured Plot for ILAW PCT-Boron Reduced PQM Model Applied to the 56 Subset V1 Validation Glasses.

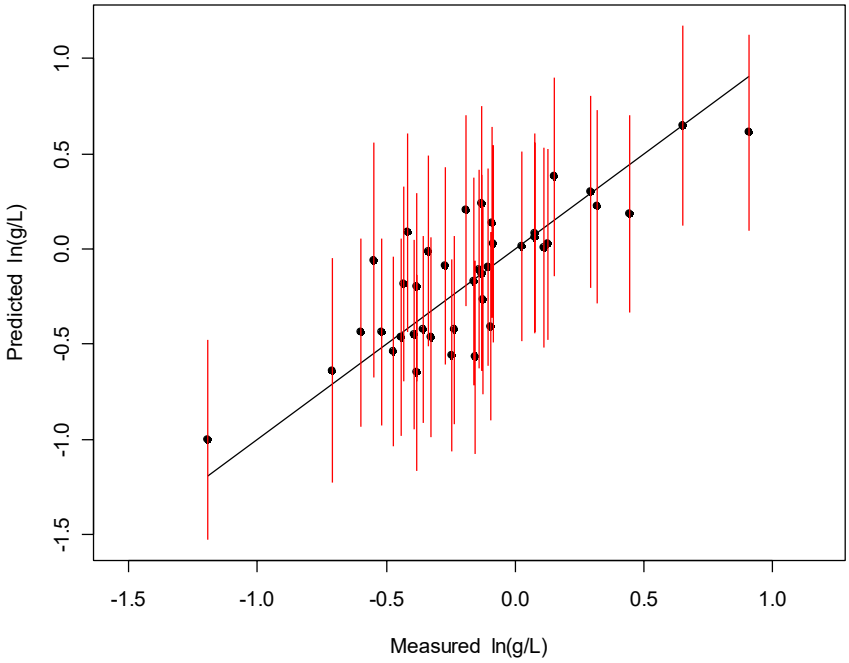


Figure 6.17. Predicted Versus Measured Plot for ILAW PCT-Boron Reduced PQM Model Applied to the 40 Subset V2 Validation Glasses.

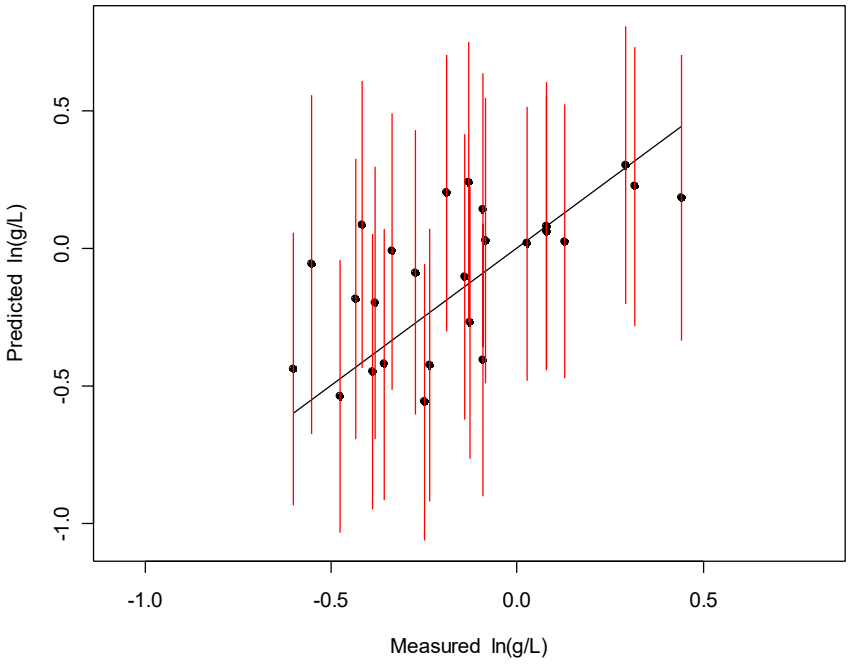


Figure 6.18. Predicted Versus Measured Plot for ILAW PCT-Boron Reduced PQM Model Applied to the 26 Subset V3 Validation Glasses.

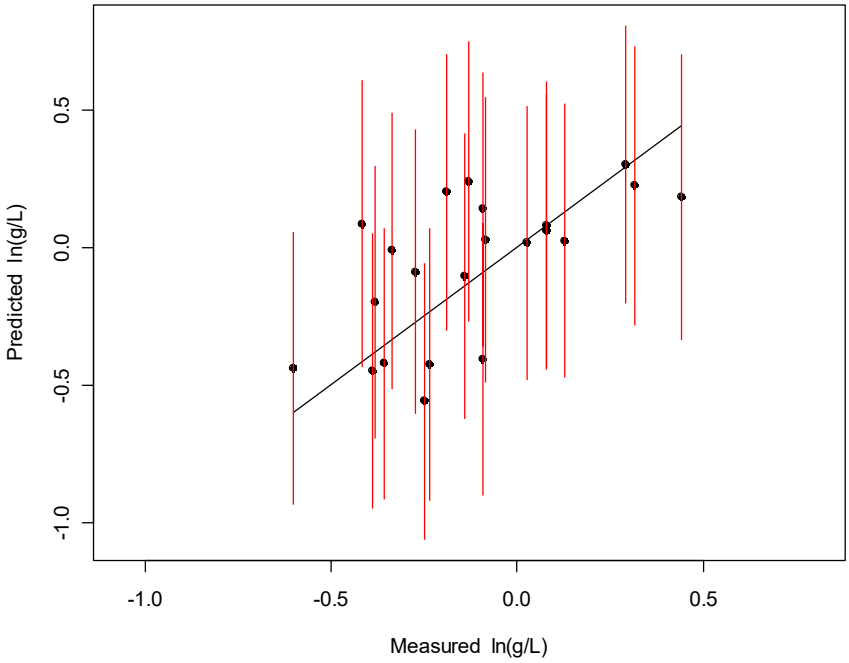


Figure 6.19. Predicted Versus Measured Plot for ILAW PCT-Boron Reduced PQM Model Applied to the 22 Subset V4 Validation Glasses.

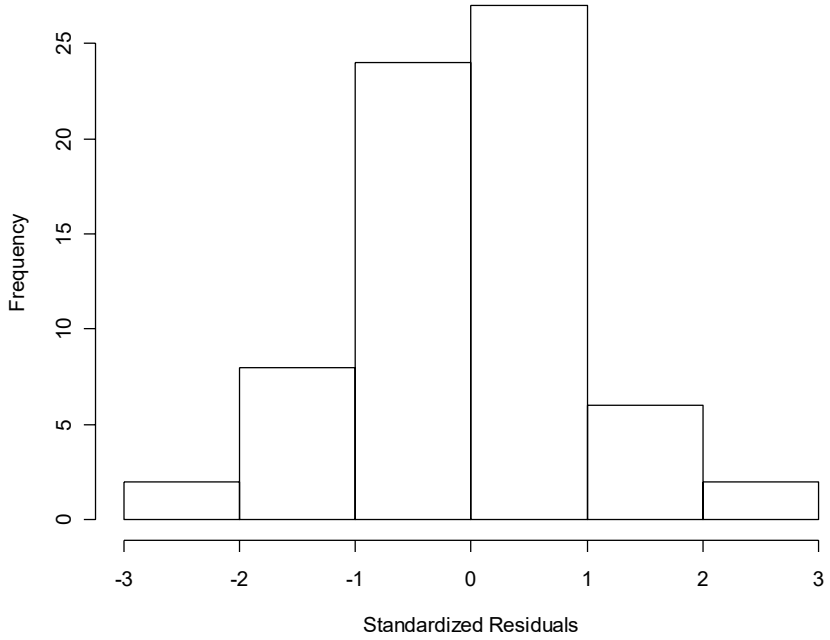


Figure 6.20. Histogram of Standardized Residuals for ILAW PCT-Sodium Reduced LM Model.

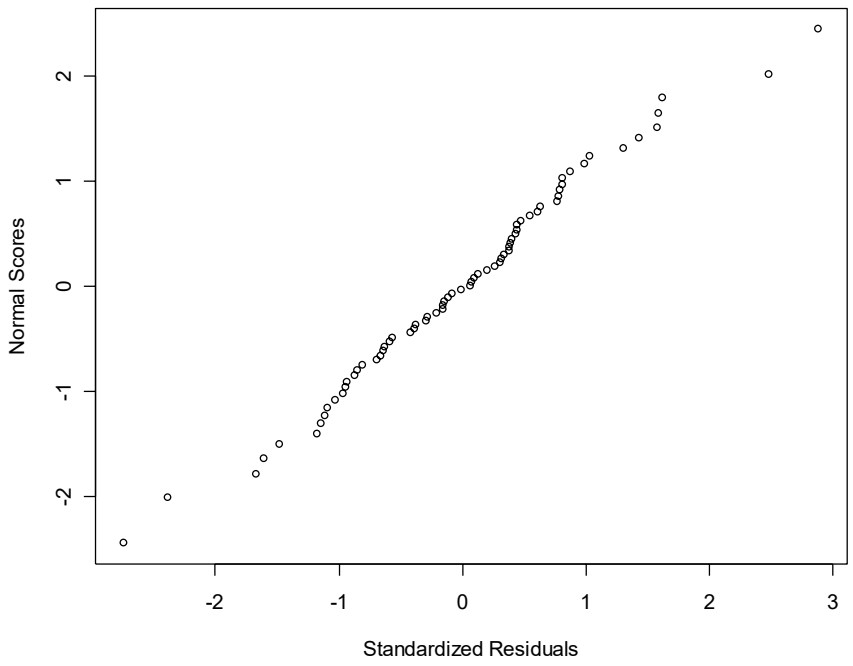


Figure 6.21. Normality Plot Associated with ILAW PCT-Sodium Reduced LM Model.

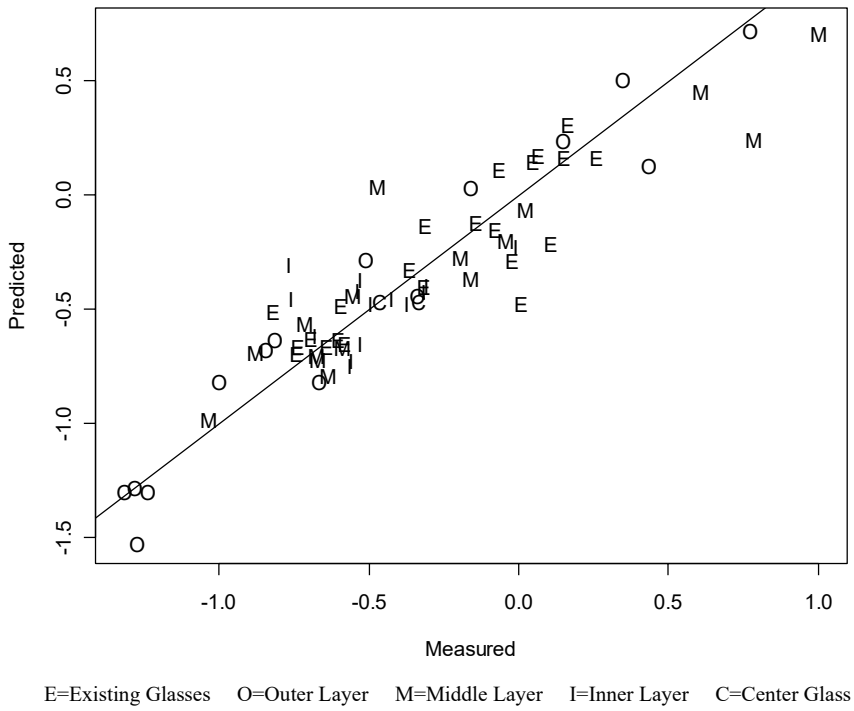


Figure 6.22. Predicted Versus Measured Plot for ILAW PCT-Sodium Reduced LM Model.

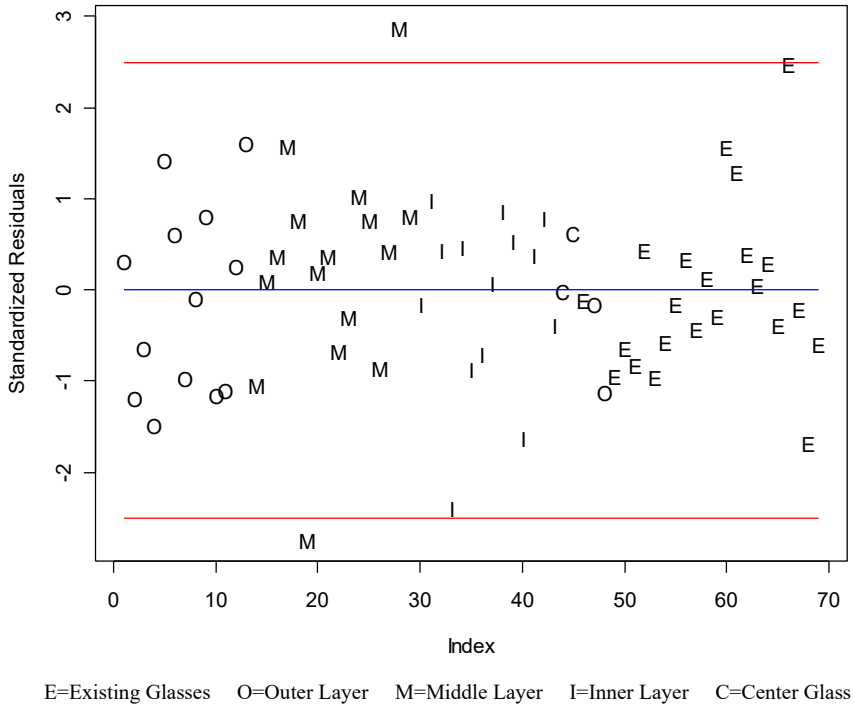


Figure 6.23. Standardized Residuals Plot for ILAW PCT-Sodium Reduced LM Model.

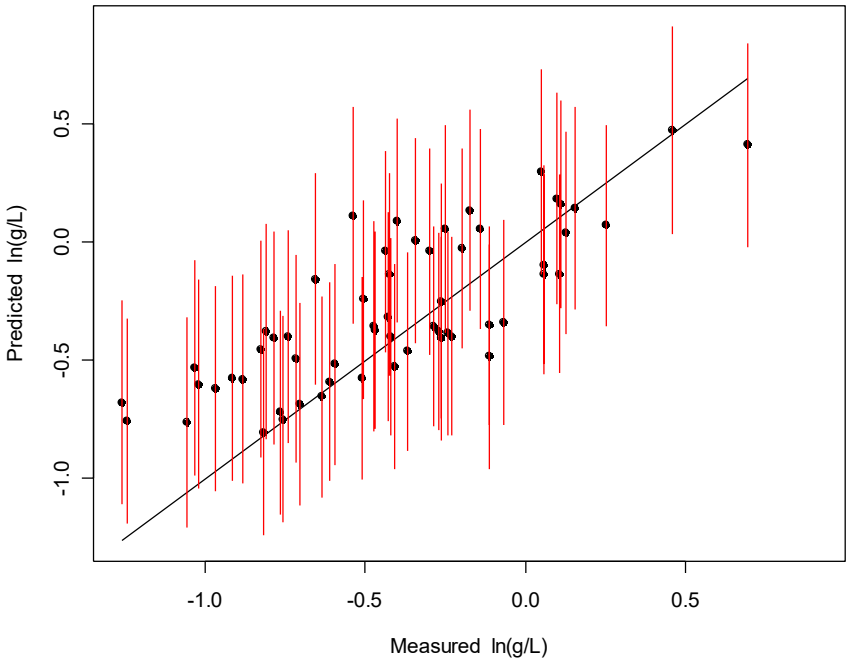


Figure 6.24. Predicted Versus Measured Plot for ILAW PCT-Sodium Reduced LM Model Applied to All 59 Validation Glasses.

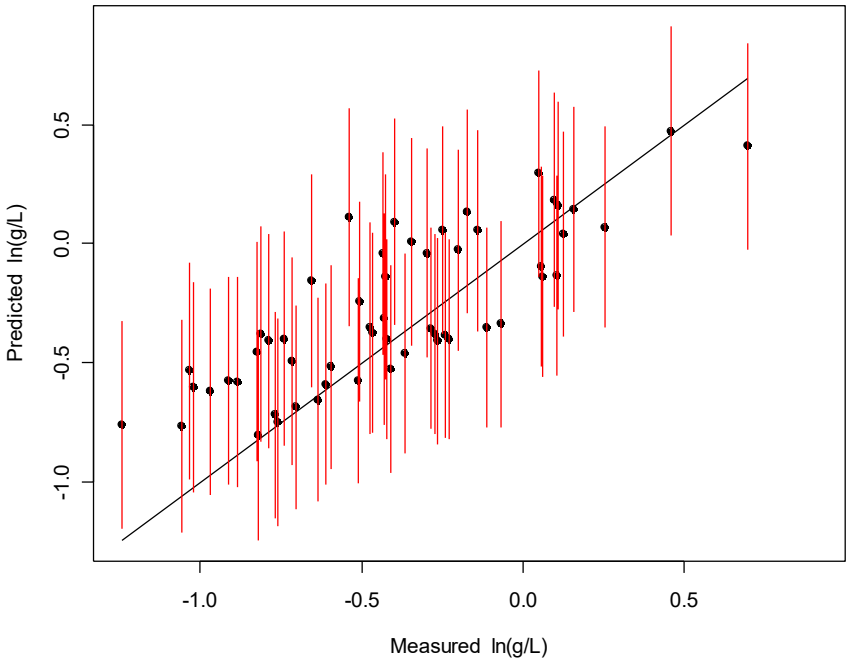


Figure 6.25. Predicted Versus Measured Plot for ILAW PCT-Sodium Reduced LM Model Applied to the 56 Subset V1 Validation Glasses.

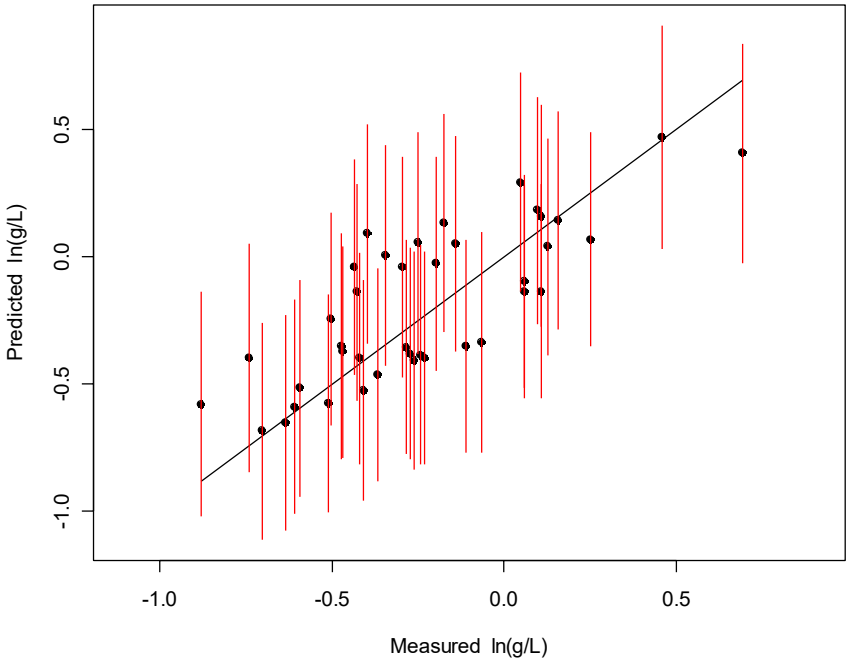


Figure 6.26. Predicted Versus Measured Plot for ILAW PCT-Sodium Reduced LM Model Applied to the 40 Subset V2 Validation Glasses.

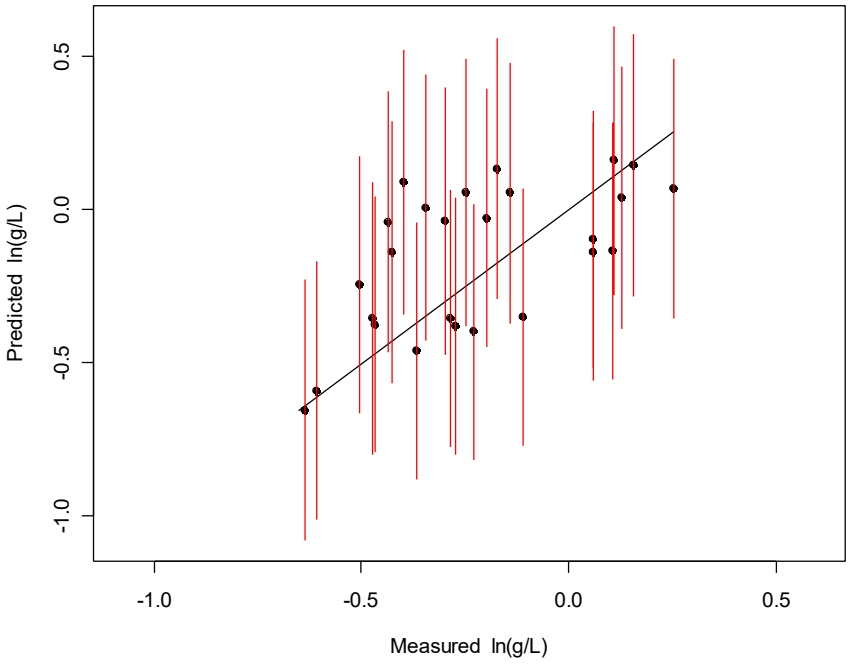


Figure 6.27. Predicted Versus Measured Plot for ILAW PCT-Sodium Reduced LM Model Applied to the 26 Subset V3 Validation Glasses.

