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Statistical Modeling and Optimization of Nuclear Waste Vitrification

Todd E. Combs

STATISTICAL MODELING AND OPTIMIZATION OF NUCLEAR WASTE VITRIFICATION

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THESIS

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THESIS APPROVAL

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Table of Contents

List of Figures

List of Tables

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Abstract

This thesis describes the development of a methodology to minimize the cost of vitrifying nuclear waste. Pacific Northwest Laboratory (PNL) regression models are used as baseline equations for modeling glass properties such as viscosity, electrical conductivity, and two types of durability. Revised PNL regression models are developed that eliminate insignificant variables from the original models. The Revised PNL regression model for electrical conductivity is shown to better predict electrical conductivity than the original PNL regression model. Neural networks are developed for viscosity and the two types of durability, PCT-B and MCC-1 B. The neural network models are shown to outperform every PNL and Revised PNL regression model in terms of predicting property values for viscosity, PCT-B, and MCC-1 B. The combined Neural Network/Revised PNL 2nd order electrical conductivity models are shown to be the best classifiers of nuclear waste glass, i.e. they have the highest probability of classifying a vitrified waste form as glass when it actually did produce glass in the laboratory. Finally, five nonlinear programs are developed with constraints containing 1) the PNL original 1st order models, 2) the PNL original 2nd order models, 3) the Revised PNL 1st order models, 4) the Revised PNL 2nd order models, and 5) the Neural Network/Revised PNL 2nd order electrical conductivity models. The Neural Network/Revised PNL 2nd order electrical conductivity nonlinear program is shown to minimize the total expected cost of vitrifying nuclear waste glass. This nonlinear program allows DOE to minimize its risk and cost of high-level nuclear waste vitrification.

STATISTICAL MODELING AND OPTIMIZATION OF NUCLEAR WASTE VITRIFICATION

1. INTRODUCTION

1.1 Historical Background

Vitrification is the process of turning an object into glass. For the purposes of this research, I will study the vitrification of nuclear waste.

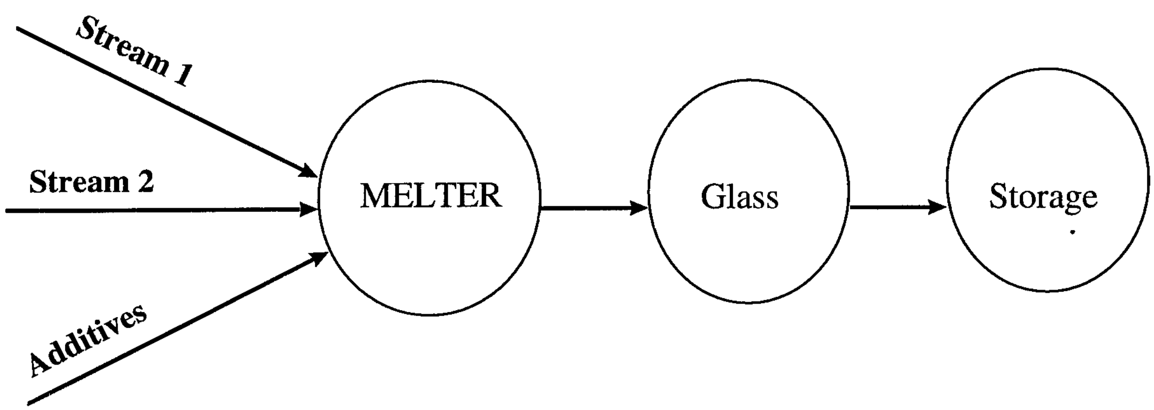

Figure 1--General Overview of Nuclear Waste Vitrification

Figure 1 displays an overview of the waste vitrification process. One or more waste streams are placed into a joule-heated melter along with any necessary chemical additives. The melter turns the waste streams and additives into a molten glass form. The glass form is poured into canisters, allowed to cool, and placed into long-term storage facilities.

Studies have been done for over two decades to characterize high-level nuclear waste glass. Pacific Northwest Laboratory established a program to characterize high-level nuclear waste glass in 1975 and published its first report on the subject in 1977 (2:1). These studies usually focus on how different compositions of glass will affect certain properties of the glass. Researchers are usually concerned with developing models to predict a nuclear waste glass's properties given its particular composition. The models generally take two forms: equations determined by the theoretical physics of glass formation or empirically derived regression equations.

Once the predictor equations have been formed, no researcher to date has attempted to take advantage of these equations in optimizing the production of nuclear waste glass with respect to cost. White et. al. developed a simple linear program within a simulation of the vitrification process, but this first attempt still did not take advantage of existing property prediction models (23:35). The constraints in their model were only approximate bounds for the components of the waste glass. This study will take the obvious next step in nuclear glass cost optimization by incorporating existing and newly developed predictor models for glass properties into a nonlinear mathematical program.

1.2 Problem Statement and Scope

The goal of this research effort is to minimize the cost of vitrifying nuclear waste glass while satisfying properties such as viscosity, electrical conductivity, durability, and glass transition temperature requirements. Linear regression (linear and nonlinear) and multilayer perceptron models are used to build a region of feasible glass composition. Nonlinear programming (NLP) is then used to search this feasible region for the optimal (lowest cost) glass composition.

The data used in this study is based on high-level nuclear waste glass (3:175-177). Therefore, the resulting NLP models are able to reliably minimize the cost of vitrifying this type of waste only. The final presentation of the research to the Department of Energy (DOE) will include models which predict feasibility and a nonlinear optimization model minimizing cost.

1.3 Research Objectives

The following research objectives must be met to solve the proposed problem:

1. Data on waste vitrification must be obtained and transformed into the proper form for prediction modeling.

2. Statistical models must be developed to determine the effects that the chemical composition of waste glass has on the four measured properties: viscosity, electrical conductivity, and two types of durability. These model should outperform existing linear or nonlinear mixture models which include the linear regression model developed by Pacific Northwest Laboratory (PNL) (3).

3. The model will produce a region of glass feasibility. A mathematical optimization program will be developed to search for the minimum cost over the feasible region formed by the model.

1.4 Thesis Organization

Chapter II will review previous studies done on vitrification, neural networks, linear regression, and mathematical programming. Chapter III will discuss the methodology that will be used to solve the existing problem. Chapter IV will present the results of the application of the methodology from Chapter III. Finally, Chapter V will discuss the conclusions that can be made from the resulting research and recommend direction for future research.

II. LITERATURE SEARCH

2.1 Vitrification of Nuclear Waste

Historically, the properties studied in a vitrification project tend to depend on what agency is completing the research. The Environmental Protection Agency states that it examines four properties to determine whether a prediction of glass can be made using historical data. The four properties the EPA examines are, "organic content of the waste, concentration of specific metal ions in the waste, concentrations of compounds in the waste that interfere with the glassmaking process, and moisture content of the waste" (1:24-6).

This differs slightly from Pacific Northwest Laboratory, which from 1989 to 1994 performed another study called the Compositional Variation Study (CVS). The goals of the study as stated in Mixture Experiment Design and Property Modeling in a Multi-Year Nuclear Waste Glass Study are as follows (3:173):

1. Make nuclear waste glass and measure viscosity, electrical conductivity, transition temperature, and two types of durability over a wide compositional range.
2. Understand glass composition effects on those five properties and develop statistical models to describe the relationships.
3. Use the statistical models to make processable waste glass that meets product requirements.

The CVS study produced a significant amount of data on glass composition and properties. This data set will be used to form the new statistical models developed in this study. Since the CVS produced empirical models exclusively, it will also be used as a benchmark to compare the models developed in this thesis.

In 1993, Pacific Northwest Laboratory initiated a shift of focus on research from vitrifying strictly high-level nuclear waste to vitrifying mixed low-level nuclear waste. Mixed waste represents a broadened challenge for vitrification because its composition is highly uncertain (5:v).

The Catholic University of America then established a broad program to study the vitrification of various nuclear wastes. The program was called the Minimum Additive Waste Stabilization (MAWS) demonstration and was conducted at DOE sites such as Hanford, Idaho National Engineering Laboratory, Oak Ridge National Laboratory (6), and Fernald (7). Ian Pegg, one of the primary scientists conducting the demonstration, states the MAWS system is innovative because 1) it views the waste streams as process resources and 2) the chemical properties of the waste streams are used to minimize the cost of purchasing necessary additive chemicals (7:2). A shortcoming of the MAWS technology developed by Catholic University is that the process today makes no attempt to use mathematical optimization methods.

It is important to note that the United States is not the only country concerned with nuclear waste treatment and disposal. For example, in Canada, Munz and Chen published a paper describing how they vitrified mixed and high-level waste in a continuous transferred arc plasma melter (4:32). One of the goals of their research was to study how quantities of waste components disappear as vitrification occurs.

2.2 Statistical Models

As defined by Devore, "Regression analysis is the part of statistics that deals with investigation of the relationship between two or more variables related in a nondeterministic fashion" (22:454). An advanced tool in regression analysis is multiple linear regression. The multiple linear regression model is a good approximator for many functions because even if the true relationship between the dependent and independent variables is unknown, "over certain ranges of the regressor (independent) variables the linear regression model is an adequate approximation" (21:110).

2.2.1 Multiple Linear Regression. As defined by Montgomery and Peck, "Regression analysis is one of the most widely used statistical techniques for analyzing multifactor data" (20:v). One form of regression analysis is multiple linear regression. In multiple linear regression, a dependent variable (one of the four property values) is modeled as the linear sum of numerous independent variables (the mass fraction of the waste components). Thus, once a model is developed the dependent variable value can be predicted given a set of independent variable values. This type of function approximation is one of the fundamental uses of linear regression.

The multiple linear regression model takes the following form:

$$y = \beta_0 + \beta_1 x_1 + \ldots + \beta_n x_n + \varepsilon \quad (21:109)$$

where y is the dependent variable, the x's are the independent variables, and ε is the random error component of the model. For this study it is important to note that "any regression model that is linear in the parameters (the β's) is a linear regression model" (21:111). This means that a regression model can form a nonlinear surface and still be considered a linear multiple regression model. Therefore, another typical linear regression model contains two-factor interactions such as the following:

$$y = \beta_0 + \beta_1 x_1 + \cdots + \beta_i x_i + \beta_{12} x_{12} + \cdots \beta_{ij} x_{ij} + \varepsilon$$

where i = 1…n, j = 1..n, and x_{ij} is the interaction term for x_i and x_j. (21:111).

The method of least squares is used to estimate the parameters of most linear regression models. A full theoretical development of the estimators ($\hat{\beta}$'s) can be found in Montgomery and Peck (21:111-123). It is very important to note that the estimators are the minimum variance unbiased estimators of the β's. This means there exists no other unbiased estimators (where $E[\hat{\beta}] = \beta$) that more closely approximate the β's.

Once a model is developed, hypothesis testing must be conducted to determine whether a model is adequate. Two types of tests are conducted: 1) Is the regression model significant and 2) Is each model parameter significant. Test 1 indicates whether multiple linear regression, in general, is a good tool to capture the relationships between the dependent and independent variables. Test 2 gives an indication of whether particular independent variables should be included in the regression model.

The hypothesis for test 1 can be written as follows:

$$\begin{aligned} &H_0: \beta_1 = \beta_2 = \cdots = \beta_n = 0 \\ &H_1: \beta_j \neq 0 \text{ for at least one j} \end{aligned} \quad (21{:}128).$$

The hypothesis for test 2 can be written as follows:

$$\begin{aligned} &H_0: \beta_j = 0 \\ &H_1: \beta_j \neq 0 \text{ for every jth variable in the model} \end{aligned} \quad (21{:}128).$$

As a part of its computational results, Minitab produces a very good statistic to test each of these hypotheses. The statistic is the p-value. As stated in Probability and Statistics for Engineering and the Sciences:

> The P-value is the smallest level of significance at which H_0 would be rejected when a specified test procedure (generally the t-test statistic) is used on a given data set. Once the P-value has been determined, the conclusion at any particular level α results from comparing the P-value to α:
>
> a. P-value $\leq \alpha \Rightarrow$ reject H_0 at level α.

b. P-value > $\alpha \Rightarrow$ do not reject H_0 at level α. (22:315).

An α of 0.05 was chosen for all hypothesis tests performed in this study.

2.2.2 Neural Networks. For the purposes of this research, a trained artificial neural network is a specific model of the well-known general field of nonlinear regression. Skapura defines neural networks as "a collection of simple, analog signal processors, connected through links called connections" (8:6). This research focuses on the multi-layered perceptron (MLP) model.

Choosing the number of layers, number of hidden nodes, and learning strategies for the MLP can be a very time consuming process. Steppe proposed a methodology for choosing the structure of an artificial neural network which allows a scientific selection of the proper neural network algorithm and can decrease development time (10).

2.3 Nonlinear Programming

Choosing the proper search mechanism to optimize a nonlinear program can be difficult. The feasible region is probably nonlinear and possibly nonconvex and may even be disconnected.

For this study, all nonlinear optimization is accomplished using a General Reduced Gradient (GRG) solver that implements Lasdon and Waren's GRG2 code (MS Excel) (24:WWWeb). The GRG2 is used because: 1) Himmelblau performed nonlinear optimization over a variety of problems of varying difficulty. The GRG is the only solver that could optimize all of the problem types (13:386-431); and 2) Microsoft Excel is a popular spreadsheet package that uses the GRG algorithm in its nonlinear optimization solver. This makes the GRG accessible to DOE engineers who have a familiarity with nonlinear optimization.

III. METHODOLOGY

The following chapter will discuss the methodology used to solve the research problem. The solution process can be broken into three main components: 1) Statistical Modeling, 2) Nonlinear Programming, and 3) Discussion of measures of effectiveness to compare the various models.

3.1 Statistical Modeling

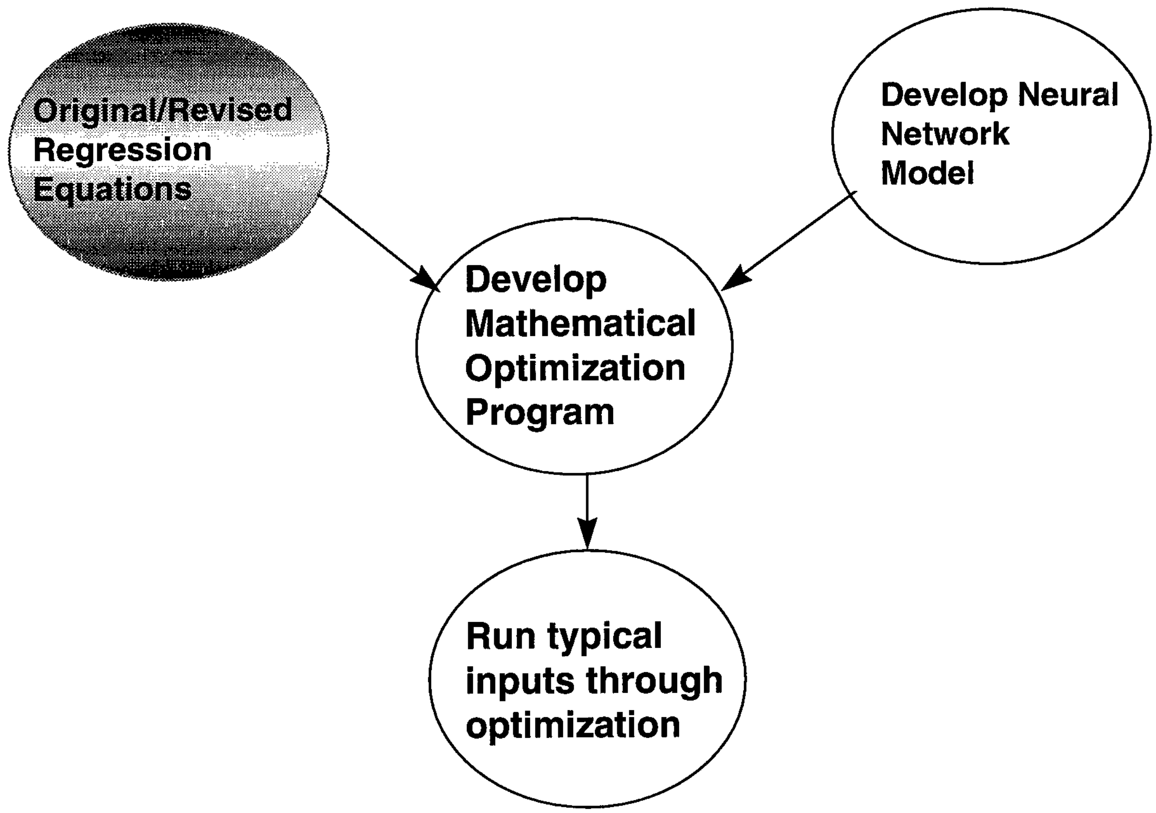

Figure 2-Modeling of PNL Original and Revised Regression Equations

Sections 3.1.1 and 3.1.2 discuss PNL's original regression equations and discuss the methodology used to revise these equations.

There are four types of glass properties modeled in this section: viscosity, electrical conductivity, and two types of durability (MCC and PCT). Transition temperature will not be modeled because although it is measured, there exists no standard range of transition temperature for a glass to be adequate. Two types of statistical tools are used to develop the four glass property models. This section of the chapter is broken into these two statistical tools: multiple linear regression and neural network modeling.

3.1.1 Pacific Northwest Laboratory Models. Piepel et al. developed baseline models for all regression analysis in this thesis (3:177-178). This paper discusses the Composition Variation Study (CVS) completed at PNL. The CVS used a general experimental design to: a) select a region of waste glass having acceptable properties and b) to investigate glasses on the exterior and interior of this region (3:173). The authors used a special form of the multiple linear regression model, the Scheffe 1st and 2nd order mixture models.

The Scheffe 1st and 2nd order mixture models have the following form:

Scheffe 1st Order Mixture Model

$$y = \sum_{i=1}^{10} b_i x_i ,$$

where b_i is the coefficient of the mass fraction of the ith component, x_i.

Scheffe 2nd Order Mixture Model

$$y = \sum_{i=1}^{10} b_i x_i + \sum_{i=1}^{10} \sum_{j \geq i}^{10} b_{ij} x_i x_j ,$$

where b_{ij} is the coefficient for the interaction term $x_i x_j$.

The models differ from the regression models previously discussed in that they contain no β_0. In addition, while they left all independent variables in the 1st order models they eliminated various two-factor interactions deemed insignificant in the 2nd order models. The data used for their analysis is found in Appendix A.

The four properties used in this thesis are as follows: viscosity (η), electrical conductivity (ε), and two types of durability (PCT B and MCC-1 B). The ten independent variables are: SiO2, B2O3, Na2O, Li2O, CaO, MgO, Fe2O3, Al2O3, ZrO2, and Others. These variables represent the mass fraction of each chemical found in the soil and additive mixture. The mass fraction is defined as the proportion of chemical found in the total mass of the soil and additive mixture. For example, if the total mixture is 100 kilograms and the mass of SiO2 is 50 kilograms, SiO2's mass fraction is 0.50. The Others variable represents 40 chemicals that also occur in high-level nuclear waste, but are not as significant as the nine explicitly stated above. The 10 independent input variables are further defined in Section 3.2.1. PNL found that they achieved the best results if a natural log transformation was performed on each dependent variable before regressing. The results for their models (in tabular form) are as follows:

Table 1. First and Reduced Second-Order Mixture Models for ln(Viscosity at 1150° C)

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
SiO2	8.968	0.237	10.987	0.254
B2O3	-6.204	0.442	-6.165	0.467
Na2O	-11.017	0.479	-26.388	2.480
Li2O	-34.239	1.069	-75.868	4.409
CaO	-7.466	0.791	-5.572	0.566
MgO	-2.776	0.874	-3.233	1.649
Fe2O3	-0.037	0.620	0.148	0.962
Al2O3	11.306	0.569	14.491	0.503
ZrO2	7.434	0.687	10.145	0.538
Others	-0.156	0.762	-2.119	0.981
B2O3 x Fe2O3			30.098	7.148
Na2O x Li2O			126.749	16.609
Na2O x MgO			29.875	12.028
Li2O x Others			78.943	20.439
MgO x Fe2O3			-39.527	13.508
Na2O x Na2O			43.574	8.890
Li2O x Li2O			296.59	41.326
R2	0.939		0.975	
R2(ADJ)	0.934		0.971	

Table 2. First and Reduced Second Order Mixture Models for ln(Elect Cond at 1150° C)

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
SiO2	0.847	0.150	0.303	0.154
B2O3	2.252	0.275	1.878	0.293
Na2O	11.040	0.307	14.543	0.419
Li2O	23.536	0.676	31.634	1.183
CaO	1.413	0.494	-0.223	0.535
MgO	1.056	0.547	0.720	0.453
Fe2O3	2.586	0.388	0.771	0.557
Al2O3	1.311	0.355	1.104	0.272
ZrO2	1.122	0.433	-0.329	0.579
Others	3.453	0.477	-5.287	2.626
Na2O x Li2O			-84.820	9.244
CaO x Fe2O3			28.333	7.013
B2O3 x Fe2O3			12.012	4.337
MgO x ZrO2			25.753	9.164
SiO2 x Others			17.260	5.403
Li2O x ZrO2			32.044	10.168
R2	0.931		0.973	
R2(ADJ)	0.926		0.969	

Table 3. First and Reduced Second Order Mixture Models for ln(PCT B)

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
SiO2	-4.303	0.568	-5.180	0.619
B2O3	11.831	1.101	13.811	1.139
Na2O	17.826	1.182	20.851	1.192
Li2O	22.970	2.665	23.454	2.188
CaO	-9.046	2.015	14.111	5.562
MgO	10.582	2.216	-36.638	14.982
Fe2O3	-3.101	1.554	-1.942	1.341
Al2O3	-25.443	1.395	-44.502	3.184
ZrO2	-10.630	1.773	-10.589	1.523
Others	0.164	1.919	2.771	1.616
SiO2 x MgO			97.566	30.293
B2O3 x CaO			-90.152	29.714
Na2O x CaO			-121.921	34.365
Al2O3 x Al2O3			126.554	17.688
R2	0.818		0.886	
R2(ADJ)	0.806		0.875	

Table 4. First and Reduced Second Order Mixture Models for ln(MCC-1 B)

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
SiO2	-0.223	0.395	-1.119	0.425
B2O3	10.039	0.747	15.430	0.985
Na2O	10.139	0.766	10.698	0.649
Li2O	12.067	1.719	13.124	1.392
CaO	3.481	1.258	-24.717	7.633
MgO	4.987	1.514	7.129	1.250
Fe2O3	5.809	1.116	6.122	0.981
Al2O3	-6.614	1.014	-12.546	2.406
ZrO2	-0.963	1.238	-1.820	1.065
Others	3.484	1.336	4.513	1.147
SiO2 x CaO			58.519	15.843
B2O3 x Al2O3			-70.216	12.270
Al2O3 x Al2O3			83.074	12.393
R2	0.675		0.794	
R2(ADJ)	0.652		0.774	

Notice the two statistics at the bottom of each row. R^2, the coefficient of multiple determination, is defined as, "A measure of the reduction in the variability of y obtained by using the regressor variables $x_1, x_2, ..., x_n$" (21:146). It takes on values between 0 and 1. Unfortunately, a large R^2 does not mean that the regression is a good fit. Extra factors will always increase the value of R^2. Because of this problem, the adjusted coefficient of multiple determination, R^2_{adj}, is often used instead to evaluate the overall regression. The adjusted coefficient of multiple determination is defined as follows:

$$\overline{R}^2_{adj} = 1 - \left(\frac{n-1}{n-p}\right)(1 - R^2_p) \quad (21:251).$$

The R^2_{adj} does not necessarily increase as you add independent variables to the model. Therefore, it will produce a better evaluation of each model.

As shown in Tables 1-4, the R^2_{adj} shows that the models for viscosity, electrical conductivity, and PCT B are all very good. Further examination of the coefficients of each model indicates that there still may be extraneous waste components in each model.

Take the shaded area in Table 1 for example. In the first order model, the coefficient for the Fe_2O_3 term is -0.037 while its standard deviation is 0.620. A statistical test may prove that the coefficient for the term is in fact, statistically equal to 0. This would lead to dropping the Fe_2O_3 term from the model.

This type of examination can be made on each model and motivates section 3.1.2 of this thesis.

3.1.2 Revised Multiple Linear Regression Models. As stated before, visual examination of each coefficient in the PNL models motivates a possible streamlining of each by eliminating excess variables. This is important because extraneous variables could skew the feasible region, and hence the results of the ensuing nonlinear program that uses the regression models.

The models were reduced using the stepwise regression, backward elimination method:

1. Regress using the general multiple linear regression models.
2. Conduct hypothesis tests 1 and 2 (from Section 2.2.1) on the model. If all tests do not reject H_0, stop.
3. After eliminating extraneous variables, regress over the new set of waste component variables. Return to step 2.

The models resulting from the stepwise regression are found in Sections 4.1.1.2 and 4.1.3 of Chapter 4.

3.1.3 Neural Network Modeling, the Multi-Layer Perceptron.

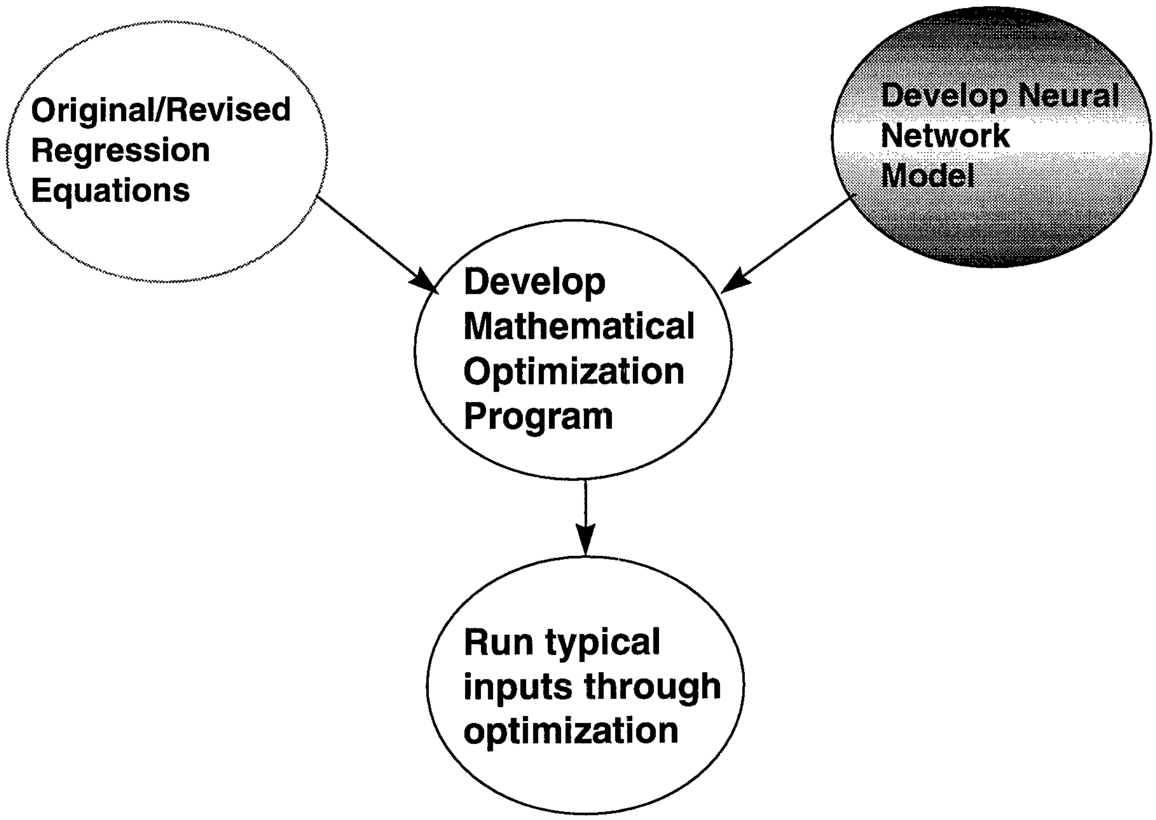

Figure 3--Modeling of Neural Networks

As seen in section 3.1.1, the second order regression models of PNL seemed to fit the data the best. There are many reasons to investigate using a multi-layer perceptron (MLP) instead of 2nd order linear regression to model the data.

First, the Pacific Northwest Laboratory's (PNL) study showed that regression equations with second order terms always modeled glass properties better than regression equations with only linear terms (3:177-78) . This indicates that the feasible glass composition region is probably nonlinear. The feasible region will be developed with a MLP because it can form nonlinear decision surfaces (9:214).

Second, the underlying population distributions for the four measured glass properties are unknown. A MLP is a nonparametric tool, and does not make the strong assumptions concerning underlying distributions that are typical of linear regression models. As Lippmann states, "They may thus prove to be more robust when distributions are generated by nonlinear processes and are strongly non-Gaussian" (12:4). The added robustness may allow the MLP to outperform the nonlinear mixture model that has been previously developed by PNL.

Third, there exists no *a priori* knowledge of the shape of the nonlinear feasible composition region. The MLP will provide a means to take data, adapt or learn from it, and build the nonlinear region.

Finally, the major reason for using an MLP is to increase the performance (data fitting) of the model. If a previous regression model had a very high R^2_{adj} value, there would be little motivation to use a more complex MLP to model the property.

There are four major concerns in developing a MLP: 1) determining how to present the data to the input layer, 2) determining what kind of network structure is optimal, 3) determining what learning algorithm to use, and 4) determining how to represent the output.

For the three modeled properties, the network is developed in the software package SNNAP (Statistical Neural Network Analysis Package) (26). SNNAP provides a proprietary expert system that suggests a network architecture to use given a particular set of data. This expert system suggested the following structure for each property:

1. All input data is standardized. This means the actual standardized input x to node i is:

$$x_i = \frac{(x_{oi} - \bar{x}_o)}{s_o}$$

where x_{oi} is the original input x_i,

$\bar{x}_o$ is the mean of all the original input values,

s_o is the standard deviation of the original input values.