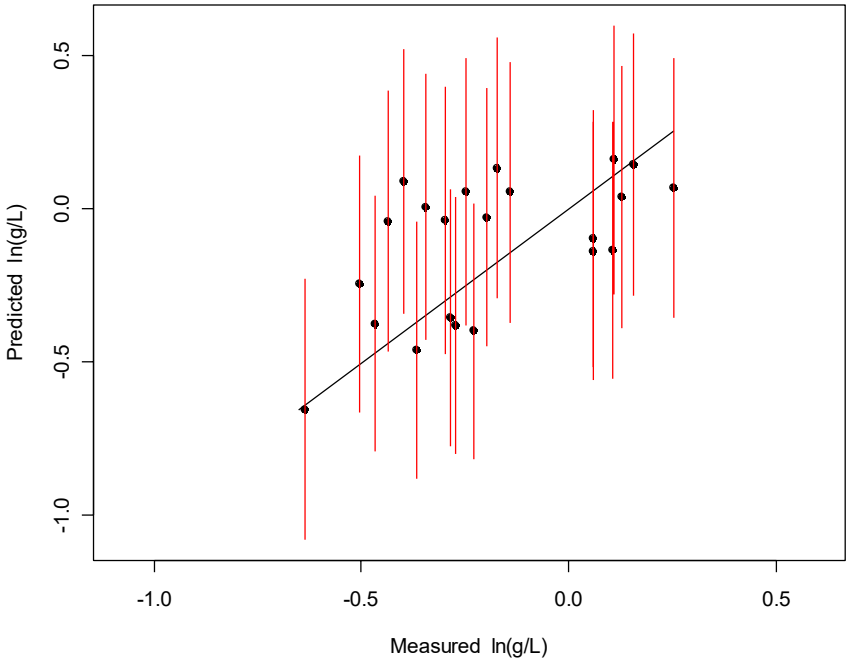


Figure 6.28. Predicted Versus Measured Plot for ILAW PCT-Sodium Reduced LM Model Applied to the 22 Subset V4 Validation Glasses.

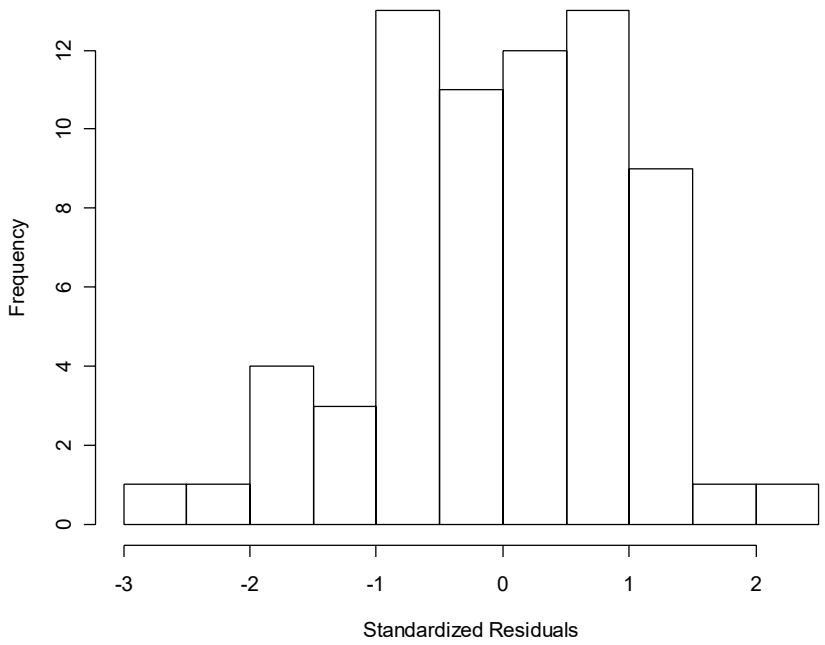


Figure 6.29. Histogram of Standardized Residuals for ILAW PCT-Sodium Reduced PQM Model.

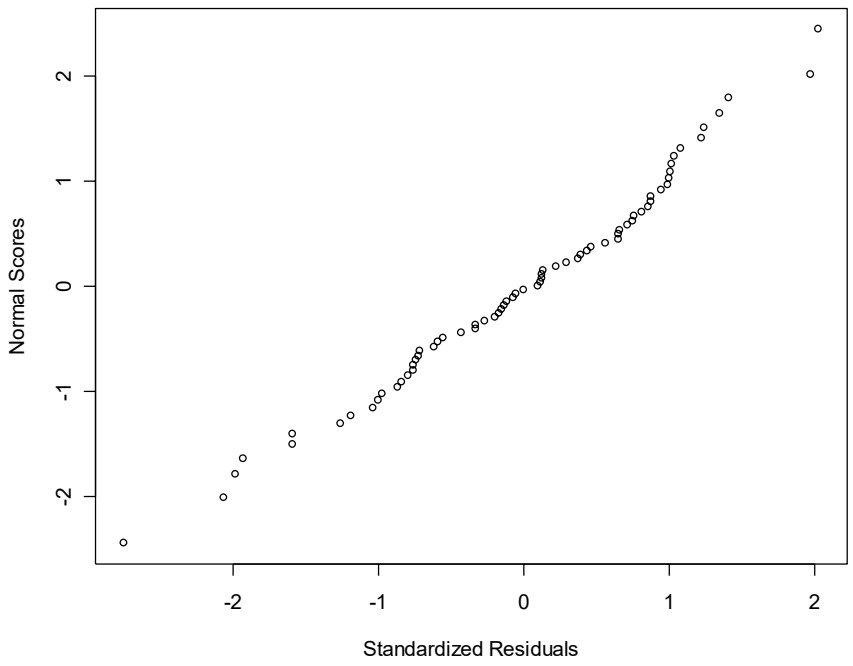


Figure 6.30. Normality Plot Associated with ILAW PCT-Sodium Reduced PQM Model.

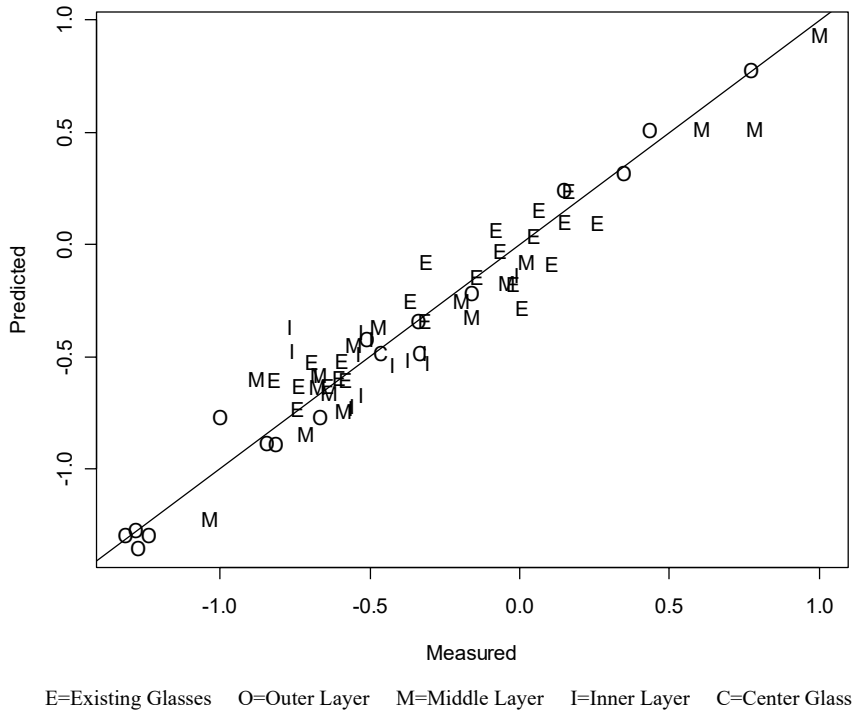


Figure 6.31. Predicted Versus Measured Plot for ILAW PCT-Sodium Reduced PQM Model.

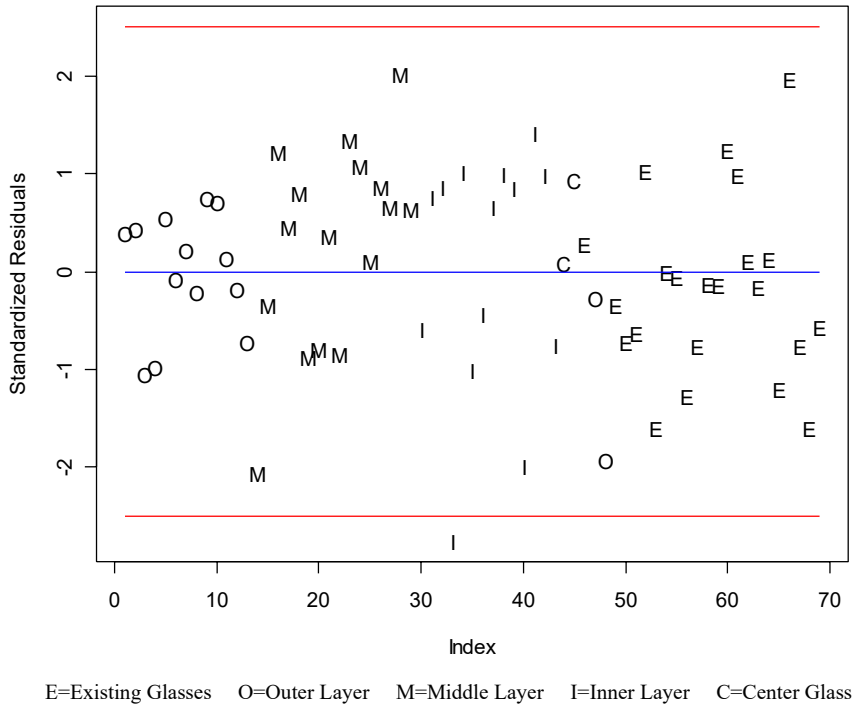


Figure 6.32. Standardized Residuals Plot for ILAW PCT-Sodium Reduced PQM Model.

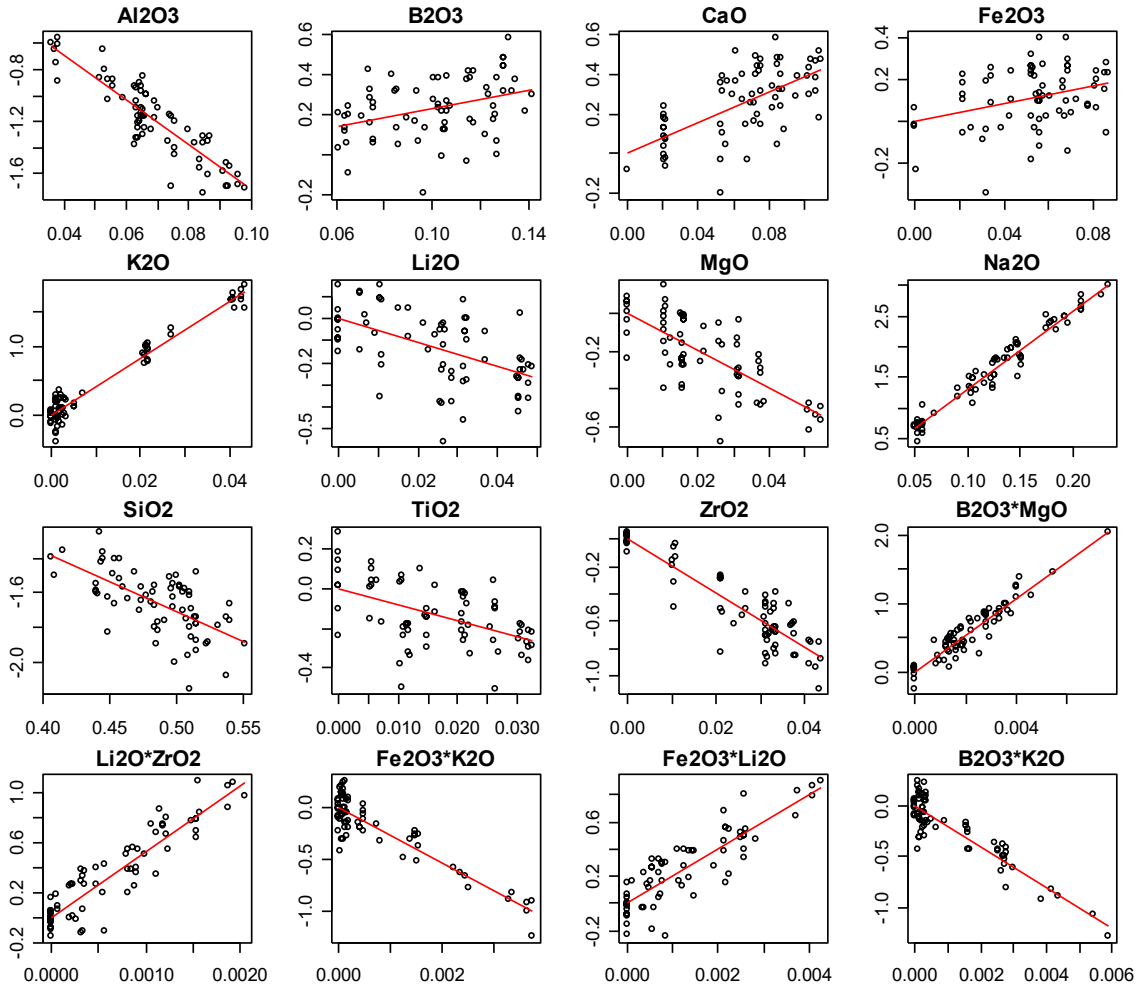


Figure 6.33. Partial Residual Plots for ILAW PCT-Sodium Reduced PQM Model.

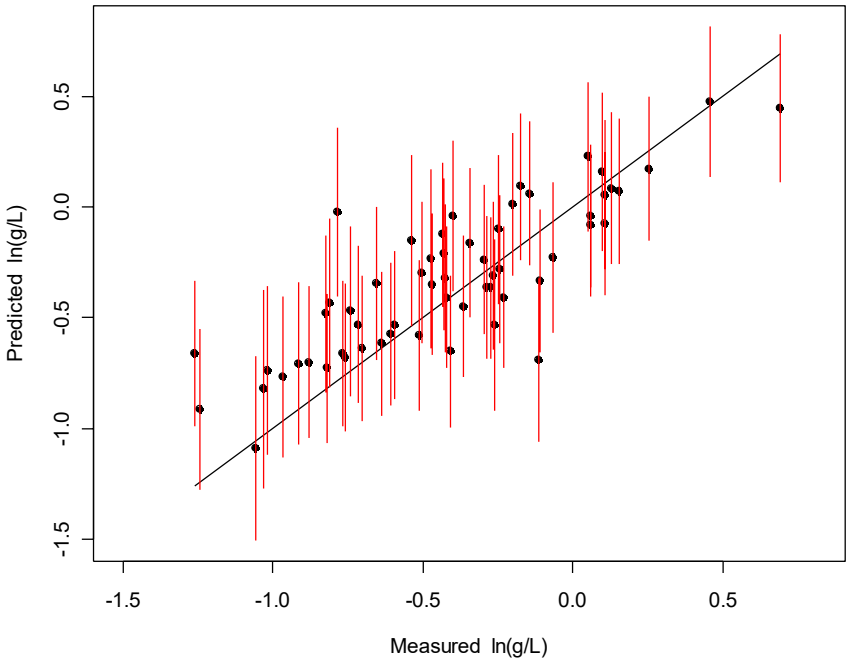


Figure 6.34. Predicted Versus Measured Plot for ILAW PCT-Sodium Reduced PQM Model Applied to All 59 Validation Glasses.

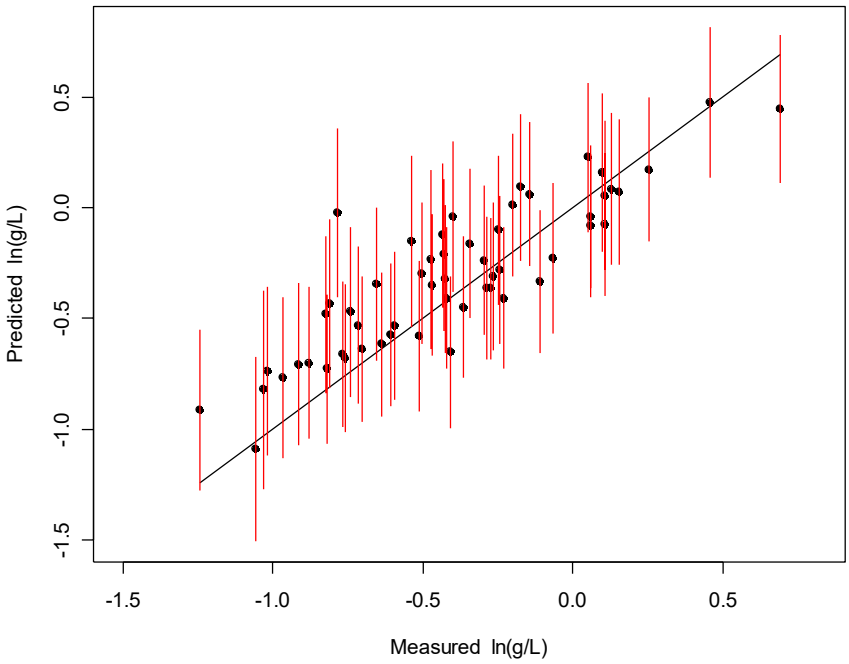


Figure 6.35. Predicted Versus Measured Plot for ILAW PCT-Sodium Reduced PQM Model Applied to the 56 Subset V1 Validation Glasses.

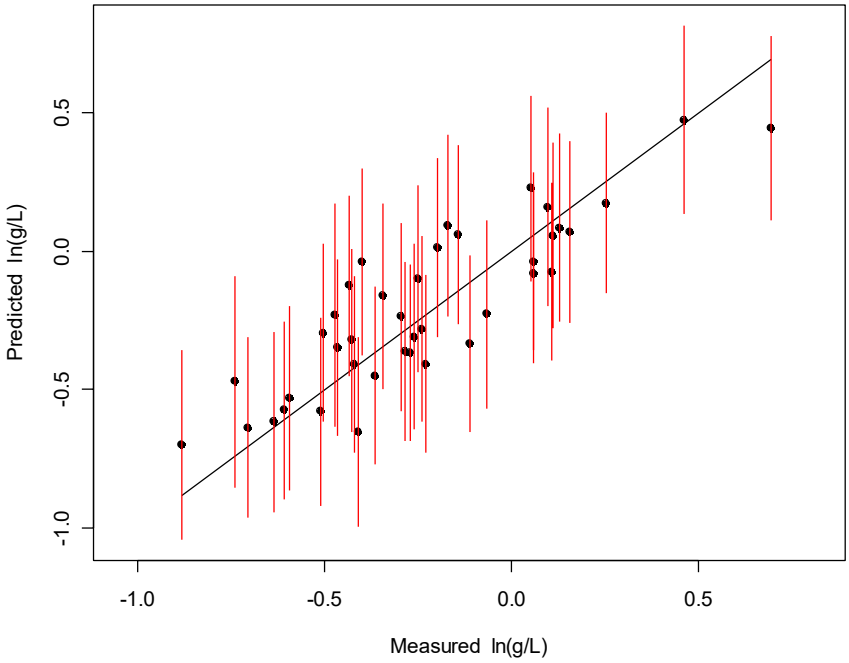


Figure 6.36. Predicted Versus Measured Plot for ILAW PCT-Sodium Reduced PQM Model Applied to the 40 Subset V2 Validation Glasses.

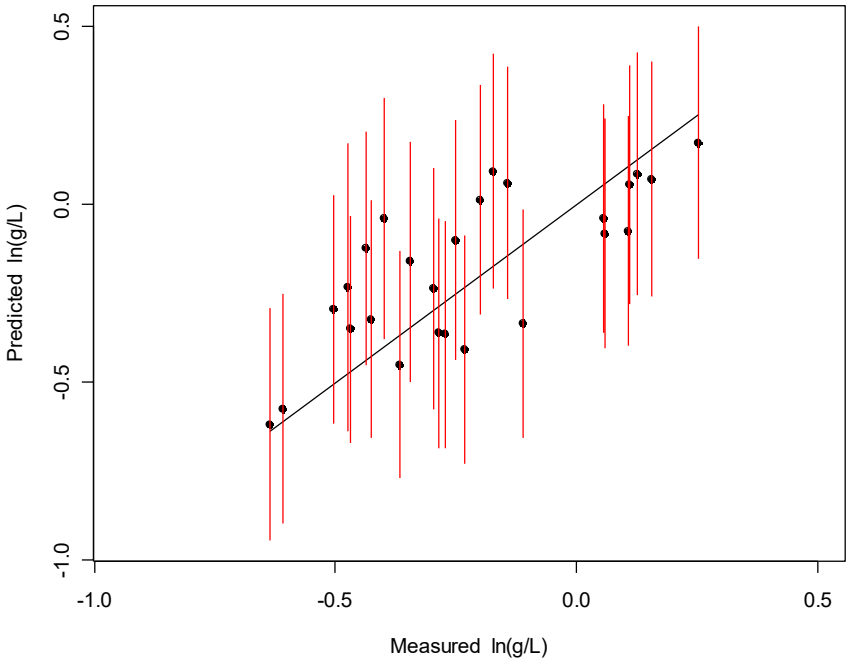


Figure 6.37. Predicted Versus Measured Plot for ILAW PCT-Sodium Reduced PQM Model Applied to the 26 Subset V3 Validation Glasses.

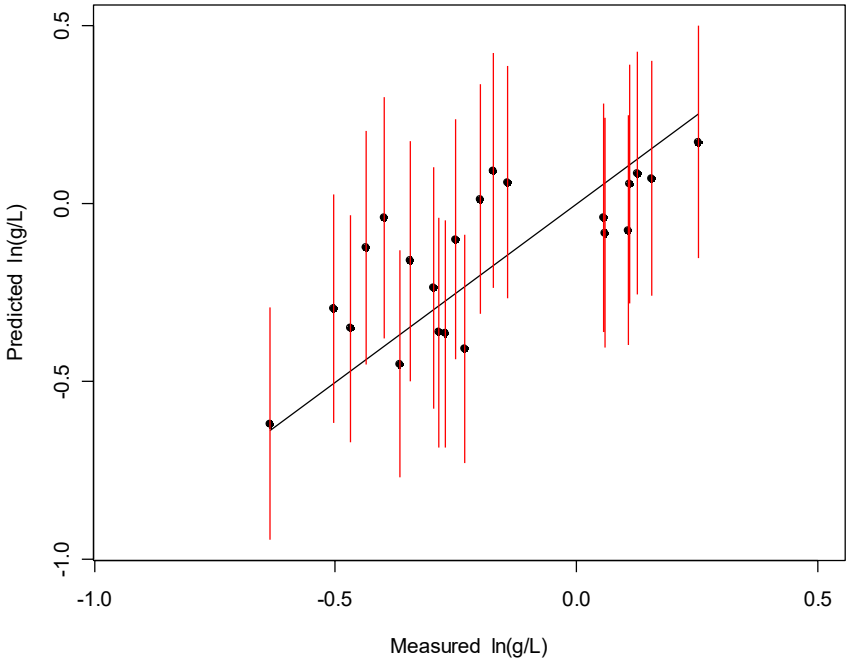


Figure 6.38. Predicted Versus Measured Plot for ILAW PCT-Sodium Reduced PQM Model Applied to the 22 Subset V4 Validation Glasses.

Appendix A

XRF Analysis Results of the Composition of the Test Matrix and Existing Matrix Glasses

Table A.1 XRF Analysis (wt%) of LAWM Test Matrix Glasses with B_2O_3 and Li_2O from DCP.

Oxide	LAWM1	LAWM2	LAWM3	LAWM4	LAWM5	LAWM6	LAWM7	LAWM8
Al_2O_3	8.43	3.32	8.44	3.26	8.52	8.37	5.25	8.71
B_2O_3	6.04	6.01	6.03	13.53	5.95	10.76	6.95	13.65
BaO	<0.01	0.06	<0.01	<0.01	0.04	<0.01	<0.01	0.04
CaO	9.56	9.98	9.95	9.33	5.55	9.36	9.55	6.45
CdO	<0.01	0.02	<0.01	<0.01	<0.01	<0.01	<0.01	0.02
Cl	0.02	0.48	0.02	0.01	0.02	0.03	0.03	0.60
Cr_2O_3	0.18	0.59	0.21	0.24	0.18	0.25	0.24	0.49
Fe_2O_3	8.44	8.93	8.72	6.15	8.20	8.52	8.49	0.45
K_2O	3.90	0.10	0.09	3.92	3.52	3.89	0.10	0.11
Li_2O	4.07	3.92	4.01	4.23	4.06	0.08	1.94	2.16
MgO	<0.01	4.91	5.07	<0.01	<0.01	4.88	4.94	5.15
Na_2O	5.67	4.91	11.44	5.46	5.69	9.60	5.81	5.75
NiO	0.02	0.07	0.03	0.03	0.02	0.04	0.04	0.05
P_2O_5	0.01	0.31	0.04	<0.01	0.02	0.01	0.04	0.37
PbO	<0.01	0.26	<0.01	<0.01	<0.01	0.24	0.24	0.26
SiO_2	45.63	47.86	40.78	41.98	49.19	41.22	52.00	45.51
SO_3	0.52	0.67	0.64	0.56	0.55	0.32	0.72	0.70
TiO_2	3.01	3.28	0.01	3.00	3.11	3.15	2.98	3.24
ZnO	4.70	4.98	1.01	4.72	0.96	0.98	1.00	4.73
ZrO_2	0.04	0.02	4.74	4.44	4.49	0.01	0.03	4.54
Sum[(a)]	100.2	100.7	101.2	100.8	100.1	101.7	100.3	103.0

(a) Sum includes B_2O_3 and Li_2O from DCP.

Table A.1 XRF Analysis (wt%) of LAWM Test Matrix Glasses with B_2O_3 and Li_2O from DCP (continued).

Oxide	LAWM9	LAWM10	LAWM11	LAWM12	LAWM13	LAWM14	LAWM15	LAWM16
Al_2O_3	3.37	8.39	3.25	3.34	3.23	3.34	8.83	7.91
B_2O_3	5.91	12.89	13.14	13.11	6.06	6.11	9.28	11.48
BaO	0.05	0.06	0.04	0.05	0.05	0.05	0.05	<0.01
CaO	9.76	10.12	8.80	0.10	9.69	2.18	0.18	7.48
CdO	0.02	0.01	<0.01	0.01	0.01	<0.01	0.02	<0.01
Cl	0.49	0.51	0.01	0.56	0.27	0.04	0.67	0.02
Cr_2O_3	0.36	0.38	0.26	0.51	0.34	0.17	0.33	0.02
Fe_2O_3	8.42	0.03	5.83	2.80	8.57	0.51	6.24	6.48
K_2O	3.53	0.08	3.86	3.86	3.65	0.10	0.09	0.19
Li_2O	2.44	4.08	4.10	4.27	0.08	1.04	0.07	2.74
MgO	<0.01	<0.01	0.00	1.98	<0.01	4.89	3.68	0.88
Na_2O	5.40	12.61	11.71	14.44	21.36	21.55	22.36	10.16
NiO	0.01	0.01	0.04	0.04	0.03	0.01	0.00	<0.01
P_2O_5	0.53	0.54	<0.01	0.58	0.29	<0.01	0.56	0.03
PbO	0.26	0.26	<0.01	0.26	0.25	<0.01	0.26	<0.01
SiO_2	49.22	40.90	47.17	42.72	40.85	52.33	44.71	44.20
SO_3	0.24	0.23	0.90	0.23	0.50	0.53	0.17	0.33
TiO_2	0.01	3.55	0.03	3.09	3.26	3.14	3.21	2.65
ZnO	5.43	1.15	0.98	4.76	2.18	4.95	0.98	4.70
ZrO_2	5.15	5.50	0.04	4.50	0.03	0.04	0.05	1.12
Sum[(a)]	100.6	101.3	100.2	101.2	100.7	101.0	101.8	100.4

(a) Sum includes B_2O_3 and Li_2O from DCP.

Table A.1 XRF Analysis (wt%) of LAWM Test Matrix Glasses with B_2O_3 and Li_2O from DCP (continued).

Oxide	LAWM17	LAWM18	LAWM19	LAWM20	LAWM21	LAWM22	LAWM23	LAWM24
Al_2O_3	4.68	7.61	7.43	4.91	4.81	7.84	4.67	7.54
B_2O_3	11.79	12.20	12.22	7.03	10.42	7.07	6.84	11.94
BaO	<0.01	0.05	0.05	0.05	<0.01	0.04	0.06	<0.01
CaO	2.21	7.74	7.92	7.90	7.69	2.11	7.72	1.97
CdO	<0.01	0.02	0.02	0.02	<0.01	0.01	0.02	<0.01
Cl	0.02	0.47	0.54	0.43	0.03	0.51	0.50	0.04
Cr_2O_3	0.17	0.58	0.56	0.35	0.16	0.56	0.37	0.18
Fe_2O_3	6.77	7.22	2.65	2.11	6.84	7.34	2.20	6.99
K_2O	1.94	0.19	1.98	1.89	1.83	1.92	1.97	2.00
Li_2O	0.54	2.78	0.58	2.07	2.70	0.56	2.69	0.71
MgO	3.56	1.05	0.93	3.45	0.84	3.51	0.82	0.97
Na_2O	17.95	10.40	13.10	16.59	9.83	16.78	10.31	17.26
NiO	0.02	0.06	0.06	0.01	0.02	0.06	0.01	0.01
P_2O_5	0.03	0.36	0.31	0.63	0.01	0.27	0.53	0.01
PbO	<0.01	0.26	0.26	0.26	<0.01	0.26	0.27	<0.01
SiO_2	42.16	42.72	43.14	43.88	43.20	42.69	48.25	47.32
SO_3	0.20	0.34	0.36	0.21	0.46	0.45	0.34	0.23
TiO_2	0.53	2.58	0.58	0.57	2.64	0.73	2.88	0.54
ZnO	4.59	1.95	4.95	4.87	4.62	4.96	5.52	1.96
ZrO_2	3.83	2.91	4.19	4.16	3.89	4.16	4.58	1.19
Sum[(a)]	101.0	101.5	101.8	101.4	100.0	101.8	100.5	100.8

(a) Sum includes B_2O_3 and Li_2O from DCP.

Table A.1 XRF Analysis (wt%) of LAWM Test Matrix Glasses with B_2O_3 and Li_2O from DCP (continued).

Oxide	LAWM25R1	LAWM26	LAWM27	LAWM28	LAWM29	LAWM30	LAWM31	LAWM32
Al_2O_3	7.64	7.74	7.42	4.97	7.09	7.47	4.77	5.08
B_2O_3	11.98	11.60[(b)]	7.34	11.70	6.95	11.87	6.96	6.98
BaO	0.05	0.05	0.05	<0.01	<0.01	<0.01	0.05	0.05
CaO	2.11	4.96	7.93	7.49	2.09	2.05	7.81	2.07
CdO	0.02	0.02	0.01	<0.01	<0.01	<0.01	0.01	0.03
Cl	0.60	0.65	0.53	0.04	0.07	0.02	0.53	0.62
Cr_2O_3	0.60	0.51	0.55	0.23	0.24	0.20	0.35	0.37
Fe_2O_3	4.50	2.42	7.12	6.99	7.03	7.10	6.78	2.14
K_2O	2.00	0.19	1.98	0.77	1.82	0.19	0.16	1.84
Li_2O	2.75	2.71[$]	0.58	0.75	2.77	2.13	2.78	2.74
MgO	3.41	0.96	3.46	1.06	3.51	0.92	0.93	3.63
Na_2O	10.06	10.64	13.26	10.08	10.78	17.40	16.31	16.47
NiO	0.07	0.05	0.06	0.03	0.03	0.03	0.00	0.01
P_2O_5	0.59	0.37	0.57	0.04	<0.01	0.03	0.55	0.57
PbO	0.26	0.26	0.26	<0.01	<0.01	<0.01	0.26	0.26
SiO_2	50.63	50.72	43.41	50.06	46.95	42.15	43.32	51.18
SO_3	0.26	0.49	0.25	0.36	0.31	0.20	0.30	0.32
TiO_2	0.57	0.55	2.70	2.51	2.50	0.63	2.75	0.56
ZnO	2.08	4.80	3.27	1.94	4.69	4.81	2.01	4.93
ZrO_2	1.15	1.08	1.18	1.18	3.91	4.03	4.20	1.21
Sum[(a)]	101.3	100.8	101.9	100.2	100.7	101.2	100.9	101.1

(a) Sum includes B_2O_3 and Li_2O from DCP
(b) revised from data set transmitted electronically in July 2003

Table A.1 XRF Analysis (wt%) of LAWM Test Matrix Glasses with B_2O_3 and Li_2O from DCP (continued).

Oxide	LAWM33R1	LAWM34	LAWM35	LAWM36	LAWM37	LAWM38	LAWM39	LAWM40
Al_2O_3	4.60	4.71	4.83	7.03	6.28	6.54	6.81	5.66
B_2O_3	11.79	8.16	11.96	11.00	10.53	8.13	9.21	10.49
BaO	<0.01	<0.01	0.05	<0.01	0.04	0.06	0.06	0.04
CaO	7.62	7.67	6.16	6.55	6.67	6.83	4.89	4.92
CdO	<0.01	<0.01	0.02	0.02	<0.01	0.02	0.01	0.00
Cl	0.02	0.02	0.53	0.24	0.02	0.55	0.57	0.20
Cr_2O_3	0.16	0.01	0.30	0.14	0.18	0.61	0.36	0.27
Fe_2O_3	6.95	6.38	4.56	4.87	5.41	3.73	3.14	5.59
K_2O	1.48	1.81	0.17	0.37	0.33	0.23	0.18	0.18
Li_2O	0.85	2.75	0.58	2.26	2.27	2.70	2.23	1.11
MgO	1.00	0.90	3.45	1.49	2.45	1.51	2.51	1.44
Na_2O	17.14	17.25	16.80	12.75	12.70	14.58	14.43	14.11
NiO	0.01	<0.01	0.01	0.00	0.02	0.08	0.00	0.03
P_2O_5	<0.01	<0.01	0.56	0.22	0.02	0.38	0.59	0.11
PbO	<0.01	<0.01	0.26	0.24	<0.01	0.26	0.26	0.25
SiO_2	42.68	42.65	43.38	46.09	45.44	48.12	48.98	47.97
SO_3	0.29	0.30	0.18	0.37	0.32	0.37	0.25	0.31
TiO_2	2.69	1.60	2.63	2.07	1.06	1.07	1.10	1.10
ZnO	1.95	1.96	1.94	3.23	3.33	3.45	3.44	3.43
ZrO_2	1.18	4.10	3.20	2.20	3.40	2.37	2.37	3.55
Sum[(a)]	100.4	100.3	101.6	101.1	100.5	101.6	101.4	100.6

(a) Sum includes B_2O_3 and Li_2O from DCP.

Table A.1 XRF Analysis (wt%) of LAWM Test Matrix Glasses with B_2O_3 and Li_2O from DCP (continued).

Oxide	LAWM41	LAWM42	LAWM43	LAWM44	LAWM45	LAWM46	LAWM47	LAWM48
Al_2O_3	6.71	5.75	6.58	5.92	6.55	5.82	6.28	6.12
B_2O_3	8.05	7.90	8.82	9.88	8.19	10.57	7.70[$]	11.08
BaO	0.06	0.05	0.06	0.04	<0.01	0.04	<0.01	0.06
CaO	7.03	4.89	4.88	6.75	5.42	6.41	6.71	5.13
CdO	0.02	0.01	0.02	<0.01	<0.01	<0.01	<0.01	0.02
Cl	0.57	0.65	0.54	0.02	0.01	0.01	0.03	0.61
Cr_2O_3	0.51	0.52	0.57	0.21	0.18	0.03	0.02	0.35
Fe_2O_3	5.62	4.50	5.71	5.61	5.40	5.30	5.04	5.05
K_2O	0.37	0.19	0.34	0.17	0.47	0.19	0.19	0.17
Li_2O	1.06	2.25	2.35	1.07	1.56	1.07	1.12[$]	1.09
MgO	2.48	1.49	2.49	1.47	1.49	2.40	2.38	1.48
Na_2O	14.71	14.46	12.43	12.23	14.95	12.10	14.01	12.31
NiO	0.05	0.04	0.06	0.03	0.02	<0.01	<0.01	0.00
P_2O_5	0.42	0.55	0.35	0.01	0.02	0.02	0.03	0.57
PbO	0.27	0.26	0.26	<0.01	<0.01	<0.01	<0.01	0.26
SiO_2	44.99	48.34	45.59	48.14	47.81	47.61	48.68	49.08
SO_3	0.34	0.30	0.39	0.29	0.31	0.20	0.31	0.26
TiO_2	1.06	2.01	2.08	2.14	2.11	1.15	1.41	2.17
ZnO	4.56	3.30	4.44	4.41	4.36	3.86	3.37	3.35
ZrO_2	2.71	3.40	3.49	2.33	2.26	3.92	3.43	2.31
Sum[(a)]	101.6	100.9	101.4	100.7	101.1	100.7	100.7	101.4

(a) Sum includes B_2O_3 and Li_2O from DCP.

Table A.1 XRF Analysis (wt%) of LAWM Test Matrix Glasses with B_2O_3 and Li_2O from DCP (continued).

Oxide	LAWM49	LAWM50	LAWM51	LAWM52	LAWM53	LAWM54R1	LAWM55	LAWM56
Al_2O_3	6.80	6.12	5.86	5.73	8.50	3.34	3.33	4.79
B_2O_3	10.94	9.64	9.56	9.71	5.77[$]	5.80	12.80	11.75
BaO	0.06	0.06	0.05	<0.01	0.04	0.06	0.04	0.05
CaO	4.89	5.87	6.02	2.01	9.71	9.51	0.21	5.96
CdO	0.02	0.01	0.01	0.00	<0.01	0.02	0.02	0.02
Cl	0.61	0.32	0.38	0.25	0.01	0.61	0.51	0.54
Cr_2O_3	0.55	0.39	0.42	0.17	0.02	0.58	0.51	0.55
Fe_2O_3	3.60	4.66	4.71	6.14	8.45	8.72	2.80	4.99
K_2O	0.20	0.27	0.30	2.57	4.01	3.87	3.79	0.17
Li_2O	1.06	1.83	1.80	0.03	4.17[$]	2.19	3.95	0.56
MgO	1.47	2.01	1.95	1.44	<0.01	<0.01	1.97	3.46
Na_2O	14.43	13.53	13.36	19.94	5.40	5.66	13.89	17.16
NiO	0.06	0.04	0.06	0.02	<0.01	0.07	0.05	0.05
P_2O_5	0.32	0.19	0.33	0.10	0.02	0.58	0.57	0.17
PbO	0.26	0.25	0.25	0.24	<0.01	0.26	0.26	0.26
SiO_2	48.06	47.51	47.40	43.97	45.02	49.36	43.03	42.69
SO_3	0.35	0.29	0.32	0.18	0.66	0.26	0.24	0.44
TiO_2	1.04	1.62	1.64	2.03	3.31	0.01	3.28	2.68
ZnO	4.39	3.89	3.95	2.92	5.11	4.93	4.79	1.97
ZrO_2	2.38	2.86	2.94	3.54	0.00	4.28	4.54	3.02
Sum[(a)]	101.5	101.4	101.3	101.0	100.2	100.1	100.6	101.3

(a) Sum includes B_2O_3 and Li_2O from DCP.

Table A.2 XRF Analysis (wt%) of Existing Matrix Glasses with B_2O_3 and Li_2O from DCP.

Oxide	LAWA44R10	LAWA53	LAWA56	LAWA88R1	LAWA102R1	LAWA126	LAWA128
Al_2O_3	6.08	6.57	6.47	6.05	5.57	5.58	5.75
B_2O_3	8.55	6.78	11.60	9.53	10.99	9.76	6.85
BaO	<0.01	<0.01	0.90[(b)]	<0.01	<0.01	<0.01	<0.01
CaO	2.03	7.87	1.95	2.00	5.15	2.03	2.13
Cl	0.57	0.47	0.44	0.24	0.21	0.17	0.15
Cr_2O_3	0.14	0.01	0.02	0.01	0.24	0.02	0.03
Cs_2O	<0.01	<0.01	<0.01	<0.01	<0.01	0.16	0.15
Fe_2O_3	7.57	7.93	8.17	5.71	6.71	5.83	6.14
K_2O	0.58	0.56	0.56	2.53	0.32	3.84	3.84
Li_2O	0.03	0.04	0.02	0.04	2.60	0.03	0.04
MgO	1.89	1.38	1.41	1.40	1.36	1.39	1.06
Na_2O	19.13	18.85	19.07	19.42	13.01	17.71	18.35
NiO	0.01	<0.01	<0.01	<0.01	0.04	<0.01	<0.01
P_2O_5	0.04	0.08	0.05	0.10	0.16	0.10	0.09
PbO	<0.01	0.24	<0.01	<0.01	<0.01	<0.01	<0.01
Re_2O_7	0.07	0.03	0.03	0.05	0.04	0.06	0.06
SeO_2	0.00	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
SiO_2	45.31	42.66	41.09	45.41	46.63	45.29	46.51
SO_3	0.09	0.62	0.52	0.19	0.67	0.31	0.30
TiO_2	2.08	1.23	1.21	2.04	1.30	2.05	2.18
ZnO	2.89	3.07	3.10	2.78	3.27	2.87	3.09
ZrO_2	3.37	3.43	3.48	3.13	3.77	3.42	3.62
Sum[(a)]	100.43	101.8	100.1	100.6	102.0	100.6	100.3

(a) Sum includes B_2O_3 and Li_2O from DCP.
(b) this was identified as a contamination during melting.

Table A.2 XRF Analysis (wt%) of Existing Matrix Glasses with B_2O_3 and Li_2O from DCP (continued).