2. The MLP's is structured as follows:

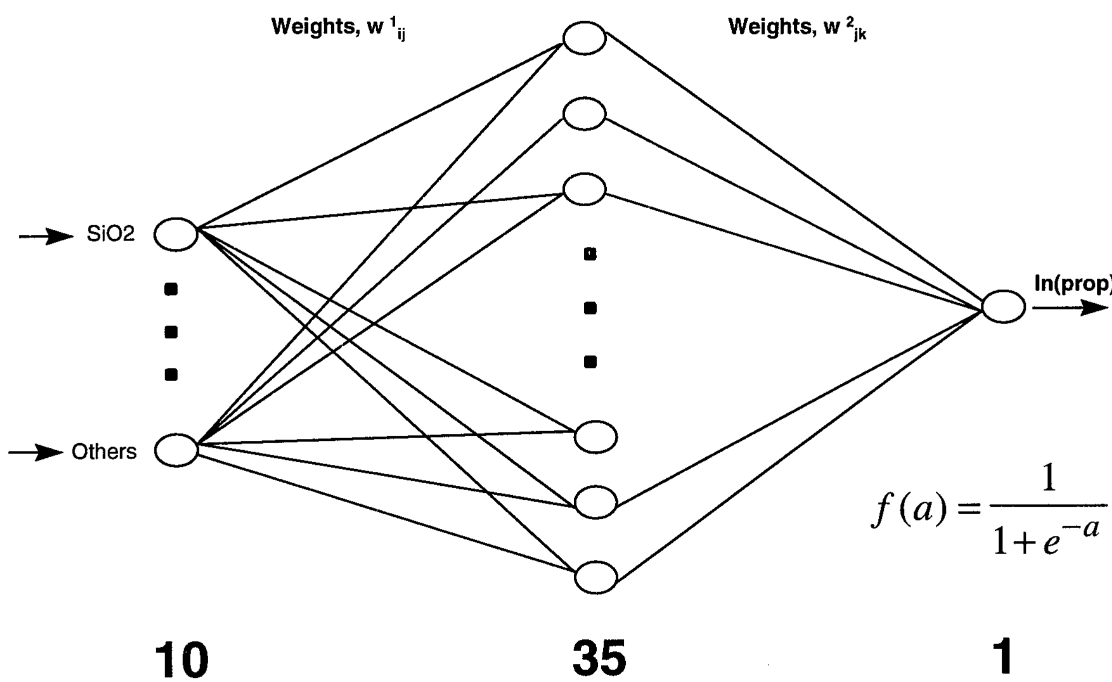

Figure 4. Structure of the Neural Network Models

The hidden layer actually has 36 nodes because it has a bias node with a permanent output (activation) of 1. The hidden layer is fully connected to the input layer with weights w_{ij}^1 and the output layer is fully connected with the hidden layer with weights w_{jk}^2.

3. The backpropagation algorithm with momentum is used for training the networks Skapura (8:31-32). A momentum term has been added to the algorithm which Skapura did not include:

a) Select the first training vector pair from the set of training vector pairs. Call this the vector pair (**x**,**y**).

b) Use the input vector, **x**, as the output from the input layer of processing elements.

c) Compute the activation to each unit on the subsequent layer as follows:

$$net_i(t) = \sum_{j=1}^{n} w_{ij}(t) o_j(t)$$

where $net_i(t)$ is the net input signal to the i^{th} unit in the network, $o_j(t)$ represents the output from the j^{th} unit in the network, the term $w_{ij}(t)$ represents the weight of the connection between the j^{th} and i^{th} unit, and the value n represents the number of other units connected to the input of the i^{th} unit.

d) Apply the appropriate activation function, f(net^h) and f(net^o), to the hidden layer and output layer. For this study, these are defined as follows:

$$f(net_i^h(t)) = \frac{1}{1+e^{-net_i^h(t)}}$$

$$f(net_i^o(t)) = net_i^o(t)$$

e) Repeat steps c and d for each layer in the network.

f) Compute the error, δ_{p1}^o, for this pattern p for the one output layer unit by using the formula:

$$\delta_{p1}^o = (y_1 - o_1) f'(net_1^o(t)).$$

$$f(net_i^o(t)) = net_i^o(t), \; f'(net_1^o(t)) = \frac{\partial net_1^o(t)}{\partial net_1^o(t)} = 1 ,$$

Therefore, $\delta_{p1}^o = (y_1 - o_1)$.

g) Compute the error, δ^h_{pj}, for all J = 35 hidden layer units using the recursive formula:

$$\delta^h_{pj} = f'(net^h_j(t))\delta^o_{p1}w_{1j}, \text{ where } f'(net^h_j(t)) = net^h_j(t)(1-net^h_j(t)).$$

$$\text{Therefore, } \delta^h_{pj} = net^h_j(t)(1-net^h_j(t))(y_1 - o_1)w_{1j}.$$

h) Update the weights to the hidden layer by using the equation:

$$w_{ji}(t+1) = w_{ji}(t) + \eta\delta^h_{pj}x_i + \alpha(w_{ji}(t) - w_{ji}(t-1)),$$

where η is a small value called the learning rate and

α is a value between 0 and 1 called the rate of momentum

i) Update the weight values to the output layer by using the equation:

$$w_{1j}(t+1) = w_{1j}(t) + \eta\delta^o_{p1}f(net^h_j) + \alpha(w_{1j}(t) - w_{1j}(t-1))$$

j) Repeat steps b through I for all (**x,y**) in the training set. Call this one training epoch.

k) Repeat steps a-j for as many epochs as it takes to reach the desired sum-squared error value. The sum-squared error calculation is as follows:

$$SSE = \sum_{p=1}^{P}(\delta_{p1})^2$$

The training is stopped when $SSE(t+1) - SSE(t) < 0.001$.

4) As was the case in the multiple regression models, the neural networks were trained to output the natural logarithms of the three modeled properties.

3.1.4 Training and Validation Sets. PNL originally used all the data to develop the regression models. The MLP requires the data to be separated into training and validation sets so the network can be checked for proper generalization (lack of memorization of input data). Comparing the MLP using half the data for training and a regression model using all the data for training would handicap the MLP. Therefore, all the statistical modeling is completed first on identical training and validation sets (Appendix B). Notice the data set for electrical conductivity was not divided. This is because no MLP was developed for this property, hence the data could stay intact to compare regression models to each other.

Finally, the original undivided data sets are used to compose final PNL regression models, Revised regression models, and MLP models. These "best" models will form the constraints used in the nonlinear optimization program. The final PNL regression models are found in Section 3.1.1, the final Revised regression models are found in Section 4.1.3, and the final MLP models are found in Appendix K. The MLP models are represented by the final weights of their hidden and output layers.

3.2 Nonlinear Programming

This section discusses the nonlinear programs developed to minimize vitrification cost.

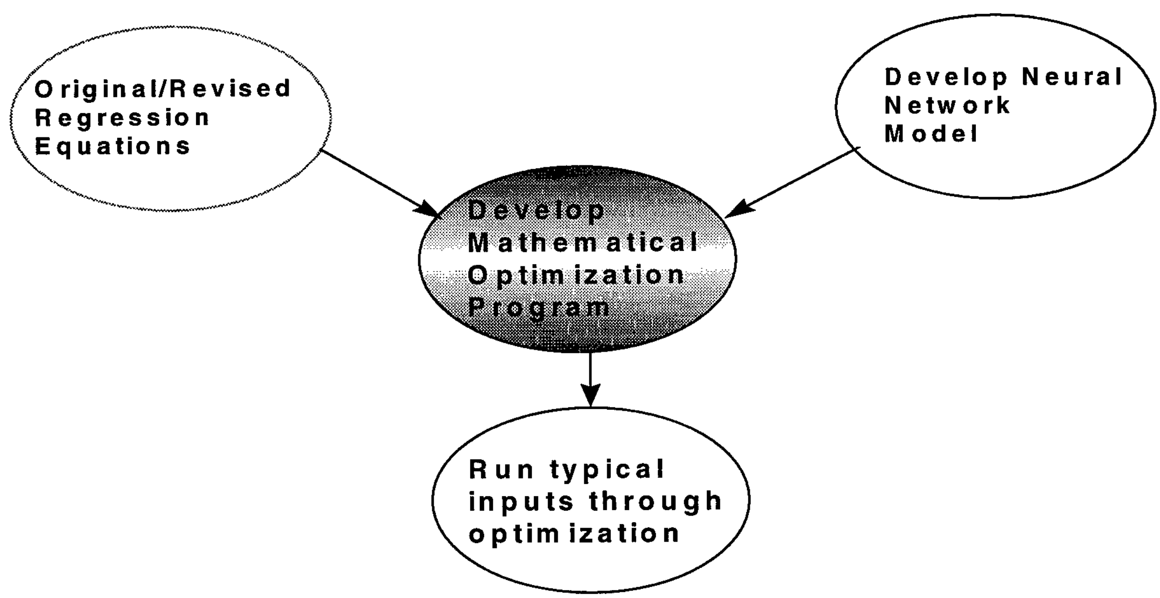

Figure 5--Developing the Nonlinear Programs

As defined by Himmelblau, "The general nonlinear problem is to find an extremum of an objective function subject to equality and/or inequality constraints. The constraints can be linear and/or nonlinear" (13:14). The following section discusses the development of the nonlinear program used to optimize the vitrification process.

3.2.1 General Form of Nonlinear Program and GRG Algorithm. The general nonlinear program is stated in the form that Lasdon and Waren's Generalized Reduced Gradient (GRG2) algorithm requires.

GRG2 requires nonlinear programs (NLP) to be placed in the following form:

Let

$g_{m+1}(X(i))$ = the objective function,

neq = the number of equality constraints,

$m - (neq+1) =$ the number of inequality constraints,

$ub(n+i)$ = the upper bound of the inequality constraints,

$lb(i) =$ the lower bound of the $X(i)$ variables, and

$ub(i)$ = the upper bound of the $X(i)$ variables.

$$\begin{aligned}
&\text{minimize } g_{m+1}(X(i)) \\
&\text{subject to } g_i(X(i)) = 0,\ i = 1,\ldots,neq \\
&0 \leq g_i(X(i)) \leq ub(n+i),\ i = neq+1,\ldots,m \\
&lb(i) \leq X(i) \leq ub(i),\ i = 1,\ldots,n
\end{aligned}$$

As stated in Chapter 2, the Excel Solver uses Lasdon and Waren's GRG2 code to optimize general NLP. The following is a brief stepwise outline of how the GRG2 conducts its optimization. The full theoretical development is found in, "Design and Testing of a Generalized Reduced Gradient Code for Nonlinear Programming," written by Lasdon et al. (25).

1. The user places the NLP in the form found in Section 3.2.1.

2. GRG2 adds slack variables to all inequality constraints and transforms them into equality constraints. This allows the inequalities to be represented by a system of equations that can later be solved.

3. GRG2 assumes nb of the original constraints in Section 3.2.1 are binding. It then uses these binding constraints to solve for nb basic variables. Basic variables are those variables whose values depend on other variables in the problem (13:275). The algorithm chooses the nb original constraints that make this system of equations solution process computationally efficient. The basic variables are now stated in terms of the n - nb remaining nonbasic variables (i.e. $x_1 = x_2+x_3-x_4$). The nonbasic variables are those variables whose values are independent of any other variable in the problem (13:275).

4. Now there is a set of basic variables (y) and a set of nonbasic variables (x). The binding constraints are now: $g(y,x) = 0$.

5. Since the y are solved in terms of x, the original objective function can be written as a function of x, F(x). This F(x) is called the reduced objective function. The problem can now be stated as follows:

minimize F(x)

subject to $l \le x \le u$, where l and u are the upper and lower bounds of the nonbasic variables.

The following example shows this process (13:287).

$$\begin{aligned} \min g_{m+1}(x) &= 4x_1 - x_2^2 - 12 \\ s.t. \quad & 25 - x_1^2 - x_2^2 = 0 \\ & 10x_1 - x_1^2 + 10x_2 - x_2^2 - 34 \ge 0 \\ & x_1 \ge 0, x_2 \ge 0 \end{aligned}$$

Take an initial starting point of x_1=2 and x_2=4. This point violates the equality constraint. Therefore, an artificial variable, x_3, is added to the equality constraint. A slack variable, x_4, is also subtracted from the inequality constraint. The problem is restated:

$$
\begin{aligned}
&\min g_{m+1}(x) = 4x_1 - x_2^2 - 12 - 10^5 x_3 \\
&s.t. \qquad 25 - x_1^2 - x_2^2 + x_3 = 0 \\
&\qquad\qquad 10x_1 - x_1^2 + 10x_2 - x_2^2 - 34 - x_4 \geq 0 \\
&\qquad\qquad x_1 \geq 0 \\
&\qquad\qquad x_2 \geq 0 \\
&\qquad\qquad -10^{10} \leq x_3 \leq 0 \\
&\qquad\qquad 0 \leq x_4 \leq 10^{10}
\end{aligned}
$$

Now, x_3 and x_4 are solved in terms of x_1 and x_2. Therefore, x_3 and x_4 are the basic variables and x_1 and x_2 are the nonbasic variables.

$$
\begin{aligned}
x_3 &= x_1^2 + x_2^2 - 25 \\
x_4 &= 10x_1 - x_1^2 + 10x_2 - x_2^2 - 34.
\end{aligned}
$$

Now F(x) is formed and the problem restated in terms of the nonbasic variables.

$$
\begin{aligned}
&\min F(x) = 4x_1 - x_2^2 - 12 - 10^5 (x_1^2 + x_2^2 - 25) \\
&s.t. \qquad x_1 \geq 0, x_2 \geq 0
\end{aligned}
$$

6. GRG then performs a one-dimensional search of F(x) using its gradient, $\nabla F(x)$, and Newton's Method. Newton's Method is an algorithm that uses second derivative information to solve an unconstrained nonlinear program (13:73). The GRG algorithm attempts to return to the feasible area at each step in the one-dimensional search. It does so by completing Newton Method iterations each time a basic variable is infeasible. As

F(x) is searched the values of the basic variables, y, are found (25:34-37). The GRG is stopped when $g_{m+1}(X^{k+1}(i)) - g_{m+1}(X^{k}(i)) \leq \varepsilon$, where ε is a user defined value.

3.2.2 Nonlinear Program. For this study, there are no equality constraints. The NLP are special forms of the general NLP (Section 3.2.1) because all the objective functions are linear. The NLP for this study take the following form:

minimize 0.0497*SIO2A + 0.0435*B2O3A + 0.3392*NA2OA + 1.378*LI2OA + 0.02998*CAOA + 0.0473*MGOA + 0.01608*NA2CO3A + 0.01868*H3BO3A + 0.01002*BORAX

subject to $2 \leq$ VISC ≤ 10
$10 \leq$ ELEC ≤ 100
PCT ≤ 8.2
MCC ≤ 28
all variables ≥ 0

The VISC, ELEC, PCT, and MCC models are found in Sections 3.1.1, 4.1.3, and Appendix K as stated previously.

The objective function consists of the 8 additives that can be added to the waste to produce "good" glass. The cost coefficients for the additives come from Aldrich Chemical Company's catalog of chemicals (26). The bounds on each property are needed for the following reasons:

1. If the viscosity of the vitrification mixture is lower than 2 Pa-s, then the mixture seeps into the bricks of the joule heater and corrodes the melter walls. If viscosity is greater than 10 Pa-s, then the mixture has a slow melting rate and is difficult to pour.
2. If electrical conductivity is less than 10 S/m, then the melter has start-up difficulties. If the electrical conductivity is higher than 100 S/m, then the current required to heat the glass exceeds the recommended maximum density for the melter electrodes.

3. If PCT is > 8.2 g/m^2 or MCC-1 B is greater than 28 g/m^2, then the glass has too high a dissolution rate and releases boron into the environment.

The constraints are the various statistical models developed in section 3.1. Five different NLPs are developed using various sets of constraints as follows:

1) Constraints consist of PNL 1st order models (Tables 1-4).

2) Constraints consist of PNL 2nd order models (Tables 1-4).

3) Constraints consist of Revised 1st order models (Tables 14-17).

4) Constraints consist of Revised 2nd order models (Tables 14-17).

5) Constraints consist of three neural network models and Revised 2nd order electrical conductivity model (Appendix K and Table 15). Each of these five sets contain models for each type of glass property. Each property has to stay within certain bounds in order to make good glass. PNL produced bounds for the constraints (11:3.2). Therefore, any of the five sets of models is considered a "constraint" because they define the area of suitable glass production.

The statistical models require mass fractions of the components. These mass fractions are defined in the following equations:

1. TOTAL = total of initial mass of components plus all additives.

2. SiO_2 = (SiO_2I+SiO_2A)/TOTAL (SiO_2I means initial mass of SiO_2I)

3. B_2O_3 = (B_2O_3I+2*BORAX+0.5*H_3BO_3)/TOTAL

4. Na_2O = (Na_2OI+BORAX+Na_2CO_3)/TOTAL

5. Li_2O = (Li_2OI+Li_2OA)/TOTAL

6. CaO = (CaOI+CaOA)/TOTAL

7. $MgO = (MgOI+MgOA)/TOTAL$

8. $Fe_2O_3 = (Fe_2O_3I)/TOTAL$

9. $Al_2O_3 = (Al_2O_3I)/TOTAL$

10. $ZrO_2 = (ZrO_2I)/TOTAL$

11. OTHERS = (OTHERSI)/TOTAL.

Finally, all mass fraction components are standardized as discussed earlier for input to the neural network models.

Given these mass fractions, the nonlinear programs are stated as follows:

1) Constraints with PNL 1st order models:

minimize 0.0497*SIO2A + 0.0435*B2O3A + 0.3392*NA2OA + 1.378*LI2OA + 0.02998*CAOA + 0.0473*MGOA + 0.01608*NA2CO3A + 0.01868*H3BO3A + 0.01002*BORAX

$$
\begin{aligned}
\textit{subject to}\quad & \mathbf{2} \le 8.968SiO_2 - 6.204B_2O_3 - 11.017Na_2O - 34.239Li_2O - 7.466CaO - 2.776MgO \\
& - 0.037Fe_2O_3 + 11.306Al_2O_3 + 7.434ZrO_2 - 0.156Others \le \mathbf{10} \\
& \mathbf{10} \le 0.847SiO_2 + 2.252B_2O_3 + 11.040Na_2O + 23.536Li_2O + 1.413CaO \\
& + 1.056MgO + 2.586Fe_2O_3 + 1.311Al_2O_3 + 1.122ZrO_2 + 3.453Others \le \mathbf{100} \\
& -4.303SiO_2 + 11.831B_2O_3 + 17.826Na_2O + 22.970Li_2O - 9.046CaO + 10.582MgO \\
& - 3.101Fe_2O_3 - 25.443Al_2O_3 - 10.630ZrO_2 + 0.164Others \le \mathbf{8.2} \\
& -0.223SiO_2 + 10.039B_2O_3 + 10.139Na_2O + 12.067Li_2O + 3.481CaO + 4.987MgO \\
& + 5.809Fe_2O_3 - 6.614Al_2O_3 - 0.963ZrO_2 + 3.484Others \le \mathbf{28} \\
& SiO_2 + B_2O_3 + Na_2O + Li_2O + CaO + MgO + Fe_2O_3 + Al_2O_3 + ZrO_2 + Others = 1 \\
& \text{all variables} \ge 0
\end{aligned}
$$

2) Constraints with PNL 2nd order models:

minimize 0.0497*SIO2A + 0.0435*B2O3A + 0.3392*NA2OA + 1.378*LI2OA +
0.02998*CAOA + 0.0473*MGOA + 0.01608*NA2CO3A +
0.01868*H3BO3A + 0.01002*BORAX

$$
\begin{aligned}
&\mathbf{2} \le 10.987SiO_2 - 6.165B_2O_3 - 26.388Na_2O - 75.868Li_2O - 5.572CaO - 3.233MgO \\
&0.148Fe_2O_3 + 14.491Al_2O_3 + 10.145ZrO_2 - 2.119Others + 30.098B_2O_3 * Fe_2O_3 \\
&+ 126.749Na_2O * Li_2O + 29.875Na_2O * MgO + 78.943Li_2O * Others \\
&- 39.527MgO * Fe_2O_3 + 43.574Na_2O * Na_2O + 296.59Li_2O * Li_2O \le \mathbf{10} \\
&\mathbf{10} \le 0.303SiO_2 + 1.878B_2O_3 + 14.543Na_2O + 31.634Li_2O - 0.223CaO \\
&+ 0.720MgO + 0.771Fe_2O_3 + 1.104Al_2O_3 - 0.329ZrO_2 - 5.287Others \\
&- 84.820Na_2O * Li_2O + 28.333CaO * Fe_2O_3 + 12.012B_2O_3 * Fe_2O_3 \\
&+ 25.753MgO * ZrO_2 + 17.260SiO_2 * Others + 32.044Li_2O * ZrO_2 \le \mathbf{100} \\
&- 5.180SiO_2 + 13.811B_2O_3 + 20.851Na_2O + 23.454Li_2O + 14.111CaO - 36.638MgO \\
&- 1.942Fe_2O_3 - 44.502Al_2O_3 - 10.589ZrO_2 + 2.771Others + 97.566SiO_2 * MgO \\
&- 90.152B_2O_3 * CaO - 121.921Na_2O * CaO - 126.554Al_2O_3 * Al_2O_3 \le \mathbf{8.2} \\
&- 1.119SiO_2 + 15.430B_2O_3 + 10.698Na_2O + 13.124Li_2O - 24.717CaO + 7.129MgO \\
&+ 6.122Fe_2O_3 - 12.546Al_2O_3 - 1.820ZrO_2 + 4.513Others + 58.519SiO_2 * CaO \\
&- 70.216B_2O_3 * Al_2O_3 + 83.074Al_2O_3 * Al_2O_3 \le \mathbf{28} \\
&SiO_2 + B_2O_3 + Na_2O + Li_2O + CaO + MgO + Fe_2O_3 + Al_2O_3 + ZrO_2 + Others = 1 \\
&\text{all variables} \ge 0
\end{aligned}
$$

3) Constraints consisting of Revised 1st Order models:

minimize 0.0497*SIO2A + 0.0435*B2O3A + 0.3392*NA2OA + 1.378*LI2OA +
0.02998*CAOA + 0.0473*MGOA + 0.01608*NA2CO3A +
0.01868*H3BO3A + 0.01002*BORAX

$$
\begin{aligned}
&\mathbf{2} \le 8.9657SiO_2 - 6.2113B_2O_3 - 11.034Na_2O - 34.290Li_2O - 7.5308CaO - 2.8496MgO \\
&+ 11.3224Al_2O_3 + 7.5083ZrO_2 \le \mathbf{10} \\
&\mathbf{10} \le 2.2587 - 1.3724SiO_2 + 8.8420Na_2O + 21.6596Li_2O - 1.2081Al_2O_3 \\
&- 1.2968ZrO_2 \le \mathbf{100} \\
&- 3.6659 + 15.3460B_2O_3 + 21.330Na_2O + 26.5710Li_2O - 5.8900CaO + 13.7370MgO \\
&- 22.5100Al_2O_3 - 7.4900ZrO_2 \le \mathbf{8.2} \\
&4.6375 - 4.7862SiO_2 + 5.2860B_2O_3 + 5.4920Na_2O + 7.360Li_2O - 11.5936Al_2O_3 \\
&- 5.7810ZrO_2 \le \mathbf{28} \\
&SiO_2 + B_2O_3 + Na_2O + Li_2O + CaO + MgO + Fe_2O_3 + Al_2O_3 + ZrO_2 + Other = 1 \\
&\text{all variables} \ge 0
\end{aligned}
$$

4) Constraints consisting of Revised 2nd Order models:

minimize 0.0497*SIO2A + 0.0435*B2O3A + 0.3392*NA2OA + 1.378*LI2OA + 0.02998*CAOA + 0.0473*MGOA + 0.01608*NA2CO3A + 0.01868*H3BO3A + 0.01002*BORAX

$$
\begin{aligned}
&\mathbf{2} \le 10.7967 SiO_2 - 6.4873 B_2O_3 - 25.8010 Na_2O - 73.996 Li_2O - 5.7882 CaO \\
&+ 14.3699 Al_2O_3 + 10.1045 ZrO_2 + 29.9500 B_2O_3 * Fe_2O_3 + 120.9600 Na_2O * Li_2O \\
&+ 44.0600 Li_2O * Others - 39.8930 MgO * Fe_2O_3 + 44.0760 Na_2O * Na_2O \\
&+ 297.2500 Li_2O * Li_2O \le \mathbf{10} \\
&\mathbf{10} \le 0.38257 + 1.13355 B_2O_3 + 14.5157 Na_2O + 33.4372 Li_2O \\
&- 94.390 Na_2O * Li_2O + 16.3778 CaO * Fe_2O_3 + 14.2337 B_2O_3 * Fe_2O_3 \\
&+ 27.9140 MgO * ZrO_2 + 5.5687 SiO_2 * Others + 0.099976 Li_2O * ZrO_2 \le \mathbf{100} \\
&-5.2717 SiO_2 + 13.909 B_2O_3 + 20.890 Na_2O + 23.992 Li_2O + 13.251 CaO - 37.540 MgO \\
&- 43.629 Al_2O_3 - 10.362 ZrO_2 + 98.980 SiO_2 * MgO - 87.110 B_2O_3 * CaO \\
&- 120.720 Na_2O * CaO - 123.090 Al_2O_3 * Al_2O_3 \le \mathbf{8.2} \\
&6.0779 - 7.301 SiO_2 + 9.199 B_2O_3 + 4.5813 Na_2O + 6.8850 Li_2O - 32.432 CaO \\
&- 18.397 Al_2O_3 - 7.605 ZrO_2 + 61.820 SiO_2 * CaO \\
&- 68.220 B_2O_3 * Al_2O_3 + 82.200 Al_2O_3 * Al_2O_3 \le \mathbf{28} \\
&SiO_2 + B_2O_3 + Na_2O + Li_2O + CaO + MgO + Fe_2O_3 + Al_2O_3 + ZrO_2 + Others = 1 \\
&\text{all variables} \ge 0
\end{aligned}
$$

5) Constraints consisting of Neural Networks and Revised 2nd Order ELEC model:

minimize 0.0497*SIO2A + 0.0435*B2O3A + 0.3392*NA2OA + 1.378*LI2OA + 0.02998*CAOA + 0.0473*MGOA + 0.01608*NA2CO3A + 0.01868*H3BO3A + 0.01002*BORAX

$$
\begin{aligned}
&\mathbf{2} \le \text{VISC calculated using weights of MLP from Appendix K} \le \mathbf{10} \\
&\mathbf{10} \le 0.38257 + 1.13355 B_2O_3 + 14.5157 Na_2O + 33.4372 Li_2O \\
&- 94.390 Na_2O * Li_2O + 16.3778 CaO * Fe_2O_3 + 14.2337 B_2O_3 * Fe_2O_3 \\
&+ 27.9140 MgO * ZrO_2 + 5.5687 SiO_2 * Others + 0.099976 Li_2O * ZrO_2 \le \mathbf{100} \\
&\text{PCT B calculated using weights of MLP from Appendix K} \le \mathbf{8.2} \\
&\text{MCC - 1 B calculated using weights of MLP from Appendix K} \le \mathbf{28} \\
&\mathrm{SiO_2 + B_2O_3 + Na_2O + Li_2O + CaO + MgO + Fe_2O_3 + Al_2O_3 + ZrO_2 + Others} = 1 \\
&\text{all variables} \ge 0
\end{aligned}
$$

3.2.3 <u>Excel Form of Nonlinear Program</u>. The NLP discussed in Section 3.2.1 takes the following tabular form in Excel. Table 5 is an example of the spreadsheet a

DOE engineer examines after mathematical optimization. The top block of the spreadsheet represents the initial mass of each waste component. The 2nd block shows the value of the additives added to the waste. For example, SIO2A = 8.106138 means that 8.1068138 kg of SiO_2 should be added to the waste stream before placing it into the melter. The 3rd block shows the costs/kg of the additives in the 2nd block. The 4th block shows the final mass fraction values of the 10 glass components. The bottom block shows the cost of the additives and the values of each glass property. An example of Excel code is given for the neural network NLP in Appendix K.

Table 5. MicroSoft Excel NLP Form

SIO2I	B2O3I	NA2OI	LI2OI	CAOI	MGOI	FE2O3I	AL2O3I	ZRO2I	OTHERSI
48.95	11.12	16.71	4.28	1.13	1.66	8.97	3.67	0.41	3.1
SIO2A	B2O3A	NA2OA	LI2OA	CAOA	MGOA	NA2CO3A	H3BO3A	BORAX	TOTAL
8.106138	0	0	0	3.5985412	0	0	0	0	111.70468
C1	C2	C3	C4	C5	C6	C7	C8	C9	
0.0497	0.0435	0.3392	1.378	0.02998	0.0473	0.01608	0.01868	0.01002	
SIO2	B2O3	NA2O	LI2O	CAO	MGO	FE2O3	AL2O3	ZRO2	OTHERS
0.5108	0.0995	0.1496	0.0383	0.0423	0.0149	0.0803	0.0329	0.0037	0.0407
OBJ FN		ELEC	LNVISC	VISC	LNPCT	PCT	LNMCC	MCC	
0.510759		40.213295	0.7027243	2.0192463	1.4267913	4.1653127	3.3322045	28	

3.3 Comparing the Models

Comparison of the various NLPs requires development of three types of measure of performance (MOP). The first two types of MOP address the statistical models themselves, while the third type of MOP addresses the final NLP models.

3.3.1 Statistical MOP. The coefficient of multiple determination, R^2, statistic and three types of probability MOP are used to compare the various statistical models. Calculations for the validation sets' R^2 are found in Appendix I.

The coefficient of multiple determination is used to compare statistical models for the following reasons:

1. The results found in Appendices C-F show that R^2 and adjusted R^2 are very close values. Therefore, it is reasonable to use R^2 itself and not its adjusted value.

2. R^2 represents the percentage of uncertainty in the model that can be tied to the regression itself. It is calculated as 1 - SSE/SST. SSE is defined as $\sum_i (y_i - \hat{y}_i)^2$, where y_i is the actual dependent data value and $\hat{y}_i$ is the dependent data value predicted by the regression model. SST is defined as $\sum_i (y_i - \overline{y}_i)^2$, the "total variation defined by the regression model" (22:531). Low values tell the modeler that the uncertainty is occurring because of reasons other than the method of least squares, i.e. the dependent and independent variables have no linear relationship. Therefore, the scientist can look at the statistic and determine whether the linear regression model is suitable.