Oxide	LAWA130	LAWB65	LAWB66	LAWB68	LAWB78	LAWB79	LAWB80
Al_2O_3	5.90	6.27	6.24	6.09	5.68	5.82	6.15
B_2O_3	8.44	9.70	9.61	7.59	11.78	11.63	11.73
BaO	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
CaO	2.22	6.54	8.00	8.28	7.31	7.34	7.29
Cl	0.17	0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Cr_2O_3	0.02	0.09	0.10	0.09	0.23	0.23	0.05
Cs2O	0.19	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Fe_2O_3	3.29	5.32	5.40	5.68	3.96	3.92	3.44
K_2O	3.64	0.36	0.35	0.36	0.28	0.29	1.89
Li_2O	0.03	3.83	3.93	3.65	2.85	3.24	3.23
MgO	0.98	2.89	3.02	2.81	2.79	2.92	2.82
Na_2O	16.65	5.86	5.63	5.32	10.08	8.75	6.25
NiO	<0.01	<0.01	<0.01	<0.01	0.03	0.03	<0.01
P_2O_5	0.11	0.02	0.02	0.06	0.05	0.05	0.06
PbO	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Re_2O_7	0.07	0.04	0.04	0.04	0.06	0.05	0.05
SeO_2	<0.01	0.00	0.00	<0.01	<0.01	<0.01	<0.01
SiO_2	47.54	49.45	49.62	49.02	47.15	48.55	49.36
SO_3	0.33	0.89	0.65	0.83	0.51	0.58	0.58
TiO_2	2.27	1.45	1.44	1.50	0.01	0.01	0.02
ZnO	4.36	4.33	2.97	4.67	4.10	4.15	4.00
ZrO_2	3.92	3.45	3.43	3.65	3.60	2.70	3.36
Sum[(a)]	100.1	100.5	100.4	99.6	100.5	100.2	100.3

(a) Sum includes B_2O_3 and Li_2O from DCP.

Table A.2 XRF Analysis (wt%) of Existing Matrix Glasses with B_2O_3 and Li_2O from DCP (continued).

Oxide	LAWB83	LAWB84	LAWB85	LAWB86	C100-G-136B	LAWC27	LAWC32
Al_2O_3	5.82	5.96	5.98	6.37	6.05	6.18	6.24
B_2O_3	9.78	9.63	10.66	11.89	10.96	11.37	9.67
BaO	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
CaO	6.95	6.57	5.39	5.61	6.06	8.46	9.07
Cl	<0.01	<0.01	0.00	0.01	0.06	0.09	0.07
Cr_2O_3	0.04	0.04	0.04	0.04	0.10	0.02	0.02
Cs2O	<0.01	<0.01	<0.01	<0.01	0.18	<0.01	<0.01
Fe_2O_3	5.70	5.41	5.62	5.26	6.65	0.08	2.62
K_2O	0.27	0.25	0.26	0.29	0.26	0.23	0.21
Li_2O	3.81	3.91	3.82	3.88	2.81	2.53	2.54
MgO	2.90	3.01	2.93	2.92	1.54	1.38	1.31
Na_2O	5.76	6.18	5.50	6.28	12.75	11.60	11.55
NiO	<0.01	<0.01	<0.01	<0.01	0.01	<0.01	<0.01
P_2O_5	0.05	0.06	0.10	0.07	0.18	0.12	0.14
PbO	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Re_2O_7	0.06	0.05	0.06	0.06	<0.01	0.07	0.04
SeO_2	0.00	0.00	0.00	0.00	<0.01	<0.01	<0.01
SiO_2	48.37	49.06	48.84	49.24	46.32	49.88	47.82
SO_3	0.49	0.44	0.49	0.43	0.42	0.41	0.38
TiO_2	1.57	1.48	1.55	0.03	1.33	1.19	1.19
ZnO	4.96	4.67	4.87	4.50	2.99	2.87	3.98
ZrO_2	3.85	3.53	3.75	3.40	3.25	3.48	3.58
Sum[(a)]	100.4	100.3	99.8	100.3	101.9	100.0	100.4

(a) Sum includes B_2O_3 and Li_2O from DCP.

Appendix B

DCP Analysis Results of the Composition of the Test Matrix and Existing Matrix Glasses

Table B.1. DCP and IC Analysis (wt%) of Test Matrix Glasses.

Oxide	LAWM1	LAWM2	LAWM3	LAWM4	LAWM5	LAWM6	LAWM7	LAWM8
Al_2O_3	8.54	3.42	8.12	3.53	8.28	7.99	4.98	8.15
B_2O_3	6.04	6.01	6.03	13.53	5.95	10.76	6.95	13.65
BaO	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.01
CaO	8.86	8.72	9.31	8.57	5.44	8.66	8.69	6.14
CdO	NA	0.02	NA	0.00	0.00	0.00	0.01	0.02
Cr_2O_3	0.20	0.55	0.21	0.25	0.16	0.25	0.26	0.33
Fe_2O_3	8.00	8.24	8.12	6.21	7.95	8.37	8.53	0.62
K_2O	3.62	0.04	0.03	3.69	3.26	3.66	0.04	0.04
Li_2O	4.07	3.92	4.01	4.23	4.06	0.08	1.94	2.16
MgO	0.04	4.44	4.41	0.03	0.02	4.46	4.48	4.61
Na_2O	4.62	4.50	10.25	4.75	4.63	7.77	4.70	4.76
NiO	0.09	0.15	0.11	0.10	0.09	0.12	0.12	0.12
P_2O_5	0.07	0.36	0.00	0.25	0.24	0.06	0.14	0.41
PbO	NA	0.05	NA	0.03	0.02	0.02	0.02	0.06
SiO_2	43.14	44.72	40.24	40.40	47.83	39.11	49.11	41.63
SO_3[(a)]	0.63	0.71	0.91	0.69	0.84	0.30	0.73	0.46
TiO_2	2.66	2.79	0.03	2.77	2.98	2.90	2.69	3.06
ZnO	4.72	4.50	0.99	4.71	1.02	0.93	0.96	4.68
ZrO_2	0.05	0.02	3.89	3.87	4.09	0.02	0.03	3.94
Sum	95.4	93.1	96.7	97.6	96.9	95.5	94.4	94.9

(a) Ion Chromatography measurement

Table B.1. DCP and IC Analysis (wt%) of Test Matrix Glasses (continued).

Oxide	LAWM9	LAWM10	LAWM11	LAWM12	LAWM13	LAWM14	LAWM15	LAWM16
Al_2O_3	3.36	8.38	3.43	3.54	3.49	3.42	8.45	7.38
B_2O_3	5.91	12.89	13.14	13.11	6.06	6.11	9.28	11.48
BaO	0.01	0.01	0.00	0.02	0.01	0.00	0.01	0.00
CaO	9.34	9.51	8.97	0.07	8.85	1.91	0.18	7.21
CdO	0.01	0.01	0.00	NA	0.01	NA	0.02	0.00
Cr_2O_3	0.31	0.33	0.28	0.47	0.32	0.19	0.30	0.02
Fe_2O_3	7.45	0.05	5.84	2.69	8.05	0.78	5.56	6.04
K_2O	3.03	0.03	3.64	3.77	3.48	0.03	0.04	0.14
Li_2O	2.44	4.08	4.10	4.27	0.08	1.04	0.07	2.74
MgO	0.02	0.02	0.05	1.80	0.04	4.31	3.21	0.98
Na_2O	4.46	11.45	10.49	11.84	18.82	19.46	18.64	9.14
NiO	0.03	0.04	0.12	0.11	0.09	0.09	0.02	0.01
P_2O_5	0.58	0.60	0.24	0.50	0.37	0.18	0.56	0.23
PbO	0.04	0.06	0.02	NA	0.03	NA	0.04	0.02
SiO_2	48.24	37.96	46.38	39.58	38.39	49.01	43.84	41.01
SO_3[(a)]	0.49	0.15	1.01	NA	0.48	0.76	0.06	0.41
TiO_2	0.02	3.06	0.03	2.80	2.84	2.67	2.89	2.45
ZnO	4.88	1.00	0.99	4.43	1.95	4.69	0.98	4.72
ZrO_2	4.17	4.12	0.04	3.97	0.03	0.04	0.05	1.09
Sum	94.8	93.8	98.8	93.1	93.4	94.7	94.2	95.1

(a) Ion Chromatography measurement
NA – Not Analyzed

Table B.1. DCP and IC Analysis (wt%) of Test Matrix Glasses (continued).

Oxide	LAWM17	LAWM18	LAWM19	LAWM20	LAWM21	LAWM22	LAWM23	LAWM24
Al_2O_3	4.43	7.05	7.12	4.65	4.67	7.49	4.64	6.93
B_2O_3	11.79	12.20	12.22	7.03	10.42	7.07	6.84	11.94
BaO	0.01	0.01	0.02	0.02	0.00	0.01	0.02	0.00
CaO	2.00	7.31	7.36	7.03	7.56	2.38	7.09	1.76
CdO	0.00	0.01	0.02	NA	0.00	0.01	0.02	0.00
Cr_2O_3	0.16	0.54	0.50	0.34	0.17	0.48	0.33	0.18
Fe_2O_3	6.47	7.13	2.69	1.96	6.56	6.60	1.90	6.51
K_2O	1.79	0.14	1.73	2.10	1.60	1.72	1.71	1.81
Li_2O	0.54	2.78	0.58	2.07	2.70	0.56	2.69	0.71
MgO	3.07	1.05	1.03	3.01	0.98	3.04	1.00	1.02
Na_2O	14.02	8.31	11.21	14.68	8.97	13.93	8.43	14.03
NiO	0.07	0.13	0.15	0.04	0.08	0.13	0.05	0.07
P_2O_5	0.10	0.52	0.45	0.56	0.17	0.37	0.51	0.18
PbO	0.02	0.06	0.05	NA	0.02	0.05	0.06	0.01
SiO_2	38.69	39.58	40.35	41.73	41.27	38.72	45.04	43.33
SO_3[(a)]	0.17	0.23	0.23	NA	0.35	0.43	0.36	0.15
TiO_2	0.51	2.36	0.55	0.57	2.47	0.69	2.42	0.52
ZnO	4.48	1.82	4.59	4.92	4.97	4.43	4.63	1.76
ZrO_2	3.20	2.39	3.36	3.30	3.54	3.21	3.55	1.02
Sum	91.5	93.6	94.2	94.0	96.5	91.3	91.3	91.9

(a) Ion Chromatography measurement
NA – Not Analyzed

Table B.1. DCP and IC Analysis (wt%) of Test Matrix Glasses (continued).

Oxide	LAWM25R1	LAWM26	LAWM27	LAWM28	LAWM29	LAWM30	LAWM31	LAWM32
Al_2O_3	7.48	7.11	7.05	4.65	7.14	7.39	4.77	4.77
B_2O_3	11.98	11.60	7.34	11.70	6.95	11.87	6.96	6.98
BaO	0.01	0.01	0.01	0.00	0.00	0.01	0.02	0.01
CaO	1.84	4.44	7.59	7.04	2.01	1.84	7.38	1.77
CdO	0.02	NA	0.01	0.00	0.00	0.00	0.01	NA
Cr_2O_3	0.56	0.44	0.50	0.23	0.23	0.23	0.32	0.33
Fe_2O_3	4.22	2.37	6.86	6.71	6.87	6.70	6.01	1.75
K_2O	1.79	0.13	1.82	0.72	1.67	0.14	0.11	1.65
Li_2O	2.75	2.71	0.58	0.75	2.77	2.13	2.78	2.74
MgO	2.99	0.99	3.20	0.99	3.09	1.04	1.04	3.05
Na_2O	9.13	8.41	10.94	8.24	9.08	14.29	14.29	13.89
NiO	0.15	0.12	0.12	0.11	0.10	0.11	0.05	0.04
P_2O_5	0.60	0.34	0.49	0.21	0.15	0.04	0.34	0.49
PbO	0.04	NA	0.05	0.02	0.01	0.02	0.06	NA
SiO_2	48.66	46.82	38.72	45.02	45.75	38.98	39.61	47.72
SO_3[(a)]	0.40	0.25	0.41	0.18	0.69	0.13	0.40	0.31
TiO_2	0.56	0.52	2.40	2.21	2.44	0.60	2.46	0.52
ZnO	1.95	4.48	2.94	1.80	4.96	4.43	1.85	4.59
ZrO_2	1.03	0.95	1.03	1.02	3.66	3.28	3.55	1.04
Sum	96.2	91.7	92.1	91.6	97.6	93.2	92.0	91.7

(a) Ion Chromatography measurement;
NA – Not Analyzed

Table B.1. DCP and IC Analysis (wt%) of Test Matrix Glasses (continued).

Oxide	LAWM33R1	LAWM34	LAWM35	LAWM36	LAWM37	LAWM38	LAWM39	LAWM40
Al_2O_3	4.79	4.66	4.71	6.57	5.99	6.56	6.43	5.41
B_2O_3	11.79	8.16	11.96	11.00	10.53	8.13	9.21	10.49
BaO	0.00	0.00	0.01	0.01	0.00	0.02	0.02	0.01
CaO	7.23	7.43	5.78	6.35	6.13	6.66	4.58	4.40
CdO	0.00	0.00	0.01	0.01	0.00	0.01	0.01	NA
Cr_2O_3	0.15	0.02	0.26	0.14	0.15	0.54	0.32	0.28
Fe_2O_3	6.39	5.78	4.00	4.63	5.08	3.63	2.84	5.20
K_2O	1.38	1.61	0.12	0.33	0.28	0.18	0.12	0.12
Li_2O	0.85	2.75	0.58	2.26	2.27	2.70	2.23	1.11
MgO	0.88	1.06	3.21	1.53	2.20	1.50	2.31	1.50
Na_2O	14.50	14.49	14.37	10.29	9.91	12.79	11.86	11.80
NiO	0.07	0.01	0.04	0.03	0.07	0.15	0.04	0.11
P_2O_5	0.15	0.00	0.49	0.31	0.08	0.49	0.38	0.14
PbO	0.02	0.02	0.06	0.03	0.02	0.05	0.06	NA
SiO_2	41.50	38.46	39.51	42.21	41.01	47.48	44.72	45.07
SO_3[(a)]	0.25	0.30	0.05	0.33	0.23	0.56	0.37	0.23
TiO_2	2.41	1.57	2.47	1.99	0.98	1.02	1.04	1.03
ZnO	1.90	1.84	1.75	3.24	3.08	3.46	3.23	3.18
ZrO_2	0.98	3.56	2.65	2.06	2.69	2.02	2.03	2.85
Sum	95.2	91.7	92.0	93.3	90.7	98.0	91.8	92.9

(a) Ion Chromatography measurement
NA – Not Analyzed

Table B.1. DCP and IC Analysis (wt%) of Test Matrix Glasses (continued).

Oxide	LAWM41	LAWM42	LAWM43	LAWM44	LAWM45	LAWM46	LAWM47	LAWM48
Al_2O_3	6.68	5.38	6.41	5.67	6.23	5.45	5.78	5.83
B_2O_3	8.05	7.90	8.82	9.88	8.19	10.57	7.70	11.08
BaO	0.02	0.01	0.02	0.00	0.00	0.00	0.00	0.02
CaO	6.72	4.38	4.52	6.25	5.17	5.84	6.17	4.81
CdO	0.01	0.02	0.02	0.01	0.01	0.00	NA	0.02
Cr_2O_3	0.47	0.45	0.51	0.23	0.17	0.03	0.02	0.32
Fe_2O_3	5.34	4.24	5.51	5.37	5.28	4.64	4.62	4.77
K_2O	0.31	0.14	0.29	0.11	0.44	0.13	0.12	0.11
Li_2O	1.06	2.25	2.35	1.07	1.56	1.07	1.12	1.09
MgO	2.22	1.47	2.28	1.47	1.56	2.22	2.19	1.52
Na_2O	12.48	11.40	10.03	9.93	11.93	9.76	12.10	9.85
NiO	0.11	0.09	0.12	0.11	0.08	0.01	0.02	0.05
P_2O_5	0.54	0.56	0.32	0.00	0.05	0.10	0.02	0.50
PbO	0.05	0.05	0.06	0.02	0.03	0.02	NA	0.05
SiO_2	43.04	43.85	42.27	44.50	45.73	42.79	45.83	44.54
SO_3[(a)]	0.63	0.22	0.41	0.20	0.30	0.16	0.15	0.11
TiO_2	1.00	1.85	1.83	1.92	1.92	1.05	1.38	2.15
ZnO	4.51	3.07	4.16	4.14	4.26	3.15	3.21	3.25
ZrO_2	2.24	2.78	2.85	1.90	1.91	3.05	2.85	2.10
Sum	95.5	90.1	92.8	92.8	94.8	90.0	93.3	92.2

(a) Ion Chromatography measurement
NA – Not Analyzed

Table B.1. DCP and IC Analysis (wt%) of Test Matrix Glasses (continued).

Oxide	LAWM49	LAWM50	LAWM51	LAWM52	LAWM53	LAWM54R1	LAWM55	LAWM56
Al_2O_3	6.29	5.92	5.57	5.69	8.11	3.46	3.38	4.70
B_2O_3	10.94	9.64	9.56	9.71	5.77	5.80	12.80	11.75
BaO	0.01	0.02	0.01	0.01	0.00	0.02	0.01	0.01
CaO	4.46	5.49	5.45	1.86	8.32	8.78	0.16	5.60
CdO	0.02	0.02	0.01	0.00	NA	0.01	0.01	0.01
Cr_2O_3	0.50	0.39	0.41	0.16	0.02	0.56	0.45	0.50
Fe_2O_3	3.58	4.58	4.50	5.60	7.31	8.16	2.67	4.65
K_2O	0.14	0.22	0.24	2.28	3.66	3.66	3.37	0.12
Li_2O	1.06	1.83	1.80	0.03	4.17	2.19	3.95	0.56
MgO	1.51	1.87	1.76	1.47	0.02	0.02	1.95	2.99
Na_2O	11.98	11.41	11.18	17.48	4.73	4.78	12.49	14.63
NiO	0.14	0.11	0.15	0.08	0.02	0.17	0.12	0.12
P_2O_5	0.28	0.20	0.25	0.31	0.08	0.56	0.65	0.29
PbO	0.06	0.06	0.06	0.01	NA	0.05	0.04	0.04
SiO_2	42.55	43.71	43.47	42.64	43.27	48.34	40.69	41.81
SO_3[(a)]	0.20	0.15	0.18	0.14	0.58	0.53	0.44	0.52
TiO_2	0.98	1.60	1.58	1.97	2.84	0.01	3.01	2.44
ZnO	4.08	3.70	3.79	2.83	4.61	4.90	4.61	1.94
ZrO_2	1.92	2.38	2.31	2.94	0.02	3.58	3.92	2.52
Sum	90.7	93.3	92.3	95.2	93.5	95.6	94.7	95.2

(a) Ion Chromatography measurement
NA – Not Analyzed

Table B.2 DCP Analysis (wt%) of Existing Matrix Glasses.

Oxide	LAWA44R10M1	LAWA53M1	LAWA56M1	LAWA88R1M1	LAWA102R1M1	LAWA126M1	LAWA128M1
Al_2O_3	5.65	6.78	6.83	5.67	6.41	5.47	5.70
B_2O_3	8.55	6.78	11.60	9.53	10.99	9.76	6.85
BaO	0.00	0.00	0.62	0.00	0.01	0.00	0.01
CaO	1.79	8.70	2.03	1.90	5.42	1.92	1.96
Cr_2O_3	0.18	0.01	0.02	0.12	0.22	0.02	0.03
Fe_2O_3	6.85	8.09	7.91	5.41	6.51	5.41	5.35
K_2O	0.62	0.57	0.56	2.38	0.28	3.69	3.63
Li_2O	0.03	0.04	0.02	0.04	2.60	0.03	0.04
MgO	1.88	1.61	1.54	1.54	1.65	1.56	1.26
Na_2O	17.86	17.22	16.77	17.76	12.06	16.21	16.71
NiO	0.08	0.01	0.01	0.06	0.11	0.01	0.01
P_2O_5	0.13	0.12	0.09	0.18	0.17	0.12	0.11
SiO_2	42.95	39.68	38.91	42.30	43.75	42.15	44.01
TiO_2	2.02	1.31	1.26	1.91	1.37	1.90	1.96
ZnO	2.72	3.02	2.90	2.71	3.07	2.80	2.93
ZrO_2	2.87	3.07	3.05	2.93	3.39	2.97	3.09
Sum	94.2	97.1	94.2	94.5	98.0	94.1	93.7

Table B.2 DCP Analysis (wt%) of Existing Matrix Glasses (continued).

Oxide	LAWA130M1	LAWB65M1	LAWB66M1	LAWB68M1	LAWB78M1	LAWB79M1	LAWB80M1
Al_2O_3	5.65	5.77	5.84	5.42	5.68	5.68	5.83
B_2O_3	8.44	9.70	9.61	7.59	11.78	11.63	11.73
BaO	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CaO	1.87	6.26	7.65	7.15	6.74	6.58	6.78
Cr_2O_3	0.02	0.09	0.10	0.09	0.22	0.22	0.05
Fe_2O_3	2.57	4.72	4.81	4.42	3.49	3.58	2.83
K_2O	3.23	0.29	0.29	0.29	0.24	0.24	1.67
Li_2O	0.03	3.83	3.93	3.65	2.85	3.24	3.23
MgO	1.18	2.58	2.60	2.39	2.58	2.51	2.58
MnO_2	0.01	0.01	0.01	0.02	0.03	0.03	0.01
Na_2O	16.4	4.93	5.01	4.66	8.21	8.04	5.71
NiO	0.01	0.01	0.01	0.01	0.11	0.10	0.01
P_2O_5	0.12	0.06	0.14	0.18	0.05	0.05	0.22
SiO_2	42.94	45.87	46.08	46.28	43.80	44.64	46.84
SrO	0	0.01	0.01	0.01	0.01	0.01	0.01
TiO_2	2.14	1.40	1.43	1.42	0.02	0.03	0.03
ZnO	3.92	4.22	2.96	4.33	3.68	3.64	3.69
ZrO_2	3.05	3.10	3.10	2.88	3.08	3.02	3.04
Sum	91.6	92.9	93.6	90.8	92.6	93.2	94.3

Table B.2 DCP Analysis (wt%) of Existing Matrix Glasses (continued).

Oxide	LAWB83M1	LAWB84M1	LAWB85M1	LAWB86M1	C100-G-136BM1	LAWC27M1	LAWC32M1
Al_2O_3	5.48	5.61	5.63	5.73	6.62	5.81	6.12
B_2O_3	9.78	9.63	10.66	11.89	10.96	11.37	9.67
BaO	0.01	0.00	0.00	0.00	0.01	0.00	0.00
CaO	5.96	6.13	4.73	5.23	6.39	7.94	7.79
Cr_2O_3	0.04	0.04	0.03	0.04	0.10	0.02	0.02
Fe_2O_3	4.93	4.69	4.59	4.84	6.70	0.14	2.09
K_2O	0.18	0.18	0.20	0.22	0.21	0.17	0.16
Li_2O	3.81	3.91	3.82	3.88	2.81	2.53	2.54
MgO	2.63	2.64	2.53	2.59	1.68	1.52	1.53
MnO_2	0.02	0.02	0.02	0.01	0.04	0.01	0.01
Na_2O	4.89	4.89	4.93	5.04	10.95	10.21	10.14
NiO	0.01	0.01	0.01	0.01	0.06	0.01	0.01
P_2O_5	0.17	0.18	0.03	0.05	0.20	0.12	0.14
SiO_2	45.60	45.01	45.06	45.25	42.95	46.23	44.65
SrO	0.00	0.00	0.00	0.01	0.00	0.00	0.01
TiO_2	1.39	1.40	1.44	0.04	1.40	1.16	1.14
ZnO	4.45	4.40	4.38	4.47	2.96	2.77	3.74
ZrO_2	2.97	3.06	2.97	3.05	2.98	2.86	2.92
Sum	92.3	91.8	91.0	92.3	97.0	92.9	92.7

Appendix C

Statistical Methods Used to Develop, Evaluate, and Validate Property-Composition Models

Appendix C

Statistical Methods Used to Develop, Evaluate, and Validate Property-Composition Models

This appendix presents various statistical methods used for developing, evaluating, and validating waste glass property-composition models. Section C.1 discusses mixture experiments, introduces two general forms of mixture experiment models, and two variants of one of the model forms appropriate for assessing the presence of "block effects". Section C.2 discusses the least squares regression methods used to fit models to data and corresponding assumptions. Section C.3 discusses the statistical methods and summary statistics used for model evaluation based on the data used to fit a model. Section C.4 discusses statistical methods for model augmentation (i.e., adding terms to a model) and model reduction (i.e., removing unneeded terms from a model). Section C.5 discusses the statistical methods and summary statistics used for model validation based on data not used to fit a model. Section C.6 discusses several statistical intervals used to assess uncertainties in model predictions.

C.1 Mixture Experiments, Model Forms, and Assessing Block Effects

A *mixture experiment* involves mixing two or more components in various proportions, and then measuring one or more responses variables for the resulting end-product mixtures. If the proportions of q mixture components are denoted x_i, $i = 1, 2, \ldots, q$, then these proportions are subject to the basic "mixture constraints"

$$0 \le x_i \le 1 \quad and \quad \sum_{i=1}^{q} x_i = 1. \tag{C.1}$$

Often in practice, the component proportions will be subject to additional single-component constraints

$$0 \le L_i \le x_i \le U_i \le 1 \tag{C.2}$$

and/or multiple-component constraints that can be written in the general form

$$\sum_{i=1}^{q} A_{ki} x_i + A_{k0} \ge 0, \quad k = 1, 2, \ldots, K. \tag{C.3}$$

In Equation (C.2) L_i and U_i denote, respectively, the lower and upper constraints on the i^{th} component ($i = 1, 2, \ldots, q$). In Equation (C.3), the A_{ki} ($i = 1, 2, \ldots, q$) and A_{k0} denote the coefficients of the k^{th} multiple-component constraint. Cornell (2002) provides a comprehensive discussion of statistical methods for the design, modeling, and data analysis of mixture experiments.

Section C.1.1 introduces the linear mixture (LM) model and partial quadratic mixture (PQM) model forms for mixture experiment data. Section C.1.2 discusses two variations of the LM model that can be used to assess modeling data collected in two or more blocks (e.g., at different times or under different conditions) for "block effects".

C.1.1 Linear and Partial Quadratic Mixture Model Forms

The LM model form is given by

$$f(y) = \sum_{i=1}^{q} b_i x_i + \varepsilon \tag{C.4}$$

while the PQM model form is given by

$$f(y) = \sum_{i=1}^{q} b_i x_i + \text{Selected}\left\{ \sum_{i=1}^{q} b_{ii} x_i^2 + \sum_{i<j}^{q-1} \sum^{q} b_{ij} x_i x_j \right\} + \varepsilon \ . \tag{C.5}$$

In Equations (C.4) and (C.5), y is a property or response variable that can be measured for each end-product mixture; $f(y)$ is some mathematical transformation of y (which could be the identity transformation); the x_i (i = 1, 2, …, q) are proportions of q components subject to the constraints in Equation (C.1) and possibly constraints of the forms in Equations (C.2) and/or (C.3); the b_i (i = 1, 2, …, q), the b_{ii} (selected), and the b_{ij} (selected) are coefficients to be estimated from data; and ε is a random error for each data point. Many statistical methods exist for the case where the ε are independent (i.e., not correlated) and normally distributed with mean 0 and standard deviation σ. In Equation (C.5), "Selected" means that only some of the terms in curly brackets are included in the model. The subset is selected using standard stepwise regression or related methods (Draper and Smith 1998; Montgomery et al. 2001). LM models and PQM models are discussed in more detail and illustrated, respectively, by Cornell (2002) and Piepel et al. (2002).

Cornell (2002) discusses many other empirical mixture model forms that can be more appropriate than models of the forms in Equations (C.4) and (C.5) in certain specialized conditions. However, models of the form in Equations (C.4) and (C.5) are widely used in many application areas (including waste glass property modeling) and have been shown to perform very well.

C.1.2 Variants of the Linear Mixture Model for Assessing Block Effects

Two variants of the LM model, useful in assessing the presence or absence of "block effects" in a modeling dataset comprised of two subsets of data collected at different times and/or locations (i.e., "blocks"), are presented in this section. These LM model variants can easily be extended for use with modeling datasets comprised of three or more subsets of data.

The following model form is applicable if: (1) the LM model accounts for the majority of the compositional dependence of $f(y)$ and (2) there is a constant difference in $f(y)$ values for one subset of data compared to the other:

$$f(y) = b_0 B + \sum_{i=1}^{q} b_i x_i + \varepsilon , \tag{C.6}$$

where $B = 0$ for one of the two subsets of modeling data, and $B = 1$ for the other subset. If there is a reason to believe one subset is unbiased and the other biased, then $B = 0$ should be used for the subset believed to be unbiased. In Equation (C.6), b_0 is a coefficient estimated from the modeling data that gives the estimated magnitude of the constant difference in $f(y)$ values between the two subsets. If the b_0 coefficient is statistically different from zero, then that is an indication there is a significant constant difference between the $f(y)$ values for one subset of the modeling data compared to the other.

The following model form is applicable if: (1) the LM model accounts for the majority of the compositional dependence of $f(y)$ and (2) the difference in $f(y)$ values for one subset of data compared to the other depends on the composition of the mixture:

$$f(y) = \sum_{i=1}^{q} b_i^0 x_i + \sum_{i=1}^{q} b_i^1 x_i B + \varepsilon , \tag{C.7}$$

where the choice of $B = 0$ or $B = 1$ is the same as previously discussed. In Equation (C.7), the b_i^0 coefficient represents the linear blending effect of the i^{th} component for the subset of modeling data represented by $B = 0$. The b_i^1 coefficient represents the change or bias in the linear blending effect of the i^{th} component for the subset of modeling data represented by $B = 1$. If any of the b_i^1 coefficients ($i = 1, 2, \ldots, q$) are statistically different from zero, that is an indication that there are compositionally-dependent differences in the $f(y)$ values for one subset of the modeling data compared to the other.

The model forms in Equations (C.6) and (C.7) are intended for use in assessing whether data collected at different times, locations, or conditions are subject to effects (biases) related to the change in time, location, or conditions of data collection. If significant bias is indicated by such models, it should ideally be confirmed by other means (e.g., results on a standard collected at different times, locations, and conditions). It is beyond the scope of this discussion to address what to do when biased data are detected and confirmed. The appropriate steps will depend on the specific situation, the intended use of the data, and any requirements or limitations regarding the use of biased (or bias-corrected) data.

C.2 Least Squares Regression Methods and Assumptions for Fitting Models

Empirical or semi-empirical property-composition models are typically fitted to data sets using unweighted least squares (ULS) or weighted least squares (WLS) regression (Draper and

Smith 1998 or Montgomery et al. 2001). The underlying assumptions of ULS and WLS regression are:

(i) The predictor variable values (e.g., mass fractions of glass components) are known or measured without uncertainty, or at least that the uncertainty is small relative to the uncertainty in response variable (glass property) values

(ii) The testing and/or measurement errors in a response variable (glass property) over a model development data set are independently distributed. For ULS regression, the additional assumption is made that the errors are identically distributed (i.e., with zero mean and the same variance). For WLS regression, the errors are also assumed to have zero mean, but the variance can be different for different data points.

(iii) The errors from (ii) are normally (Gaussian) distributed.

Regarding assumption (i), the true composition of glasses in a model development data set are generally not known, and so any representation of glass composition selected (e.g., target compositions, analyzed compositions, or adjusted and normalized versions of analyzed compositions) will be subject to uncertainty. Weier and Piepel (2002) discuss a procedure for performing adjustments and weighted normalization of analyzed glass compositions that corrects for biases and reduces uncertainties in analyzed glass compositions. As long as representations of glass composition do not have significant biases (or those biases are appropriately corrected), it is generally expected that uncertainties will be small compared to uncertainties in glass property values. Further, uncertainties in glass compositions are expected to be small compared to errors in using empirical or semi-empirical model forms to approximate the true (but unknown) property-composition relationships. Hence, assumption (i) is sufficiently satisfied for most waste glass property-composition modeling situations.

The portion of assumption (ii) having to do with the independence of errors in testing and measuring properties may not be completely satisfied when model development data sets are comprised of subsets of data generated at different times or locations (e.g., different laboratories). There is the potential for errors in testing and measuring properties to vary for different subsets of data, and be more alike within the same subset of data. However, this issue has generally not been a problem in many past property-composition modeling efforts. If needed, *generalized least squares* methods that account for correlations among data points could be applied.

The "identically distributed" portion of assumption (ii) for ULS regression is not valid for some properties, because the variance of errors in testing and measurement of properties depends on the value of the property. For example, the variances of viscosity and durability results for waste glasses tend to increase as the values of these properties increase. In cases where the identically distributed (equal variance) assumption is violated, it can often be remedied by applying an appropriate mathematical transformation to the property values (e.g., a logarithmic transformation). The Box-Cox family of transformations contains transformations (including the logarithmic transformation) appropriate for many models (see Draper and Smith 1998). Such transformations also often yield better fitting empirical or semi-empirical property-composition

models. In some cases, a property transformation used in a particular model form may be preferred for some reason (e.g., provides a better fit), but does not satisfy the constant variance assumption of (ii). Or, it may be that the difference in variances across response values in the modeling data set cannot be rectified by a response transformation. In such cases, other regression methods such as WLS regression or generalized linear models (Myers et al. 2002) could be applied.

The assumption of normally distributed measurement and testing errors in the measured response variable values allows the use of normal theory regression tests and uncertainty equations associated with the fitted regression model. For example, normal theory confidence intervals and prediction intervals can be used (see Section C.6).

As discussed in preceding text, ULS regression requires that all response values for the modeling data have constant variance (i.e., uncertainty). WLS regression accounts for response values having different variations by using a weight for each data point (w_i). Often, w_i is chosen to be proportional to the reciprocal of the variance (squared standard deviation) of the response for the i^{th} data point (y_i).

$$w_i = \frac{\lambda}{Var(y_i)} = \frac{\lambda}{[SD(y_i)]^2}$$

where λ is a proportionality constant (which could be 1). Thus, in such a WLS regression the weighted response values $\sqrt{w_i}\, y_i$ then have equal variance. However, other methods for selecting weights can be applicable for various situations.

In summary, assumptions of ULS regression may not be completely satisfied for typical property-composition data sets and models. Violations of the constant variance assumption for property values over a modeling data set can sometimes be addressed by appropriate property transformations so that ULS regression may be used. Other violations may be small enough that ULS regression methods can still be used without significant consequence. However, if there are large enough differences in variances of property values across a modeling data set that cannot be addressed by a property transformation, then WLS regression methods should be used.

C.3 Statistical Methods for Model Evaluation

There are many statistical methods (both numerical and graphical) for assessing models. *Evaluation methods* assess a model with the data used to develop the model. Such data are referred to as *model development data*. The goals of model evaluation are to assess: (1) how well a model fits the data used to develop it, (2) how well the least squares or other regression method assumptions are satisfied (see Section C.2), and (3) whether there are any outlying or influential data points that significantly affect the fitted model. Problems detected by model evaluation such as violation of assumptions, detection of outlying data points, or detection of model inadequacy require implementing various remedies in the model development process until the problem(s) are corrected. When the model being evaluated acceptably fits the data used to develop the model, *model validation* methods should be applied using data not used to develop the model.

Such data are referred to as *model validation data*. If model validation data are not available, *crossvalidation methods* can be applied using the model development data. Crossvalidation methods leave out one or more data points at a time, so that some of the data are used for model development and some for model validation. Such methods are also referred to as data-splitting validation methods, where part of the data is used for model development and evaluation, while the other part is used for validation. Draper and Smith (1998) and Montgomery et al. (2001) discuss statistical methods for evaluating and validating models.

Model evaluation techniques include predicted versus measured (PvM) property plots, standardized residual plots, outlier diagnostics, three R^2 statistics, root mean squared error (*RMSE*), and statistical lack-of-fit (LOF) tests. Each of these is explained briefly below. The following notation is used in the subsequent descriptions and definitions:

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

p = the number of parameters in a model form estimated via regression on the data,

y_i = the measured property value (mathematically transformed, if appropriate for the model form used) for the i^{th} data point,

$\hat{y}_i$ = the predicted property value (mathematically transformed, if appropriate for the model form used) for the i^{th} data point made using the model fitted to all n data points,

r_i = the residual for the i^{th} data point = $y_i - \hat{y}_i$,

$\hat{y}_{(i)}$ = the predicted property value (mathematically transformed, if appropriate for the model form used) for the i^{th} data point made using a model fitted to all n data points except the i^{th},

w_i = the weight applied to the i^{th} data point in cases where WLS regression is used. Typically, w_i is proportional to the reciprocal of the variance of the response variable for the i^{th} data point,

$\bar{y}$ = the unweighted average (mean) of the n measured property values (mathematically transformed, if appropriate for the model form used),

$\bar{y}_w$ = the weighted average (mean) of the n measured property values (mathematically transformed, if appropriate for the model form used)

$$\bar{y}_w = \frac{\sum_{i=1}^{n} w_i y_i}{\sum_{i=1}^{n} w_i} \tag{C.8}$$

The model evaluation methods are now briefly described.

- *Predicted versus measured (PvM) property plots* show how well model predicted values $\hat{y}_i$ compare to the measured values y_i for the glasses in the model development data set. Predicted property values $\hat{y}_i$ are plotted on the *y*-axis and measured property values y_i are plotted on the *x*-axis. A line with slope one is included in the plot for reference purposes, and represents the ideal of predicted values equaling measured values. Plotted points falling above this line correspond to glasses for which the model over-predicts the property, while plotted points falling below this line represent glasses for which the model under-predicts the property. A preponderance of plotted points in a portion of the plot falling above or below the line indicates that the model tends to yield biased predictions for that range of property values. Plotted points far from the line are outlying or potentially influential data points.

  For WLS regression, an *ordinary (unweighted) PvM plot* of $\hat{y}_i$ versus y_i could be viewed as is done for ULS regression. Or, a *weighted PvM plot* of $\sqrt{w_i}\,\hat{y}_i$ versus $\sqrt{w_i}\,y_i$ could be viewed. The unweighted PvM plot has the advantage of retaining the units of the response (or its transformation), but the disadvantage that points with smaller weights (i.e., higher uncertainties) may appear farther from the line with slope one. However, rather than considering this a disadvantage, it may be better thought of as showing the penalty paid in obtaining predictions having more uncertainty for modeling data points with smaller weights (i.e., higher uncertainty). The weighted PvM plot would show the model predictive performance for the modeling data points after accounting for (i.e., removing the scatter due to) the differing weights (i.e., uncertainties).

- *RMSE* is given by

$$RMSE_U = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{n-p}} \tag{C.9a}$$

  for ULS regression, and by

$$RMSE_W = \sqrt{\frac{\sum_{i=1}^{n} w_i(\hat{y}_i - y_i)^2}{n-p}} \tag{C.9b}$$

  for WLS regression. If the fitted model is adequate and does not have a statistically significant lack-of-fit, this statistic provides an estimate of the experimental and measurement uncertainty standard deviation associated with melting glasses and measuring the associated property. The statistic *RMSE* is included as standard output in most regression software, and has units the same as the property values y_i (including any mathematical transformation of the property in the model form) for ULS regression and the units of $\sqrt{w_i}\,y_i$ for WLS regression.

- *Standardized residual plots* display standardized residuals (s_i, differences in predicted and measured property values divided by their standard deviations) versus various quantities, such as: glass component mass fractions (x_i), predicted property values ($\hat{y}_i$), or an index associated with each data point. The formula for a standardized residual is given by

$$s_i = \frac{r_i}{RMSE_U \left[1 - \boldsymbol{a}_i^T \left(\boldsymbol{A}^T \boldsymbol{A} \right)^{-1} \boldsymbol{a}_i \right]^{0.5}} \tag{C.10a}$$

for ULS regression, and by

$$s_i = \frac{\sqrt{w_i} r_i}{RMSE_W \left[1 - w_i \boldsymbol{a}_i^T \left(\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A} \right)^{-1} \boldsymbol{a}_i \right]^{0.5}} \tag{C.10b}$$

for WLS regression. In Equations (C.10a) and (C.10b): s_i, w_i, and r_i are as previously described; $RMSE_U$ and $RMSE_W$ are respectively given by Equations (C.9a) and (C.9b); $\boldsymbol{a}_i$ is the composition (column) vector for the i^{th} modeling data point expanded in the form of the model; $\boldsymbol{A}$ is an $n \times p$ matrix of the compositions in the modeling data set expanded in the form of the model; and $\boldsymbol{W}$ is an $n \times n$ matrix with the weights w_i along the main diagonal, and zeros elsewhere.

Patterns in the s_i versus $\hat{y}_i$ plot can indicate a violation of the least squares regression assumptions and suggest a property transformation to remedy the situation. Patterns in the s_i versus x_i plots can indicate inadequacies of the model or least squares assumptions. Standardized residuals are typically used in residual plots because the majority should fall within the range of ± 2.0 or 2.5. Comparing standardized residuals to such a range provides an easy criterion for judging whether a data point is possibly outlying or influential.

- *Normality plots* display normal scores versus the ordered (from smallest to largest) standardized residuals (from Equations (C.10a) or (C.10b) for ULS and WLS regression, respectively) for the n data points used to fit the model being assessed. Normal scores are the expected values of a sample of size n from standard normal distribution (with mean 0 and standard deviation 1). The plotted points are compared to the ideal of a straight line corresponding to a normal distribution. A straight middle portion of the plot with curved "tails" on each end of the plot indicate the presence of outlying data points, which cause a heavier-tailed distribution than the normal distribution.

- *Outlier diagnostics and plots* indicate data points that are outlying or influential with respect to property value or composition. There are too many of these diagnostics and plots to discuss here, but several produced by the R software (Ihaka and Gentleman 1996) and the SAS software (2001) were considered in this work. Draper and Smith (1998) and Montgomery et al. (2001) discuss outlier diagnostics and plots for ULS regression, but

software such as R and SAS produce the appropriate weighted versions of diagnostics and plots for WLS as well as ULS regression.

- *R^2 statistics* quantify the proportion of variation in the property values y_i (for ULS regression) or weighted property values $\sqrt{w_i}\,y_i$ (for WLS regression) accounted for by the fitted model. Three R^2 statistics are used, as discussed later in this section.