3.3.2 Probability MOPs. Three types of probabilities are used to compare the statistical models. All the probabilities are calculated by using the tables in Appendix J. The first is the probability of correctly classifying the vitrified waste as glass or not glass, P(correct classify). There are 113 glasses in the total database that have all four property values measured. Each set of glass inputs is tested to see if each individual predicted property value falls within its feasible bounds. If any property is infeasible, the glass is classified as "not glass". This is then compared to the actual glass classification to determine proper classification.

If the inputs are misclassified, two errors can occur. These two types of errors drive the use of the final two probability MOP. The first type of error is predicting that vitrifying the inputs will not produce glass (without additives) when the vitrified inputs actually did produce glass, P(pred not glass|glass). This will cause the NLP to tell DOE to add unnecessary chemicals to the waste stream. The second type of error is predicting that vitrifying the inputs will produce glass (without additives) when the vitrified inputs actually did not produce glass, P(pred glass|not glass). This will cause DOE to run the joule heaters without adding any chemicals, and adequate glass will not result. This is the worst type of error because the operation is run for an unuseful day, hence wasting money. Chemicals will have to be added on a second day and the process re-run. The ideal statistical model has a high P(correct classify) and P(pred not glass|glass) >> P(pred glass|not glass).

3.3.3 NLP MOP. Since the objective of the NLP is to minimize cost, the obvious choice for MOP is some type of cost. Therefore, expected cost is the MOP for the NLP.

Expected total cost of vitrification is defined as follows:

E(Total Cost) = (Expected Cost of Additives + Fixed Cost of Running Plant)*E(X),

where X = number of times the waste stream is vitrified before a successful glass is made.

After the NLP is solved, the model predicts that the final glass components make "good" glass. The one error that occurs "post-optimization" is predicting glass when the final mass fraction components do not make glass.

The distribution of X, the number of trials before the first success in a sequence of independent Bernoulli trials of probability p (probability of success on each trial), is geometric. X has the following probability distribution function:

Let p = the probability of predicting glass given that the final components do make glass.

$$p(x) = \begin{cases} (1-p)^{x-1}p & x = 1,2,3,\ldots \\ 0 & \text{otherwise} \end{cases} \quad (22:88)$$

The expected value of X, E(X), is $1/p$ (22:96).

Therefore, expected total cost is now calculated as follows:

E(Total Cost) = (Expected Cost of Additives + Fixed Cost of Running Plant)*($1/p$).

Note that Expected Cost of Additives = f(P(pred not glass|glass)). The probability is wrapped up in the Expected Cost of Additives (ECOA) because the error simply causes unnecessary chemicals to be added to the waste. Those additives are used in calculating ECOA. A small P(pred not glass|glass) will yield a smaller value for ECOA.

The ideal situation occurs when an NLP produces the smallest ECOA **and** E(X). The worst case occurs when the NLP produces the largest ECOA and E(X). Using this model, DOE would have the highest percentage of reprocessing, and when it added chemicals it would do so at the highest average cost. To choose the NLP that has the best E(Total Cost), both ECOA and E(X) have to be examined simultaneously.

IV. RESULTS

4.1 Statistical Modeling Results

The following section presents the results from the statistical modeling efforts of this study.

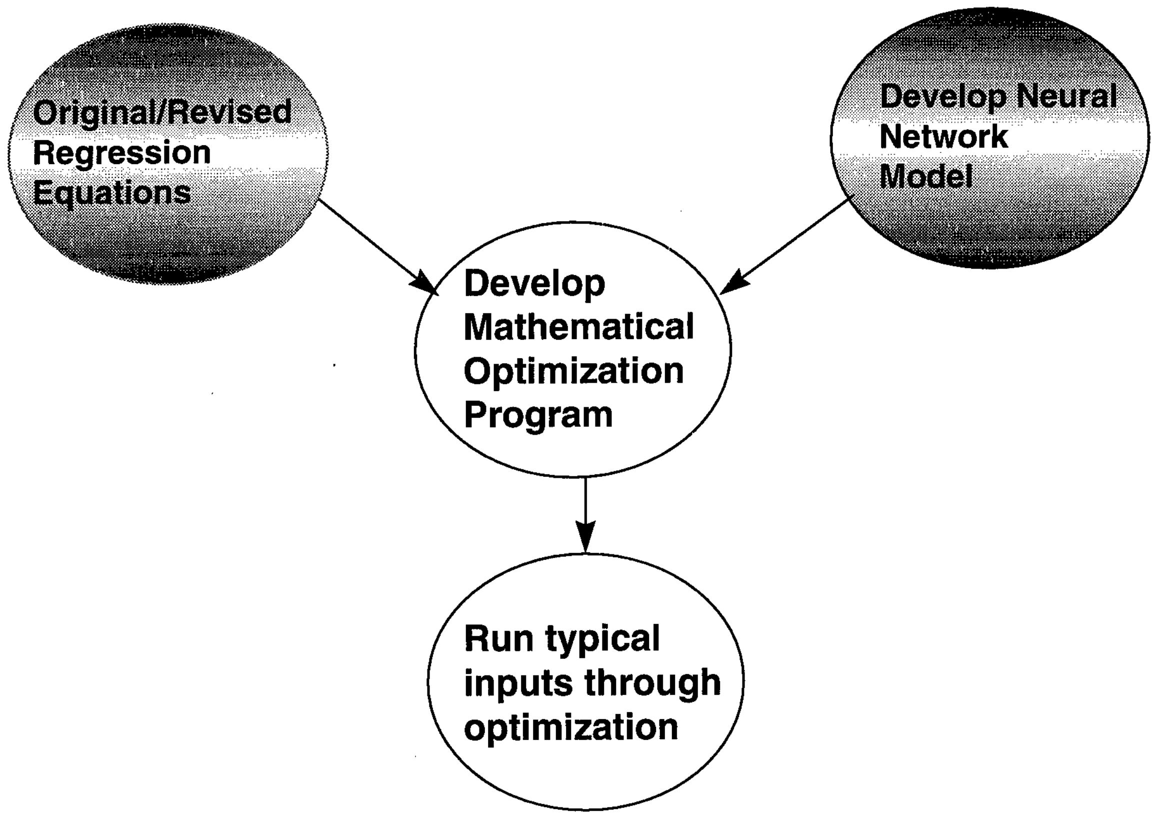

Figure 6--Results of Statistical Modeling

4.1.1 Modeling of Training Sets. As discussed in Section 3.1.3, the original PNL and Revised PNL regression equations are developed for each data set used to train the neural networks. This allows a fair comparison of all the regression equations and the neural networks.

4.1.1.1 Regression on Training Sets Using PNL Models. This section contains the results of using the original PNL models to regress on the training sets. These models are then revised using stepwise regression (Section 4.1.1.2). Notice that there is no training set regression for electrical conductivity. This is because a stepwise regression completed on all data points produces a revised PNL electrical conductivity model with an R^2 of 99.9%. A neural network cannot beat this performance, therefore no multi-layer perceptron is developed for electrical conductivity.

Table 6. PNL First and Second Order Models for Viscosity Training Set

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
SiO2	8.8121	0.2691	10.6283	0.2531
B2O3	-6.1954	0.4463	-6.2945	0.3814
Na2O	-10.8000	0.6253	-24.819	2.5750
Li2O	-34.5030	1.248	-77.478	4.5230
CaO	-6.3084	0.8096	-5.0912	0.4546
MgO	-1.9434	0.8768	-2.180	1.3350
Fe2O3	0.0609	0.6224	0.6936	0.7788
Al2O3	11.1117	0.6904	14.1206	0.4768
ZrO2	7.8691	0.7163	10.4672	0.4805
Others	-0.7670	0.7553	-2.7285	0.7210
B2O3 x Fe2O3			29.1740	5.1780
Na2O x Li2O			122.5600	19.9700
Na2O x MgO			22.6210	8.9400
Li2O x Others			88.5700	17.4400
MgO x Fe2O3			-44.7200	10.4800
Na2O x Na2O			42.4980	9.0430
Li2O x Li2O			339.7500	40.8000

Table 7. PNL First and Second Order Models for PCT-B Training Set

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
SiO2	-3.1399	0.9125	-4.7800	1.0480
B2O3	10.244	1.5190	12.6840	1.6050
Na2O	15.091	2.1130	19.0620	2.1560
Li2O	18.595	4.3030	19.7800	3.5430
CaO	-10.0240	2.7840	14.5990	8.6430
MgO	9.5410	3.0300	-50.9900	20.5500
Fe2O3	-2.1340	2.1080	-0.4110	1.9100
Al2O3	-26.6650	2.3840	-43.2760	5.4980
ZrO2	-8.8760	2.4760	-7.6650	2.2180
Others	2.1150	2.5950	5.4930	2.2530
SiO2 x MgO			121.7600	41.3600
B2O3 x CaO			-100.5300	41.2300
Na2O x CaO			-151.6300	52.8000
Al2O3 x Al2O3			145.4600	38.7700

Table 8. PNL First and Second Order Models for MCC-1 Training Set

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
SiO2	0.3018	0.4474	0.1036	0.5635
B2O3	9.0717	0.8043	13.2080	1.2500
Na2O	9.0333	0.9918	9.1767	0.9007
Li2O	9.2790	2.0510	10.1860	1.8230
CaO	7.3270	1.2510	-11.0110	9.6560
MgO	6.4490	1.5080	7.1690	1.3230
Fe2O3	5.1000	1.1540	4.6210	1.1850
Al2O3	-6.9410	1.4030	-15.1590	3.6830
ZrO2	-0.5070	1.3770	-1.9840	1.3370
Others	0.4520	1.3590	1.8150	1.3490
SiO2 x CaO			33.9800	19.4500
B2O3 x Al2O3			-49.9300	15.5800
Al2O3 x Al2O3			89.2700	22.0800

4.1.1.2 <u>Regression on Training Sets Using Revised PNL Models</u>. The stepwise modeling efforts of the various training sets are found in Appendices C-F. The two hypothesis tests discussed in Section 3.1.1 are completed on the PNL models. If a p-value is > 0.05 for a particular waste component, that variable is eliminated in the Revised regression models. The final models are as follows:

Table 9. Revised PNL First and Second Order Models for Viscosity Training Set

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
Constant			-2.5969	0.6120
SiO2	8.6000	0.2316	13.2282	0.6794
B2O3	-6.1712	0.4518	-3.6852	0.7302
Na2O	-10.8403	0.6391	-22.1830	2.7100
Li2O	-34.6290	1.2730	-74.6640	4.4320
CaO	-5.5507	0.7483	-2.5294	0.7876
MgO				
Fe2O3			3.2198	0.8841
Al2O3	11.2714	0.6695	16.6586	0.7453
ZrO2	8.0675	0.7104	13.0175	0.6917
Others				
B2O3 x Fe2O3			29.0850	5.1240
Na2O x Li2O			122.0900	19.7500
Na2O x MgO			25.0410	5.6580
Li2O x Others			85.6500	15.2200
MgO x Fe2O3			-42.8120	8.8910
Na2O x Na2O			42.2380	8.9310
Li2O x Li2O			339.8600	40.4200

Table 10. Revised First and Second Order Models for PCT-B Training Set

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
Constant	-1.3624	0.5934	5.8660	2.2260
SiO2			-10.2020	2.7700
B2O3	10.7110	1.9580	6.1240	2.5880
Na2O	15.1520	2.6880	12.2380	2.6990
Li2O	18.0200	4.9920	14.1090	4.3030
CaO	-13.4490	2.8640		
MgO			-56.2100	21.3300
Fe2O3			-6.2960	2.5410
Al2O3	-25.7650	2.4510	-50.7690	5.5530
ZrO2	-8.4440	2.6460	-13.5650	2.8160
Others				
SiO2 x MgO			115.1300	40.9100
B2O3 x CaO			-66.6300	25.4900
Na2O x CaO			-106.8800	30.9700
Al2O3 x Al2O3			158.6900	36.6700

Table 11. Revised PNL First and Second Order Models for MCC-1 Training Set

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
Constant			1.7322	0.2624
SiO2				
B2O3	9.2714	0.6850	11.1870	1.3990
Na2O	9.4281	0.6952	6.3700	1.1310
Li2O	10.0950	1.5440	6.7760	2.1340
CaO	7.5530	1.1950		
MgO	6.5960	1.4510	3.7940	1.4030
Fe2O3	5.5081	0.9021		
Al2O3	-6.5880	1.0020	-23.1140	3.5790
ZrO2			-5.7950	1.2620
Others				
SiO2 x CaO				
B2O3 x Al2O3			-53.4400	16.7300
Al2O3 x Al2O3			123.9800	21.9100

Tables 9-11 show that there are nonsignificant variables left in the original PNL models that are eliminated in the revised regression models. For example, the shaded areas in Table 6 indicate that Mgo, Fe_2O_3 and Others all seem to be insignificant. The stepwise regression showed this by eliminating them from the Revised PNL regression model for viscosity (see shaded areas in Table 9).

4.1.1.3 Neural Network Modeling Results. The neural networks for each parameter are developed using the training set and the following parameters:

Table 12. Parameters Used for Neural Network--Training Set

	ln(viscosity)	ln(PCT-B)	ln(MCC-1 B)
learning rate	0.000944	0.000500	0.001328
momentum	0.9500	0.9500	0.9500
# of epochs trained	3071	482	972

4.1.2 Statistics for Training and Validation Set Models. The following table presents the resulting R^2 statistics for all training and validation sets.

Table 13. R^2 Statistics for Training and Validation Set Models

	Training	Validation
PNL 1st Order VISC	0.958634	0.900706
Revised 1st Order VISC	0.953909	0.889256
PNL 2nd Order VISC	0.990429	0.938008
Revised 2nd Order VISC	0.990000	0.938238
MLP VISC Model	0.998600	0.946300
PNL 1st Order PCT B	0.783881	0.676223
Revised 1st Order PCT B	0.730000	0.603272
PNL 2nd Order PCT B	0.866581	0.679495
Revised 2nd Order PCT B	0.864000	0.616962
MLP PCT-B Model	0.960500	0.727100
PNL 1st Order MCC-1 B	0.709254	0.105532
Revised 1st Order MCC-1 B	0.704916	0.113086
PNL 2nd Order MCC-1 B	0.793147	0.358522
Revised 2nd Order MCC-1 B	0.716000	0.138776
MLP MCC-1 B Model	0.963200	0.637400

The results from the validation sets indicate that the 1st order regression models may not be adequate in predicting future glass property values. This is especially true for MCC-1 B. R^2 values of 0.105532 and 0.113086 indicate that a linear model is not appropriate for modeling this property. The 2nd order models do a better job of generalization, but they still poorly perform for the MCC property. The R^2 values are only increased to 0.358522 and 0.138776 respectively. Note that the revised models did not increase the property modeling performance. NLPs will still be formed using these models to determine if using a smaller number of variables in each equation changes the feasible region and possibly lowers optimiztion costs. The neural network models are clearly the best. They have the highest training and validation R^2 values. They outperform every regression model, especially for the PCT and MCC properties.

4.1.3 <u>Final Revised PNL and Neural Network Models</u>. The following equations (in tabular form) are the final Revised PNL and Neural Network models that serve as constraints in the NLP models. Shaded areas indicate variables existing in the original PNL models, but eliminated by stepwise regression for the revised regression models. The original PNL Model also serve as constraints in a NLP model, but they are already displayed in Tables 1-4 in Chapter 3.

Table 14. Final Revised PNL First and Second Order Models for Viscosity

Model	1st-Order Model		2nd-Order Model	
Term	Coefficient	Standard Dev	Coefficient	Standard Dev
SiO2	8.9657	0.1988	10.7967	0.2562
B2O3	-6.2113	0.4399	-6.4873	0.3559
Na2O	-11.0340	0.4782	-25.8010	2.3470
Li2O	-34.2900	1.0600	-73.9960	4.2710
CaO	-7.5308	0.7900	-5.78820	0.5832
MgO	-2.8496	0.8764		
Fe2O3				
Al2O3	11.3224	0.5088	14.3699	0.4596
ZrO2	7.5083	0.6708	10.1045	0.5206
Others				
B2O3 x Fe2O3			29.9500	4.3410
Na2O x Li2O			120.9600	15.8700
Na2O x MgO				
Li2O x Others			44.0600	11.4600
MgO x Fe2O3			-39.8930	8.2440
Na2O x Na2O			44.0760	8.6940
Li2O x Li2O			297.2500	42.8500

Table 15. Final Revised PNL First and Second Order Models for Electrical Conductivity

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
Constant	2.2587	0.1917	0.38257	0.01626
SiO2	-1.3724	0.3240		
B2O3			1.13355	0.04340
Na2O	8.8420	0.3467	14.5157	0.0906
Li2O	21.6596	0.6891	33.4372	0.2158
CaO				
MgO				
Fe2O3				
Al2O3	-1.2081	0.3565		
ZrO2	-1.2968	0.4603		
Others				
Na2O x Li2O			-94.3090	1.7020
CaO x Fe2O3			16.3778	0.7669
B2O3 x Fe2O3			14.2337	0.4371
MgO x ZrO2			27.9140	1.3590
SiO2 x Others			5.5687	0.1224
Li2O x ZrO2			0.099976	0.001748

Table 16. Final Revised First and Second Order Models for PCT-B

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
Constant	-3.6659	0.3680		
SiO2			-5.2717	0.5021
B2O3	15.3460	1.3190	13.9090	1.1540
Na2O	21.3330	1.4310	20.8900	1.2040
Li2O	26.5710	2.8760	23.9920	2.2090
CaO	-5.8900	2.1180	13.2510	5.6100
MgO	13.7370	2.3370	-37.5400	13.8100
Fe2O3				
Al2O3	-22.5100	1.2630	-43.6290	3.1390
ZrO2	-7.4900	1.8080	-10.3620	1.4750
Others				
SiO2 x MgO			98.9800	27.8300
B2O3 x CaO			-87.1100	30.1200
Na2O x CaO			-120.7200	34.6200
Al2O3 x Al2O3			123.0900	17.8900

Table 17. Final Revised PNL First and Second Order Models for MCC-1

Model Term	1st-Order Model Coefficient	1st-Order Model Standard Dev	2nd-Order Model Coefficient	2nd-Order Model Standard Dev
Constant	4.6375	0.7071	6.0779	0.7096
SiO2	-4.7862	0.9939	-7.3010	1.0340
B2O3	5.2860	1.0470	9.1990	1.1510
Na2O	5.4920	1.0900	4.5813	0.9442
Li2O	7.360	1.8360	6.8850	1.5440
CaO			-32.4320	7.8820
MgO				
Fe2O3				
Al2O3	-11.5936	0.8782	-18.3970	2.2960
ZrO2	-5.7810	1.2170	-7.6050	1.0220
Others				
SiO2 x CaO			61.8200	15.7400
B2O3 x Al2O3			-68.2200	12.2600
Al2O3 x Al2O3			82.2000	12.1100

Table 18 shows the parameters used to train the final neural network models. The final data is trained approximately the same number of epochs as the training models. This is purposely done to avoid memorizing the data. Memorizing the data hinders the neural networks capability to predict future glass production.

Table 18. Parameters Used for Final Neural Network Models

	ln(viscosity)	ln(PCT-B)	ln(MCC-1 B)
learning rate	0.000944	0.000769	0.001145
momentum	0.9500	0.9500	0.9500
# of epochs trained	3000	400	1500

Complex mathematical equations are developed in spreadsheet form to enable the neural networks to be used in the NLP. The spreadsheet of the weights used to build these equations for each neural network is found in Appendix K.

4.1.4 Statistics for Final Models. The following table presents the resulting R^2 statistics for final statistical models.

Table 19. Final Model R^2 Results

	Final R^2 (entire data set used for modeling)
PNL 1st Order VISC	0.939
Revised 1st Order VISC	0.939
PNL 2nd Order VISC	0.975
Revised 2nd Order VISC	0.972
MLP VISC Model	0.992
PNL 1st Order ELEC	0.931
Revised 1st Order ELEC	0.924
PNL 2nd Order ELEC	0.973
Revised 2nd Order ELEC	0.999
PNL 1st Order PCT B	0.818
Revised 1st Order PCT B	0.813
PNL 2nd Order PCT B	0.886
Revised 2nd Order PCT B	0.881
MLP PCT-B Model	0.962
PNL 1st Order MCC-1 B	0.675
Revised 1st Order MCC-1 B	0.666
PNL 2nd Order MCC-1 B	0.794
Revised 2nd Order MCC-1 B	0.789
MLP MCC-1 B Model	0.966

The shaded areas in Tables 19 indicate the models that modeled each property the best: Revised PNL 2nd Order regression model for electrical conductivity and the neural network models for the other three properties. The neural networks clearly outperform all regression models for the durability properties, PCT-B and MCC-1 B.

The following tables are referred to as confusion matrices. They show how the final models classified the 113 glasses represented in Appendix J. The matrices are used to calculate the 3 probability MOP discussed in Section 3.3.2 and the p used in the geometric distribution of Section 3.3.3.

Table 20. Confusion Matrix--PNL 1st Order Model

Actual		Predicted: Glass	Predicted: Not Glass
	Glass	60	2
	Not Glass	8	43

Table 21. Confusion Matrix--PNL 2nd Order Model

Actual		Predicted: Glass	Predicted: Not Glass
	Glass	58	4
	Not Glass	5	46

Table 22. Confusion Matrix--Revised 1st Order Model

Actual		Predicted: Glass	Predicted: Not Glass
	Glass	60	2
	Not Glass	10	41

Table 23. Confusion Matrix--Revised 2nd Order Model

Actual		Predicted: Glass	Predicted: Not Glass
	Glass	58	4
	Not Glass	5	46

Table 24. Confusion Matrix--Neural Network Model

Actual		Predicted: Glass	Predicted: Not Glass
	Glass	58	4
	Not Glass	2	49

The confusion matrices are used to calculate the following probability MOPs described in Chapter 3. After optimization with the NLP, the only column of the confusion matrix used is the Predicted (Glass) column. This is because the NLP constraints force the final mass fractions of the waste components to have values that predict that glass is produced. The p value for the geometric distribution is calculated using this column. For example, the Neural Network model in Table 24 has a p value of 58/60. The Neural Network model's E(X) is $1/p$, or 1.0345.

Table 25. Probability MOPs for Statistical Models

	P(correct classify)	P(not glass|glass)	P(glass|not glass)
PNL 1st Order Model	0.9115	0.0177	0.0708
PNL 2nd Order Model	0.9204	0.0354	0.0442
Revised 1st Order Model	0.8938	0.0177	0.0885
Revised 2nd Order Model	0.9204	0.0354	0.0442
MLP Model	0.9469	0.0354	0.0177

One point of Table 25 is very prominent. The neural network models (with the Revised 2nd order ELEC) outperform all other models with the highest P(correct classify) and a much lower P(glass|not glass). If the NLP results show that it has the lowest average cost as well, it will clearly outdistance all other models for selection as the best alternative for DOE.

4.2 Nonlinear Optimization Results.

This section analyses the results of the optimization of 10 nuclear waste stream vitrifications.

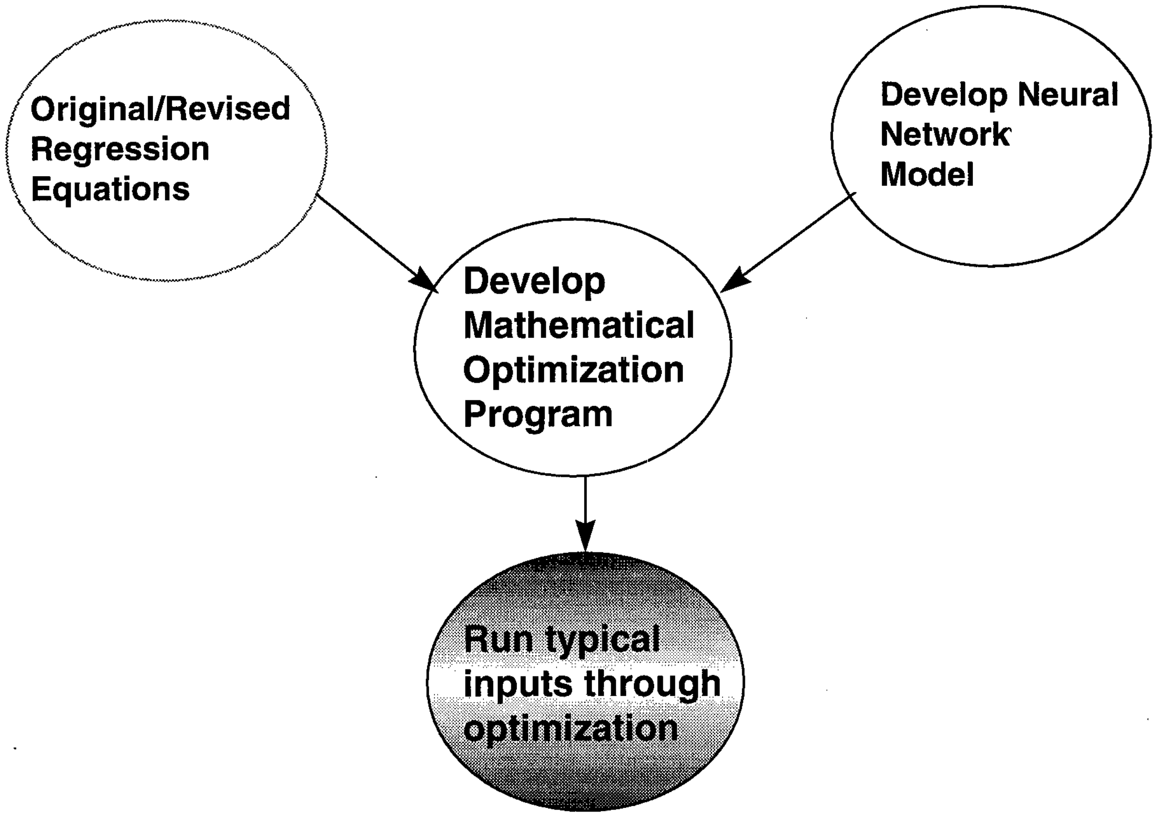

Figure 7--Nonlinear Optimization of 10 Waste Streams

The following ten waste inputs are optimized with the nonlinear MicroSoft Excel programs.

Table 26. Ten Glass Inputs to be Optimized

Input	SIO2I	B2O3	NA2O	LI2OI	CAOI	MGOI	FE2O3I	AL2O3I	ZRO2I	OTHERSI
1	50.40	13.55	7.97	6.96	0.07	0.02	0.46	16.40	0.01	4.16
2	48.95	11.12	16.71	4.28	1.13	1.66	8.97	3.67	0.41	3.10
3	43.91	20.00	6.75	1.00	8.00	0.00	2.00	0.00	8.34	10.00
4	57.00	20.00	9.00	1.00	2.00	8.00	2.00	0.00	0.00	1.00
5	55.00	5.00	5.00	7.00	10.00	0.00	2.00	15.00	0.00	1.00
6	55.89	5.00	12.11	7.00	0.00	8.00	2.00	0.00	0.00	10.00
7	50.18	6.00	18.00	6.32	4.00	0.50	10.50	2.00	0.50	2.00
8	54.79	16.00	5.00	1.21	0.50	0.50	10.50	2.00	0.50	9.00
9	52.81	6.64	12.00	7.30	0.00	0.00	2.00	16.25	1.75	1.25
10	48.95	11.12	16.71	4.28	1.13	1.66	8.97	3.67	0.41	3.10

The resulting costs, means, and standard deviations of the optimization are found in the following two tables:

Table 27. Results of Optimizing 10 Glass Inputs ($)

	1	2	3	4	5	6	7	8	9	10
PNL 1st Order	0	0.537	0.057	0.428	0.012	0.284	0.623	0.125	0.006	0.537
PNL 2nd Order	0	0.491	1.289	7.176	0.017	1.206	0.634	2.515	0.014	0.491
Rev 1st Order	0	0.476	0.378	0.446	0.012	0.253	0.590	0.137	0.006	0.476
Rev 2nd Order	0	0.434	0.609	4.769	0.016	0.923	0.558	2.934	0.014	0.434
MLP	0.0024	0.510	0.558	0.054	0.018	0.224	0.452	0.076	0.011	0.510

Table 27 shows the total cost of the additives ($) for each model and each waste input. The output from waste input #1 shows that the MLP is the only model to avoid making the error of classifying the final waste form as glass when it actually is not glass. This is apparent because it is the only model that added chemicals to the waste stream with a cost equal to $0.0024.

Table 28. Mean and Standard Deviation of Optimization Results ($)

	Mean	Standard Deviation
PNL 1st Order	0.2612	0.2511
PNL 2nd Order	1.3837	2.1777
Rev 1st Order	0.2778	0.2254
Rev 2nd Order	1.0670	1.5574
MLP	0.2420	0.2385

As seen from Table 28, the PNL 1st Order, Revised 1st Order, and MLP models have the lowest mean cost and standard deviations. The 2nd order regression models have the highest cost and highest standard deviations. The high standard deviations indicate that the results from these models are not as predictable as the other 3 models. The high mean costs and low predictability is a risk to the DOE.

Notice that the MLP model has the lowest mean cost and a small standard deviation of 0.2385. This indicates that the MLP provides a low cost, low risk alternative to the DOE. The expected total cost MOE from Section 3.3.2 is restated here:

E(Total Cost) = (Expected Cost of Additives + Fixed Cost of Running Plant)*(1/ p).

The following table shows calculated total expected costs for the PNL, Revised PNL, and Neural Network/Revised PNL 2nd Order ELEC models.

Table 29. Calculation of Total Expected Cost of Vitrification

	E(Total Cost)
PNL 1st Order	(0.2612+Fixed Cost)*1.1333
PNL 2nd Order	(1.3837+Fixed Cost)*1.0862
Revised PNL 1st Order	(0.2778+Fixed Cost)*1.1667
Revised PNL 2nd Order	(1.0670+Fixed Cost)*1.0862
Neural Net/Rev 2nd Order ELEC	(0.2420+Fixed Cost)*1.0345

To minimize expected total cost, the best case situation occurs when ECOA and E(X) are minimized. The MLP/Revised 2nd Order ELEC nonlinear program demonstrates the optimal performance. The MLP has both the lowest average cost and lowest E(X). In addition, it has the highest P(correct classify). This means the DOE could use this tool and be very confident in its results.

V. RECOMMENDATION/CONCLUSION

5.1 Recommendations

The statistical and nonlinear programming tools developed in this thesis provide a means for DOE engineers to minimize the expected cost of vitrifying high level nuclear glass. The DOE goal is to minimize the cost of vitrifying its high-level nuclear waste. With this goal in mind, the recommendation is to optimize the additive values by using the nonlinear program with MLP/Combs 2nd Order ELEC constraints. This program has the lowest mean cost, lowest E(X), and highest P(correct classify). Therefore, it will provide the lowest cost, lowest risk DOE vitrification solution.

5.2 Contributions to Sponsor

This optimization study provides a good solution to the DOE problem of minimizing its costs when vitrifying high-level nuclear waste. The study has made three major contributions in solving this problem. One, the neural networks provide better statistical models for predicting property values (viscosity, PCT B, MCC-1 B) given a set of waste component inputs. Two, a nonlinear optimization program (Appendix K shows an example for the neural network nonlinear program) has been developed in MicroSoft Excel to minimize the cost of vitrifying nuclear waste given various statistical models. The program will output the following:

1. Type and amount of additive chemicals.
2. Final mass fraction values of waste components.
3. Cost of the additives.

Finally, the study provides a lowest cost, lowest risk program for optimizing high-level waste vitrification. The MLP NLP has been shown to provide the lowest cost solution while minimizing the risk of producing glass with infeasible property values.

5.3 Recommendations for further research.

While completing this study, a two other opportunities for further research have been identified. A brief description of each follows below.

5.3.1 Study of Mixed Waste. This data concentrated on modeling the property values of high-level nuclear wastes and optimizing its vitrification process at 1150° C. Work should now be completed on vitrifying DOE mixed waste at varying temperature values. Models could then be developed to optimize the vitrification of any type of waste in any temperature range.

5.3.2 Neural Network Modeling of NLP Surface. This study took many statistical models and used them in nonlinear programs. Now, there exists Excel programs to optimize the vitrification. So given a set of inputs, the NLP have to be run to obtain optimal additive values. The process could be streamlined by taking the existing NLPs and solving them for a great number of different inputs. Then a new neural network could be developed which mapped waste component inputs to the NLP outputs. This would decrease the complexity of the whole optimization process for DOE. There would no longer be a need for running optimization code. A spreadsheet model could be developed to model the neural network. Then DOE could change the input cells in the model and obtain optimal cost and additive values.

APPENDIX A--Data on Waste Glass

This Appendix is a compilation of all the waste component and property data that is used in this study.

SiO2	B2O3	Na2O	Li2O	CaO	MgO	Fe2O3	Al2O3	ZrO2	Others	Visc	Elec	PCT-B	MCC-1 B
48.01	11.42	10.03	3.76	2.75	3.63	5.68	6.36	4.29	4.07	5.78	18.65	0.521	12.47
55	5	5	7	10	0	2	15	0	1	13.29	25.97	0.066	7.46
42	20	5	7	0	8	2	14	1	1	2.39	35.64	0.864	15.57
57	20	9	1	2	8	2	0	0	1	8.7	9.11	20.64	189.71
57	5	7	7	0	0	15	8	0	1	13.24	30.74	0.355	11.48
44	20	5	7	0	0	2	0	12	10	2.01	47.29	6.113	121.3
57	5	9.64	1	10	0	3.36	0	13	1	72.88	6.87	0.287	10.995
53.63	5	8.37	1	0	8	15	0	8	1	29.26	8.84	1.238	17.875
42	19.62	5.38	1	0	8	14	0	0	10	4.06	8.37	10.99	158.72
57	8.51	9.49	1	0	0	2	12	0	10	83.83	20.61	0.127	2.745
42	15.49	7.51	1	10	0	2	14	0	8	14.5	7.47	0.099	8.25
42	17.64	7.36	7	10	0	15	0	0	1	0.42	65.44	4.662	118.48
57	20	18.62	1	0	0	2	0.38	0	1	3.31	34.17	14.07	690.515
42	20	18.62	1	0	0	2	2.38	13	1	3.42	34.92	9.847	73.635
55.89	5	12.11	7	0	8	2	0	0	10	2.55	58.2	18.78	210.285
43.27	5	18.73	1	0	8	8.58	14.42	0	1	17.81	26.36	0.523	16.85
45.45	5	14.55	1	10	0	14	0	0	10	2.23	28.53	2.235	39.1
42.14	5	11.86	7	2	8	2	0	13	9	1.87	65.5	11.24	24.055
48.01	11.42	10.03	3.76	2.75	3.63	5.68	6.36	4.29	4.07	5.76	24.27	0.523	13.025
48.01	11.42	10.03	3.76	2.75	3.63	5.68	6.36	4.29	4.07	5.71	26.88	0.455	12.505
57	20	9	1	2	8	2	0	0	1	9.36	8.05	18.85	205.79
53.63	5	8.37	1	0	8	15	0	8	1	38.11	9.24	1.119	17.36
51.53	9.56	10.52	3.75	2.89	0.84	11.79	4.56	0.63	3.93	5.69	28.03	0.525	15.37
52.26	8.74	7	6	0	5	4	8	1	8	7.74	32.55	0.312	12.24
50.17	7	8.83	6	7	0	4.5	11	3	2.5	6.26	33.08	0.128	8.44
46.45	13.2	7	4.35	7	1	4.5	10.32	3.68	2.5	5.56	22.36	0.137	8.87
56	10.95	7	5.36	7	0	4	6.19	1	2.5	6.37	23.43	0.158	9.73
47.51	15.9	10.1	2	3.48	0	4	8	1	8	8.18	17	0.284	10.405
53.73	7	7	3.82	7	0.46	12	1.59	1	6.41	6.19	19.63	1.185	17.475
48.14	17	7	5.91	0.94	0	4	9.53	1	6.48	4.26	30.39	0.74	5.02
51.15	7	9.85	6	0	5	11.4	6.1	1	2.5	4.36	38.78	0.484	18.505
54.31	9.44	9.24	6	0	0	7.12	1.38	10	2.5	7.3	35.84	0.56	13.2
46.94	17	13.06	2	0	0	6.69	10.43	1	2.88	8.99	23.58	1.332	12.275
49.15	7.51	8.33	6	7	1	4	1	9.35	6.65	3.07	35.3	1.587	19.85
46.83	17	7	4.66	7	1	4	9.01	1	2.5	3.38	23.26	0.194	9.86
49.37	7	16.92	2.25	3	5	4	8.96	1	2.5	7.27	33.95	0.36	13.36
46	13.13	8.02	4.86	5	2	4	2.43	10	4.57	2.97	27.4	1.656	15.095
47.29	7	17	2.14	6.01	0	4	7.56	1	8	4.47	35.85	0.331	25.1
53.53	10.53	11.25	3.75	0.83	0.84	7.19	2.31	3.85	5.92	6.57	27.54	2.937	18.085
48.01	11.42	10.03	3.76	2.75	3.63	5.68	6.36	4.29	4.07	5.37	26.06	0.495	12.325
53.53	10.53	11.25	3.75	0.83	0.84	7.19	2.31	3.85	5.92	6.41	28.34	2.578	19.72
53.28	10.48	11.29	3.73	0.82	0.84	7.33	2.35	3.92	5.96	6.76	27.55	1.99	13.69
57	5	10.31	6.69	0	0	6	1	13	1	12.31	38.08	0.347	8.425
57	13.14	5	7	0	8	2	6.86	0	1	6.01	31.58	3.854	11.805
57	5	7.35	7	0	8	2	3.65	0	10	5.92	37.02	9.646	15.595

57	5.22	20	1	8	0	2	5.78	0	1	9.91	34.97	0.173	11.21
44.64	20	7.36	7	0	0	2	9.61	0	9.39	1.99	40.91	4.522	19.855
50.59	5	8.41	7	8	0	15	0.33	0	5.67	1.35	50.7	4.662	34.5
44.31	20	5.12	7	8	0	2	2.57	10	1	1.26	34.3	1.628	39.145
54.63	5	20	1.55	0	8	2	7.82	0	1	14.41	36.98	3.27	11.22
56.19	5	20	1.26	0	0	2	5.55	0	10	13.44	43.25	5.144	9.835
43.91	20	6.75	1	8	0	2	0	8.34	10	5.32	6.89	1.286	42.285
51.9	20	8.32	1	0	0	13.2	4.58	0	1	27.42	10.85	6.512	24.435
57	18.43	5	3.31	8	0	2	5.26	0	1	10.3	10.96	0.411	47.02
54.45	5	20	4.28	0	0	2	0.27	13	1	8.07	57.11	9.646	16.62
42	5.44	20	3.64	0	8	2	8.92	0	10	2.15	60.94	1.723	14.51
42	17.43	20	3.69	0	0	2	13.88	0	1	1.79	52.63	4.34	29.24
42	5	20	4.28	8	0	6.32	13.4	0	1	2.82	57.81	0.32	11.61
54.21	5	8.91	7	8	0	15	0.88	0	1	1.91	39.89	0.48	21.09
57	8.39	10.61	7	0	0	2	14	0	1	12.34	41.6	0.246	9.635
51.47	11.09	10.44	1	0	8	14.28	2.72	0	1	12.02	13.62	1.119	23.645
48.38	5	13.62	7	0	8	7.42	2.58	7	1	1.98	61.14	12.7	16.3
50.4	6.39	15	4.21	2	5	2	10	2	3	6.88	38.09	0.337	12.205
53.25	6.94	7.81	7	5	2	3	10	2	3	6.2	30.87	0.177	9.425
56.75	5	6.25	7	3.2	3.8	10	3	2	3	5.51	31.9	1.694	14.31
50.7	14.77	5	6.53	2	3	3	5	7	3	4.43	31.42	0.767	11.33
57	10.78	5	6.99	5	2	2	6.23	2	3	6.08	28.6	0.255	10.275
52.99	11.06	5	5.95	2	5	3.08	5.92	2	7	6.03	25	0.5	11.6
52.64	12.59	5.77	7	2	2	2	7.46	2	6.54	4.7	34.77	0.317	10.985
52.94	5	12.77	4.29	5	2	2	4	5	7	6.64	26.65	1.159	11.555
47	14.42	9.68	3.9	5	2	2	8.54	2	5.46	3.94	22.48	0.307	10.625
50.73	13.57	9.57	4.13	2	2	5.15	7.85	2	3	6.46	23.38	0.303	11.35
48.01	11.42	10.03	3.76	2.75	3.63	5.68	6.36	4.29	4.07	5.71	24.81	0.442	11.43
53.28	10.48	11.29	3.73	0.82	0.84	7.33	2.35	3.92	5.96	7.07	28.3	1.764	12.35
60	8.17	4.5	7.88	0.08	0.09	7.2	2.33	3.85	5.9	9.22	35.17	0.557	10.075
53.28	10.48	11.29	3.73	0.82	0.84	7.33	2.35	3.92	5.96	6.26	27.02	1.342	15.905
53.28	10.48	11.29	3.73	0.82	0.84	7.33	2.35	3.92	5.96	6.12	27.83	1.419	17.23
53.28	10.48	11.29	3.73	0.82	0.84	7.33	2.35	3.92	5.96	6.74	28.13	1.164	15.28
39	20	5	7	2	8	2	15	1	1	1.85	32.87	0.778	13.15
43.8	17.18	12.68	7.27	3.75	0.05	2	11.5	0.75	1.02	1.15	48.41	1.591	11.975
52.81	8.76	17.25	7.43	0.63	0.05	2	9.25	0.75	1.07	2.61	68.96	1.624	16.52
52.81	6.64	12	7.3	0	0	2	16.25	1.75	1.25	12.9	45.69	0.222	10.895
55.79	17.65	11.25	1.56	5	0.05	2	5	0.75	0.95	9.95	15.18	1.002	12.39
32.32	17.17	19	0.51	10	0	2	18	0	1	2.38	34.05	0.332	9.645
56.97	5.09	9.25	6.42	0.25	0.08	8.12	2.88	4.31	6.63	8.89	39.53	0.379	12.315
53.44	11.28	8.6	6.97	0.07	0.04	0.13	1.96	15.5	2.03	8.2	36.43	0.335	9.405
51.75	9.17	12.11	5.23	0.97	0.61	3.88	11.8	0.26	4.22	8.24	37.74	0.21	11.745
45.96	15.87	10.86	5.83	0.24	0.01	0.04	20.43	0	0.76	8.97	36.2	0.512	11.145
50.4	13.55	7.97	6.96	0.07	0.02	0.46	16.4	0.01	4.16	17.05	35.28	0.308	10.56
56.6	7.81	6.64	7.13	0.79	0.32	3.34	8.16	0.05	9.16	22.15	36.01	0.226	9.88
48.54	14.18	8.12	6.91	0.08	0.08	0.8	18.19	0.05	3.05	10.8	36.97	0.312	11.56
56.97	5.09	9.25	6.42	0.25	0.08	8.12	2.88	4.31	6.63	8.5	38.46	0.411	12
51.75	9.17	12.11	5.23	0.97	0.61	3.88	11.8	0.26	4.22	7.81	36.88	0.21	11.745
50.4	13.55	7.97	6.96	0.07	0.02	0.46	16.4	0.01	4.16	8.67	36.85	0.244	6.645
56.6	7.81	6.64	7.13	0.79	0.32	3.34	8.16	0.05	9.16	9.55	35.4	0.226	9.88
48.54	14.18	8.12	6.91	0.08	0.08	0.8	18.19	0.05	3.05	8.66	36.4	0.278	8.62

50.18	6	18	6.32	4	0.5	10.5	2	0.5	2	1.18	80.23	14.87	26.53
45.5	6	18	7	0.5	0.5	0.5	2	11	9	1.55	85.62	9.512	49.575
56	16	5	2.54	0.5	4	6.99	2	4.97	2	28.12	9.96	0.934	32.15
54.79	16	5	1.21	0.5	0.5	10.5	2	0.5	9	57.26	10.44	0.744	32.15
50.74	16	5	1.76	0.5	4	10.5	2	7.5	2	66.25	8.08	0.764	45.215
44	6	17.34	7	0.5	4	10.5	2	0.5	8.16	0.69	19.24	16.61	107.18
56	9.5	18	7	0.5	4	0.5	2	0.5	2	1.58	76.39	44	643.09
49	9.51	18	6.99	4	0.5	0.5	2	0.5	9	0.74	94.09	34.66	37.19
45.5	6	18	7	0.5	0.5	10.5	2	8	2	1.19	81.62	12.46	30.01
44	6	18	7	0.5	2	0.5	17	0.5	4.5	4.02	72.19	0.456	18.49
47.64	6	18	1.36	4	0.5	0.5	17	0.5	4.5	29.69	30.93	0.115	8.305
49.83	8	18	1.8	1.37	0.5	2.5	9.87	6.13	2	17.98	34.12	0.178	9.445
45.97	6	14.03	7	4	0.5	2.5	10.5	7.5	2	3.57	56.7	0.308	9.11
44	11.71	18	1	4	0.5	10.5	2	6.29	2	2.78	36.92	1.716	38.44
56	16	5.42	7	0.5	0.5	10.08	2	0.5	2	3.65	32.58	5.577	29.14
56	16	10.5	1	0.5	4	0.5	2	0.5	9	14.31	12.9	8.642	44.21
44	16	10	7	0.5	4	0.5	2	7	9	1	54.07	18.59	86.415
44	13.37	12.79	7	0.98	0.5	9.86	2	0.5	9	0.64	73.54	13.23	216.45
44	16	18	5.26	4	0.5	2.71	7.03	0.5	2	0.81	68.27	4.07	87.42
48.95	11.12	16.71	4.28	1.13	1.66	8.97	3.67	0.41	3.1	1.6	54.06	9.976	49.16
48.01	11.42	10.03	3.76	2.75	3.63	5.68	6.36	4.29	4.07	5.55	25.08	0.493	12.53
53.28	10.48	11.29	3.73	0.82	0.84	7.33	2.35	3.92	5.96	7.25	24.56	1.434	12.89
42	17.43	20	3.69	0	0	2	13.88	0	1	1.9	59.92	4.52	30.44
52.03	9.69	9.8	3.56	0.97	0.77	10.19	5.23	1.99	5.77	8.53	19.71	0.232	13.94
53.29	7.4	6.26	5.96	0.35	0.12	12.29	2.86	4.43	7.04	6.85	27.21	0.326	14.125
48.95	11.12	16.71	4.28	1.13	1.66	8.97	3.67	0.41	3.1	1.51	58.16	8.644	90.76
53.53	10.53	11.25	3.75	0.83	0.84	7.19	2.31	3.85	5.92			2.672	19.238
41	13.37	14.28	4.76	1.05	1.07	9.13	2.93	4.89	7.52			6.073	52.909
45	12.46	13.32	4.44	0.98	0.99	8.51	2.73	4.56	7.01			5.548	30.967
49	11.56	12.35	4.12	0.91	0.92	7.89	2.54	4.23	6.5			4.59	22.669
57	9.74	10.41	3.47	0.77	0.78	6.65	2.14	3.56	5.48			1.651	13.37
56.84	5	11.95	3.98	0.88	0.89	7.63	2.45	4.09	6.29			0.788	12.54
50.86	15	10.69	3.56	0.79	0.8	6.83	2.2	3.66	5.62			2.144	22.722
47.86	20	10.06	3.35	0.74	0.75	6.43	2.07	3.44	5.29			5.707	90.836
57.3	11.27	5	4.01	0.89	0.9	7.7	2.47	4.12	6.34			0.314	10.128
51.27	10.09	15	3.59	0.8	0.81	6.89	2.21	3.69	5.67			6.135	25.972
48.25	9.49	20	3.38	0.75	0.76	6.48	2.08	3.47	5.34			14.4	98.259
55.06	10.83	11.57	1	0.85	0.86	7.4	2.38	3.96	6.09			0.612	12.767
52.28	10.28	10.99	6	0.81	0.82	7.02	2.26	3.76	5.78			7.116	20.331
51.72	10.17	10.87	7	0.8	0.81	6.95	2.23	3.72	5.72			9.406	29.404
52.9	10.41	11.12	3.71	2	0.83	7.11	2.28	3.81	5.85			3.012	19.768
53.98	10.62	11.35	3.78	0.84	0	7.25	2.33	3.88	5.97			1.59	19.983
52.9	10.41	11.12	3.71	0.82	2	7.11	2.28	3.81	5.85			3.63	20.386
54.8	10.78	11.52	3.84	0.85	0.86	7.36	0	3.94	6.06			3.803	56.673
52.06	10.24	10.94	3.65	0.81	0.82	6.99	5	3.74	5.76			0.291	13.502
49.32	9.7	10.36	3.46	0.77	0.77	6.62	10	3.55	5.45			0.199	10.11
46.58	9.16	9.79	3.26	0.72	0.73	6.26	15	3.35	5.15			0.193	9.302
53.28	10.48	11.29	3.73	0.82	0.84	7.33	2.35	3.92	5.96			1.473	15.648

APPENDIX B--Training and Validation Data Sets

This Appendix displays the data sets used for training and validation of viscosity, PCT B and MCC-1 B.

Table 1. Training Set for Viscosity

SIO2	B2O3		LI2O			FE2O3	AL2O3	ZRO2	OTHERS	VISC	LNVISC
0.4801	0.1142	0.1003	0.04	0.028	0.0363	0.0568	0.0636	0.0429	0.0407	5.78	1.754404
0.55	0.05	0.05	0.07	0.1	0	0.02	0.15	0	0.01	13.29	2.587012
0.42	0.2	0.05	0.07	0	0.08	0.02	0.14	0.01	0.01	2.39	0.871293
0.57	0.2	0.09	0.01	0.02	0.08	0.02	0	0	0.01	8.7	2.163323
0.57	0.05	0.07	0.07	0	0	0.15	0.08	0	0.01	13.24	2.583243
0.44	0.2	0.05	0.07	0	0	0.02	0	0.12	0.1	2.01	0.698135
0.57	0.05	0.0964	0.01	0.1	0	0.0336	0	0.13	0.01	72.88	4.288814
0.5363	0.05	0.0837	0.01	0	0.08	0.15	0	0.08	0.01	29.26	3.376221
0.42	0.1962	0.0538	0.01	0	0.08	0.14	0	0	0.1	4.06	1.401183
0.57	0.0851	0.0949	0.01	0	0	0.02	0.12	0	0.1	83.83	4.428791
0.42	0.1549	0.0751	0.01	0.1	0	0.02	0.14	0	0.08	14.5	2.674149
0.42	0.1764	0.0736	0.07	0.1	0	0.15	0	0	0.01	0.42	-0.8675
0.57	0.2	0.1862	0.01	0	0	0.02	0.0038	0	0.01	3.31	1.196948
0.42	0.2	0.1862	0.01	0	0	0.02	0.0238	0.13	0.01	3.42	1.229641
0.5589	0.05	0.1211	0.07	0	0.08	0.02	0	0	0.1	2.55	0.936093
0.4327	0.05	0.1873	0.01	0	0.08	0.0858	0.1442	0	0.01	17.81	2.87976
0.4545	0.05	0.1455	0.01	0.1	0	0.14	0	0	0.1	2.23	0.802002
0.4214	0.05	0.1186	0.07	0.02	0.08	0.02	0	0.13	0.09	1.87	0.625938
0.4801	0.1142	0.1003	0.04	0.028	0.0363	0.0568	0.0636	0.0429	0.0407	5.76	1.750937
0.4801	0.1142	0.1003	0.04	0.028	0.0363	0.0568	0.0636	0.0429	0.0407	5.71	1.742219
0.57	0.2	0.09	0.01	0.02	0.08	0.02	0	0	0.01	9.36	2.236445
0.5363	0.05	0.0837	0.01	0	0.08	0.15	0	0.08	0.01	38.11	3.640477
0.5153	0.0956	0.1052	0.04	0.029	0.0084	0.1179	0.0456	0.0063	0.0393	5.69	1.73871
0.5226	0.0874	0.07	0.06	0	0.05	0.04	0.08	0.01	0.08	7.74	2.046402
0.5017	0.07	0.0883	0.06	0.07	0	0.045	0.11	0.03	0.025	6.26	1.83418
0.4645	0.132	0.07	0.04	0.07	0.01	0.045	0.1032	0.0368	0.025	5.56	1.715598
0.56	0.1095	0.07	0.05	0.07	0	0.04	0.0619	0.01	0.025	6.37	1.851599
0.4751	0.159	0.101	0.02	0.035	0	0.04	0.08	0.01	0.08	8.18	2.101692
0.5373	0.07	0.07	0.04	0.07	0.0046	0.12	0.0159	0.01	0.0641	6.19	1.822935
0.4814	0.17	0.07	0.06	0.009	0	0.04	0.0953	0.01	0.0648	4.26	1.449269
0.5115	0.07	0.0985	0.06	0	0.05	0.114	0.061	0.01	0.025	4.36	1.472472
0.5431	0.0944	0.0924	0.06	0	0	0.0712	0.0138	0.1	0.025	7.3	1.987874
0.4694	0.17	0.1306	0.02	0	0	0.0669	0.1043	0.01	0.0288	8.99	2.196113
0.4915	0.0751	0.0833	0.06	0.07	0.01	0.04	0.01	0.0935	0.0665	3.07	1.121678
0.4683	0.17	0.07	0.05	0.07	0.01	0.04	0.0901	0.01	0.025	3.38	1.217876
0.4937	0.07	0.1692	0.02	0.03	0.05	0.04	0.0896	0.01	0.025	7.27	1.983756
0.46	0.1313	0.0802	0.05	0.05	0.02	0.04	0.0243	0.1	0.0457	2.97	1.088562
0.4729	0.07	0.17	0.02	0.06	0	0.04	0.0756	0.01	0.08	4.47	1.497388
0.5353	0.1053	0.1125	0.04	0.008	0.0084	0.0719	0.0231	0.0385	0.0592	6.57	1.882514
0.4801	0.1142	0.1003	0.04	0.028	0.0363	0.0568	0.0636	0.0429	0.0407	5.37	1.680828
0.5353	0.1053	0.1125	0.04	0.008	0.0084	0.0719	0.0231	0.0385	0.0592	6.41	1.857859
0.5328	0.1048	0.1129	0.04	0.008	0.0084	0.0733	0.0235	0.0392	0.0596	6.76	1.911023
0.57	0.05	0.1031	0.07	0	0	0.06	0.01	0.13	0.01	12.31	2.510412
0.57	0.1314	0.05	0.07	0	0.08	0.02	0.0686	0	0.01	6.01	1.793425
0.57	0.05	0.0735	0.07	0	0.08	0.02	0.0365	0	0.1	5.92	1.778336
0.57	0.0522	0.2	0.01	0.08	0	0.02	0.0578	0	0.01	9.91	2.293544
0.4464	0.2	0.0736	0.07	0	0	0.02	0.0961	0	0.0939	1.99	0.688135
0.5059	0.05	0.0841	0.07	0.08	0	0.15	0.0033	0	0.0567	1.35	0.300105
0.4431	0.2	0.0512	0.07	0.08	0	0.02	0.0257	0.1	0.01	1.26	0.231112
0.5463	0.05	0.2	0.02	0	0.08	0.02	0.0782	0	0.01	14.41	2.667922
0.5619	0.05	0.2	0.01	0	0	0.02	0.0555	0	0.1	13.44	2.598235
0.4391	0.2	0.0675	0.01	0.08	0	0.02	0	0.0834	0.1	5.32	1.671473
0.519	0.2	0.0832	0.01	0	0	0.132	0.0458	0	0.01	27.42	3.311273
0.57	0.1843	0.05	0.03	0.08	0	0.02	0.0526	0	0.01	10.3	2.332144
0.5445	0.05	0.2	0.04	0	0	0.02	0.0027	0.13	0.01	8.07	2.088153
0.42	0.0544	0.2	0.04	0	0.08	0.02	0.0892	0	0.1	2.15	0.765468
0.42	0.1743	0.2	0.04	0	0	0.02	0.1388	0	0.01	1.79	0.582216
0.42	0.05	0.2	0.04	0.08	0	0.0632	0.134	0	0.01	2.82	1.036737
0.5421	0.05	0.0891	0.07	0.08	0	0.15	0.0088	0	0.01	1.91	0.647103
0.57	0.0839	0.1061	0.07	0	0	0.02	0.14	0	0.01	12.34	2.512846
0.5147	0.1109	0.1044	0.01	0	0.08	0.1428	0.0272	0	0.01	12.02	2.486572

0.4838	0.05	0.1362	0.07	0	0.08	0.0742	0.0258	0.07	0.01	1.98	0.683097
0.504	0.0639	0.15	0.04	0.02	0.05	0.02	0.1	0.02	0.03	6.88	1.928619