- A *statistical lack-of-fit (LOF) test* checks whether the differences (for ULS regression) or weighted differences (for WLS regression) 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[1] are required to perform statistical LOF tests. This process is conducted using a LOF F-test given by

$$F = \frac{(\text{SSE} - \text{SSPE})/(n - p - f)}{\text{SSPE}/f} = \frac{\left[\left(\sum_{i=1}^{n}(\hat{y}_i - y_i)^2 - \sum_{k=1}^{K}\sum_{j=1}^{m_k}(y_{kj} - \bar{y}_k)^2\right)\Big/(n-p-f)\right]}{\sum_{k=1}^{K}\sum_{j=1}^{m_k}(y_{kj} - \bar{y}_k)^2\Big/f} \tag{C.11a}$$

for ULS regression, and by

$$F = \frac{(\text{SSE} - \text{SSPE})/(n - p - f)}{\text{SSPE}/f} = \frac{\left[\left(\sum_{i=1}^{n} w_i(\hat{y}_i - y_i)^2 - \sum_{k=1}^{K}\sum_{j=1}^{m_k} w_j(y_{kj} - \bar{y}_k)^2\right)\Big/(n-p-f)\right]}{\sum_{k=1}^{K}\sum_{j=1}^{m_k} w_j(y_{kj} - \bar{y}_k)^2\Big/f} \tag{C.11b}$$

for WLS regression. In Equations (C.11a) and C.11b): SSE = sum of squares error; SSPE = sum of squared pure error (i.e., from replicates); n and p are as described previously such that $n–p$ is the degrees of freedom for SSE; and the degrees 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

[1] To be appropriate replicate data points, two or more glass samples of the same composition must be batched and melted at different times, and have their properties measured at different times. It is insufficient, for example, to batch and melt a glass once, and measure its properties several times (because the batching and melting sources of uncertainty are not included in the data). Similarly, replicate samples should not be measured at the same time (or close in time) because all sources of measurement uncertainty will not be included in the data.

set, $k = 1, 2, \ldots, K$. In practice, if the F-test is statistically significant at a significance level of 0.05 or smaller (i.e., 95% confidence or higher), then it would be concluded that the fitted model has a statistically significant LOF for the modeling dataset. See Draper and Smith (1998) or Montgomery et al. (2001) for additional discussion of the statistical test for model LOF.

Even when a fitted model has a statistically significant LOF, the LOF may not be "practically significant". An example of such a situation is when a fitted model yields biased predictions for higher and/or lower values of a property or in a particular subregion of compositions, but the model will not be applied to such areas in practice. Another example is when the model fits the data very well (e.g., $R^2 > 0.95$) without bias over the model's region of validity, but the LOF is statistically significant because the experimental and measurement uncertainty is very small (e.g., because glasses can be batched, melted, and properties measured with excellent repeatability). Finally, a statistically significant LOF may not be practically significant if the uncertainty in model predictions is considerably smaller than uncertainty that can be tolerated and still meet requirements.

The model evaluation techniques discussed in the preceding bullets are included in, or can be obtained from, the output of the R software (Ihaka and Gentleman 1996) and SAS software (2001). See Draper and Smith (1998) or Montgomery et al. (2001) for further discussion of the concepts.

Three different R^2 statistics are useful in evaluating models fitted to glass property-composition data. The *(ordinary) R^2 statistic* is given by

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2} \tag{C.12a}$$

for ULS regression, and by

$$R^2 = 1 - \frac{\sum_{i=1}^{n} w_i (\hat{y}_i - y_i)^2}{\sum_{i=1}^{n} w_i (y_i - \bar{y}_w)^2} \tag{C.12b}$$

for WLS regression, where $\bar{y}_w$ in Equation (C.12b) is the weighted mean whose formula is given in Equation (C.8). R^2 is interpreted as the fraction of variability in the unweighted (for ULS regression) or weighted (for WLS regression) property data (transformed if appropriate) accounted for by the fitted model. The *adjusted R^2 statistic* is given by

$$R_A^2 = 1 - \frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2 \Big/ (n-p)}{\sum_{i=1}^{n} (y_i - \bar{y})^2 \Big/ (n-1)} \tag{C.13a}$$

for ULS regression, and by

$$R_A^2 = 1 - \frac{\sum_{i=1}^{n} w_i(\hat{y}_i - y_i)^2 \Big/ (n-p)}{\sum_{i=1}^{n} w_i(y_i - \bar{y}_w)^2 \Big/ (n-1)} \qquad \text{(C.13b)}$$

for WLS regression. R_A^2 is interpreted as the adjusted fraction of variability in the unweighted or weighted property data (transformed if appropriate) accounted for by the fitted model. The adjustment is for the number of parameters (p) and number of data points (n) used in fitting the model. The *predicted R^2 statistic* is given by

$$R_P^2 = 1 - \frac{\sum_{i=1}^{n} (\hat{y}_{(i)} - y_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}, \qquad \text{(C.14a)}$$

for ULS regression, and by

$$R_P^2 = 1 - \frac{\sum_{i=1}^{n} w_i(\hat{y}_{(i)} - y_i)^2}{\sum_{i=1}^{n} w_i(y_i - \bar{y}_w)^2}, \qquad \text{(C.14b)}$$

for WLS regression. R_P^2 is interpreted as the leave-one-out crossvalidation fraction of variability in the unweighted or weighted property data (transformed if appropriate) accounted for by the fitted model. This statistic is calculated by a method equivalent to leaving each data point out of the model fit, and then evaluating how well the model predicts the property for that data point. R_P^2 estimates the fraction of variability that would be explained in predicting new observations drawn from the same composition space.

Generally R^2 statistics take values between 0 and 1. However, R_A^2 and R_P^2 can take negative values for a poor fitting model, a model that contains many more terms than needed to fit the data, or a model fitted to data with one or more very influential data points. Among the three R^2 statistics, typically $R^2 > R_A^2 > R_P^2$. More than a minor difference between R^2 and R_A^2 indicates that the model may contain more terms than needed to achieve the same goodness of fit. A substantial difference between R^2 and R_P^2 is indicative of one or more data points being very influential in determining the fit of the model. Some reduction from R^2 to R_P^2 is expected because R^2 corresponds to using all data to fit the model, whereas R_P^2 corresponds to leaving each data point out of the fit when evaluating the performance of the model for that point. In general, a model will tend to predict better for data used to fit it than for data not used to fit it. R_P^2 is a crossvalidation evaluation method.

C.4 Statistical Methods for Model Reduction and Augmentation

Section C.4.1 discusses methods for identifying and removing unnecessary terms from mixture experiment models. Section C.4.2 discusses methods for augmenting linear mixture models with quadratic terms.

C.4.1 Statistical Methods for Reducing Mixture Experiment Models

In evaluating a fitted regression model, it may often be determined that there are unnecessary terms in the model. Such terms may not improve, and can even degrade, the predictive performance of the model in applications to data not used to develop the model.

The most basic statistical method to identify unnecessary terms in a model is a *t-test* to perform a hypothesis test of whether the coefficient of a model term is statistically different from zero. The t-test computes a t-statistic equal to a model coefficient divided by the standard deviation of the coefficient. The t-statistic is then compared to the Student-t probability distribution to determine the probability of getting a t-statistic at least that large. The resulting probability is referred to as a *p-value*, and represents the probability of incorrectly deciding a coefficient is significantly different than zero. Most regression software outputs estimated model coefficients, coefficient standard deviations, t-statistics, and p-values. Typically, practitioners require a p-value to be smaller than 0.05 or 0.01 as strong evidence that the coefficient is significantly different than zero, and thus that the corresponding model term is needed. If there are not too many potentially unnecessary terms in a model, a practitioner can assess the t-statistics and p-values for the coefficients in a "full" model, and remove the model term whose coefficient is least statistically significant. Then, the model would be refitted without that term, and the t-statistics and p-values again considered, deleting the model term with the least statistically significant coefficient. This process continues until all terms in the model have p-values lower than 0.05, say. *Backward elimination* (Draper and Smith 1998, Montgomery et al. 2001) is a widely used statistical method for removing unneeded terms from a model. This method basically automates the process just described, where the practitioner sets a stopping criterion.

Unfortunately, there are some model forms for which the model reduction methods just described are inappropriate. In general, these are model forms where a model coefficient being small (e.g., near zero) does not imply the corresponding model term is unneeded. That, is some model forms may have terms with significant effects even though the coefficients of those terms are small. One class of models in this category relevant to this work is the class of *mixture experiment models* (Cornell 2002), of which LM and PQM models are given in Section C.1.1. The LM model (or the linear blending portion of a PQM model) is of the form $\sum_{i=1}^{q} b_i x_i$, where the b_i are coefficients and the x_i are proportions of the mixture components (e.g., mass fractions of waste glass components) that must sum to one (i.e., $\sum_{i=1}^{q} x_i = 1$). When each x_i can vary from zero to one, the coefficient b_i represents the estimated response variable value for pure component i [i.e., when $x_i = 1$ and $x_j = 0$ ($j \neq i$)]. When the ranges of the mixture component proportions x_i are constrained, each b_i represents extrapolated response values for pure component i. Because

hypotheses concerning LM model coefficients (or the coefficients of linear terms in PQM models) equaling zero are not related to the importance or non-importance of a given component, it is inappropriate to use t-tests or the standard backward elimination method to reduce the linear portion of a mixture experiment model. However, mixture models can contain nonlinear terms in the components (such as in the PQM model form discussed in Section C.1.1), and it is appropriate to use t-tests or the standard stepwise, forward, or backward elimination *variable selection methods* (see Draper and Smith 1998 or Montgomery et al. 2001) on such terms.

A special backward elimination method for mixture experiments could be used to reduce linear mixture models and linear portions of mixture models. The reduction method is performed in stages. In the first stage, each mixture component in turn is dropped from the model, the remaining mixture component proportions are renormalized to sum to one, and then a linear mixture model without the dropped component is fitted to the data. The dropped mixture component that causes the smallest increase in the error sums of squares (the quantity being minimized in ULS regression) is then the first component to be permanently dropped from the model. Similar stages continue, with one component dropped at the end of each stage, until dropping a component causes the full-reduced model F-test (Draper and Smith 1998, Montgomery et al. 2001) to declare a statistically significant increase in the error sum of squares. This then signals the stopping point for the backward elimination algorithm. After each component is dropped, the remaining components are renormalized according to the mixture experiment definition that a response variable depends only on the relative proportions of the mixture components that affect the response variable (Cornell 2002). Hence, only the normalized proportions of components affecting the response are used in developing mixture experiment models.

C.4.2 Statistical Methods for Adding Terms to Models

It is often of interest to add additional terms onto a starting model in the hopes of improving the predictive performance of the starting model. For example, a linear mixture model may be considered as a starting model. However, if it has a significant LOF, adding nonlinear composition terms may be considered in hopes of improving the predictive performance of the model. *Stepwise regression* is the most commonly used method to add terms to an existing starting model. In stepwise regression, certain terms can be forced into the model, and a candidate list of possible terms to add is identified. The procedure identifies the term from the candidate list that, if added to the model, would yield the greatest reduction in the error sum of squares (i.e., the sum of squared differences in measured and model-predicted values across the modeling data set). If the reduction is statistically significant, that term is added to the model. Stepwise regression proceeds in stages, with one additional term being added at each stage unless the user-selected stopping criterion is reached. After adding a term, stepwise regression checks all other terms in the model to assess if they are still statistically significant. If not, a term can be removed during a stage.

The stepwise regression algorithm requires that a significance level be specified for terms to enter the model, and that a significance level be specified for terms to remain in the model. In each iteration of a stepwise regression application, t-tests are conducted for each term already in the model and for terms being considered for inclusion in the model. To describe the results of

these t-tests, a p-value is calculated for each of the terms. Loosely speaking, the p-values represent the probability that the respective model terms do not make a significant contribution to the predictive ability of the model. Terms whose corresponding p-values are small (often <0.05 is considered sufficiently small) are considered important in the model. The significance levels specified for the stepwise regression algorithm indicate how small p-values must be for the corresponding terms to be included in the model. The statistical literature generally indicates that the stepwise algorithm is somewhat liberal in allowing terms into models. Yet, models containing unnecessary terms are undesirable because they tend to have inflated prediction variance. Thus, it is typically advisable to use tight significance levels such as 0.05 or 0.01 when applying the stepwise regression algorithm.

One particular variation of stepwise regression that can be used to select terms for model building is what the SAS statistical software package (SAS 2001) refers to as the Maximum R-squared Improvement (MAXR) selection method. For the MAXR criterion (as with other criteria for stepwise regression), terms can enter and leave (being replaced by another term) the model. Sequential changes to the model are based on maximal increases to the model's R^2 value, and MAXR tries to find the "best" model having a specified numbers of terms. However, MAXR is not the same as the "best subsets" algorithm because it does not consider all possible models with a given number of terms. Therefore, MAXR is not guaranteed to find the model with the highest R^2 value among all models having a given number of terms. This method tends to have a better chance of finding more nearly optimal models than does the stepwise selection method using other criteria (Freund and Littell, 1995). The MAXR method does not require significance levels to control term selection, but does require the user to identify any terms to force into the model and to specify the number of terms to include in models being considered.

The standard stepwise regression procedure (regardless of the criterion used for model term selection) is not appropriate for linear mixture models or linear portions of other mixture experiment models for similar reasons as described previously with regard to the standard backward elimination method. However, it is appropriate for adding nonlinear mixture terms or non-mixture terms to mixture models.

C.5 Statistical Methods for Model Validation

Model validation methods assess how well a fitted model predicts property values for glasses not used in fitting the model. The glasses used for validation ideally should be in the same composition region as the data used to fit the property-composition models, because (in general) fitted empirical and semi-empirical models should not be used to extrapolate much beyond the region covered by the modeling data. Also, ideally the validation data should be evenly distributed over the model composition region of model validity to properly assess predictive ability over the region. However, this is difficult to achieve in practice because validation data is typically not designed, but often consists of whatever extra data are available.

Validation generally consists of using a fitted model to predict property values for a set of validation data, and then comparing the predicted property values to the measured values from the validation database. Assessment of these comparisons is aided by plotting the predicted

versus the measured property values for each data point. Such *predicted versus measured plots* are the same as described in Section C.3, except model validation data are used instead of model development data. Also, similarly as described in Section C.3, *unweighted PvM plots* or *weighted PvM plots* may be produced and viewed to validate models fitted by WLS regression.

Statistical comparisons of predicted and measured response values are also useful to see if differences are larger than their expected uncertainties. One such comparison is the *validation* R^2 statistic, which in general is given by

$$R_V^2 = 1 - \frac{\sum_{i=1}^{n} (\hat{y}_i - y_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}. \qquad \text{(C.15a)}$$

However, in cases where WLS regression is used to fit the model and corresponding weights are available, a weighted version of the *validation* R^2 statistics is given by

$$R_V^2 = 1 - \frac{\sum_{i=1}^{n} w_i (\hat{y}_i - y_i)^2}{\sum_{i=1}^{n} w_i (y_i - \bar{y}_w)^2}. \qquad \text{(C.15b)}$$

R_V^2 is interpreted as the fraction of variability in the unweighted or weighted property values (transformed if appropriate) in the validation data accounted for by the fitted model. Note that R_V^2 is defined exactly the same as the ordinary R^2 defined in Equations (C.12a) and (C.12b), except that model validation data are used to assess model predictive performance instead of the model development data. Hence, the y_i, $\hat{y}_i$, $\bar{y}$, w_i, and $\bar{y}_w$ values in Equations (C.15a) and (C.15b) correspond to the model validation data.

Generally $R_V^2 \le R_P^2 \le R_A^2 \le R^2 \le 1$. However, R_V^2 can take negative values (when a model predicts a validation set very poorly) and can take values larger than R_P^2, R_A^2, or R^2 (when a model predicts a particular validation dataset better than estimated by these statistics based on the modeling data).

Another useful statistical technique, which can be combined with the plot of predicted versus measured property values for the validation data set, is to include error bars consisting of 95% two-sided prediction intervals (95% PIs) on the predicted values. Then, if the error bar for a given validation data point overlaps a line with slope one superimposed on the PvM plot, the model is validated for that data point. Draper and Smith (1998) and Montgomery et al. (2001) provide additional discussion of 95% PIs for regression models. The formulas for a 95% two-sided PI in the ULS and WLS cases are given in Section C.6 following.

C.6 Statistical Methods for Describing Uncertainties in Model Predictions

Several types of statistical intervals are available to describe the uncertainty associated with model predictions. Each type of statistical interval has a particular interpretation. The following two types of statistical intervals are used to describe the uncertainty associated with model predictions at a single specific composition.

A *100(1–α)% upper confidence interval (UCI)* for the true mean response value for a given glass composition $\boldsymbol{x} = (x_1, x_2, \ldots, x_q)$ is given by

$$\begin{aligned} \hat{y}(\boldsymbol{x}) + t_{1-\alpha,n-p}\sqrt{\boldsymbol{a}^T \boldsymbol{C}_U \ \boldsymbol{a}} &= \hat{y}(\boldsymbol{x}) + t_{1-\alpha,n-p}\sqrt{\boldsymbol{a}^T [(\boldsymbol{A}^T \boldsymbol{A})^{-1} MSE_U]\, \boldsymbol{a}} \\ &= \hat{y}(\boldsymbol{x}) + t_{1-\alpha,n-p} RMSE_U \sqrt{\boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{a}} \end{aligned}, \qquad \text{(C.16a)}$$

for ULS regression, and by

$$\begin{aligned} \hat{y}(\boldsymbol{x}) + t_{1-\alpha,n-p}\sqrt{\boldsymbol{a}^T \boldsymbol{C}_W \ \boldsymbol{a}} &= \hat{y}(\boldsymbol{x}) + t_{1-\alpha,n-p}\sqrt{\boldsymbol{a}^T [(\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A})^{-1} MSE_W]\, \boldsymbol{a}} \\ &= \hat{y}(\boldsymbol{x}) + t_{1-\alpha,n-p} RMSE_W \sqrt{\boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A})^{-1} \boldsymbol{a}} \end{aligned}, \qquad \text{(C.16b)}$$

for WLS regression. In Equations (C.16a) and (C.16b)

$\hat{y}(\boldsymbol{x})$ = the model predicted value at composition $\boldsymbol{x}$,

$100(1-\alpha)$ = the desired confidence (e.g., 90%) for the confidence interval, where α denotes the significance level (e.g., $\alpha = 0.10$ for 90% confidence),

$t_{1-\alpha,n-p}$ = the $100(1-\alpha)$-percentile of the Student's t-distribution with n-p degrees of freedom,

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

p = the number of parameters estimated in the model,

$\boldsymbol{C}_U$ = the estimated variance-covariance matrix for a model fitted by ULS regression = $(\boldsymbol{A}^T \boldsymbol{A})^{-1} MSE_U$,

$\boldsymbol{C}_W$ = the estimated variance-covariance matrix for a model fitted by WLS regression = $(\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A})^{-1} MSE_W$,

$\boldsymbol{a}^T$ = the vector transpose of the glass composition vector $\boldsymbol{x}$ expanded in the form of the model,

$\boldsymbol{A}^T$ = the matrix transpose of the composition matrix (used to estimate the model coefficients via regression) expanded in the form of the model,

$\boldsymbol{W}$ = an $n \times n$ diagonal weight matrix with entries w_i, $i = 1, 2, \ldots, n$ (i.e., the weights associated with the model development set of n data points),

MSE = mean squared error, which is obtained from the ULS (MSE_U) or WLS (MSE_W) regression fit of the model,

RMSE = the root mean squared error = $\sqrt{MSE}$, with $RMSE_U$ and $RMSE_W$ resulting from ULS and WLS regression fits of a model, respectively.

A 100(1−α)% UCI is appropriate when an uncertainty statement is desired about the true mean response for a given composition $\boldsymbol{x}$.

A *100(1−α)% two-sided prediction interval (PI)* for an individual response value for a given composition $\boldsymbol{x}$ is given by

$$\hat{y}(\boldsymbol{x}) \mp t_{1-\alpha/2,n-p}\sqrt{MSE_U + \boldsymbol{a}^T \boldsymbol{C}_U \boldsymbol{a}} = \hat{y}(\boldsymbol{x}) \mp t_{1-\alpha/2,n-p} RMSE_U \sqrt{1 + \boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{a}}\,, \quad \text{(C.17a)}$$

for ULS regression, and by

$$\hat{y}(\boldsymbol{x}) \mp t_{1-\alpha/2,n-p}\sqrt{\frac{MSE_W}{w_i} + \boldsymbol{a}^T \boldsymbol{C}_W \boldsymbol{a}} = \hat{y}(\boldsymbol{x}) \mp t_{1-\alpha/2,n-p} RMSE_W \sqrt{\frac{1}{w_i} + \boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A})^{-1} \boldsymbol{a}}\,, \quad \text{(C.17b)}$$

for WLS regression, where the notation is defined as in the preceding UCI definition. Note that the w_i under the square root applies when PIs are calculated for modeling data, validation data, or application data (i.e., data used in applying the models and PIs) with weights. In situations where validation or application data do not have weights, w_i should be set to 1. A 100(1−α)% PI is appropriately used when comparing a model predicted response value for a given composition to an individual measurement of the response for that composition. This type of application arises in validating the predictive performance of a model for one or more glass compositions not used to fit the model. Specifically, Equations (C.17a) and (C.17b) can be used to produce 95% PIs displayed as error bars in PvM plots, as described at the end of Section C.5.