Table 2. Validation Set for Viscosity

SIO2	B2O3	NA2O	LI2O			FE2O3	AL2O3	ZRO2	OTHERS	VISC	LNVISC
0.55671	0.18221	0.10704	0.00911	0.04471	0.072885	0.018221	0	0	0.009111	6.2	1.824549
0.5325	0.0694	0.0781	0.07	0.05	0.02	0.03	0.1	0.02	0.03	6.2	1.824549
0.5675	0.05	0.0625	0.07	0.032	0.038	0.1	0.03	0.02	0.03	5.51	1.706565
0.507	0.1477	0.05	0.0653	0.02	0.03	0.03	0.05	0.07	0.03	4.43	1.4884
0.57	0.1078	0.05	0.0699	0.05	0.02	0.02	0.0623	0.02	0.03	6.08	1.805005
0.5299	0.1106	0.05	0.0595	0.02	0.05	0.0308	0.0592	0.02	0.07	6.03	1.796747
0.5264	0.1259	0.0577	0.07	0.02	0.02	0.02	0.0746	0.02	0.0654	4.7	1.547563
0.5294	0.05	0.1277	0.0429	0.05	0.02	0.02	0.04	0.05	0.07	6.64	1.893112
0.47	0.1442	0.0968	0.039	0.05	0.02	0.02	0.0854	0.02	0.0546	3.94	1.371181
0.5073	0.1357	0.0957	0.0413	0.02	0.02	0.0515	0.0785	0.02	0.03	6.46	1.865629
0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.043	0.0407	5.71	1.742219
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.039	0.0596	7.07	1.95586
0.6	0.0817	0.045	0.0788	0.0008	0.0009	0.072	0.0233	0.039	0.059	9.22	2.221375
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.039	0.0596	6.26	1.83418
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.039	0.0596	6.12	1.811562
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.039	0.0596	6.74	1.90806
0.39	0.2	0.05	0.07	0.02	0.08	0.02	0.15	0.01	0.01	1.85	0.615186
0.438	0.1718	0.1268	0.0727	0.0375	0.0005	0.02	0.115	0.008	0.0102	1.15	0.139762
0.5281	0.0876	0.1725	0.0743	0.0063	0.0005	0.02	0.0925	0.008	0.0107	2.61	0.95935
0.5281	0.0664	0.12	0.073	0	0	0.02	0.1625	0.018	0.0125	12.9	2.557227
0.5579	0.1765	0.1125	0.0156	0.05	0.0005	0.02	0.05	0.008	0.0095	9.95	2.297573
0.3232	0.1717	0.19	0.0051	0.1	0	0.02	0.18	0	0.01	2.38	0.8671
0.5697	0.0509	0.0925	0.0642	0.0025	0.0008	0.0812	0.0288	0.043	0.0663	8.89	2.184927
0.5344	0.1128	0.086	0.0697	0.0007	0.0004	0.0013	0.0196	0.155	0.0203	8.2	2.104134
0.5175	0.0917	0.1211	0.0523	0.0097	0.0061	0.0388	0.118	0.003	0.0422	8.24	2.109
0.4596	0.1587	0.1086	0.0583	0.0024	0.0001	0.0004	0.2043	0	0.0076	8.97	2.193886
0.504	0.1355	0.0797	0.0696	0.0007	0.0002	0.0046	0.164	1E-04	0.0416	17.05	2.83615
0.566	0.0781	0.0664	0.0713	0.0079	0.0032	0.0334	0.0816	5E-04	0.0916	22.15	3.097837
0.4854	0.1418	0.0812	0.0691	0.0008	0.0008	0.008	0.1819	5E-04	0.0305	10.8	2.379546
0.5697	0.0509	0.0925	0.0642	0.0025	0.0008	0.0812	0.0288	0.043	0.0663	8.5	2.140066
0.5175	0.0917	0.1211	0.0523	0.0097	0.0061	0.0388	0.118	0.003	0.0422	7.81	2.055405
0.504	0.1355	0.0797	0.0696	0.0007	0.0002	0.0046	0.164	1E-04	0.0416	8.67	2.159869
0.566	0.0781	0.0664	0.0713	0.0079	0.0032	0.0334	0.0816	5E-04	0.0916	9.55	2.256541
0.4854	0.1418	0.0812	0.0691	0.0008	0.0008	0.008	0.1819	5E-04	0.0305	8.66	2.158715
0.5018	0.06	0.18	0.0632	0.04	0.005	0.105	0.02	0.005	0.02	1.18	0.165514
0.455	0.06	0.18	0.07	0.005	0.005	0.005	0.02	0.11	0.09	1.55	0.438255
0.56	0.16	0.05	0.0254	0.005	0.04	0.0699	0.02	0.05	0.02	28.12	3.336481
0.5479	0.16	0.05	0.0121	0.005	0.005	0.105	0.02	0.005	0.09	57.26	4.047602
0.5074	0.16	0.05	0.0176	0.005	0.04	0.105	0.02	0.075	0.02	66.25	4.193435
0.44	0.06	0.1734	0.07	0.005	0.04	0.105	0.02	0.005	0.0816	0.69	-0.37106
0.56	0.095	0.18	0.07	0.005	0.04	0.005	0.02	0.005	0.02	1.58	0.457425
0.49	0.0951	0.18	0.0699	0.04	0.005	0.005	0.02	0.005	0.09	0.74	-0.30111
0.455	0.06	0.18	0.07	0.005	0.005	0.105	0.02	0.08	0.02	1.19	0.173953
0.44	0.06	0.18	0.07	0.005	0.02	0.005	0.17	0.005	0.045	4.02	1.391282
0.4764	0.06	0.18	0.0136	0.04	0.005	0.005	0.17	0.005	0.045	29.69	3.39081
0.4983	0.08	0.18	0.018	0.0137	0.005	0.025	0.0987	0.061	0.02	17.98	2.88926
0.4597	0.06	0.1403	0.07	0.04	0.005	0.025	0.105	0.075	0.02	3.57	1.272566
0.44	0.1171	0.18	0.01	0.04	0.005	0.105	0.02	0.063	0.02	2.78	1.022451
0.56	0.16	0.0542	0.07	0.005	0.005	0.1008	0.02	0.005	0.02	3.65	1.294727
0.56	0.16	0.105	0.01	0.005	0.04	0.005	0.02	0.005	0.09	14.31	2.660959
0.44	0.16	0.1	0.07	0.005	0.04	0.005	0.02	0.07	0.09	1	0
0.44	0.1337	0.1279	0.07	0.0098	0.005	0.0986	0.02	0.005	0.09	0.64	-0.44629
0.44	0.16	0.18	0.0526	0.04	0.005	0.0271	0.0703	0.005	0.02	0.81	-0.21072
0.4895	0.1112	0.1671	0.0428	0.0113	0.0166	0.0897	0.0367	0.004	0.031	1.6	0.470004
0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.043	0.0407	5.55	1.713798
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.039	0.0596	7.25	1.981001
0.42	0.1743	0.2	0.0369	0	0	0.02	0.1388	0	0.01	1.9	0.641854
0.5203	0.0969	0.098	0.0356	0.0097	0.0077	0.1019	0.0523	0.02	0.0577	8.53	2.143589
0.5329	0.074	0.0626	0.0596	0.0035	0.0012	0.1229	0.0286	0.044	0.0704	6.85	1.924249
0.4895	0.1112	0.1671	0.0428	0.0113	0.0166	0.0897	0.0367	0.004	0.031	1.51	0.41211

Table 3. Training Set for PCT B

SIO2	B2O3	NA2O	LI2O		MGO	FE2O3	AL2O3	ZRO2	OTHERS	PCT	LNPCT
0.46270	0.19850	0.115182	0.048313	0.048324	0.087705	0.015119	0	0	0.00756	0.557	-0.58519
0.6	0.0817	0.045	0.0788	0.0008	0.0009	0.072	0.0233	0.0385	0.059	0.557	-0.58519
0.5226	0.0874	0.07	0.06	0	0.05	0.04	0.08	0.01	0.08	0.304	-1.19073
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	2.761	1.015593
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	1.342	0.294161
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	1.419	0.349952
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	1.164	0.151862
0.39	0.2	0.05	0.07	0.02	0.08	0.02	0.15	0.01	0.01	0.778	-0.25103
0.438	0.1718	0.1268	0.0727	0.0375	0.0005	0.02	0.115	0.0075	0.0102	1.591	0.464363
0.5281	0.0876	0.1725	0.0743	0.0063	0.0005	0.02	0.0925	0.0075	0.0107	1.624	0.484892
0.5281	0.0664	0.12	0.073	0	0	0.02	0.1625	0.0175	0.0125	0.222	-1.50508
0.5579	0.1765	0.1125	0.0156	0.05	0.0005	0.02	0.05	0.0075	0.0095	1.002	0.001998
0.3232	0.1717	0.19	0.0051	0.1	0	0.02	0.18	0	0.01	0.332	-1.10262
0.5697	0.0509	0.0925	0.0642	0.0025	0.0008	0.0812	0.0288	0.0431	0.0663	0.379	-0.97022
0.5344	0.1128	0.086	0.0697	0.0007	0.0004	0.0013	0.0196	0.1548	0.0203	0.335	-1.09362
0.5175	0.0917	0.1211	0.0523	0.0097	0.0061	0.0388	0.118	0.0026	0.0422	0.21	-1.56065
0.4596	0.1587	0.1086	0.0583	0.0024	0.0001	0.0004	0.2043	0	0.0076	0.512	-0.66943
0.504	0.1355	0.0797	0.0696	0.0007	0.0002	0.0046	0.164	0.0001	0.0416	0.308	-1.17766
0.566	0.0781	0.0664	0.0713	0.0079	0.0032	0.0334	0.0816	0.0005	0.0916	0.226	-1.48722
0.4854	0.1418	0.0812	0.0691	0.0008	0.0008	0.008	0.1819	0.0005	0.0305	0.312	-1.16475
0.5697	0.0509	0.0925	0.0642	0.0025	0.0008	0.0812	0.0288	0.0431	0.0663	0.411	-0.88916
0.5175	0.0917	0.1211	0.0523	0.0097	0.0061	0.0388	0.118	0.0026	0.0422	0.21	-1.56065
0.504	0.1355	0.0797	0.0696	0.0007	0.0002	0.0046	0.164	0.0001	0.0416	0.244	-1.41059
0.566	0.0781	0.0664	0.0713	0.0079	0.0032	0.0334	0.0816	0.0005	0.0916	0.226	-1.48722
0.4854	0.1418	0.0812	0.0691	0.0008	0.0008	0.008	0.1819	0.0005	0.0305	0.278	-1.28013
0.5018	0.06	0.18	0.0632	0.04	0.005	0.105	0.02	0.005	0.02	14.87	2.699413
0.455	0.06	0.18	0.07	0.005	0.005	0.005	0.02	0.11	0.09	9.512	2.252554
0.56	0.16	0.05	0.0254	0.005	0.04	0.0699	0.02	0.0497	0.02	0.934	-0.06828
0.5479	0.16	0.05	0.0121	0.005	0.005	0.105	0.02	0.005	0.09	0.744	-0.29571
0.5074	0.16	0.05	0.0176	0.005	0.04	0.105	0.02	0.075	0.02	0.764	-0.26919
0.44	0.06	0.1734	0.07	0.005	0.04	0.105	0.02	0.005	0.0816	16.61	2.810186
0.56	0.095	0.18	0.07	0.005	0.04	0.005	0.02	0.005	0.02	44	3.78419
0.49	0.0951	0.18	0.0699	0.04	0.005	0.005	0.02	0.005	0.09	34.65	3.545471
0.455	0.06	0.18	0.07	0.005	0.005	0.105	0.02	0.08	0.02	12.46	2.522524
0.44	0.06	0.18	0.07	0.005	0.02	0.005	0.17	0.005	0.045	0.456	-0.78526
0.4764	0.06	0.18	0.0136	0.04	0.005	0.005	0.17	0.005	0.045	0.115	-2.16282
0.4983	0.08	0.18	0.018	0.0137	0.005	0.025	0.0987	0.0613	0.02	0.178	-1.72597
0.4597	0.06	0.1403	0.07	0.04	0.005	0.025	0.105	0.075	0.02	0.308	-1.17766
0.44	0.1171	0.18	0.01	0.04	0.005	0.105	0.02	0.0629	0.02	1.716	0.539996
0.56	0.16	0.0542	0.07	0.005	0.005	0.1008	0.02	0.005	0.02	5.577	1.718651
0.56	0.16	0.105	0.01	0.005	0.04	0.005	0.02	0.005	0.09	8.642	2.156634
0.44	0.16	0.1	0.07	0.005	0.04	0.005	0.02	0.07	0.09	18.59	2.922624
0.44	0.1337	0.1279	0.07	0.0098	0.005	0.0986	0.02	0.005	0.09	13.22	2.58226
0.44	0.16	0.18	0.0526	0.04	0.005	0.0271	0.0703	0.005	0.02	4.07	1.403643
0.4895	0.1112	0.1671	0.0428	0.0113	0.0166	0.0897	0.0367	0.0041	0.031	9.976	2.300182
0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407	0.493	-0.70725
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	1.434	0.360468
0.42	0.1743	0.2	0.0369	0	0	0.02	0.1388	0	0.01	4.52	1.508512
0.5203	0.0969	0.098	0.0356	0.0097	0.0077	0.1019	0.0523	0.0199	0.0577	0.232	-1.46102
0.5329	0.074	0.0626	0.0596	0.0035	0.0012	0.1229	0.0286	0.0443	0.0704	0.326	-1.12086
0.4895	0.1112	0.1671	0.0428	0.0113	0.0166	0.0897	0.0367	0.0041	0.031	8.644	2.156865
0.5353	0.1053	0.1125	0.0375	0.0083	0.0084	0.0719	0.0231	0.0385	0.0592	2.672	0.982827
0.41	0.1337	0.1428	0.0476	0.0105	0.0107	0.0913	0.0293	0.0489	0.0752	6.073	1.803853
0.45	0.1246	0.1332	0.0444	0.0098	0.0099	0.0851	0.0273	0.0456	0.0701	5.548	1.713438
0.49	0.1156	0.1235	0.0412	0.0091	0.0092	0.0789	0.0254	0.0423	0.065	4.59	1.52388
0.57	0.0974	0.1041	0.0347	0.0077	0.0078	0.0665	0.0214	0.0356	0.0548	1.651	0.501381
0.5684	0.05	0.1195	0.0398	0.0088	0.0089	0.0763	0.0245	0.0409	0.0629	0.788	-0.23826
0.5086	0.15	0.1069	0.0356	0.0079	0.008	0.0683	0.022	0.0366	0.0562	2.144	0.762673
0.4786	0.2	0.1006	0.0335	0.0074	0.0075	0.0643	0.0207	0.0344	0.0529	5.707	1.741693
0.573	0.1127	0.05	0.0401	0.0089	0.009	0.077	0.0247	0.0412	0.0634	0.314	-1.15836
0.5127	0.1009	0.15	0.0359	0.008	0.0081	0.0689	0.0221	0.0369	0.0567	6.135	1.81401
0.4825	0.0949	0.2	0.0338	0.0075	0.0076	0.0648	0.0208	0.0347	0.0534	14.4	2.667228
0.5506	0.1083	0.1157	0.01	0.0085	0.0086	0.074	0.0238	0.0396	0.0609	0.612	-0.49102
0.5228	0.1028	0.1099	0.06	0.0081	0.0082	0.0702	0.0226	0.0376	0.0578	7.116	1.962346
0.5172	0.1017	0.1087	0.07	0.008	0.0081	0.0695	0.0223	0.0372	0.0572	9.406	2.241348
0.529	0.1041	0.1112	0.0371	0.02	0.0083	0.0711	0.0228	0.0381	0.0585	3.012	1.102604
0.5398	0.1062	0.1135	0.0378	0.0084	0	0.0725	0.0233	0.0388	0.0597	1.59	0.463734
0.529	0.1041	0.1112	0.0371	0.0082	0.02	0.0711	0.0228	0.0381	0.0585	3.63	1.289233
0.548	0.1078	0.1152	0.0384	0.0085	0.0086	0.0736	0	0.0394	0.0606	3.803	1.33579
0.5206	0.1024	0.1094	0.0365	0.0081	0.0082	0.0699	0.05	0.0374	0.0576	0.291	-1.23443
0.4932	0.097	0.1036	0.0346	0.0077	0.0077	0.0662	0.1	0.0355	0.0545	0.199	-1.61445
0.4658	0.0916	0.0979	0.0326	0.0072	0.0073	0.0626	0.15	0.0335	0.0515	0.193	-1.64507
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	1.473	0.387301
0.37	0.1428	0.1525	0.0508	0.0113	0.0114	0.0975	0.0313	0.0522	0.0803	5.567	1.716856

Table 4. Validation Set for PCT B

SIO2	B2O3	NA2O	LI2O	CAO	MGO	FE2O3	AL2O3	ZRO2	OTHERS	PCT	LNPCT
0.46270	0.19850	0.115182	0.048313	0.048324	0.087705	0.01511	0	0	0.00756	0.557	-0.58519
0.6	0.0817	0.045	0.0788	0.0008	0.0009	0.072	0.0233	0.0385	0.059	0.557	-0.58519
0.5226	0.0874	0.07	0.06	0	0.05	0.04	0.08	0.01	0.08	0.304	-1.19073
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	2.761	1.015593
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	1.342	0.294161
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	1.419	0.349952
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	1.164	0.151862
0.39	0.2	0.05	0.07	0.02	0.08	0.02	0.15	0.01	0.01	0.778	-0.25103
0.438	0.1718	0.1268	0.0727	0.0375	0.0005	0.02	0.115	0.0075	0.0102	1.591	0.464363
0.5281	0.0876	0.1725	0.0743	0.0063	0.0005	0.02	0.0925	0.0075	0.0107	1.624	0.484892
0.5281	0.0664	0.12	0.073	0	0	0.02	0.1625	0.0175	0.0125	0.222	-1.50508
0.5579	0.1765	0.1125	0.0156	0.05	0.0005	0.02	0.05	0.0075	0.0095	1.002	0.001998
0.3232	0.1717	0.19	0.0051	0.1	0	0.02	0.18	0	0.01	0.332	-1.10262
0.5697	0.0509	0.0925	0.0642	0.0025	0.0008	0.0812	0.0288	0.0431	0.0663	0.379	-0.97022
0.5344	0.1128	0.086	0.0697	0.0007	0.0004	0.0013	0.0196	0.1548	0.0203	0.335	-1.09362
0.5175	0.0917	0.1211	0.0523	0.0097	0.0061	0.0388	0.118	0.0026	0.0422	0.21	-1.56065
0.4596	0.1587	0.1086	0.0583	0.0024	0.0001	0.0004	0.2043	0	0.0076	0.512	-0.66943
0.504	0.1355	0.0797	0.0696	0.0007	0.0002	0.0046	0.164	0.0001	0.0416	0.308	-1.17766
0.566	0.0781	0.0664	0.0713	0.0079	0.0032	0.0334	0.0816	0.0005	0.0916	0.226	-1.48722
0.4854	0.1418	0.0812	0.0691	0.0008	0.0008	0.008	0.1819	0.0005	0.0305	0.312	-1.16475
0.5697	0.0509	0.0925	0.0642	0.0025	0.0008	0.0812	0.0288	0.0431	0.0663	0.411	-0.88916
0.5175	0.0917	0.1211	0.0523	0.0097	0.0061	0.0388	0.118	0.0026	0.0422	0.21	-1.56065
0.504	0.1355	0.0797	0.0696	0.0007	0.0002	0.0046	0.164	0.0001	0.0416	0.244	-1.41059
0.566	0.0781	0.0664	0.0713	0.0079	0.0032	0.0334	0.0816	0.0005	0.0916	0.226	-1.48722
0.4854	0.1418	0.0812	0.0691	0.0008	0.0008	0.008	0.1819	0.0005	0.0305	0.278	-1.28013
0.5018	0.06	0.18	0.0632	0.04	0.005	0.105	0.02	0.005	0.02	14.871	2.699413
0.455	0.06	0.18	0.07	0.005	0.005	0.005	0.02	0.11	0.09	9.512	2.252554
0.56	0.16	0.05	0.0254	0.005	0.04	0.0699	0.02	0.0497	0.02	0.934	-0.06828
0.5479	0.16	0.05	0.0121	0.005	0.005	0.105	0.02	0.005	0.09	0.744	-0.29571
0.5074	0.16	0.05	0.0176	0.005	0.04	0.105	0.02	0.075	0.02	0.764	-0.26919
0.44	0.06	0.1734	0.07	0.005	0.04	0.105	0.02	0.005	0.0816	16.613	2.810186
0.56	0.095	0.18	0.07	0.005	0.04	0.005	0.02	0.005	0.02	44	3.78419
0.49	0.0951	0.18	0.0699	0.04	0.005	0.005	0.02	0.005	0.09	34.656	3.545471
0.455	0.06	0.18	0.07	0.005	0.005	0.105	0.02	0.08	0.02	12.46	2.522524
0.44	0.06	0.18	0.07	0.005	0.02	0.005	0.17	0.005	0.045	0.456	-0.78526
0.4764	0.06	0.18	0.0136	0.04	0.005	0.005	0.17	0.005	0.045	0.115	-2.16282
0.4983	0.08	0.18	0.018	0.0137	0.005	0.025	0.0987	0.0613	0.02	0.178	-1.72597
0.4597	0.06	0.1403	0.07	0.04	0.005	0.025	0.105	0.075	0.02	0.308	-1.17766
0.44	0.1171	0.18	0.01	0.04	0.005	0.105	0.02	0.0629	0.02	1.716	0.539996
0.56	0.16	0.0542	0.07	0.005	0.005	0.1008	0.02	0.005	0.02	5.577	1.718651
0.56	0.16	0.105	0.01	0.005	0.04	0.005	0.02	0.005	0.09	8.642	2.156634
0.44	0.16	0.1	0.07	0.005	0.04	0.005	0.02	0.07	0.09	18.59	2.922624
0.44	0.1337	0.1279	0.07	0.0098	0.005	0.0986	0.02	0.005	0.09	13.227	2.58226
0.44	0.16	0.18	0.0526	0.04	0.005	0.0271	0.0703	0.005	0.02	4.07	1.403643
0.4895	0.1112	0.1671	0.0428	0.0113	0.0166	0.0897	0.0367	0.0041	0.031	9.976	2.300182
0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407	0.493	-0.70725
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	1.434	0.360468
0.42	0.1743	0.2	0.0369	0	0	0.02	0.1388	0	0.01	4.52	1.508512
0.5203	0.0969	0.098	0.0356	0.0097	0.0077	0.1019	0.0523	0.0199	0.0577	0.232	-1.46102
0.5329	0.074	0.0626	0.0596	0.0035	0.0012	0.1229	0.0286	0.0443	0.0704	0.326	-1.12086
0.4895	0.1112	0.1671	0.0428	0.0113	0.0166	0.0897	0.0367	0.0041	0.031	8.644	2.156865
0.5353	0.1053	0.1125	0.0375	0.0083	0.0084	0.0719	0.0231	0.0385	0.0592	2.672	0.982827
0.41	0.1337	0.1428	0.0476	0.0105	0.0107	0.0913	0.0293	0.0489	0.0752	6.073	1.803853
0.45	0.1246	0.1332	0.0444	0.0098	0.0099	0.0851	0.0273	0.0456	0.0701	5.548	1.713438
0.49	0.1156	0.1235	0.0412	0.0091	0.0092	0.0789	0.0254	0.0423	0.065	4.59	1.52388
0.57	0.0974	0.1041	0.0347	0.0077	0.0078	0.0665	0.0214	0.0356	0.0548	1.651	0.501381
0.5684	0.05	0.1195	0.0398	0.0088	0.0089	0.0763	0.0245	0.0409	0.0629	0.788	-0.23826
0.5086	0.15	0.1069	0.0356	0.0079	0.008	0.0683	0.022	0.0366	0.0562	2.144	0.762673
0.4786	0.2	0.1006	0.0335	0.0074	0.0075	0.0643	0.0207	0.0344	0.0529	5.707	1.741693
0.573	0.1127	0.05	0.0401	0.0089	0.009	0.077	0.0247	0.0412	0.0634	0.314	-1.15836
0.5127	0.1009	0.15	0.0359	0.008	0.0081	0.0689	0.0221	0.0369	0.0567	6.135	1.81401
0.4825	0.0949	0.2	0.0338	0.0075	0.0076	0.0648	0.0208	0.0347	0.0534	14.4	2.667228
0.5506	0.1083	0.1157	0.01	0.0085	0.0086	0.074	0.0238	0.0396	0.0609	0.612	-0.49102
0.5228	0.1028	0.1099	0.06	0.0081	0.0082	0.0702	0.0226	0.0376	0.0578	7.116	1.962346
0.5172	0.1017	0.1087	0.07	0.008	0.0081	0.0695	0.0223	0.0372	0.0572	9.406	2.241348
0.529	0.1041	0.1112	0.0371	0.02	0.0083	0.0711	0.0228	0.0381	0.0585	3.012	1.102604
0.5398	0.1062	0.1135	0.0378	0.0084	0	0.0725	0.0233	0.0388	0.0597	1.59	0.463734
0.529	0.1041	0.1112	0.0371	0.0082	0.02	0.0711	0.0228	0.0381	0.0585	3.63	1.289233
0.548	0.1078	0.1152	0.0384	0.0085	0.0086	0.0736	0	0.0394	0.0606	3.803	1.33579
0.5206	0.1024	0.1094	0.0365	0.0081	0.0082	0.0699	0.05	0.0374	0.0576	0.291	-1.23443
0.4932	0.097	0.1036	0.0346	0.0077	0.0077	0.0662	0.1	0.0355	0.0545	0.199	-1.61445
0.4658	0.0916	0.0979	0.0326	0.0072	0.0073	0.0626	0.15	0.0335	0.0515	0.193	-1.64507
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	1.473	0.387301
0.37	0.1428	0.1525	0.0508	0.0113	0.0114	0.0975	0.0313	0.0522	0.0803	5.567	1.716856

Table 5. Training Set for MCC-1 B

SIO2	B2O3		LI2O		MGO	FE2O3	AL2O3	ZRO2	OTHERS		LNMCC
0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407	12.47	2.523326
0.55	0.05	0.05	0.07	0.1	0	0.02	0.15	0	0.01	7.46	2.009555
0.42	0.2	0.05	0.07	0	0.08	0.02	0.14	0.01	0.01	15.57	2.745346
0.57	0.05	0.07	0.07	0	0	0.15	0.08	0	0.01	11.48	2.440606
0.57	0.05	0.0964	0.01	0.1	0	0.0336	0	0.13	0.01	10.995	2.397441
0.5363	0.05	0.0837	0.01	0	0.08	0.15	0	0.08	0.01	17.875	2.883403
0.57	0.0851	0.0949	0.01	0	0	0.02	0.12	0	0.1	2.745	1.009781
0.42	0.1549	0.0751	0.01	0.1	0	0.02	0.14	0	0.08	8.25	2.110213
0.42	0.1764	0.0736	0.07	0.1	0	0.15	0	0	0.01	118.48	4.774744
0.42	0.2	0.1862	0.01	0	0	0.02	0.0238	0.13	0.01	73.635	4.29912
0.4327	0.05	0.1873	0.01	0	0.08	0.0858	0.1442	0	0.01	16.85	2.824351
0.4545	0.05	0.1455	0.01	0.1	0	0.14	0	0	0.1	39.1	3.666122
0.4214	0.05	0.1186	0.07	0.02	0.08	0.02	0	0.13	0.09	24.055	3.180343
0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407	13.025	2.566871
0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407	12.505	2.526129
0.5363	0.05	0.0837	0.01	0	0.08	0.15	0	0.08	0.01	17.36	2.854169
0.5153	0.0956	0.1052	0.0375	0.0289	0.0084	0.1179	0.0456	0.0063	0.0393	15.37	2.732418
0.5226	0.0874	0.07	0.06	0	0.05	0.04	0.08	0.01	0.08	12.24	2.504709
0.5017	0.07	0.0883	0.06	0.07	0	0.045	0.11	0.03	0.025	8.44	2.132982
0.4645	0.132	0.07	0.0435	0.07	0.01	0.045	0.1032	0.0368	0.025	8.87	2.182675
0.56	0.1095	0.07	0.0536	0.07	0	0.04	0.0619	0.01	0.025	9.73	2.275214
0.4751	0.159	0.101	0.02	0.0348	0	0.04	0.08	0.01	0.08	10.405	2.342286
0.5373	0.07	0.07	0.0382	0.07	0.0046	0.12	0.0159	0.01	0.0641	17.475	2.860771
0.4814	0.17	0.07	0.0591	0.0094	0	0.04	0.0953	0.01	0.0648	5.02	1.61343
0.5115	0.07	0.0985	0.06	0	0.05	0.114	0.061	0.01	0.025	18.505	2.918041
0.5431	0.0944	0.0924	0.06	0	0	0.0712	0.0138	0.1	0.025	13.2	2.580217
0.4694	0.17	0.1306	0.02	0	0	0.0669	0.1043	0.01	0.0288	12.275	2.507565
0.4915	0.0751	0.0833	0.06	0.07	0.01	0.04	0.01	0.0935	0.0665	19.85	2.988204
0.4683	0.17	0.07	0.0466	0.07	0.01	0.04	0.0901	0.01	0.025	9.86	2.288486
0.4937	0.07	0.1692	0.0225	0.03	0.05	0.04	0.0896	0.01	0.025	13.36	2.592265
0.46	0.1313	0.0802	0.0486	0.05	0.02	0.04	0.0243	0.1	0.0457	15.095	2.714364
0.4729	0.07	0.17	0.0214	0.0601	0	0.04	0.0756	0.01	0.08	25.1	3.222868
0.5353	0.1053	0.1125	0.0375	0.0083	0.0084	0.0719	0.0231	0.0385	0.0592	18.085	2.895083
0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407	12.325	2.51163
0.5353	0.1053	0.1125	0.0375	0.0083	0.0084	0.0719	0.0231	0.0385	0.0592	19.72	2.981633
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	13.69	2.616666
0.57	0.05	0.1031	0.0669	0	0	0.06	0.01	0.13	0.01	8.425	2.131203
0.57	0.1314	0.05	0.07	0	0.08	0.02	0.0686	0	0.01	11.805	2.468523
0.57	0.05	0.0735	0.07	0	0.08	0.02	0.0365	0	0.1	15.595	2.74695
0.57	0.0522	0.2	0.01	0.08	0	0.02	0.0578	0	0.01	11.21	2.416806
0.4464	0.2	0.0736	0.07	0	0	0.02	0.0961	0	0.0939	19.855	2.988456
0.5059	0.05	0.0841	0.07	0.08	0	0.15	0.0033	0	0.0567	34.5	3.540959
0.4431	0.2	0.0512	0.07	0.08	0	0.02	0.0257	0.1	0.01	39.145	3.667273
0.5463	0.05	0.2	0.0155	0	0.08	0.02	0.0782	0	0.01	11.22	2.417698
0.5619	0.05	0.2	0.0126	0	0	0.02	0.0555	0	0.1	9.835	2.285947
0.4391	0.2	0.0675	0.01	0.08	0	0.02	0	0.0834	0.1	42.285	3.744432
0.519	0.2	0.0832	0.01	0	0	0.132	0.0458	0	0.01	24.435	3.196017
0.57	0.1843	0.05	0.0331	0.08	0	0.02	0.0526	0	0.01	47.02	3.850573
0.5445	0.05	0.2	0.0428	0	0	0.02	0.0027	0.13	0.01	16.62	2.810607
0.42	0.0544	0.2	0.0364	0	0.08	0.02	0.0892	0	0.1	14.51	2.674838
0.42	0.1743	0.2	0.0369	0	0	0.02	0.1388	0	0.01	29.24	3.375538
0.42	0.05	0.2	0.0428	0.08	0	0.0632	0.134	0	0.01	11.61	2.451867
0.5421	0.05	0.0891	0.07	0.08	0	0.15	0.0088	0	0.01	21.09	3.048799
0.57	0.0839	0.1061	0.07	0	0	0.02	0.14	0	0.01	9.635	2.265402
0.5147	0.1109	0.1044	0.01	0	0.08	0.1428	0.0272	0	0.01	23.645	3.163152
0.4838	0.05	0.1362	0.07	0	0.08	0.0742	0.0258	0.07	0.01	16.3	2.791165
0.504	0.0639	0.15	0.0421	0.02	0.05	0.02	0.1	0.02	0.03	12.205	2.501846
0.5325	0.0694	0.0781	0.07	0.05	0.02	0.03	0.1	0.02	0.03	9.425	2.243366
0.5675	0.05	0.0625	0.07	0.032	0.038	0.1	0.03	0.02	0.03	14.31	2.660959
0.507	0.1477	0.05	0.0653	0.02	0.03	0.03	0.05	0.07	0.03	11.33	2.427454
0.57	0.1078	0.05	0.0699	0.05	0.02	0.02	0.0623	0.02	0.03	10.275	2.329714
0.5299	0.1106	0.05	0.0595	0.02	0.05	0.0308	0.0592	0.02	0.07	11.6	2.451005
0.5264	0.1259	0.0577	0.07	0.02	0.02	0.02	0.0746	0.02	0.0654	10.985	2.396531
0.5294	0.05	0.1277	0.0429	0.05	0.02	0.02	0.04	0.05	0.07	11.555	2.447118
0.47	0.1442	0.0968	0.039	0.05	0.02	0.02	0.0854	0.02	0.0546	10.625	2.36321
0.5073	0.1357	0.0957	0.0413	0.02	0.02	0.0515	0.0785	0.02	0.03	11.35	2.429218
0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407	11.43	2.436241
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	12.35	2.513656
0.6	0.0817	0.045	0.0788	0.0008	0.0009	0.072	0.0233	0.0385	0.059	10.075	2.310057
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	15.905	2.766634

Table 6. Validation Set for MCC-1 B

SIO2	B2O3		LI2O			FE2O3	AL2O3	ZRO2	OTHERS		LNMCC
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	17.23	2.846652
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	15.28	2.726545
0.39	0.2	0.05	0.07	0.02	0.08	0.02	0.15	0.01	0.01	13.15	2.576422
0.438	0.1718	0.1268	0.0727	0.0375	0.0005	0.02	0.115	0.0075	0.0102	11.975	2.482821
0.5281	0.0876	0.1725	0.0743	0.0063	0.0005	0.02	0.0925	0.0075	0.0107	16.52	2.804572
0.5281	0.0664	0.12	0.073	0	0	0.02	0.1625	0.0175	0.0125	10.895	2.388304
0.5579	0.1765	0.1125	0.0156	0.05	0.0005	0.02	0.05	0.0075	0.0095	12.39	2.51689
0.3232	0.1717	0.19	0.0051	0.1	0	0.02	0.18	0	0.01	9.645	2.26644
0.5697	0.0509	0.0925	0.0642	0.0025	0.0008	0.0812	0.0288	0.0431	0.0663	12.315	2.510818
0.5344	0.1128	0.086	0.0697	0.0007	0.0004	0.0013	0.0196	0.1548	0.0203	9.405	2.241241
0.5175	0.0917	0.1211	0.0523	0.0097	0.0061	0.0388	0.118	0.0026	0.0422	11.745	2.463428
0.4596	0.1587	0.1086	0.0583	0.0024	0.0001	0.0004	0.2043	0	0.0076	11.145	2.410991
0.504	0.1355	0.0797	0.0696	0.0007	0.0002	0.0046	0.164	0.0001	0.0416	10.56	2.357073
0.566	0.0781	0.0664	0.0713	0.0079	0.0032	0.0334	0.0816	0.0005	0.0916	9.88	2.290513
0.4854	0.1418	0.0812	0.0691	0.0008	0.0008	0.008	0.1819	0.0005	0.0305	11.56	2.447551
0.5697	0.0509	0.0925	0.0642	0.0025	0.0008	0.0812	0.0288	0.0431	0.0663	12	2.484907
0.5175	0.0917	0.1211	0.0523	0.0097	0.0061	0.0388	0.118	0.0026	0.0422	11.745	2.463428
0.504	0.1355	0.0797	0.0696	0.0007	0.0002	0.0046	0.164	0.0001	0.0416	6.645	1.893865
0.566	0.0781	0.0664	0.0713	0.0079	0.0032	0.0334	0.0816	0.0005	0.0916	9.88	2.290513
0.4854	0.1418	0.0812	0.0691	0.0008	0.0008	0.008	0.1819	0.0005	0.0305	8.62	2.154085
0.5018	0.06	0.18	0.0632	0.04	0.005	0.105	0.02	0.005	0.02	26.53	3.278276
0.455	0.06	0.18	0.07	0.005	0.005	0.005	0.02	0.11	0.09	49.575	3.903487
0.56	0.16	0.05	0.0254	0.005	0.04	0.0699	0.02	0.0497	0.02	32.15	3.470412
0.5479	0.16	0.05	0.0121	0.005	0.005	0.105	0.02	0.005	0.09	32.15	3.470412
0.5074	0.16	0.05	0.0176	0.005	0.04	0.105	0.02	0.075	0.02	45.215	3.811429
0.44	0.06	0.1734	0.07	0.005	0.04	0.105	0.02	0.005	0.0816	107.18	4.67451
0.49	0.0951	0.18	0.0699	0.04	0.005	0.005	0.02	0.005	0.09	37.19	3.61604
0.455	0.06	0.18	0.07	0.005	0.005	0.105	0.02	0.08	0.02	30.01	3.401531
0.44	0.06	0.18	0.07	0.005	0.02	0.005	0.17	0.005	0.045	18.49	2.91723
0.4764	0.06	0.18	0.0136	0.04	0.005	0.005	0.17	0.005	0.045	8.305	2.116858
0.4983	0.08	0.18	0.018	0.0137	0.005	0.025	0.0987	0.0613	0.02	9.445	2.245486
0.4597	0.06	0.1403	0.07	0.04	0.005	0.025	0.105	0.075	0.02	9.11	2.209373
0.44	0.1171	0.18	0.01	0.04	0.005	0.105	0.02	0.0629	0.02	38.44	3.649099
0.56	0.16	0.0542	0.07	0.005	0.005	0.1008	0.02	0.005	0.02	29.14	3.372112
0.56	0.16	0.105	0.01	0.005	0.04	0.005	0.02	0.005	0.09	44.21	3.788951
0.44	0.16	0.1	0.07	0.005	0.04	0.005	0.02	0.07	0.09	86.415	4.459161
0.44	0.1337	0.1279	0.07	0.0098	0.005	0.0986	0.02	0.005	0.09	216.45	5.37736
0.44	0.16	0.18	0.0526	0.04	0.005	0.0271	0.0703	0.005	0.02	87.42	4.470724
0.4895	0.1112	0.1671	0.0428	0.0113	0.0166	0.0897	0.0367	0.0041	0.031	49.16	3.89508
0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407	12.53	2.528126
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	12.89	2.556452
0.42	0.1743	0.2	0.0369	0	0	0.02	0.1388	0	0.01	30.44	3.415758
0.5203	0.0969	0.098	0.0356	0.0097	0.0077	0.1019	0.0523	0.0199	0.0577	13.94	2.634762
0.5329	0.074	0.0626	0.0596	0.0035	0.0012	0.1229	0.0286	0.0443	0.0704	14.125	2.647946
0.4895	0.1112	0.1671	0.0428	0.0113	0.0166	0.0897	0.0367	0.0041	0.031	90.76	4.508219
0.5353	0.1053	0.1125	0.0375	0.0083	0.0084	0.0719	0.0231	0.0385	0.0592	19.238	2.956887
0.41	0.1337	0.1428	0.0476	0.0105	0.0107	0.0913	0.0293	0.0489	0.0752	52.909	3.968573
0.45	0.1246	0.1332	0.0444	0.0098	0.0099	0.0851	0.0273	0.0456	0.0701	30.967	3.432922
0.49	0.1156	0.1235	0.0412	0.0091	0.0092	0.0789	0.0254	0.0423	0.065	22.669	3.120998
0.57	0.0974	0.1041	0.0347	0.0077	0.0078	0.0665	0.0214	0.0356	0.0548	13.37	2.593013
0.5684	0.05	0.1195	0.0398	0.0088	0.0089	0.0763	0.0245	0.0409	0.0629	12.54	2.528924
0.5086	0.15	0.1069	0.0356	0.0079	0.008	0.0683	0.022	0.0366	0.0562	22.722	3.123334
0.4786	0.2	0.1006	0.0335	0.0074	0.0075	0.0643	0.0207	0.0344	0.0529	90.836	4.509056
0.573	0.1127	0.05	0.0401	0.0089	0.009	0.077	0.0247	0.0412	0.0634	10.128	2.315304
0.5127	0.1009	0.15	0.0359	0.008	0.0081	0.0689	0.0221	0.0369	0.0567	25.972	3.257019
0.4825	0.0949	0.2	0.0338	0.0075	0.0076	0.0648	0.0208	0.0347	0.0534	98.259	4.587607
0.5506	0.1083	0.1157	0.01	0.0085	0.0086	0.074	0.0238	0.0396	0.0609	12.767	2.546864
0.5228	0.1028	0.1099	0.06	0.0081	0.0082	0.0702	0.0226	0.0376	0.0578	20.331	3.012147
0.5172	0.1017	0.1087	0.07	0.008	0.0081	0.0695	0.0223	0.0372	0.0572	29.404	3.381131
0.529	0.1041	0.1112	0.0371	0.02	0.0083	0.0711	0.0228	0.0381	0.0585	19.768	2.984064
0.5398	0.1062	0.1135	0.0378	0.0084	0	0.0725	0.0233	0.0388	0.0597	19.983	2.994882
0.529	0.1041	0.1112	0.0371	0.0082	0.02	0.0711	0.0228	0.0381	0.0585	20.386	3.014848
0.548	0.1078	0.1152	0.0384	0.0085	0.0086	0.0736	0	0.0394	0.0606	56.673	4.037298
0.5206	0.1024	0.1094	0.0365	0.0081	0.0082	0.0699	0.05	0.0374	0.0576	13.502	2.602838
0.4932	0.097	0.1036	0.0346	0.0077	0.0077	0.0662	0.1	0.0355	0.0545	10.11	2.313525
0.4658	0.0916	0.0979	0.0326	0.0072	0.0073	0.0626	0.15	0.0335	0.0515	9.302	2.230229
0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596	15.648	2.750343

APPENDIX C--PNL 1st Order Regression of Glass Properties, Training

This Appendix displays the resulting Pacific Northwest Laboratory 1st Order viscosity, PCT B, and MCC-1 B models after regression on the appropriate training sets from Appendix B.

1. PNL 1st Order Regression on Viscosity Training Set

LNVISC = 8.81 SIO2 - 6.20 B2O3 - 10.8 NA2O - 34.5 LI2O - 6.31 CAO - 1.94 MGO + 0.061 FE2O3 + 11.1 AL2O3 + 7.87 ZRO2 - 0.767 OTHERS

Predictor	Coef	Stdev	t-ratio	p
Noconstant				
SIO2	8.8121	0.2691	32.75	0.000
B2O3	-6.1954	0.4463	-13.88	0.000
NA2O	-10.8000	0.6253	-17.27	0.000
LI2O	-34.503	1.248	-27.65	0.000
CAO	-6.3084	0.8096	-7.79	0.000
MGO	-1.9434	0.8768	-2.22	0.031
FE2O3	0.0609	0.6224	0.10	0.922
AL2O3	11.1117	0.6904	16.09	0.000
ZRO2	7.8691	0.7163	10.99	0.000
OTHERS	-0.7670	0.7553	-1.02	0.315

s = 0.2074

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	10	253.262	25.326	588.57	0.000
Error	53	2.281	0.043		
Total	63	255.542			

SOURCE	DF	SEQ SS
SIO2	1	210.458
B2O3	1	2.868
NA2O	1	0.653
LI2O	1	23.745
CAO	1	1.774
MGO	1	0.658
FE2O3	1	1.150
AL2O3	1	6.590
ZRO2	1	5.321
OTHERS	1	0.044

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
7	0.570	4.2888	3.7135	0.1105	0.5753	3.28R
12	0.420	-0.8675	-1.2312	0.1162	0.3637	2.12R
53	0.519	3.3113	2.6001	0.0892	0.7112	3.80R

2. PNL 1st Order Regression on PCT B Training Set

LNPCT = - 3.14 SIO2 + 10.2 B2O3 + 15.1 NA2O + 18.6 LI2O - 10.0 CAO + 9.54 MGO
- 2.13 FE2O3 - 26.7 AL2O3 - 8.88 ZRO2 + 2.12 OTHERS

Predictor	Coef	Stdev	t-ratio	p
Noconstant				
SIO2	-3.1399	0.9125	-3.44	0.001
B2O3	10.244	1.519	6.74	0.000
NA2O	15.091	2.113	7.14	0.000
LI2O	18.595	4.303	4.32	0.000
CAO	-10.024	2.784	-3.60	0.001
MGO	9.541	3.030	3.15	0.002
FE2O3	-2.134	2.108	-1.01	0.315
AL2O3	-26.665	2.384	-11.18	0.000
ZRO2	-8.876	2.476	-3.58	0.001
OTHERS	2.115	2.595	0.82	0.418

s = 0.7275
Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	10	123.056	12.306	23.25	0.000
Error	64	33.874	0.529		
Total	74	156.930			

SOURCE	DF	SEQ SS
SIO2	1	0.135
B2O3	1	7.893
NA2O	1	9.320
LI2O	1	0.255
CAO	1	22.512
MGO	1	7.481
FE2O3	1	3.056
AL2O3	1	64.909
ZRO2	1	7.143
OTHERS	1	0.352

Unusual Observations

Obs.	SIO2	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
2	0.550	-2.7181	-4.1822	0.3251	1.4641	2.25R

46	0.570	-1.7545	-0.4154	0.3130	-1.3390	-2.04R
53	0.519	1.8736	0.3790	0.3052	1.4947	2.26R

R denotes an obs. with a large st. resid.

3. PNL 1st Order Regression on MCC-1 B Training Set

LNMCC = 0.302 SIO2 + 9.07 B2O3 + 9.03 NA2O + 9.28 LI2O + 7.33 CAO + 6.45 MGO + 5.10 FE2O3 - 6.94 AL2O3 - 0.51 ZRO2 + 0.45 OTHERS

Predictor	Coef	Stdev	t-ratio	p
Noconstant				
SIO2	0.3018	0.4474	0.67	0.502
B2O3	9.0717	0.8043	11.28	0.000
NA2O	9.0333	0.9918	9.11	0.000
LI2O	9.279	2.051	4.53	0.000
CAO	7.327	1.251	5.86	0.000
MGO	6.449	1.508	4.28	0.000
FE2O3	5.100	1.154	4.42	0.000
AL2O3	-6.941	1.403	-4.95	0.000
ZRO2	-0.507	1.377	-0.37	0.714
OTHERS	0.452	1.359	0.33	0.741

s = 0.3283

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	10	523.846	52.385	485.97	0.000
Error	60	6.468	0.108		
Total	70	530.313			

SOURCE	DF	SEQ SS
SIO2	1	495.359
B2O3	1	7.827
NA2O	1	4.416
LI2O	1	0.892
CAO	1	2.424
MGO	1	1.806
FE2O3	1	6.529
AL2O3	1	4.557
ZRO2	1	0.024
OTHERS	1	0.012

Unusual Observations

Obs.	SIO2	LNMCC	Fit	Stdev.Fit	Residual	St.Resid
10	0.420	4.2991	3.5914	0.1734	0.7078	2.54R

24	0.481	1.6134	2.5039	0.0968	-0.8904	-2.84R
48	0.570	3.8506	2.9304	0.1597	0.9202	3.21R

R denotes an obs. with a large st. resid.

APPENDIX D--PNL 2nd Order Regression of Glass Properties, Training

This Appendix displays the resulting Pacific Northwest Laboratory 2nd Order viscosity, PCT B, and MCC-1 B models after regression on the appropriate training sets from Appendix B.

1. PNL 2nd Order Regression on Viscosity Training Set

LNVISC = 10.6 SIO2 - 6.29 B2O3 - 24.8 NA2O - 77.5 LI2O - 5.09 CAO - 2.18 MGO
+ 0.694 FE2O3 + 14.1 AL2O3 + 10.5 ZRO - 2.73 OTHERS + 29.2 BXFE
+ 123 NAXLI + 22.6 NAXMG + 88.6 LIXOTH - 44.7 MGXFE + 42.5 NAXNA
+ 340 LIXLI

Predictor	Coef	Stdev	t-ratio	p
Noconstant				
SIO2	10.6283	0.2531	42.00	0.000
B2O3	-6.2945	0.3814	-16.50	0.000
NA2O	-24.819	2.575	-9.64	0.000
LI2O	-77.478	4.523	-17.13	0.000
CAO	-5.0912	0.4546	-11.20	0.000
MGO	-2.180	1.335	-1.63	0.109
FE2O3	0.6936	0.7788	0.89	0.378
AL2O3	14.1206	0.4768	29.62	0.000
ZRO	10.4672	0.4805	21.78	0.000
OTHERS	-2.7285	0.7210	-3.78	0.000
BXFE	29.174	5.178	5.63	0.000
NAXLI	122.56	19.97	6.14	0.000
NAXMG	22.621	8.940	2.53	0.015
LIXOTH	88.57	17.44	5.08	0.000
MGXFE	-44.72	10.48	-4.27	0.000
NAXNA	42.498	9.043	4.70	0.000
LIXLI	339.75	40.80	8.33	0.000

s = 0.1071
Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	17	255.015	15.001	1307.66	0.000
Error	46	0.528	0.011		
Total	63	255.542			

SOURCE	DF	SEQ SS
SIO2	1	210.458
B2O3	1	2.868

NA2O	1	0.653
LI2O	1	23.745
CAO	1	1.774
MGO	1	0.658
FE2O3	1	1.150
AL2O3	1	6.590
ZRO	1	5.321
OTHERS	1	0.044
BXFE	1	0.392
NAXLI	1	0.010
NAXMG	1	0.130
LIXOTH	1	0.134
MGXFE	1	0.062
NAXNA	1	0.230
LIXLI	1	0.795

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
7	0.570	4.2888	4.0286	0.0649	0.2602	3.05R
16	0.433	2.8798	2.6751	0.0683	0.2047	2.48R
58	0.420	1.0367	0.8721	0.0709	0.1646	2.05R

R denotes an obs. with a large st. resid.

2. PNL 2nd Order Regression on PCT Training Set

The regression equation is

LNPCT = - 4.78 SIO2 + 12.7 B2O3 + 19.1 NA2O + 19.8 LI2O + 14.6 CAO - 51.0 MGO
- 0.41 FE2O3 - 43.3 AL2O3 - 7.66 ZRO + 5.49 OTHERS + 122 SIXMG
- 101 B2XCA - 152 NAXCA + 145 ALXAL

Predictor	Coef	Stdev	t-ratio	p
Noconstant				
SIO2	-4.780	1.048	-4.56	0.000
B2O3	12.684	1.605	7.90	0.000
NA2O	19.062	2.156	8.84	0.000
LI2O	19.780	3.543	5.58	0.000
CAO	14.599	8.643	1.69	0.096
MGO	-50.99	20.55	-2.48	0.016
FE2O3	-0.411	1.910	-0.22	0.830
AL2O3	-43.276	5.498	-7.87	0.000
ZRO	-7.665	2.218	-3.46	0.001
OTHERS	5.493	2.253	2.44	0.018
SIXMG	121.76	41.36	2.94	0.005
B2XCA	-100.53	41.23	-2.44	0.018
NAXCA	-151.63	52.80	-2.87	0.006
ALXAL	145.46	38.77	3.75	0.000

s = 0.5904

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	14	136.0182	9.7156	27.88	0.000
Error	60	20.9116	0.3485		
Total	74	156.9298			

SOURCE	DF	SEQ SS
SIO2	1	0.1345
B2O3	1	7.8934
NA2O	1	9.3202
LI2O	1	0.2549
CAO	1	22.5119
MGO	1	7.4811
FE2O3	1	3.0556
AL2O3	1	64.9094
ZRO	1	7.1431
OTHERS	1	0.3517
SIXMG	1	1.5251
B2XCA	1	1.4146

NAXCA	1	5.1161
ALXAL	1	4.9064

Unusual Observations

Obs.	SIO2	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
51	0.562	1.6378	0.5974	0.2954	1.0404	2.04R
53	0.519	1.8736	0.1636	0.2663	1.7101	3.25R
59	0.542	-0.7340	0.4348	0.2695	-1.1688	-2.23R
62	0.484	2.5417	1.4042	0.2302	1.1375	2.09R

R denotes an obs. with a large st. resid.

3. PNL 2nd Order Regression on MCC-1 B Training Set

The regression equation is
LNMCC = 0.104 SIO2 + 13.2 B2O3 + 9.18 NA2O + 10.2 LI2O - 11.0 CAO + 7.17 MGO
+ 4.62 FE2O3 - 15.2 AL2O3 - 1.98 ZRO + 1.81 OTHERS + 34.0 SIXCA
- 49.9 BXAL + 89.3 ALXAL

Predictor	Coef	Stdev	t-ratio	p
Noconstant				
SIO2	0.1036	0.5635	0.18	0.855
B2O3	13.208	1.250	10.56	0.000
NA2O	9.1767	0.9007	10.19	0.000
LI2O	10.186	1.823	5.59	0.000
CAO	-11.011	9.656	-1.14	0.259
MGO	7.169	1.323	5.42	0.000
FE2O3	4.621	1.185	3.90	0.000
AL2O3	-15.159	3.683	-4.12	0.000
ZRO	-1.984	1.337	-1.48	0.143
OTHERS	1.815	1.349	1.35	0.184
SIXCA	33.98	19.45	1.75	0.086
BXAL	-49.93	15.58	-3.20	0.002
ALXAL	89.27	22.08	4.04	0.000

s = 0.2841
Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	13	525.712	40.439	500.94	0.000
Error	57	4.601	0.081		
Total	70	530.313			

SOURCE	DF	SEQ SS
SIO2	1	495.359
B2O3	1	7.827
NA2O	1	4.416
LI2O	1	0.892
CAO	1	2.424
MGO	1	1.806
FE2O3	1	6.529
AL2O3	1	4.557
ZRO	1	0.024
OTHERS	1	0.012
SIXCA	1	0.037
BXAL	1	0.509

ALXAL	1	1.320

Unusual Observations

Obs.	SIO2	LNMCC	Fit	Stdev.Fit	Residual	St.Resid
4	0.570	2.4406	1.9449	0.1471	0.4957	2.04R
10	0.420	4.2991	3.8003	0.1692	0.4988	2.19R
24	0.481	1.6134	2.4294	0.0906	-0.8160	-3.03R
32	0.473	3.2229	2.4656	0.1011	0.7573	2.85R
48	0.570	3.8506	3.0339	0.1464	0.8167	3.35R

APPENDIX E--Revised 1st Order Regression of Glass Properties, Training

This Appendix displays the stepwise regression used to form the Revised PNL 1st Order viscosity, PCT B, and MCC-1 B models (using the appropriate training set).

1. Revised 1st Order Regression on Training Set for Viscosity

LNVISC = - 0.767 + 9.58 SIO2 - 5.43 B2O3 - 10.0 NA2O - 33.7 LI2O - 5.54 CAO - 1.18 MGO + 0.828 FE2O3 + 11.9 AL2O3 + 8.64 ZRO

Predictor	Coef	Stdev	t-ratio	p
Constant	-0.7667	0.7553	-1.01	0.315
SIO2	9.5787	0.8449	11.34	0.000
B2O3	-5.4287	0.9148	-5.93	0.000
NA2O	-10.033	1.017	-9.87	0.000
LI2O	-33.736	1.528	-22.08	0.000
CAO	-5.542	1.124	-4.93	0.000
MGO	-1.177	1.169	-1.01	0.319
FE2O3	0.8276	0.9254	0.89	0.375
AL2O3	11.8784	0.9599	12.38	0.000
ZRO	8.6358	0.9938	8.69	0.000

s = 0.2074 R-sq = 95.9% R-sq(adj) = 95.2%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	9	52.8515	5.8724	136.47	0.000
Error	53	2.2806	0.0430		
Total	62	55.1321			

SOURCE	DF	SEQ SS
SIO2	1	16.8613
B2O3	1	0.2012
NA2O	1	0.0160
LI2O	1	20.4055
CAO	1	2.6055
MGO	1	1.9528
FE2O3	1	4.1824
AL2O3	1	3.3773
ZRO	1	3.2496

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid

7	0.570	4.2888	3.7135	0.1105	0.5753	3.28R
12	0.420	-0.8675	-1.2313	0.1162	0.3638	2.12R
53	0.519	3.3113	2.6001	0.0892	0.7112	3.80R

LNVISC = - 0.696 + 9.52 SIO2 - 5.51 B2O3 - 10.1 NA2O - 33.8 LI2O - 5.05 CAO + 11.6 AL2O3 + 8.48 ZRO

Predictor	Coef	Stdev	t-ratio	p
Constant	-0.6959	0.4346	-1.60	0.115
SIO2	9.5245	0.6209	15.34	0.000
B2O3	-5.5143	0.6057	-9.10	0.000
NA2O	-10.1433	0.7661	-13.24	0.000
LI2O	-33.782	1.363	-24.79	0.000
CAO	-5.0470	0.8023	-6.29	0.000
AL2O3	11.6356	0.6984	16.66	0.000
ZRO	8.4796	0.7465	11.36	0.000

s = 0.2101   R-sq = 95.6%   R-sq(adj) = 95.0%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	7	52.7042	7.5292	170.56	0.000
Error	55	2.4280	0.0441		
Total	62	55.1321			

SOURCE	DF	SEQ SS
SIO2	1	16.8613
B2O3	1	0.2012
NA2O	1	0.0160
LI2O	1	20.4055
CAO	1	2.6055
AL2O3	1	6.9187
ZRO	1	5.6960

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
7	0.570	4.2888	3.7394	0.1109	0.5494	3.08R
12	0.420	-0.8675	-1.2843	0.1057	0.4168	2.30R
53	0.519	3.3113	2.4956	0.0671	0.8156	4.10R

R denotes an obs. with a large st. resid.

LNVISC = 8.60 SIO2 - 6.17 B2O3 - 10.8 NA2O - 34.6 LI2O - 5.55 CAO + 11.3 AL2O3 + 8.07 ZRO

Predictor	Coef	Stdev	t-ratio	p
Noconstant				
SIO2	8.6000	0.2316	37.13	0.000
B2O3	-6.1712	0.4518	-13.66	0.000
NA2O	-10.8403	0.6391	-16.96	0.000
LI2O	-34.629	1.273	-27.20	0.000
CAO	-5.5507	0.7483	-7.42	0.000
AL2O3	11.2714	0.6695	16.84	0.000
ZRO	8.0675	0.7104	11.36	0.000

s = 0.2130

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	7	253.001	36.143	796.50	0.000
Error	56	2.541	0.045		
Total	63	255.542			

SOURCE	DF	SEQ SS
SIO2	1	210.458
B2O3	1	2.868
NA2O	1	0.653
LI2O	1	23.745
CAO	1	1.774
AL2O3	1	7.652
ZRO	1	5.851

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
7	0.570	4.2888	3.6959	0.1090	0.5929	3.24R
12	0.420	-0.8675	-1.2535	0.1053	0.3860	2.08R
53	0.519	3.3113	2.4972	0.0680	0.8141	4.03R

2. Revised 1st Order Regression on Training Set for PCT B

LNPCT = 2.11 - 5.25 SIO2 + 8.13 B2O3 + 13.0 NA2O + 16.5 LI2O - 12.1 CAO + 7.43 MGO - 4.25 FE2O3 - 28.8 AL2O3 - 11.0 ZRO

Predictor	Coef	Stdev	t-ratio	p
Constant	2.113	2.595	0.81	0.419
SIO2	-5.252	2.906	-1.81	0.075
B2O3	8.132	3.137	2.59	0.012
NA2O	12.979	3.484	3.72	0.000
LI2O	16.483	5.252	3.14	0.003
CAO	-12.136	3.859	-3.15	0.003
MGO	7.429	4.030	1.84	0.070
FE2O3	-4.247	3.132	-1.36	0.180
AL2O3	-28.778	3.292	-8.74	0.000
ZRO	-10.989	3.421	-3.21	0.002

s = 0.7275   R-sq = 78.4%   R-sq(adj) = 75.3%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	9	122.862	13.651	25.79	0.000
Error	64	33.875	0.529		
Total	73	156.737			

SOURCE	DF	SEQ SS
SIO2	1	0.501
B2O3	1	7.975
NA2O	1	15.246
LI2O	1	3.434
CAO	1	14.776
MGO	1	14.082
FE2O3	1	12.958
AL2O3	1	48.428
ZRO	1	5.462

Unusual Observations

Obs.	SIO2	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
2	0.550	-2.7181	-4.1821	0.3251	1.4640	2.25R
46	0.570	-1.7545	-0.4153	0.3130	-1.3392	-2.04R
53	0.519	1.8736	0.3790	0.3052	1.4946	2.26R

LNPCT = - 1.36 + 10.7 B2O3 + 15.2 NA2O + 18.0 LI2O - 13.4 CAO - 25.8 AL2O3 - 8.44 ZRO

Predictor	Coef	Stdev	t-ratio	p
Constant	-1.3624	0.5934	-2.30	0.025
B2O3	10.711	1.958	5.47	0.000
NA2O	15.152	2.688	5.64	0.000
LI2O	18.020	4.992	3.61	0.001
CAO	-13.449	2.864	-4.70	0.000
AL2O3	-25.765	2.451	-10.51	0.000
ZRO	-8.444	2.646	-3.19	0.002

s = 0.7947 R-sq = 73.0% R-sq(adj) = 70.6%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	6	114.427	19.071	30.20	0.000
Error	67	42.310	0.631		
Total	73	156.737			

SOURCE	DF	SEQ SS
B2O3	1	8.354
NA2O	1	13.523
LI2O	1	2.562
CAO	1	17.163
AL2O3	1	66.394
ZRO	1	6.431

Unusual Observations

Obs.	B2O3	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
18	0.050	2.4193	0.8649	0.2831	1.5544	2.09R
43	0.050	-1.0584	0.5855	0.2826	-1.6439	-2.21R
45	0.050	2.2665	0.6078	0.2433	1.6587	2.19R
46	0.052	-1.7545	-0.1579	0.2927	-1.5966	-2.16R

3. Revised 1st Order Regression on Training Set for MCC-1 B

LNMCC = 0.45 - 0.15 SIO2 + 8.62 B2O3 + 8.58 NA2O + 8.83 LI2O + 6.87 CAO
+ 6.00 MGO + 4.65 FE2O3 - 7.39 AL2O3 - 0.96 ZRO

Predictor	Coef	Stdev	t-ratio	p
Constant	0.452	1.359	0.33	0.741
SIO2	-0.150	1.574	-0.10	0.924
B2O3	8.620	1.677	5.14	0.000
NA2O	8.581	1.782	4.82	0.000
LI2O	8.827	2.459	3.59	0.001
CAO	6.875	1.888	3.64	0.001
MGO	5.997	2.058	2.91	0.005
FE2O3	4.649	1.494	3.11	0.003
AL2O3	-7.392	1.677	-4.41	0.000
ZRO	-0.959	1.670	-0.57	0.568

s = 0.3283 R-sq = 70.9% R-sq(adj) = 66.6%
Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	9	15.7774	1.7530	16.26	0.000
Error	60	6.4677	0.1078		
Total	69	22.2451			

SOURCE	DF	SEQ SS
SIO2	1	3.3329
B2O3	1	0.3211
NA2O	1	0.1419
LI2O	1	0.0263
CAO	1	0.7286
MGO	1	0.4857
FE2O3	1	6.4196
AL2O3	1	4.2858
ZRO	1	0.0355

Unusual Observations

Obs.	SIO2	LNMCC	Fit	Stdev.Fit	Residual	St.Resid
10	0.420	4.2991	3.5914	0.1734	0.7078	2.54R
24	0.481	1.6134	2.5039	0.0968	-0.8904	-2.84R
48	0.570	3.8506	2.9304	0.1597	0.9202	3.21R

$$LNMCC = 0.233 + 8.77\ B2O3 + 8.71\ NA2O + 8.95\ LI2O + 7.11\ CAO + 6.15\ MGO + 5.10\ FE2O3 - 6.70\ AL2O3$$

Predictor	Coef	Stdev	t-ratio	p
Constant	0.2332	0.3236	0.72	0.474
B2O3	8.7672	0.9809	8.94	0.000
NA2O	8.711	1.216	7.17	0.000
LI2O	8.954	2.216	4.04	0.000
CAO	7.110	1.348	5.27	0.000
MGO	6.154	1.581	3.89	0.000
FE2O3	5.099	1.068	4.77	0.000
AL2O3	-6.697	1.017	-6.58	0.000

s = 0.3240 R-sq = 70.7% R-sq(adj) = 67.4%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	7	15.7355	2.2479	21.41	0.000
Error	62	6.5096	0.1050		
Total	69	22.2451			

SOURCE	DF	SEQ SS
B2O3	1	1.7376
NA2O	1	0.9347
LI2O	1	0.0922
CAO	1	1.3205
MGO	1	0.9043
FE2O3	1	6.1958
AL2O3	1	4.5503

Unusual Observations

Obs.	B2O3	LNMCC	Fit	Stdev.Fit	Residual	St.Resid
10	0.200	4.2991	3.6408	0.1519	0.6584	2.30R
24	0.170	1.6134	2.4952	0.0881	-0.8817	-2.83R
48	0.184	3.8506	2.8995	0.1054	0.9511	3.10R

The regression equation is

$$LNMCC = 9.27\ B2O3 + 9.43\ NA2O + 10.1\ LI2O + 7.55\ CAO + 6.60\ MGO + 5.51\ FE2O3 - 6.59\ AL2O3$$

Predictor	Coef	Stdev	t-ratio	p

Noconstant

B2O3	9.2714	0.6850	13.54	0.000
NA2O	9.4281	0.6952	13.56	0.000
LI2O	10.095	1.544	6.54	0.000
CAO	7.553	1.195	6.32	0.000
MGO	6.596	1.451	4.54	0.000
FE2O3	5.5081	0.9021	6.11	0.000
AL2O3	-6.588	1.002	-6.57	0.000

s = 0.3228

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	7	523.749	74.821	718.10	0.000
Error	63	6.564	0.104		
Total	70	530.313			

SOURCE	DF	SEQ SS
B2O3	1	436.363
NA2O	1	56.261
LI2O	1	11.711
CAO	1	3.867
MGO	1	2.878
FE2O3	1	8.168
AL2O3	1	4.503

Unusual Observations

Obs.	B2O3	LNMCC	Fit	Stdev.Fit	Residual	St.Resid
10	0.200	4.2991	3.6641	0.1478	0.6350	2.21R
24	0.170	1.6134	2.4962	0.0877	-0.8828	-2.84R
29	0.170	2.2885	2.9280	0.0798	-0.6395	-2.04R
48	0.184	3.8506	2.8822	0.1023	0.9684	3.16R

R denotes an obs. with a large st. resid.