At times it is desirable to describe the uncertainty associated with predictions obtained for a specified group of compositions. For example, a statement may be desired that indicates with high confidence that the predicted response value for every composition $\boldsymbol{x}$ in a specified group of compositions (or composition region) is below a particular regulatory limit. Such a confidence statement requires a statistical interval called a simultaneous upper confidence interval. The formula for a *100(1−α)% upper simultaneous confidence interval (SUCI)* is given by

$$\hat{y}(\boldsymbol{x}) + \sqrt{pF_{1-2\alpha;p,n-p}}\sqrt{\boldsymbol{a}^T \boldsymbol{C}_U \boldsymbol{a}} = \hat{y}(\boldsymbol{x}) + RMSE_U \sqrt{pF_{1-2\alpha;p,n-p}}\sqrt{\boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{a}} \quad \text{(C.18a)}$$

for ULS regression, and by

$$\hat{y}(\boldsymbol{x}) + \sqrt{pF_{1-2\alpha;p,n-p}}\sqrt{\boldsymbol{a}^T \boldsymbol{C}_W \boldsymbol{a}} = \hat{y}(\boldsymbol{x}) + RMSE_W \sqrt{pF_{1-2\alpha;p,n-p}}\sqrt{\boldsymbol{a}^T (\boldsymbol{A}^T \boldsymbol{W} \boldsymbol{A})^{-1} \boldsymbol{a}} \quad \text{(C.18b)}$$

for WLS regression. In Equations (C.18a) and (C.18b):

$\hat{y}(\boldsymbol{x})$ = the predicted response for each composition $\boldsymbol{x}$ in the specified composition set or region,

$F_{1-2\alpha,p,n-p}$ = the $100(1-2\alpha)$-percentile of the F-distribution with p and $n-p$ degrees of freedom.

The remaining notation in Equations (C.18a) and (C.18b) is the same as defined previously.

Equations (C.16), (C.17), and (C.18) yield statistical intervals in transformed units when a transformed property is modeled. For example, a natural logarithm transformation of a response y [i.e., ln(y)] is often used for property-composition models. Hence, the statistical intervals calculated using the preceding equations would be in ln(y) units. The statistical intervals can be transformed back to the original units of y by exponentiating the endpoint(s) of the statistical interval. However, the process of back-transforming (exponentiating) a statistical interval can change its interpretation. For example, if a 90% UCI in ln(y) units has the value "v", the back-transformed 90% UCI in the original units of y is given by e^{v}. The 90% UCI in units of ln(y) is a statement about the true mean response in ln(y) units for a given glass composition $\boldsymbol{x}$. However, the resulting back-transformed interval is a 90% UCI on the true median response value for the given composition $\boldsymbol{x}$, under the assumption that experimental errors in the data used to develop the model are lognormally distributed. This assumption corresponds to the assumption of the natural-log-transformed response data being normally distributed. This change in interpretation occurs because the mean and median of a normal distribution are the same, but the mean of a lognormal distribution is larger than the median of a lognormal distribution.

Hence, back-transforming a 90% UCI on a mean response for a given composition $\boldsymbol{x}$ (in ln-units) yields a 90% UCI on the median response for a given composition $\boldsymbol{x}$ in original units, which in turn underestimates a 90% UCI on the mean response for a given composition $\boldsymbol{x}$ in original units. Back-transforming *100(1–α)% SUCIs* given by Equation (C.18) in log-transformed units has a similar change in interpretation. Whereas the original *100(1–α)% SUCIs* are statements about the true mean values of responses in log-transformed response units for multiple compositions $\boldsymbol{x}$, the back-transformed *100(1–α)% SUCIs* are statements about the true median values of responses in original response units for multiple compositions $\boldsymbol{x}$. However, a *100(1–α)% PI* given by Equation (C.17) in log-transformed units does not have a change in interpretation when back-transforming, because the original statement (in log-transformed units) and the back-transformed statement (in original units) are both about a true individual response value.

Alternatives exist to using normal-theory-based Equations (C.16) through (C.18) and back-transforming them when a transformed response variable is modeled. One alternative is to modify the statistical interval equations so that the statistical statement is about the true mean response value in the original units for a given composition $\boldsymbol{x}$ [Equation C.16)] or set of compositions $\boldsymbol{x}$ [Equation (C.18)]. Although this type of alternative is discussed in the literature for non-regression problems (e.g., Gilbert 1987), no references were found for the regression context. Another alternative, the *generalized linear model* regression approach (Myers et al. 2002), avoids directly transforming the response variable and instead uses the transformation

indirectly. These alternative approaches were not pursued in this work. However, the interested reader may refer to the references given.

Note that Equations (C.16) through (C.18) require knowledge of the variance-covariance matrix $\boldsymbol{C}_U = MSE_U(\boldsymbol{A}^T\boldsymbol{A})^{-1}$ for ULS regression and $\boldsymbol{C}_W = MSE_W(\boldsymbol{A}^T\boldsymbol{W}\boldsymbol{A})^{-1}$ for WLS regression. The MSE_U and MSE_W are mean squared errors equal to the squares of $RMSE_U$ and $RMSE_W$ given by Equations (C.9a) and (C.9b). This information is included in the regression software output that comes with the estimates of the p model coefficients. A variance-covariance matrix is a $p \times p$ matrix with coefficient variances along the diagonal, and covariances between coefficient pairs in the off-diagonal entries.

References

Cornell, J.A. (2002), *Experiments with Mixtures*, Third Edition, John Wiley and Sons, NY.

Draper, N.R. and Smith, H. (1998). *Applied Regression Analysis*, Third Edition, John Wiley and Sons, Inc., New York, NY.

Freund, R.J. and Littell, R.C. (1995). *SAS System for Regression*, Second Edition, SAS Institute, Inc., Cary. NC.

Gilbert, R. O. (1987). *Statistical Methods for Environmental Pollution Monitoring*, Van Nostrand Reinhold, New York.

Ihaka, R. and Gentleman, R. (1996). "R: A Language for Data Analysis and Graphics", *Journal of Computational and Graphical Statistics*, 5, 299-314.

Montgomery, D.C., Peck, E.A., and Vining, G.G. (2001), *Introduction to Linear Regression Analysis*, Third Edition, John Wiley and Sons, New York.

Myers, R.H., Montgomery, D.C., and Vining, G.G. (2002), *Generalized Linear Models: With Applications in Engineering and the Sciences*, John Wiley and Sons, New York.

Piepel, G.F., Szychowski, J.M. and Loeppky, J.L. (2002), "Augmenting Scheffé Linear Mixture Models with Squared and/or Crossproduct Terms", *Journal of Quality Technology*, 34, 297-314.

SAS (2001). *SAS Release 8.2*, SAS Institute, Inc., Cary. NC.

Weier, D.R. and Piepel, G.F. (2003). *Methodology for Adjusting and Normalizing Analyzed Glass Compositions*, PNWD-3260 (WTP-RPT-049), Battelle—Pacific Northwest Division, Richland, WA, March 2003.

APPENDIX D

Variance-Covariance Matrices Associated With Coefficients of Phase 1 ILAW PCT and VHT Models

APPENDIX D

Variance-Covariance Matrices Associated With Coefficients of Phase 1 ILAW PCT and VHT Model

This appendix contains the variance-covariance matrices for the VHT and PCT property-composition models for ILAW glasses that are recommended in this report.

Tables D.1 and D.2, respectively, contain the variance-covariance matrices for the two recommended ln(VHT Alteration Depth) models: (1) the 14-term linear mixture (LM) model given in Table 5.6, and (2) the 22-term partial quadratic mixture (PQM) model given in Table 5.8.

Tables D.3 and D.4, respectively, contain the variance-covariance matrices for the two recommended ln(PCT-Boron) models: (1) the 11-term reduced LM model given in Table 6.11, and (2) the 14-term reduced PQM model given in Table 6.13. Tables D.5 and D.6, respectively, contain the variance-covariance matrices for the two recommended ln(PCT-Sodium) models: (1) the 11-term reduced LM model given in Table 6.19, and (2) the 16-term reduced PQM model given in Table 6.21.

Table D.1. Variance-Covariance Matrix Associated With the Estimated Coefficients of the ILAW VHT LM Model

	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SO_3	SiO_2	TiO_2	ZnO	ZrO_2	Others
Al_2O_3	61.289	-8.691	3.228	2.896	-11.808	-25.530	-9.461	-8.801	-77.981	-3.450	-6.471	2.457	19.321	-6.741
B_2O_3	-8.691	26.979	-1.763	9.011	8.288	3.422	-1.417	-1.335	42.965	-5.310	-7.087	-0.945	-7.505	19.654
CaO	3.228	-1.763	25.032	-3.353	0.016	-15.142	1.620	2.183	-33.680	-2.551	-11.346	4.422	2.587	-14.007
Fe_2O_3	2.896	9.011	-3.353	41.285	-16.510	-0.461	-6.413	-5.964	-96.148	-4.504	-2.999	2.836	10.562	28.046
K_2O	-11.808	8.288	0.016	-16.510	82.729	28.858	26.662	6.421	9.076	-2.013	-20.892	-9.537	-21.745	7.220
Li_2O	-25.530	3.422	-15.142	-0.461	28.858	149.168	19.322	25.297	-175.874	-5.526	-0.513	-3.889	-50.269	14.292
MgO	-9.461	-1.417	1.620	-6.413	26.662	19.322	77.282	4.610	-88.100	-3.278	6.582	3.436	-2.817	-11.474
Na_2O	-8.801	-1.335	2.183	-5.964	6.421	25.297	4.610	13.238	66.068	-2.772	-8.491	4.965	-17.613	-6.666
SO_3	-77.981	42.965	-33.680	-96.148	9.076	-175.874	-88.100	66.068	4534.105	-24.760	-239.828	-4.049	-66.934	89.403
SiO_2	-3.450	-5.310	-2.551	-4.504	-2.013	-5.526	-3.278	-2.772	-24.760	4.796	0.723	-8.215	-1.675	-5.674
TiO_2	-6.471	-7.087	-11.346	-2.999	-20.892	-0.513	6.582	-8.491	-239.828	0.723	167.056	13.386	35.777	-14.007
ZnO	2.457	-0.945	4.422	2.836	-9.537	-3.889	3.436	4.965	-4.049	-8.215	13.386	84.397	-12.331	-16.380
ZrO_2	19.321	-7.505	2.587	10.562	-21.745	-50.269	-2.817	-17.613	-66.934	-1.675	35.777	-12.331	127.073	-9.104
Others	-6.741	19.654	-14.007	28.046	7.220	14.292	-11.474	-6.666	89.403	-5.674	-14.007	-16.380	-9.104	201.145

Table D.2. Variance-Covariance Matrix Associated With the Estimated Coefficients of the ILAW VHT PQM Model

	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SO_3	SiO_2	TiO_2	ZnO
Al_2O_3	113.828	-1.193	-443.559	-19.264	208.424	44.453	29.941	30.197	-76.481	-33.420	44.085	17.557
B_2O_3	-1.193	118.698	0.710	-27.645	55.482	-19.495	23.108	-9.133	432.437	-22.023	70.055	10.549
CaO	-443.559	0.710	4459.342	310.723	-534.317	-565.049	-431.705	-369.745	442.232	282.641	-404.033	-285.594
Fe_2O_3	-19.264	-27.645	310.723	207.007	32.360	-38.944	-7.125	-31.612	-218.910	5.308	-33.590	-25.414
K_2O	208.424	55.482	-534.317	32.360	1432.330	18.078	150.641	18.502	2121.178	-71.956	173.142	154.411
Li_2O	44.453	-19.495	-565.049	-38.944	18.078	167.295	21.301	69.155	-620.920	-36.878	-11.559	30.463
MgO	29.941	23.108	-431.705	-7.125	150.641	21.301	277.661	28.082	-656.933	-43.867	265.040	62.720
Na_2O	30.197	-9.133	-369.745	-31.612	18.502	69.155	28.082	40.939	-219.853	-24.013	12.656	26.734
SO_3	-76.481	432.437	442.232	-218.910	2121.178	-620.920	-656.933	-219.853	32133.689	86.995	-996.705	206.351
SiO_2	-33.420	-22.023	282.641	5.308	-71.956	-36.878	-43.867	-24.013	86.995	27.599	-48.091	-27.727
TiO_2	44.085	70.055	-404.033	-33.590	173.142	-11.559	265.040	12.656	-996.705	-48.091	409.499	59.110
ZnO	17.557	10.549	-285.594	-25.414	154.411	30.463	62.720	26.734	206.351	-27.727	59.110	99.804
ZrO_2	12.225	26.704	-249.651	-71.504	-128.683	11.204	-7.866	15.043	-137.008	-13.881	30.389	2.853
Others	-13.909	0.105	-419.874	-5.242	8.866	69.121	179.428	41.515	-238.677	-37.314	109.623	80.657
Mg*Ti	-688.870	-1343.644	6967.981	-257.909	-6298.682	1903.939	-8757.361	210.261	21095.088	966.561	-11245.704	-1539.299
Al*K	-2482.487	-384.074	-101.034	-808.851	-14495.261	882.415	-413.746	471.499	-30795.454	232.872	-996.247	-312.494
Ca*Fe	656.185	152.426	-8610.547	-2921.266	-640.081	1134.751	393.894	790.337	-1025.364	-309.738	694.824	570.967
K*Zn	-533.629	-898.794	5021.967	265.772	-12170.533	-255.183	-2267.731	-378.174	-8650.599	858.525	-2731.454	-3224.093
B*Ca	368.097	-1220.711	-5149.304	-212.656	530.334	610.951	-368.033	412.235	14397.769	34.097	-1290.510	264.583
B*S	147.438	-5522.539	-5655.825	2393.223	-20669.003	6382.439	6675.352	2881.822	-309995.803	-969.630	8013.272	-1274.261
Mg*Ot	1547.665	-305.781	1604.566	550.033	1217.197	-1170.948	-5879.079	-681.420	12778.391	576.660	-3134.980	-2442.339
Ca*Si	894.699	230.821	-8461.646	-336.062	1199.497	1070.254	1058.675	702.910	-4505.053	-646.822	1148.823	562.024

	ZrO_2	Others	Mg*Ti	Al*K	Ca*Fe	K*Zn	B*Ca	B*S	Mg*Ot	Ca*Si
Al_2O_3	12.225	-13.909	-688.870	-2482.487	656.185	-533.629	368.097	147.438	1547.665	894.699
B_2O_3	26.704	0.105	-1343.644	-384.074	152.426	-898.794	-1220.711	-5522.539	-305.781	230.821
CaO	-249.651	-419.874	6967.981	-101.034	-8610.547	5021.967	-5149.304	-5655.825	1604.566	-8461.646
Fe_2O_3	-71.504	-5.242	-257.909	-808.851	-2921.266	265.772	-212.656	2393.223	550.033	-336.062
K_2O	-128.683	8.866	-6298.682	-14495.261	-640.081	-12170.533	530.334	-20669.003	1217.197	1199.497
Li_2O	11.204	69.121	1903.939	882.415	1134.751	-255.183	610.951	6382.439	-1170.948	1070.254
MgO	-7.866	179.428	-8757.361	-413.746	393.894	-2267.731	-368.033	6675.352	-5879.079	1058.675
Na_2O	15.043	41.515	210.261	471.499	790.337	-378.174	412.235	2881.822	-681.420	702.910
SO_3	-137.008	-238.677	21095.088	-30795.454	-1025.364	-8650.599	14397.769	-309995.803	12778.391	-4505.053
SiO_2	-13.881	-37.314	966.561	232.872	-309.738	858.525	34.097	-969.630	576.660	-646.822
TiO_2	30.389	109.623	-11245.704	-996.247	694.824	-2731.454	-1290.510	8013.272	-3134.980	1148.823
ZnO	2.853	80.657	-1539.299	-312.494	570.967	-3224.093	264.583	-1274.261	-2442.339	562.024
ZrO_2	113.567	-13.127	256.601	1849.518	1313.467	419.483	-39.272	360.660	1220.260	454.581
Others	-13.127	389.566	-2894.300	1923.220	545.160	-2373.485	358.245	5489.616	-11748.678	833.061
Mg*Ti	256.601	-2894.300	425877.106	42710.709	-1613.590	98313.981	29730.374	-178021.417	51760.496	-23099.232
Al*K	1849.518	1923.220	42710.709	194556.976	18162.903	62648.601	-6639.187	323696.166	-64304.459	330.296
Ca*Fe	1313.467	545.160	-1613.590	18162.903	49736.137	-3634.523	10067.958	4848.772	-2801.412	12306.669
K*Zn	419.483	-2373.485	98313.981	62648.601	-3634.523	217820.023	7684.770	54401.278	64551.675	-13600.138
B*Ca	-39.272	358.245	29730.374	-6639.187	10067.958	7684.770	33928.822	-130198.800	14671.817	3614.696
B*S	360.660	5489.616	-178021.417	323696.166	4848.772	54401.278	-130198.800	3226486.902	-239516.271	45435.353
Mg*Ot	1220.260	-11748.678	51760.496	-64304.459	-2801.412	64551.675	14671.817	-239516.271	536318.597	-5789.555
Ca*Si	454.581	833.061	-23099.232	330.296	12306.669	-13600.138	3614.696	45435.353	-5789.555	17968.042

Note: Products such as Mg*Ti are actually products of oxides, MgO*TiO_2. The elemental format was used to save space in the table headings.

Table D.3. Variance-Covariance Matrix Associated With the Estimated Coefficients of the ILAW PCT-Boron Reduced LM Model

	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SiO_2	TiO_2	ZrO_2
Al_2O_3	5.957	-1.443	-0.036	-0.887	-0.183	-1.145	-1.218	-0.540	-0.088	-2.314	-0.251
B_2O_3	-1.443	2.813	-0.111	0.628	0.798	0.201	0.992	0.051	-0.508	0.660	-0.584
CaO	-0.036	-0.111	2.582	-0.438	0.062	-1.219	0.506	0.500	-0.314	-0.898	-0.322
$F_{e2}O_3$	-0.887	0.628	-0.438	3.193	-1.155	0.478	0.207	0.089	-0.302	-0.582	0.067
K_2O	-0.183	0.798	0.062	-1.155	7.840	1.029	3.015	0.266	-0.434	-0.750	-0.176
Li_2O	-1.145	0.201	-1.219	0.478	1.029	12.357	0.646	2.257	-0.959	0.242	-1.207
MgO	-1.218	0.992	0.506	0.207	3.015	0.646	8.569	0.357	-0.758	-0.192	1.069
Na_2O	-0.540	0.051	0.500	0.089	0.266	2.257	0.357	1.108	-0.397	-0.291	-0.411
SiO_2	-0.088	-0.508	-0.314	-0.302	-0.434	-0.959	-0.758	-0.397	0.411	-0.185	-0.261
TiO_2	-2.314	0.660	-0.898	-0.582	-0.750	0.242	-0.192	-0.291	-0.185	15.253	2.493
ZrO_2	-0.251	-0.584	-0.322	0.067	-0.176	-1.207	1.069	-0.411	-0.261	2.493	9.111

Table D.4. Variance-Covariance Matrix Associated With the Estimated Coefficients of the ILAW PCT-Boron Reduced PQM Model

	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SiO_2	TiO_2	ZrO_2	B*Mg	Li*Zr	Fe*Li
Al_2O_3	4.160	0.132	-0.343	-1.005	-0.034	-2.170	4.731	-0.852	-0.043	-1.746	0.237	-61.845	1.014	8.489
B_2O_3	0.132	3.944	-0.695	-1.033	0.599	-3.481	11.901	-1.006	-0.313	-0.205	1.162	-126.097	-20.697	37.461
CaO	-0.343	-0.695	2.017	-0.941	0.063	-3.262	-4.436	0.922	-0.147	-0.533	-1.629	52.700	44.143	40.861
Fe_2O_3	-1.005	-1.033	-0.941	7.771	-0.867	16.827	-0.147	-0.656	-0.318	0.454	1.552	1.761	-87.641	-255.801
K_2O	-0.034	0.599	0.063	-0.867	4.937	-0.935	2.241	0.186	-0.216	-0.667	-1.332	-5.970	45.413	7.611
Li_2O	-2.170	-3.481	-3.262	16.827	-0.935	67.900	2.762	-1.478	-1.532	4.292	18.375	-10.520	-770.984	-754.079
MgO	4.731	11.901	-4.436	-0.147	2.241	2.762	72.895	-7.061	-0.672	-2.568	12.527	-756.321	-269.016	-139.959
Na_2O	-0.852	-1.006	0.922	-0.656	0.186	-1.478	-7.061	1.580	-0.184	-0.093	-2.282	80.845	59.949	48.476
SiO_2	-0.043	-0.313	-0.147	-0.318	-0.216	-1.532	-0.672	-0.184	0.281	-0.208	-0.841	1.490	24.552	7.062
TiO_2	-1.746	-0.205	-0.533	0.454	-0.667	4.292	-2.568	-0.093	-0.208	9.885	3.443	30.141	-78.177	-33.127
ZrO_2	0.237	1.162	-1.629	1.552	-1.332	18.375	12.527	-2.282	-0.841	3.443	23.693	-111.659	-626.741	-113.574
B*Mg	-61.845	-126.097	52.700	1.761	-5.970	-10.520	-756.321	80.845	1.490	30.141	-111.659	8489.722	2263.913	1595.341
Li*Zr	1.014	-20.697	44.143	-87.641	45.413	-770.984	-269.016	59.949	24.552	-78.177	-626.741	2263.913	22248.652	5194.522
Fe*Li	8.489	37.461	40.861	-255.801	7.611	-754.079	-139.959	48.476	7.062	-33.127	-113.574	1595.341	5194.522	11641.429

Note: Products such as B*Mg are actually products of oxides, B_2O_3*MgO. The elemental format was used to save space in the table headings.