APPENDIX F--Revised 2nd Order Regression of Glass Properties, Training

This Appendix displays the stepwise regression used to form the Revised PNL 2nd Order viscosity, PCT B, and MCC-1 B models (using the appropriate training set).

1. Revised 2nd Order Regression on Training Set for Viscosity

LNVISC = - 2.73 + 13.4 SIO2 - 3.57 B2O3 - 22.1 NA2O - 74.8 LI2O - 2.36 CAO
+ 0.55 MGO + 3.42 FE2O3 + 16.8 AL2O3 + 13.2 ZRO + 29.2 BXFE
+ 123 NAXLI + 22.6 NAXMG + 88.6 LIXOTH - 44.7 MGXFE + 42.5 NAXNA
+ 340 LIXLI

Predictor	Coef	Stdev	t-ratio	p
Constant	-2.7276	0.7211	-3.78	0.000
SIO2	13.3557	0.7759	17.21	0.000
B2O3	-3.5670	0.8102	-4.40	0.000
NA2O	-22.090	2.748	-8.04	0.000
LI2O	-74.751	4.481	-16.68	0.000
CAO	-2.3640	0.9239	-2.56	0.014
MGO	0.546	1.555	0.35	0.727
FE2O3	3.421	1.060	3.23	0.002
AL2O3	16.8480	0.9254	18.21	0.000
ZRO	13.1947	0.8613	15.32	0.000
BXFE	29.176	5.179	5.63	0.000
NAXLI	122.55	19.98	6.13	0.000
NAXMG	22.624	8.941	2.53	0.015
LIXOTH	88.55	17.44	5.08	0.000
MGXFE	-44.72	10.49	-4.26	0.000
NAXNA	42.491	9.044	4.70	0.000
LIXLI	339.78	40.80	8.33	0.000

s = 0.1071 R-sq = 99.0% R-sq(adj) = 98.7%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	16	54.6043	3.4128	297.45	0.000
Error	46	0.5278	0.0115		
Total	62	55.1321			

SOURCE	DF	SEQ SS
SIO2	1	16.8613
B2O3	1	0.2012
NA2O	1	0.0160

LI2O	1	20.4055
CAO	1	2.6055
MGO	1	1.9528
FE2O3	1	4.1824
AL2O3	1	3.3773
ZRO	1	3.2496
BXFE	1	0.3915
NAXLI	1	0.0097
NAXMG	1	0.1304
LIXOTH	1	0.1343
MGXFE	1	0.0617
NAXNA	1	0.2297
LIXLI	1	0.7956

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
7	0.570	4.2888	4.0286	0.0649	0.2602	3.05R
16	0.433	2.8798	2.6751	0.0683	0.2047	2.48R
58	0.420	1.0367	0.8721	0.0709	0.1647	2.05R

LNVISC = - 2.60 + 13.2 SIO2 - 3.69 B2O3 - 22.2 NA2O - 74.7 LI2O - 2.53 CAO
+ 3.22 FE2O3 + 16.7 AL2O3 + 13.0 ZRO + 29.1 BXFE + 122 NAXLI
+ 25.0 NAXMG + 85.7 LIXOTH - 42.8 MGXFE + 42.2 NAXNA + 340 LIXLI

Predictor	Coef	Stdev	t-ratio	p
Constant	-2.5969	0.6120	-4.24	0.000
SIO2	13.2282	0.6794	19.47	0.000
B2O3	-3.6852	0.7302	-5.05	0.000
NA2O	-22.183	2.710	-8.19	0.000
LI2O	-74.664	4.432	-16.85	0.000
CAO	-2.5294	0.7876	-3.21	0.002
FE2O3	3.2198	0.8841	3.64	0.001
AL2O3	16.6586	0.7453	22.35	0.000
ZRO	13.0175	0.6917	18.82	0.000
BXFE	29.085	5.124	5.68	0.000
NAXLI	122.09	19.75	6.18	0.000
NAXMG	25.041	5.658	4.43	0.000
LIXOTH	85.65	15.22	5.63	0.000
MGXFE	-42.812	8.891	-4.82	0.000
NAXNA	42.238	8.931	4.73	0.000
LIXLI	339.86	40.42	8.41	0.000

s = 0.1061   R-sq = 99.0%   R-sq(adj) = 98.7%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	15	54.6029	3.6402	323.30	0.000
Error	47	0.5292	0.0113		
Total	62	55.1321			

SOURCE	DF	SEQ SS
SIO2	1	16.8613
B2O3	1	0.2012
NA2O	1	0.0160
LI2O	1	20.4055
CAO	1	2.6055
FE2O3	1	3.1792
AL2O3	1	4.5966
ZRO	1	4.9427
BXFE	1	0.4052
NAXLI	1	0.0091
NAXMG	1	0.0022
LIXOTH	1	0.2716
MGXFE	1	0.0830

NAXNA	1	0.2279
LIXLI	1	0.7960

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
7	0.570	4.2888	4.0230	0.0624	0.2658	3.10R
16	0.433	2.8798	2.6788	0.0668	0.2010	2.44R
58	0.420	1.0367	0.8617	0.0638	0.1750	2.06R

R denotes an obs. with a large st. resid.

2. Revised 2nd Order Regression on Training Set for PCT

LNPCT = 5.49 - 10.3 SIO2 + 7.19 B2O3 + 13.6 NA2O + 14.3 LI2O + 9.11 CAO
- 56.5 MGO - 5.90 FE2O3 - 48.8 AL2O3 - 13.2 ZRO + 122 SIXMG
- 101 BXCA - 152 NAXCA + 145 ALXAL

Predictor	Coef	Stdev	t-ratio	p
Constant	5.490	2.253	2.44	0.018
SIO2	-10.269	2.769	-3.71	0.000
B2O3	7.194	2.780	2.59	0.012
NA2O	13.572	2.983	4.55	0.000
LI2O	14.290	4.303	3.32	0.002
CAO	9.110	8.712	1.05	0.300
MGO	-56.47	21.42	-2.64	0.011
FE2O3	-5.902	2.567	-2.30	0.025
AL2O3	-48.766	5.870	-8.31	0.000
ZRO	-13.156	2.841	-4.63	0.000
SIXMG	121.74	41.36	2.94	0.005
BXCA	-100.53	41.23	-2.44	0.018
NAXCA	-151.63	52.81	-2.87	0.006
ALXAL	145.45	38.77	3.75	0.000

s = 0.5904 R-sq = 86.7% R-sq(adj) = 83.8%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	13	135.823	10.448	29.97	0.000
Error	60	20.914	0.349		
Total	73	156.737			

SOURCE	DF	SEQ SS
SIO2	1	0.501
B2O3	1	7.975
NA2O	1	15.246
LI2O	1	3.434
CAO	1	14.776
MGO	1	14.082
FE2O3	1	12.958
AL2O3	1	48.428
ZRO	1	5.462
SIXMG	1	1.524
BXCA	1	1.415
NAXCA	1	5.116
ALXAL	1	4.906

Unusual Observations

Obs.	SIO2	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
51	0.562	1.6378	0.5973	0.2954	1.0406	2.04R
53	0.519	1.8736	0.1636	0.2663	1.7100	3.25R
59	0.542	-0.7340	0.4349	0.2695	-1.1689	-2.23R
62	0.484	2.5417	1.4043	0.2302	1.1374	2.09R

LNPCT = 5.87 - 10.2 SIO2 + 6.12 B2O3 + 12.2 NA2O + 14.1 LI2O - 54.2 MGO
- 6.30 FE2O3 - 50.8 AL2O3 - 13.6 ZRO + 115 SIXMG - 66.6 BXCA
- 107 NAXCA + 159 ALXAL

Predictor	Coef	Stdev	t-ratio	p
Constant	5.866	2.226	2.64	0.011
SIO2	-10.202	2.770	-3.68	0.000
B2O3	6.124	2.588	2.37	0.021
NA2O	12.238	2.699	4.53	0.000
LI2O	14.109	4.303	3.28	0.002
MGO	-54.21	21.33	-2.54	0.014
FE2O3	-6.296	2.541	-2.48	0.016
AL2O3	-50.769	5.553	-9.14	0.000
ZRO	-13.565	2.816	-4.82	0.000
SIXMG	115.13	40.91	2.81	0.007
BXCA	-66.63	25.49	-2.61	0.011
NAXCA	-106.88	30.97	-3.45	0.001
ALXAL	158.69	36.67	4.33	0.000

s = 0.5908 R-sq = 86.4% R-sq(adj) = 83.7%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	12	135.442	11.287	32.33	0.000
Error	61	21.295	0.349		
Total	73	156.737			

SOURCE	DF	SEQ SS
SIO2	1	0.501
B2O3	1	7.975
NA2O	1	15.246
LI2O	1	3.434
MGO	1	27.644
FE2O3	1	14.091
AL2O3	1	46.737
ZRO	1	1.998
SIXMG	1	0.792
BXCA	1	6.961
NAXCA	1	3.525
ALXAL	1	6.537

Unusual Observations

Obs.	SIO2	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
51	0.562	1.6378	0.6099	0.2954	1.0279	2.01R

53	0.519	1.8736	0.1315	0.2647	1.7422	3.30R
62	0.484	2.5417	1.3885	0.2299	1.1532	2.12R

3. Revised 2nd Order Regression on Training Set for MCC-1 B

LNMCC = 1.82 - 1.71 SIO2 + 11.4 B2O3 + 7.36 NA2O + 8.37 LI2O - 12.8 CAO
+ 5.35 MGO + 2.81 FE2O3 - 17.0 AL2O3 - 3.80 ZRO + 34.0 SIXCA
- 49.9 BXAL + 89.3 ALXAL

Predictor	Coef	Stdev	t-ratio	p
Constant	1.815	1.349	1.35	0.184
SIO2	-1.712	1.712	-1.00	0.321
B2O3	11.392	1.668	6.83	0.000
NA2O	7.361	1.613	4.56	0.000
LI2O	8.370	2.142	3.91	0.000
CAO	-12.83	10.38	-1.24	0.222
MGO	5.353	1.849	2.89	0.005
FE2O3	2.806	1.358	2.07	0.043
AL2O3	-16.975	3.775	-4.50	0.000
ZRO	-3.799	1.585	-2.40	0.020
SIXCA	33.99	19.45	1.75	0.086
BXAL	-49.94	15.58	-3.20	0.002
ALXAL	89.27	22.08	4.04	0.000

s = 0.2841 R-sq = 79.3% R-sq(adj) = 75.0%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	12	17.6437	1.4703	18.21	0.000
Error	57	4.6014	0.0807		
Total	69	22.2451			

SOURCE	DF	SEQ SS
SIO2	1	3.3329
B2O3	1	0.3211
NA2O	1	0.1419
LI2O	1	0.0263
CAO	1	0.7286
MGO	1	0.4857
FE2O3	1	6.4196
AL2O3	1	4.2858
ZRO	1	0.0355
SIXCA	1	0.0373
BXAL	1	0.5091
ALXAL	1	1.3199

Unusual Observations

Obs.	SIO2	LNMCC	Fit	Stdev.Fit	Residual	St.Resid
4	0.570	2.4406	1.9449	0.1471	0.4957	2.04R
10	0.420	4.2991	3.8003	0.1692	0.4988	2.19R
24	0.481	1.6134	2.4295	0.0906	-0.8160	-3.03R
32	0.473	3.2229	2.4656	0.1011	0.7573	2.85R
48	0.570	3.8506	3.0339	0.1464	0.8167	3.35R

$$LNMCC = 1.41 + 11.4\ B2O3 + 6.67\ NA2O + 7.27\ LI2O + 3.69\ MGO + 1.83\ FE2O3 - 20.3\ AL2O3 - 4.61\ ZRO - 53.6\ BXAL + 113\ ALXAL$$

Predictor	Coef	Stdev	t-ratio	p
Constant	1.4068	0.3444	4.08	0.000
B2O3	11.431	1.397	8.18	0.000
NA2O	6.675	1.141	5.85	0.000
LI2O	7.274	2.143	3.39	0.001
MGO	3.689	1.393	2.65	0.010
FE2O3	1.827	1.268	1.44	0.155
AL2O3	-20.252	4.066	-4.98	0.000
ZRO	-4.612	1.496	-3.08	0.003
BXAL	-53.61	16.58	-3.23	0.002
ALXAL	112.56	23.12	4.87	0.000

s = 0.3190   R-sq = 72.6%   R-sq(adj) = 68.4%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	9	16.1392	1.7932	17.62	0.000
Error	60	6.1058	0.1018		
Total	69	22.2451			

SOURCE	DF	SEQ SS
B2O3	1	1.7376
NA2O	1	0.9347
LI2O	1	0.0922
MGO	1	0.0850
FE2O3	1	5.3872
AL2O3	1	4.5778
ZRO	1	0.1813
BXAL	1	0.7306
ALXAL	1	2.4127

Unusual Observations

Obs.	B2O3	LNMCC	Fit	Stdev.Fit	Residual	St.Resid
7	0.085	1.0098	1.7655	0.1305	-0.7557	-2.60R
24	0.170	1.6134	2.4978	0.0887	-0.8844	-2.89R
32	0.070	3.2229	2.3529	0.0940	0.8700	2.85R
48	0.184	3.8506	2.8510	0.1188	0.9996	3.38R

LNMCC = 1.73 + 11.2 B2O3 + 6.37 NA2O + 6.78 LI2O + 3.79 MGO - 23.1 AL2O3 - 5.79 ZRO - 53.4 BXAL + 124 ALXAL

Predictor	Coef	Stdev	t-ratio	p
Constant	1.7322	0.2624	6.60	0.000
B2O3	11.187	1.399	8.00	0.000
NA2O	6.370	1.131	5.63	0.000
LI2O	6.776	2.134	3.18	0.002
MGO	3.794	1.403	2.70	0.009
AL2O3	-23.114	3.579	-6.46	0.000
ZRO	-5.795	1.262	-4.59	0.000
BXAL	-53.44	16.73	-3.19	0.002
ALXAL	123.98	21.91	5.66	0.000

s = 0.3218   R-sq = 71.6%   R-sq(adj) = 67.9%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	8	15.9279	1.9910	19.23	0.000
Error	61	6.3171	0.1036		
Total	69	22.2451			

SOURCE	DF	SEQ SS
B2O3	1	1.7376
NA2O	1	0.9347
LI2O	1	0.0922
MGO	1	0.0850
AL2O3	1	8.0516
ZRO	1	1.0665
BXAL	1	0.6434
ALXAL	1	3.3169

Unusual Observations

Obs.	B2O3	LNMCC	Fit	Stdev.Fit	Residual	St.Resid
3	0.200	2.7453	2.7058	0.2058	0.0396	0.16 X
7	0.085	1.0098	1.8225	0.1255	-0.8127	-2.74R
10	0.200	4.2991	3.7359	0.1771	0.5632	2.10R
24	0.170	1.6134	2.4799	0.0886	-0.8665	-2.80R
32	0.070	3.2229	2.3637	0.0946	0.8591	2.79R
48	0.184	3.8506	2.9459	0.0998	0.9046	2.96R

APPENDIX G--Revised Final 1st Order Regression of Glass Properties

This Appendix displays the stepwise regression used to form the FINAL Revised PNL 1st Order viscosity, electrical conductivity, PCT B, and MCC-1 B models (using the appropriate data set from Appendix A).

1. Revised Final 1st Order Modeling for Viscosity

LNVISC = - 0.128 + 9.11 SIO2 - 6.08 B2O3 - 10.9 NA2O - 34.1 LI2O - 7.40 CAO - 2.72 MGO + 0.083 FE2O3 + 11.4 AL2O3 + 7.61 ZRO2

Predictor	Coef	Stdev	t-ratio	p
Constant	-0.1277	0.7680	-0.17	0.868
SIO2	9.1117	0.8748	10.42	0.000
B2O3	-6.0835	0.8975	-6.78	0.000
NA2O	-10.9035	0.9214	-11.83	0.000
LI2O	-34.144	1.392	-24.53	0.000
CAO	-7.405	1.088	-6.81	0.000
MGO	-2.725	1.156	-2.36	0.020
FE2O3	0.0825	0.9288	0.09	0.929
AL2O3	11.4170	0.8477	13.47	0.000
ZRO2	7.6142	0.9707	7.84	0.000

s = 0.2551 R-sq = 93.9% R-sq(adj) = 93.4%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	9	112.849	12.539	192.66	0.000
Error	112	7.289	0.065		
Total	121	120.138			

SOURCE	DF	SEQ SS
SIO2	1	34.679
B2O3	1	0.222
NA2O	1	1.955
LI2O	1	39.357
CAO	1	6.140
MGO	1	5.115
FE2O3	1	12.842
AL2O3	1	8.535
ZRO2	1	4.004

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid

7	0.570	4.2888	3.6214	0.1111	0.6674	2.91R
53	0.519	3.3113	2.6697	0.0867	0.6415	2.67R
89	0.504	2.8362	2.2627	0.0620	0.5735	2.32R
90	0.566	3.0978	2.2669	0.0634	0.8309	3.36R
100	0.548	4.0476	3.1573	0.0795	0.8903	3.67R
101	0.507	4.1934	3.0382	0.0714	1.1553	4.72R

R denotes an obs. with a large st. resid.

LNVISC = - 0.045 + 9.03 SIO2 - 6.17 B2O3 - 11.0 NA2O - 34.2 LI2O - 7.49 CAO
- 2.81 MGO + 11.3 AL2O3 + 7.53 ZRO2 - 0.083 OTHERS

Predictor	Coef	Stdev	t-ratio	p
Constant	-0.0451	0.6236	-0.07	0.942
SIO2	9.0291	0.7665	11.78	0.000
B2O3	-6.1661	0.7390	-8.34	0.000
NA2O	-10.9862	0.7886	-13.93	0.000
LI2O	-34.226	1.236	-27.68	0.000
CAO	-7.487	1.052	-7.11	0.000
MGO	-2.807	1.093	-2.57	0.012
AL2O3	11.3344	0.6529	17.36	0.000
ZRO2	7.5316	0.8282	9.09	0.000
OTHERS	-0.0827	0.9289	-0.09	0.929

s = 0.2551   R-sq = 93.9%   R-sq(adj) = 93.4%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	9	112.849	12.539	192.66	0.000
Error	112	7.289	0.065		
Total	121	120.138			

SOURCE	DF	SEQ SS
SIO2	1	34.679
B2O3	1	0.222
NA2O	1	1.955
LI2O	1	39.357
CAO	1	6.140
MGO	1	5.115
AL2O3	1	18.960
ZRO2	1	6.421
OTHERS	1	0.001

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
7	0.570	4.2888	3.6214	0.1111	0.6674	2.91R
53	0.519	3.3113	2.6698	0.0867	0.6415	2.67R
89	0.504	2.8362	2.2627	0.0620	0.5735	2.32R
90	0.566	3.0978	2.2669	0.0634	0.8309	3.36R
100	0.548	4.0476	3.1573	0.0795	0.8903	3.67R
101	0.507	4.1934	3.0382	0.0714	1.1553	4.72R

R denotes an obs. with a large st. resid.

LNVISC = - 0.077 + 9.06 SIO2 - 6.14 B2O3 - 11.0 NA2O - 34.2 LI2O - 7.45 CAO - 2.77 MGO + 11.4 AL2O3 + 7.56 ZRO2

Predictor	Coef	Stdev	t-ratio	p
Constant	-0.0768	0.5095	-0.15	0.880
SIO2	9.0619	0.6690	13.55	0.000
B2O3	-6.1372	0.6609	-9.29	0.000
NA2O	-10.9557	0.7074	-15.49	0.000
LI2O	-34.204	1.207	-28.34	0.000
CAO	-7.4495	0.9592	-7.77	0.000
MGO	-2.773	1.018	-2.72	0.007
AL2O3	11.3617	0.5736	19.81	0.000
ZRO2	7.5606	0.7578	9.98	0.000

s = 0.2540   R-sq = 93.9%   R-sq(adj) = 93.5%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	8	112.848	14.106	218.66	0.000
Error	113	7.290	0.065		
Total	121	120.138			

SOURCE	DF	SEQ SS
SIO2	1	34.679
B2O3	1	0.222
NA2O	1	1.955
LI2O	1	39.357
CAO	1	6.140
MGO	1	5.115
AL2O3	1	18.960
ZRO2	1	6.421

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
7	0.570	4.2888	3.6214	0.1106	0.6674	2.92R
53	0.519	3.3113	2.6657	0.0734	0.6456	2.66R
89	0.504	2.8362	2.2633	0.0613	0.5728	2.32R
90	0.566	3.0978	2.2699	0.0539	0.8280	3.34R
100	0.548	4.0476	3.1585	0.0780	0.8891	3.68R
101	0.507	4.1934	3.0356	0.0649	1.1578	4.72R

R denotes an obs. with a large st. resid.

LNVISC = 8.97 SIO2 - 6.21 B2O3 - 11.0 NA2O - 34.3 LI2O - 7.53 CAO - 2.85 MGO + 11.3 AL2O3 + 7.51 ZRO2

Predictor	Coef	Stdev	t-ratio	p
Noconstant				
SIO2	8.9657	0.1988	45.11	0.000
B2O3	-6.2113	0.4399	-14.12	0.000
NA2O	-11.0340	0.4782	-23.07	0.000
LI2O	-34.290	1.060	-32.35	0.000
CAO	-7.5308	0.7900	-9.53	0.000
MGO	-2.8496	0.8764	-3.25	0.002
AL2O3	11.3224	0.5088	22.25	0.000
ZRO2	7.5083	0.6708	11.19	0.000

s = 0.2529

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	8	470.686	58.836	919.93	0.000
Error	114	7.291	0.064		
Total	122	477.978			

SOURCE	DF	SEQ SS
SIO2	1	377.227
B2O3	1	2.535
NA2O	1	10.964
LI2O	1	42.627
CAO	1	3.691
MGO	1	1.763
AL2O3	1	23.867
ZRO2	1	8.013

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
7	0.570	4.2888	3.6163	0.1048	0.6725	2.92R
53	0.519	3.3113	2.6685	0.0706	0.6427	2.65R
89	0.504	2.8362	2.2628	0.0609	0.5733	2.34R
90	0.566	3.0978	2.2710	0.0532	0.8269	3.34R
100	0.548	4.0476	3.1640	0.0689	0.8837	3.63R
101	0.507	4.1934	3.0381	0.0625	1.1553	4.71R

R denotes an obs. with a large st. resid.

2. Revised Final 1st Order Modeling for Electrical Conductivity

LNELEC = 3.44 - 2.60 SIO2 - 1.18 B2O3 + 7.64 NA2O + 20.1 LI2O - 2.04 CAO - 2.39 MGO - 0.833 FE2O3 - 2.15 AL2O3 - 2.35 ZRO2

Predictor	Coef	Stdev	t-ratio	p
Constant	3.4389	0.4759	7.23	0.000
SIO2	-2.5975	0.5449	-4.77	0.000
B2O3	-1.1758	0.5549	-2.12	0.036
NA2O	7.6351	0.5671	13.46	0.000
LI2O	20.1276	0.8593	23.42	0.000
CAO	-2.0428	0.6724	-3.04	0.003
MGO	-2.3920	0.7118	-3.36	0.001
FE2O3	-0.8333	0.5717	-1.46	0.148
AL2O3	-2.1512	0.5280	-4.07	0.000
ZRO2	-2.3473	0.6042	-3.88	0.000

s = 0.1570 R-sq = 93.2% R-sq(adj) = 92.6%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	9	37.3656	4.1517	168.43	0.000
Error	111	2.7362	0.0247		
Total	120	40.1017			

SOURCE	DF	SEQ SS
SIO2	1	2.2643
B2O3	1	7.3093
NA2O	1	3.5054
LI2O	1	23.6161
CAO	1	0.0161
MGO	1	0.0650
FE2O3	1	0.1423
AL2O3	1	0.0750
ZRO2	1	0.3720

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
6	0.440	3.8563	3.5532	0.0604	0.3031	2.09R
7	0.570	1.9272	2.2994	0.0694	-0.3722	-2.64R
9	0.420	2.1247	2.4213	0.0672	-0.2966	-2.09R
10	0.570	3.0258	2.5093	0.0582	0.5165	3.54R
11	0.420	2.0109	2.4183	0.0595	-0.4074	-2.80R
12	0.420	4.1811	3.7821	0.0705	0.3990	2.84R
52	0.439	1.9301	2.4039	0.0602	-0.4739	-3.27R

LNELEC = 2.61 - 1.76 SIO2 - 0.343 B2O3 + 8.47 NA2O + 21.0 LI2O - 1.21 CAO
- 1.56 MGO - 1.32 AL2O3 - 1.51 ZRO2 + 0.833 OTHERS

Predictor	Coef	Stdev	t-ratio	p
Constant	2.6056	0.3868	6.74	0.000
SIO2	-1.7642	0.4780	-3.69	0.000
B2O3	-0.3425	0.4571	-0.75	0.455
NA2O	8.4684	0.4855	17.44	0.000
LI2O	20.9609	0.7645	27.42	0.000
CAO	-1.2095	0.6500	-1.86	0.065
MGO	-1.5588	0.6730	-2.32	0.022
AL2O3	-1.3179	0.4085	-3.23	0.002
ZRO2	-1.5139	0.5164	-2.93	0.004
OTHERS	0.8333	0.5717	1.46	0.148

s = 0.1570 R-sq = 93.2% R-sq(adj) = 92.6%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	9	37.3656	4.1517	168.43	0.000
Error	111	2.7362	0.0247		
Total	120	40.1017			

SOURCE	DF	SEQ SS
SIO2	1	2.2643
B2O3	1	7.3093
NA2O	1	3.5054
LI2O	1	23.6161
CAO	1	0.0161
MGO	1	0.0650
AL2O3	1	0.1827
ZRO2	1	0.3543
OTHERS	1	0.0524

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
6	0.440	3.8563	3.5532	0.0604	0.3031	2.09R
7	0.570	1.9272	2.2994	0.0694	-0.3722	-2.64R
9	0.420	2.1247	2.4213	0.0672	-0.2966	-2.09R
10	0.570	3.0258	2.5093	0.0582	0.5165	3.54R
11	0.420	2.0109	2.4183	0.0595	-0.4074	-2.80R
12	0.420	4.1811	3.7821	0.0705	0.3990	2.84R
52	0.439	1.9301	2.4039	0.0602	-0.4739	-3.27R

LNELEC = 2.35 - 1.45 SIO2 + 8.75 NA2O + 21.5 LI2O - 1.05 MGO - 1.33 AL2O3 - 1.41 ZRO2

Predictor	Coef	Stdev	t-ratio	p
Constant	2.3460	0.1951	12.02	0.000
SIO2	-1.4498	0.3230	-4.49	0.000
NA2O	8.7549	0.3460	25.30	0.000
LI2O	21.5175	0.6856	31.38	0.000
MGO	-1.0534	0.5569	-1.89	0.061
AL2O3	-1.3341	0.3588	-3.72	0.000
ZRO2	-1.4119	0.4593	-3.07	0.003

s = 0.1614 R-sq = 92.6% R-sq(adj) = 92.2%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	6	37.1312	6.1885	237.50	0.000
Error	114	2.9705	0.0261		
Total	120	40.1017			

SOURCE	DF	SEQ SS
SIO2	1	2.2643
NA2O	1	8.0923
LI2O	1	26.3335
MGO	1	0.0355
AL2O3	1	0.1594
ZRO2	1	0.2462

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
6	0.440	3.8563	3.4827	0.0510	0.3736	2.44R
7	0.570	1.9272	2.3953	0.0566	-0.4681	-3.10R
10	0.570	3.0258	2.4056	0.0460	0.6202	4.01R
11	0.420	2.0109	2.4230	0.0506	-0.4121	-2.69R
21	0.570	2.0857	2.4385	0.0471	-0.3528	-2.29R
52	0.439	1.9301	2.3978	0.0510	-0.4677	-3.05R
80	0.438	3.8797	4.2209	0.0331	-0.3412	-2.16R
81	0.528	4.2335	4.5549	0.0385	-0.3213	-2.05R

R denotes an obs. with a large st. resid.