Table D.5. Variance-Covariance Matrix Associated With the Estimated Coefficients of the ILAW PCT-Sodium Reduced LM Model

	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SiO_2	TiO_2	ZrO_2
Al_2O_3	2.639	-0.639	-0.016	-0.393	-0.081	-0.507	-0.540	-0.239	-0.039	-1.025	-0.111
B_2O_3	-0.639	1.246	-0.049	0.278	0.354	0.089	0.439	0.023	-0.225	0.292	-0.259
CaO	-0.016	-0.049	1.144	-0.194	0.027	-0.540	0.224	0.221	-0.139	-0.398	-0.143
Fe_2O_3	-0.393	0.278	-0.194	1.414	-0.512	0.212	0.091	0.039	-0.134	-0.258	0.029
K_2O	-0.081	0.354	0.027	-0.512	3.473	0.456	1.336	0.118	-0.192	-0.332	-0.078
Li_2O	-0.507	0.089	-0.540	0.212	0.456	5.474	0.286	1.000	-0.425	0.107	-0.535
MgO	-0.540	0.439	0.224	0.091	1.336	0.286	3.796	0.158	-0.336	-0.085	0.473
Na_2O	-0.239	0.023	0.221	0.039	0.118	1.000	0.158	0.491	-0.176	-0.129	-0.182
SiO_2	-0.039	-0.225	-0.139	-0.134	-0.192	-0.425	-0.336	-0.176	0.182	-0.082	-0.116
TiO_2	-1.025	0.292	-0.398	-0.258	-0.332	0.107	-0.085	-0.129	-0.082	6.756	1.104
ZrO_2	-0.111	-0.259	-0.143	0.029	-0.078	-0.535	0.473	-0.182	-0.116	1.104	4.036

Table D.6. Variance-Covariance Matrix Associated With the Estimated Coefficients of the ILAW PCT-Sodium Reduced PQM Model

	Al_2O_3	B_2O_3	CaO	Fe_2O_3	K_2O	Li_2O	MgO	Na_2O	SiO_2	TiO_2	ZrO_2
Al_2O_3	2.338	-1.251	-0.172	-0.209	-5.412	-0.336	-0.051	-0.432	0.171	-0.669	0.569
B_2O_3	-1.251	4.481	-0.222	-0.866	12.190	-2.711	9.325	-0.255	-0.541	-0.214	-0.572
CaO	-0.172	-0.222	0.880	-0.262	1.734	-1.527	-1.991	0.378	-0.075	-0.211	-0.937
Fe_2O_3	-0.209	-0.866	-0.262	3.856	3.297	6.695	-1.670	-0.340	-0.084	0.266	-0.086
K_2O	-5.412	12.190	1.734	3.297	107.574	-10.936	9.837	0.359	-1.971	-0.244	-14.020
Li_2O	-0.336	-2.711	-1.527	6.695	-10.936	29.398	0.116	-0.651	-0.443	1.794	8.995
MgO	-0.051	9.325	-1.991	-1.670	9.837	0.116	38.747	-2.622	-0.887	-1.368	5.147
Na_2O	-0.432	-0.255	0.378	-0.340	0.359	-0.651	-2.622	0.672	-0.100	-0.051	-0.946
SiO_2	0.171	-0.541	-0.075	-0.084	-1.971	-0.443	-0.887	-0.100	0.177	-0.070	-0.173
TiO_2	-0.669	-0.214	-0.211	0.266	-0.244	1.794	-1.368	-0.051	-0.070	4.138	1.391
ZrO_2	0.569	-0.572	-0.937	-0.086	-14.020	8.995	5.147	-0.946	-0.173	1.391	11.754
B*Mg	-9.528	-87.675	23.109	13.647	-74.321	3.970	-382.552	31.135	5.496	14.959	-45.912
Li*Zr	-8.917	12.531	24.606	-17.923	328.419	-352.129	-117.470	24.603	6.581	-31.295	-305.448
Fe*K	-1.106	0.003	-15.202	-58.698	-590.276	56.063	101.120	4.428	1.603	-6.151	96.346
Fe*Li	-4.058	32.085	17.121	-110.564	59.698	-320.842	-30.939	21.288	0.598	-14.706	-51.454
B*K	55.599	-121.511	-8.155	-1.608	-715.478	73.291	-151.962	-5.550	18.169	3.387	78.535

	B*Mg	Li*Zr	Fe*K	Fe*Li	B*K
Al_2O_3	-9.528	-8.917	-1.106	-4.058	55.599
B_2O_3	-87.675	12.531	0.003	32.085	-121.511
CaO	23.109	24.606	-15.202	17.121	-8.155
Fe_2O_3	13.647	-17.923	-58.698	-110.564	-1.608
K_2O	-74.321	328.419	-590.276	59.698	-715.478
Li_2O	3.970	-352.129	56.063	-320.842	73.291
MgO	-382.552	-117.470	101.120	-30.939	-151.962
Na_2O	31.135	24.603	4.428	21.288	-5.550
SiO_2	5.496	6.581	1.603	0.598	18.169
TiO_2	14.959	-31.295	-6.151	-14.706	3.387
ZrO_2	-45.912	-305.448	96.346	-51.454	78.535
B*Mg	4080.911	985.624	-810.415	444.984	1222.864
Li*Zr	985.624	10323.527	-2355.079	2240.077	-1719.814
Fe*K	-810.415	-2355.079	6311.016	136.593	2176.393
Fe*Li	444.984	2240.077	136.593	4957.526	-658.094
B*K	1222.864	-1719.814	2176.393	-658.094	5960.074

Note: Products such as B*Mg are actually products of oxides, B_2O_3*MgO. The elemental format was used to save space in the table headings.

R&T Subcontractor Document Review Record

1) To Be Completed by Cognizant R&T Personnel		
Document Number VSL-04R4480-2	Revision 0	Document Title Final Report: Phase 1 ILAW PCT & VHT Model Development
Test Spec: 24590-LAW-TSP-RT-01-013, Rev 1 24590-WTP-TSP-RT-02-001, Rev. 0		Scoping Statement(s): VSL-21Law Glass Property Composition Modeling VSL-22, LAW Processing Properties Models

R&T Contact:	Keith Abel	MS5-L	371-3086	11/30/04
	Name (Print)	MSIN	Telephone Number	Date

Review Distribution

Organization	Contact	MSIN	Required?
Process Operations	D McLaughlin	MS4-B2	Yes ☒ No ☐
Quality Assurance	M Mitchell	MS14-4B	Yes ☐ No ☒
Environmental and Nuclear Safety	E Sauceda	MS4-C1	Yes ☐ No ☒
Commissioning and Training	K Vacca	MS12-B	Yes ☐ No ☒
Engineering	M Ongpin	MS4-A2	Yes ☒ No ☐
R&T Functional Manager	C Musick	MS1-B	Yes ☒ No ☐
Subcontracts	L S Jenkins	MS14-3A	Yes ☐ No ☒
			Yes ☐ No ☐
			Yes ☐ No ☐
			Yes ☐ No ☐

Comments Due By: 12/14/04

Required Reviewers are required to respond to the R&T Contact.

2) To be Completed by Reviewer

Reviewer	E. SAUCEDA/POC	EFNS	12/15/04
	Name (Print)	Organization	Date

☒ Accepted, No Comments	☐ Accepted, Comments Not Significant	☐ Significant Comments, Form 24590-MGT-F00006 Attached	☐ Significant Comments, Comments Marked on Document

3) To be Completed by Reviewer*

My significant comments have been addressed.

Acceptance: _____ _____ _____

Print/Type Name *Signature* *Date*

* *An e-mail to the R&T contact stating that significant comments are addressed can substitute for this acceptance.*

Abel, Keith H.

From: Sauceda, Ermelinda
Sent: Wednesday, December 15, 2004 12:56 PM
To: Abel, Keith H.
Subject: RE: Document Review for VSL Report: Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. 0

No comments from E&NS

-----Original Message-----
From: Abel, Keith H.
Sent: Wednesday, December 15, 2004 8:32 AM
To: Sauceda, Ermelinda
Subject: FW: Document Review for VSL Report: Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. 0
Importance: High

Emmy,

Will there be any comments from ES&H?

Thanks,

Keith

-----Original Message-----
From: Abel, Keith H.
Sent: Monday, December 13, 2004 8:47 AM
To: Sauceda, Ermelinda; Mitchell, Michelle; Ongpin, Maria; Vacca, Karen; Jenkins, L. S (Scot)
Cc: Reed, Ronald D; Bostic, Lee; Wells, Kenneth R; Doyle, Jeanette; Damerow, Frederick; Musick, Chris A; Vienna, John; 'Joseph H Westsik Jr (E-mail)'; Gimpel, Rod; Pillai, Rathini; Westsik, Joseph
Subject: RE: Document Review for VSL Report: Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. 0

Just a note of reminder. Comments are due by tomorrow on the report listed above.

Thank you for your assistance.

Keith Abel

-----Original Message-----
From: Abel, Keith H.
Sent: Tuesday, November 30, 2004 7:46 AM
To: Sauceda, Ermelinda; Mitchell, Michelle; Ongpin, Maria; Vacca, Karen; Jenkins, L. S (Scot)
Cc: Reed, Ronald D; Bostic, Lee; Wells, Kenneth R; Doyle, Jeanette; Damerow, Frederick; Musick, Chris A; Vienna, John; Joseph H Westsik Jr (E-mail); Gimpel, Rod; Pillai, Rathini; Westsik, Joseph
Subject: Document Review for VSL Report: Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. 0

We are requesting your assistance in review and finalization of the joint Battelle/VSL report ***Phase 1 ILAW PCT and VHT Model Development***, **VSL-04R4480-2, Rev. A.** The Document Review Record Form, the Comment Resolution Form for comments and an electronic version of the report are attached. This report describes initial experimental work at VSL and PCT and VHT model development by VSL and Battelle staff for ILAW glasses. We appreciate your assistance in finalizing this document.

Comments are due no later than December 14, 2004

If you have any questions regarding this review request, please contact me(371-3086) or Chris Musick (371-3881)

Please provide comments using the attached electronic DRR and CRF, if required, by e-mail back to me.

Thank you for your assistance in the review and finalization of this document.

Keith Abel

<< File: VSL PCT VHT Report Doc Rev Rec 11 04.doc >> << File: VSL PCT VHT Commnt Res Form 1104.doc >> << File: LAW PCT VHT Model Report RevA.pdf >>

Abel, Keith H.

From: Wells, Kenneth R
Sent: Monday, December 13, 2004 12:05 PM
To: Abel, Keith H.
Subject: RE: Document Review for VSL Report: Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. 0

No comments from Ken Wells.

-----Original Message-----
From: Abel, Keith H.
Sent: Monday, December 13, 2004 8:47 AM
To: Sauceda, Ermelinda; Mitchell, Michelle; Ongpin, Maria; Vacca, Karen; Jenkins, L. S (Scot)
Cc: Reed, Ronald D; Bostic, Lee; Wells, Kenneth R; Doyle, Jeanette; Damerow, Frederick; Musick, Chris A; Vienna, John; 'Joseph H Westsik Jr (E-mail)'; Gimpel, Rod; Pillai, Rathini; Westsik, Joseph
Subject: RE: Document Review for VSL Report: Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. 0

Just a note of reminder. Comments are due by tomorrow on the report listed above.

Thank you for your assistance.

Keith Abel

-----Original Message-----
From: Abel, Keith H.
Sent: Tuesday, November 30, 2004 7:46 AM
To: Sauceda, Ermelinda; Mitchell, Michelle; Ongpin, Maria; Vacca, Karen; Jenkins, L. S (Scot)
Cc: Reed, Ronald D; Bostic, Lee; Wells, Kenneth R; Doyle, Jeanette; Damerow, Frederick; Musick, Chris A; Vienna, John; Joseph H Westsik Jr (E-mail); Gimpel, Rod; Pillai, Rathini; Westsik, Joseph
Subject: Document Review for VSL Report: Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. 0

We are requesting your assistance in review and finalization of the joint Battelle/VSL report ***Phase 1 ILAW PCT and VHT Model Development***, **VSL-04R4480-2, Rev. A.** The Document Review Record Form, the Comment Resolution Form for comments and an electronic version of the report are attached. This report describes initial experimental work at VSL and PCT and VHT model development by VSL and Battelle staff for ILAW glasses. We appreciate your assistance in finalizing this document.

Comments are due no later than December 14, 2004

If you have any questions regarding this review request, please contact me(371-3086) or Chris Musick (371-3881)

Please provide comments using the attached electronic DRR and CRF, if required, by e-mail back to me.

Thank you for your assistance in the review and finalization of this document.

Keith Abel

<< File: VSL PCT VHT Report Doc Rev Rec 11 04.doc >> << File: VSL PCT VHT Commnt Res Form 1104.doc >> << File: LAW PCT VHT Model Report RevA.pdf >>

Abel, Keith H.

From: Vienna, John
Sent: Monday, December 13, 2004 12:56 PM
To: Abel, Keith H.
Subject: RE: Document Review for VSL Report: Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. 0

No comments.

-----Original Message-----
From: Abel, Keith H.
Sent: Monday, December 13, 2004 8:47 AM
To: Sauceda, Ermelinda; Mitchell, Michelle; Ongpin, Maria; Vacca, Karen; Jenkins, L. S (Scot)
Cc: Reed, Ronald D; Bostic, Lee; Wells, Kenneth R; Doyle, Jeanette; Damerow, Frederick; Musick, Chris A; Vienna, John; 'Joseph H Westsik Jr (E-mail)'; Gimpel, Rod; Pillai, Rathini; Westsik, Joseph
Subject: RE: Document Review for VSL Report: Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. 0

Just a note of reminder. Comments are due by tomorrow on the report listed above.

Thank you for your assistance.

Keith Abel

-----Original Message-----
From: Abel, Keith H.
Sent: Tuesday, November 30, 2004 7:46 AM
To: Sauceda, Ermelinda; Mitchell, Michelle; Ongpin, Maria; Vacca, Karen; Jenkins, L. S (Scot)
Cc: Reed, Ronald D; Bostic, Lee; Wells, Kenneth R; Doyle, Jeanette; Damerow, Frederick; Musick, Chris A; Vienna, John; Joseph H Westsik Jr (E-mail); Gimpel, Rod; Pillai, Rathini; Westsik, Joseph
Subject: Document Review for VSL Report: Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. 0

We are requesting your assistance in review and finalization of the joint Battelle/VSL report ***Phase 1 ILAW PCT and VHT Model Development***, **VSL-04R4480-2, Rev. A.** The Document Review Record Form, the Comment Resolution Form for comments and an electronic version of the report are attached. This report describes initial experimental work at VSL and PCT and VHT model development by VSL and Battelle staff for ILAW glasses. We appreciate your assistance in finalizing this document.

Comments are due no later than December 14, 2004

If you have any questions regarding this review request, please contact me(371-3086) or Chris Musick (371-3881)

Please provide comments using the attached electronic DRR and CRF, if required, by e-mail back to me.

Thank you for your assistance in the review and finalization of this document.

Keith Abel

<< File: VSL PCT VHT Report Doc Rev Rec 11 04.doc >> << File: VSL PCT VHT Commnt Res Form 1104.doc >> << File: LAW PCT VHT Model Report RevA.pdf >>

Abel, Keith H.

From: Babel, Carol A [Carol_A_Babel@RL.gov]
Sent: Monday, December 13, 2004 3:46 PM
To: Abel, Keith H.
Subject: RE: Document Review for VSL Report: Phase 1 ILAW PCT and VHT Mode l De velopment, VSL-04R4480-2, Rev. 0

Keith,

Thank you for the opportunity to review the draft final report, "Phase 1 ILAW PCT and VHT Model Development," VSL-04R4480-2, Rev. 0. I have completed my review and have no comments at this time.

Carol Babel, 373-9281
LAW Federal Area Engineer, ORP/WED

-----Original Message-----
From: Abel, Keith H. [mailto:khabel@bechtel.com]
Sent: Tuesday, November 30, 2004 7:56 AM
To: Babel, Carol A; Abdul, Wahed
Cc: Westsik, Joseph; Musick, Chris A; Doyle, Jeanette; Damerow, Frederick
Subject: Document Review for VSL Report: Phase 1 ILAW PCT and VHT Model De velopment, VSL-04R4480-2, Rev. 0

Carol & Wahed,

We are requesting your assistance in review of the joint Battelle VSL report Phase 1 ILAW PCT and VHT Model Development, VSL-04R4480-2, Rev. A. The Document Review Record Form, the Comment Resolution Form for comments and an electronic version of the report are attached. This report describes initial experimental work at VSL and PCT and VHT model development by VSL and Battelle staff for ILAW glasses. We appreciate your assistance in finalizing this document.

Comments are due no later than December 14, 2004

If you have any questions regarding this review request, please contact me(371-3086) or Chris Musick (371-3881)

Please provide comments using the attached electronic DRR and CRF, if required, by e-mail back to me.

Thank you for your assistance in the review and finalization of this document.

Keith Abel
<<VSL PCT VHT Report Doc Rev Rec 11 04.doc>>
<<VSL PCT VHT Commnt Res Form 1104.doc>> <<LAW PCT VHT Model Report RevA.pdf>>

Abel, Keith H.

From: Abel, Keith H.
Sent: Tuesday, January 18, 2005 8:09 AM
To: Abel, Keith H.
Subject: VSL/PNL Report VSL-04R4480-2, Final Report: Phase I ILAW PCT & VHT Model Development, Rev. 0

I concur with the responses provided for comment resolution. The report should be revised as stated, finalized and submitted for final project acceptance.

Keith

R+T

Abel, Keith H.

From: Westsik, Joseph
Sent: Tuesday, January 18, 2005 8:02 AM
To: Abel, Keith H.
Subject: RE: VSL/PNL responses on ILAW PCT VHT report

Keith,
I concur with the comment responses for the report *Phase 1 ILAW PCT and VHT Model Development*, VSL-04R4480-2.

Joe

-----Original Message-----
From: Abel, Keith H.
Sent: Tuesday, January 18, 2005 6:56 AM
To: Westsik, Joseph; Joseph H Westsik Jr (E-mail)
Subject: VSL/PNL responses on ILAW PCT VHT report

<< File: VSL PCT VHT Commnt Responses 1104 jhw .doc >>
Joe,

Here are the responses to your comments on the report. Let me know if your comments are resolved.

Thanks,

Keith

Abel, Keith H.

From: Pillai, Rathini
Sent: Tuesday, January 18, 2005 2:19 PM
To: Abel, Keith H.
Cc: Ongpin, Maria; Mclaughlin, Doris
Subject: RE: Comment Response on ILAW PCT VHT Report draft

Engineering concurs on VSL-04R4480-2

-----Original Message-----
From: Abel, Keith H.
Sent: Tuesday, January 18, 2005 1:53 PM
To: Pillai, Rathini
Subject: RE: Comment Response on ILAW PCT VHT Report draft

Rathini,

I stopped up and got Rod's signature for resolution, he was the only commenter, for the Engineering comments on VSL-04R4480-2 "Final Report: Phase I ILAW PCT and VHT Model Development".

Please forward the Engineering concurrence for Comment Resolution so that I can have the contractor finalize the document.

Thanks,

Keith
371-3086

-----Original Message-----
From: Abel, Keith H.
Sent: Tuesday, January 18, 2005 9:06 AM
To: Pillai, Rathini
Subject: FW: Comment Response on ILAW PCT VHT Report draft

Rathini,

FYI. I sent this to Rod this morning for his concurrence. Forgot you on original transmittal, so am forwarding now...

Keith

-----Original Message-----
From: Abel, Keith H.
Sent: Tuesday, January 18, 2005 6:59 AM
To: Gimpel, Rod
Subject: Comment Response on ILAW PCT VHT Report draft

<< File: VSL PCTVHT Commnt Responses 1104 rg.doc >>

Rod,

Attached are the VSL and PNL responses to your comments on the draft. Please review and let me know if your comments are resolved or whether you need additional changes in the draft.

Thanks,

Keith

R&T Technology Issues Summary

Test Report Title: Phase 1 ILAW PCT and VHT Model Development

Test Report Number: VSL-04R4480-2 Rev 0

Prepared By: Keith Abel / Joe Westsik **Date:** February 8, 2005

Signature: K A J. Westsik

Does the Testing or Report reveal any new discoveries, technology issues, or suggest potential follow-on work?	**Yes**	**No**
	☒	☐

If yes, describe the suggested activity.

This document describes the initial development of models to describe VHT and PCT behavior in relation to chemical composition for ILAW glasses. The Research and Technology program plan for ILAW VHT and PCT contains follow-on work to finalize model development and validate the models after the development phase. The final models and model validation will be reported in a subsequent document.

If appropriate, is a Request for Technology Development attached.	**Yes**	**No**
	☐	☒

Additional comments (include researcher recommendations):