LNELEC = 2.26 - 1.37 SIO2 + 8.84 NA2O + 21.7 LI2O - 1.21 AL2O3 - 1.30 ZRO2

Predictor	Coef	Stdev	t-ratio	p
Constant	2.2587	0.1917	11.78	0.000
SIO2	-1.3724	0.3240	-4.24	0.000
NA2O	8.8420	0.3467	25.50	0.000
LI2O	21.6596	0.6891	31.43	0.000
AL2O3	-1.2081	0.3565	-3.39	0.001
ZRO2	-1.2968	0.4603	-2.82	0.006

s = 0.1632 R-sq = 92.4% R-sq(adj) = 92.0%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	5	37.0380	7.4076	278.05	0.000
Error	115	3.0637	0.0266		
Total	120	40.1017			

SOURCE	DF	SEQ SS
SIO2	1	2.2643
NA2O	1	8.0923
LI2O	1	26.3335
AL2O3	1	0.1365
ZRO2	1	0.2114

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
6	0.440	3.8563	3.4575	0.0498	0.3988	2.57R
7	0.570	1.9272	2.3769	0.0564	-0.4497	-2.94R
10	0.570	3.0258	2.3872	0.0454	0.6386	4.07R
11	0.420	2.0109	2.3938	0.0487	-0.3829	-2.46R
12	0.420	4.1811	3.8493	0.0578	0.3319	2.17R
21	0.570	2.0857	2.4888	0.0392	-0.4032	-2.54R
52	0.439	1.9301	2.3614	0.0478	-0.4313	-2.76R
80	0.438	3.8797	4.2048	0.0324	-0.3251	-2.03R

R denotes an obs. with a large st. resid.

3. Revised Final 1st Order Modeling for PCT B

LNPCT = 0.16 - 4.46 SIO2 + 11.7 B2O3 + 17.7 NA2O + 22.8 LI2O - 9.21 CAO
+ 10.4 MGO - 3.27 FE2O3 - 25.6 AL2O3 - 10.8 ZRO2

Predictor	Coef	Stdev	t-ratio	p
Constant	0.163	1.919	0.09	0.932
SIO2	-4.465	2.168	-2.06	0.041
B2O3	11.666	2.264	5.15	0.000
NA2O	17.659	2.316	7.62	0.000
LI2O	22.803	3.459	6.59	0.000
CAO	-9.208	2.659	-3.46	0.001
MGO	10.419	2.851	3.65	0.000
FE2O3	-3.272	2.394	-1.37	0.174
AL2O3	-25.606	2.107	-12.15	0.000
ZRO2	-10.792	2.487	-4.34	0.000

s = 0.6621 R-sq = 81.8% R-sq(adj) = 80.6%
Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	9	270.428	30.048	68.55	0.000
Error	137	60.056	0.438		
Total	146	330.484			

SOURCE	DF	SEQ SS
SIO2	1	5.320
B2O3	1	8.202
NA2O	1	57.966
LI2O	1	18.008
CAO	1	9.759
MGO	1	31.953
FE2O3	1	52.193
AL2O3	1	78.773
ZRO2	1	8.254

Unusual Observations

Obs.	SIO2	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
2	0.550	-2.7181	-4.0569	0.2370	1.3388	2.17R
45	0.570	2.2665	0.9295	0.2209	1.3371	2.14R
46	0.570	-1.7545	-0.2948	0.2332	-1.4597	-2.36R
48	0.506	1.5394	0.2574	0.2200	1.2821	2.05R
53	0.519	1.8736	0.2720	0.2132	1.6016	2.56R
90	0.460	-0.6694	-2.0437	0.1893	1.3743	2.17R

LNPCT = - 1.83 - 2.50 SIO2 + 13.8 B2O3 + 19.7 NA2O + 25.2 LI2O - 7.49 CAO
+ 12.3 MGO - 23.4 AL2O3 - 8.69 ZRO2

Predictor	Coef	Stdev	t-ratio	p
Constant	-1.834	1.248	-1.47	0.144
SIO2	-2.502	1.629	-1.54	0.127
B2O3	13.767	1.667	8.26	0.000
NA2O	19.697	1.778	11.08	0.000
LI2O	25.172	3.003	8.38	0.000
CAO	-7.494	2.352	-3.19	0.002
MGO	12.287	2.510	4.89	0.000
AL2O3	-23.445	1.397	-16.79	0.000
ZRO2	-8.694	1.963	-4.43	0.000

s = 0.6642 R-sq = 81.6% R-sq(adj) = 80.5%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	8	269.610	33.701	76.40	0.000
Error	138	60.874	0.441		
Total	146	330.484			

SOURCE	DF	SEQ SS
SIO2	1	5.320
B2O3	1	8.202
NA2O	1	57.966
LI2O	1	18.008
CAO	1	9.759
MGO	1	31.953
AL2O3	1	129.746
ZRO2	1	8.655

Unusual Observations

Obs.	SIO2	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
2	0.550	-2.7181	-4.0404	0.2374	1.3223	2.13R
45	0.570	2.2665	0.7658	0.1862	1.5007	2.35R
46	0.570	-1.7545	-0.3044	0.2338	-1.4501	-2.33R
53	0.519	1.8736	0.4382	0.1756	1.4355	2.24R
90	0.460	-0.6694	-1.9984	0.1870	1.3290	2.09R

$$LNPCT = - 3.67 + 15.3\ B2O3 + 21.3\ NA2O + 26.6\ LI2O - 5.89\ CAO + 13.7\ MGO - 22.5\ AL2O3 - 7.49\ ZRO2$$

Predictor	Coef	Stdev	t-ratio	p
Constant	-3.6659	0.3680	-9.96	0.000
B2O3	15.346	1.319	11.64	0.000
NA2O	21.333	1.431	14.91	0.000
LI2O	26.571	2.876	9.24	0.000
CAO	-5.890	2.118	-2.78	0.006
MGO	13.737	2.337	5.88	0.000
AL2O3	-22.510	1.263	-17.82	0.000
ZRO2	-7.490	1.808	-4.14	0.000

s = 0.6674   R-sq = 81.3%   R-sq(adj) = 80.3%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	7	268.569	38.367	86.13	0.000
Error	139	61.915	0.445		
Total	146	330.484			

SOURCE	DF	SEQ SS
B2O3	1	12.109
NA2O	1	54.173
LI2O	1	12.976
CAO	1	15.923
MGO	1	23.501
AL2O3	1	142.245
ZRO2	1	7.642

Unusual Observations

Obs.	B2O3	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
45	0.050	2.2665	0.8067	0.1852	1.4598	2.28R
46	0.052	-1.7545	-0.1048	0.1953	-1.6497	-2.58R
48	0.050	1.5394	0.2100	0.1999	1.3295	2.09R
53	0.200	1.8736	0.4129	0.1757	1.4608	2.27R
90	0.159	-0.6694	-1.9763	0.1874	1.3068	2.04R

R denotes an obs. with a large st. resid.

4. Revised Final 1st Order Modeling for MCC-1 B

LNMCC = 3.49 - 3.71 SIO2 + 6.55 B2O3 + 6.65 NA2O + 8.58 LI2O - 0.00 CAO
+ 1.50 MGO + 2.32 FE2O3 - 10.1 AL2O3 - 4.45 ZRO2

Predictor	Coef	Stdev	t-ratio	p
Constant	3.485	1.336	2.61	0.010
SIO2	-3.709	1.548	-2.40	0.018
B2O3	6.553	1.571	4.17	0.000
NA2O	6.654	1.616	4.12	0.000
LI2O	8.582	2.230	3.85	0.000
CAO	-0.004	1.757	-0.00	0.998
MGO	1.502	1.971	0.76	0.448
FE2O3	2.324	1.538	1.51	0.133
AL2O3	-10.100	1.383	-7.30	0.000
ZRO2	-4.448	1.605	-2.77	0.006

s = 0.4095 R-sq = 67.5% R-sq(adj) = 65.2%
Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	9	44.1841	4.9093	29.27	0.000
Error	127	21.3018	0.1677		
Total	136	65.4859			

SOURCE	DF	SEQ SS
SIO2	1	6.5411
B2O3	1	1.4246
NA2O	1	4.2441
LI2O	1	0.9481
CAO	1	0.0355
MGO	1	0.8685
FE2O3	1	18.2358
AL2O3	1	10.5979
ZRO2	1	1.2884

Unusual Observations

Obs.	SIO2	LNMCC	Fit	Stdev.Fit	Residual	St.Resid
2	0.550	2.0096	1.2378	0.1537	0.7718	2.03R
24	0.481	1.6134	2.8730	0.0823	-1.2596	-3.14R
48	0.570	3.8506	2.7109	0.1482	1.1397	2.99R
74	0.438	2.4828	3.3067	0.1028	-0.8239	-2.08R
95	0.507	3.8114	2.9043	0.1172	0.9071	2.31R
107	0.440	5.3774	4.1939	0.1210	1.1835	3.02R
126	0.482	4.5876	3.7362	0.0901	0.8514	2.13R

LNMCC = 4.64 - 4.79 SIO2 + 5.29 B2O3 + 5.49 NA2O + 7.36 LI2O - 11.6 AL2O3 - 5.78 ZRO2

Predictor	Coef	Stdev	t-ratio	p
Constant	4.6375	0.7071	6.56	0.000
SIO2	-4.7862	0.9939	-4.82	0.000
B2O3	5.286	1.047	5.05	0.000
NA2O	5.492	1.090	5.04	0.000
LI2O	7.360	1.836	4.01	0.000
AL2O3	-11.5936	0.8782	-13.20	0.000
ZRO2	-5.781	1.217	-4.75	0.000

s = 0.4100   R-sq = 66.6%   R-sq(adj) = 65.1%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	6	43.6288	7.2715	43.25	0.000
Error	130	21.8571	0.1681		
Total	136	65.4859			

SOURCE	DF	SEQ SS
SIO2	1	6.5411
B2O3	1	1.4246
NA2O	1	4.2441
LI2O	1	0.9481
AL2O3	1	26.6787
ZRO2	1	3.7922

Unusual Observations

Obs.	SIO2	LNMCC	Fit	Stdev.Fit	Residual	St.Resid
10	0.420	4.2991	3.7532	0.1664	0.5460	1.46 X
24	0.481	1.6134	2.8887	0.0705	-1.2752	-3.16R
48	0.570	3.8506	2.7919	0.1067	1.0587	2.67R
74	0.438	2.4828	3.3040	0.0953	-0.8212	-2.06R
95	0.507	3.8114	2.7934	0.0997	1.0181	2.56R
107	0.440	5.3774	4.1950	0.1084	1.1823	2.99R
115	0.489	4.5082	3.6659	0.0783	0.8423	2.09R
126	0.482	4.5876	3.7351	0.0895	0.8525	2.13R

R denotes an obs. with a large st. resid.
X denotes an obs. whose X value gives it large influence.

APPENDIX H--Revised Final 2nd Order Regression of Glass Properties

This Appendix displays the stepwise regression used to form the FINAL Revised PNL 2nd Order viscosity, electrical conductivity, PCT B, and MCC-1 B models (using the appropriate data set from Appendix A).

1. Revised Final 2nd Order Modeling for Viscosity

LNVISC = - 2.10 + 13.1 SIO2 - 4.06 B2O3 - 24.3 NA2O - 73.9 LI2O - 3.47 CAO
- 1.13 MGO + 2.26 FE2O3 + 16.6 AL2O3 + 12.3 ZRO2 + 30.1 BXFE
+ 43.6 NAXNA + 127 NAXLI + 30.0 NAXMG + 298 LIXLI + 78.7 LIXOTH
- 39.7 MGXFE

Predictor	Coef	Stdev	t-ratio	p
Constant	-2.1048	0.9911	-2.12	0.036
SIO2	13.097	1.074	12.20	0.000
B2O3	-4.063	1.098	-3.70	0.000
NA2O	-24.305	2.768	-8.78	0.000
LI2O	-73.903	4.414	-16.74	0.000
CAO	-3.472	1.206	-2.88	0.005
MGO	-1.134	1.995	-0.57	0.571
FE2O3	2.255	1.402	1.61	0.111
AL2O3	16.608	1.164	14.27	0.000
ZRO2	12.286	1.125	10.92	0.000
BXFE	30.059	7.224	4.16	0.000
NAXNA	43.590	9.014	4.84	0.000
NAXLI	126.79	16.81	7.54	0.000
NAXMG	29.99	12.16	2.47	0.015
LIXLI	298.25	42.02	7.10	0.000
LIXOTH	78.71	20.69	3.80	0.000
MGXFE	-39.74	13.67	-2.91	0.004

s = 0.1709   R-sq = 97.4%   R-sq(adj) = 97.1%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	16	117.0725	7.3170	250.62	0.000
Error	105	3.0655	0.0292		
Total	121	120.1380			

SOURCE	DF	SEQ SS
SIO2	1	34.6787
B2O3	1	0.2221

NA2O	1	1.9554
LI2O	1	39.3568
CAO	1	6.1396
MGO	1	5.1149
FE2O3	1	12.8422
AL2O3	1	8.5352
ZRO2	1	4.0040
BXFE	1	0.8216
NAXNA	1	0.3479
NAXLI	1	0.9248
NAXMG	1	0.2291
LIXLI	1	1.3070
LIXOTH	1	0.3465
MGXFE	1	0.2468

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
9	0.420	1.4012	1.5898	0.1211	-0.1886	-1.56 X
89	0.504	2.8362	2.2696	0.0455	0.5665	3.44R
90	0.566	3.0978	2.4167	0.0554	0.6812	4.21R
100	0.548	4.0476	3.7257	0.0840	0.3219	2.16R
101	0.507	4.1934	3.5411	0.0722	0.6523	4.21R

R denotes an obs. with a large st. resid.
X denotes an obs. whose X value gives it large influence.

LNVISC = - 0.540 + 11.5 SIO2 - 6.09 B2O3 - 24.9 NA2O - 75.4 LI2O - 4.95 CAO
+ 15.0 AL2O3 + 10.7 ZRO2 - 1.66 OTHERS + 36.1 BXFE + 41.0 NAXNA
+ 125 NAXLI + 11.6 NAXMG + 299 LIXLI + 79.6 LIXOTH - 46.3 MGXFE

Predictor	Coef	Stdev	t-ratio	p
Constant	-0.5405	0.9150	-0.59	0.556
SIO2	11.4898	0.9354	12.28	0.000
B2O3	-6.0866	0.7769	-7.83	0.000
NA2O	-24.862	2.934	-8.47	0.000
LI2O	-75.355	4.903	-15.37	0.000
CAO	-4.951	1.110	-4.46	0.000
AL2O3	15.0295	0.8290	18.13	0.000
ZRO2	10.7055	0.9126	11.73	0.000
OTHERS	-1.661	1.385	-1.20	0.233
BXFE	36.120	6.583	5.49	0.000
NAXNA	40.992	9.025	4.54	0.000
NAXLI	124.66	16.99	7.34	0.000
NAXMG	11.646	7.640	1.52	0.130
LIXLI	298.57	42.55	7.02	0.000
LIXOTH	79.63	20.95	3.80	0.000
MGXFE	-46.32	13.40	-3.46	0.001

s = 0.1730   R-sq = 97.4%   R-sq(adj) = 97.0%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	15	116.9645	7.7976	260.46	0.000
Error	106	3.1735	0.0299		
Total	121	120.1380			

SOURCE	DF	SEQ SS
SIO2	1	34.6787
B2O3	1	0.2221
NA2O	1	1.9554
LI2O	1	39.3568
CAO	1	6.1396
AL2O3	1	21.9748
ZRO2	1	8.0421
OTHERS	1	0.0504
BXFE	1	1.2205
NAXNA	1	0.3710
NAXLI	1	0.9294
NAXMG	1	0.0669

LIXLI	1	1.2588
LIXOTH	1	0.3404
MGXFE	1	0.3577

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
9	0.420	1.4012	1.6525	0.1181	-0.2514	-1.99 X
89	0.504	2.8362	2.2443	0.0441	0.5919	3.54R
90	0.566	3.0978	2.4049	0.0558	0.6929	4.23R
98	0.455	0.4383	0.7600	0.0733	-0.3217	-2.05R
100	0.548	4.0476	3.6997	0.0839	0.3479	2.30R
101	0.507	4.1934	3.5601	0.0725	0.6334	4.03R
110	0.440	1.0225	1.3450	0.0654	-0.3225	-2.01R

R denotes an obs. with a large st. resid.
X denotes an obs. whose X value gives it large influence.

LNVISC = - 0.807 + 11.6 SIO2 - 5.87 B2O3 - 23.9 NA2O - 72.3 LI2O - 4.94 CAO
+ 15.0 AL2O3 + 10.7 ZRO2 + 33.9 BXFE + 40.5 NAXNA + 116 NAXLI
+ 290 LIXLI + 55.8 LIXOTH - 30.1 MGXFE

Predictor	Coef	Stdev	t-ratio	p
Constant	-0.8068	0.6285	-1.28	0.202
SIO2	11.6219	0.6917	16.80	0.000
B2O3	-5.8667	0.5996	-9.78	0.000
NA2O	-23.903	2.767	-8.64	0.000
LI2O	-72.256	4.469	-16.17	0.000
CAO	-4.9358	0.8826	-5.59	0.000
AL2O3	14.9694	0.6542	22.88	0.000
ZRO2	10.6872	0.6895	15.50	0.000
BXFE	33.850	5.288	6.40	0.000
NAXNA	40.490	9.108	4.45	0.000
NAXLI	115.68	16.35	7.07	0.000
LIXLI	289.85	43.11	6.72	0.000
LIXOTH	55.76	14.62	3.81	0.000
MGXFE	-30.13	11.20	-2.69	0.008

s = 0.1760   R-sq = 97.2%   R-sq(adj) = 96.9%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	13	116.7927	8.9841	290.05	0.000
Error	108	3.3452	0.0310		
Total	121	120.1380			

SOURCE	DF	SEQ SS
SIO2	1	34.6787
B2O3	1	0.2221
NA2O	1	1.9554
LI2O	1	39.3568
CAO	1	6.1396
AL2O3	1	21.9748
ZRO2	1	8.0421
BXFE	1	0.7621
NAXNA	1	0.3106
NAXLI	1	1.0054
LIXLI	1	1.1393
LIXOTH	1	0.9815
MGXFE	1	0.2242

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid
7	0.570	4.2888	3.9725	0.0840	0.3164	2.05R
9	0.420	1.4012	1.7713	0.0968	-0.3701	-2.52R
16	0.433	2.8798	2.4977	0.0748	0.3821	2.40R
89	0.504	2.8362	2.2596	0.0444	0.5765	3.38R
90	0.566	3.0978	2.4108	0.0565	0.6871	4.12R
98	0.455	0.4383	0.7694	0.0743	-0.3311	-2.08R
100	0.548	4.0476	3.7080	0.0842	0.3396	2.20R
101	0.507	4.1934	3.5154	0.0699	0.6780	4.20R

R denotes an obs. with a large st. resid.

LNVISC = 10.8 SIO2 - 6.49 B2O3 - 25.8 NA2O - 74.0 LI2O - 5.79 CAO + 14.4 AL2O3
+ 10.1 ZRO2 + 29.9 BXFE + 44.1 NAXNA + 121 NAXLI + 297 LIXLI
+ 44.1 LIXOTH - 39.9 MGXFE

Predictor	Coef	Stdev	t-ratio	p
Noconstant				
SIO2	10.7967	0.2562	42.15	0.000
B2O3	-6.4873	0.3559	-18.23	0.000
NA2O	-25.801	2.347	-10.99	0.000
LI2O	-73.996	4.271	-17.32	0.000
CAO	-5.7882	0.5832	-9.92	0.000
AL2O3	14.3699	0.4596	31.27	0.000
ZRO2	10.1045	0.5206	19.41	0.000
BXFE	29.950	4.341	6.90	0.000
NAXNA	44.076	8.694	5.07	0.000
NAXLI	120.96	15.87	7.62	0.000
LIXLI	297.25	42.85	6.94	0.000
LIXOTH	44.06	11.46	3.84	0.000
MGXFE	-39.893	8.244	-4.84	0.000

s = 0.1765
Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	13	474.581	36.506	1171.63	0.000
Error	109	3.396	0.031		
Total	122	477.978			

SOURCE	DF	SEQ SS
SIO2	1	377.227
B2O3	1	2.535
NA2O	1	10.964
LI2O	1	42.627
CAO	1	3.691
AL2O3	1	24.638
ZRO2	1	8.328
BXFE	1	0.232
NAXNA	1	0.662
NAXLI	1	1.273
LIXLI	1	1.157
LIXOTH	1	0.517
MGXFE	1	0.730

Unusual Observations

Obs.	SIO2	LNVISC	Fit	Stdev.Fit	Residual	St.Resid

7	0.570	4.2888	3.9480	0.0820	0.3408	2.18R
9	0.420	1.4012	1.7760	0.0971	-0.3749	-2.54R
10	0.570	4.4288	4.7745	0.0656	-0.3457	-2.11R
16	0.433	2.8798	2.5087	0.0745	0.3711	2.32R
89	0.504	2.8362	2.2468	0.0433	0.5894	3.44R
90	0.566	3.0978	2.3869	0.0536	0.7110	4.23R
98	0.455	0.4383	0.7637	0.0744	-0.3254	-2.03R
101	0.507	4.1934	3.5240	0.0697	0.6694	4.13R

R denotes an obs. with a large st. resid.

2. Revised Final 2nd Order Modeling for Electrical Conductivity

LNELEC = - 9.47 + 9.93 SIO2 + 11.2 B2O3 + 24.0 NA2O + 40.8 LI2O + 8.68 CAO + 9.79 MGO + 8.89 FE2O3 + 10.9 AL2O3 + 8.98 ZRO2 - 94.5 NAXLI + 42.2 CAXFE + 19.3 BXFE + 38.6 MGXZR + 24.7 SIXOTH + 43.3 LIXZR

Predictor	Coef	Stdev	t-ratio	p
Constant	-9.470	4.135	-2.29	0.024
SIO2	9.931	3.994	2.49	0.014
B2O3	11.190	4.362	2.57	0.012
NA2O	24.044	4.244	5.67	0.000
LI2O	40.826	4.384	9.31	0.000
CAO	8.685	4.490	1.93	0.056
MGO	9.786	4.404	2.22	0.028
FE2O3	8.895	4.402	2.02	0.046
AL2O3	10.895	4.269	2.55	0.012
ZRO2	8.981	4.341	2.07	0.041
NAXLI	-94.49	14.68	-6.44	0.000
CAXFE	42.24	10.98	3.85	0.000
BXFE	19.283	6.850	2.82	0.006
MGXZR	38.59	14.51	2.66	0.009
SIXOTH	24.693	8.555	2.89	0.005
LIXZR	43.28	16.14	2.68	0.009

s = 0.1622   R-sq = 93.1%   R-sq(adj) = 92.1%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	15	37.5252	2.5017	95.12	0.000
Error	106	2.7878	0.0263		
Total	121	40.3130			

SOURCE	DF	SEQ SS
SIO2	1	2.0872
B2O3	1	6.7194
NA2O	1	3.3538
LI2O	1	22.3609
CAO	1	0.0004
MGO	1	0.1194
FE2O3	1	0.0183
AL2O3	1	0.0303
ZRO2	1	0.1344
NAXLI	1	1.5893

CAXFE	1	0.3515
BXFE	1	0.2168
MGXZR	1	0.1716
SIXOTH	1	0.1828
LIXZR	1	0.1891

Unusual Observations

Obs.	SIO2	LNELEC	Fit	Stdev.Fit	Residual	St.Resid
10	0.570	3.0258	2.6696	0.0762	0.3561	2.49R
12	0.420	4.1811	4.2665	0.1171	-0.0854	-0.76 X
14	0.420	3.5531	3.4908	0.1025	0.0622	0.49 X
18	0.421	4.1821	4.2697	0.1223	-0.0877	-0.82 X
102	0.440	2.9570	4.1365	0.0679	-1.1795	-8.01R

R denotes an obs. with a large st. resid.
X denotes an obs. whose X value gives it large influence.

$$LNELEC = - 5.31 + 5.60\ SIO2 + 7.20\ B2O3 + 19.9\ NA2O + 37.0\ LI2O + 5.12\ CAO + 6.01\ MGO + 6.12\ FE2O3 + 6.38\ AL2O3 + 4.93\ ZRO2 - 85.0\ NAXLI + 27.4\ CAXFE + 12.1\ BXFE + 25.8\ MGXZR + 17.3\ SIXOTH + 32.0\ LIXZR$$

121 cases used 1 cases contain missing values

Predictor	Coef	Stdev	t-ratio	p
Constant	-5.310	2.632	-2.02	0.046
SIO2	5.601	2.545	2.20	0.030
B2O3	7.198	2.773	2.60	0.011
NA2O	19.911	2.700	7.38	0.000
LI2O	37.030	2.785	13.30	0.000
CAO	5.116	2.849	1.80	0.075
MGO	6.011	2.797	2.15	0.034
FE2O3	6.119	2.788	2.19	0.030
AL2O3	6.376	2.719	2.34	0.021
ZRO2	4.933	2.760	1.79	0.077
NAXLI	-85.029	9.300	-9.14	0.000
CAXFE	27.424	7.030	3.90	0.000
BXFE	12.100	4.363	2.77	0.007
MGXZR	25.811	9.221	2.80	0.006
SIXOTH	17.272	5.434	3.18	0.002
LIXZR	31.98	10.23	3.13	0.002

s = 0.1024 R-sq = 97.3% R-sq(adj) = 96.9%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	15	39.0004	2.6000	247.90	0.000
Error	105	1.1013	0.0105		
Total	120	40.1017			

SOURCE	DF	SEQ SS
SIO2	1	2.2643
B2O3	1	7.3093
NA2O	1	3.5054
LI2O	1	23.6161
CAO	1	0.0161
MGO	1	0.0650
FE2O3	1	0.1423
AL2O3	1	0.0750
ZRO2	1	0.3720
NAXLI	1	1.1640
CAXFE	1	0.1303

BXFE	1	0.0796
MGXZR	1	0.0725
SIXOTH	1	0.0859
LIXZR	1	0.1025

Unusual Observations

Obs.	SIO2	LNELEC	Fit	Stdev.Fit	Residual	St.Resid
1	0.480	2.92585	3.14406	0.01442	-0.21821	-2.15R
6	0.440	3.85630	3.67552	0.05091	0.18078	2.03R
10	0.570	3.02578	2.56691	0.04879	0.45887	5.10R
12	0.420	4.18113	4.16525	0.07440	0.01589	0.23 X
14	0.420	3.55306	3.47948	0.06471	0.07358	0.93 X
16	0.433	3.27185	3.46589	0.04845	-0.19405	-2.15R
18	0.421	4.18205	4.24241	0.07724	-0.06036	-0.90 X
21	0.570	2.08567	2.27135	0.04595	-0.18568	-2.03R

R denotes an obs. with a large st. resid.

X denotes an obs. whose X value gives it large influence.

LNELEC = - 0.587 + 1.05 SIO2 + 2.25 B2O3 + 15.1 NA2O + 32.5 LI2O + 1.03 MGO
+ 1.20 FE2O3 + 1.52 AL2O3 - 88.3 NAXLI + 28.7 CAXFE + 12.1 BXFE
+ 25.2 MGXZR + 7.56 SIXOTH + 31.3 LIXZR

121 cases used 1 cases contain missing values

Predictor	Coef	Stdev	t-ratio	p
Constant	-0.5875	0.3505	-1.68	0.097
SIO2	1.0504	0.4036	2.60	0.011
B2O3	2.2519	0.4743	4.75	0.000
NA2O	15.1254	0.5473	27.64	0.000
LI2O	32.459	1.182	27.46	0.000
MGO	1.0283	0.4993	2.06	0.042
FE2O3	1.1984	0.6108	1.96	0.052
AL2O3	1.5175	0.4396	3.45	0.001
NAXLI	-88.301	9.168	-9.63	0.000
CAXFE	28.688	5.906	4.86	0.000
BXFE	12.078	4.377	2.76	0.007
MGXZR	25.240	9.154	2.76	0.007
SIXOTH	7.5603	0.8729	8.66	0.000
LIXZR	31.255	8.365	3.74	0.000

s = 0.1030   R-sq = 97.2%   R-sq(adj) = 96.8%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	13	38.9661	2.9974	282.41	0.000
Error	107	1.1357	0.0106		
Total	120	40.1017			

SOURCE	DF	SEQ SS
SIO2	1	2.2643
B2O3	1	7.3093
NA2O	1	3.5054
LI2O	1	23.6161
MGO	1	0.0318
FE2O3	1	0.1667
AL2O3	1	0.0538
NAXLI	1	1.0454
CAXFE	1	0.0142
BXFE	1	0.1400
MGXZR	1	0.0137
SIXOTH	1	0.6572
LIXZR	1	0.1482

Unusual Observations

Obs.	SIO2	LNELEC	Fit	Stdev.Fit	Residual	St.Resid
1	0.480	2.92585	3.14104	0.01399	-0.21520	-2.11R
10	0.570	3.02578	2.53665	0.04573	0.48912	5.30R
12	0.420	4.18113	4.14279	0.07274	0.03834	0.53 X
16	0.433	3.27185	3.46026	0.04861	-0.18841	-2.07R
18	0.421	4.18205	4.26414	0.07533	-0.08209	-1.17 X
21	0.570	2.08567	2.27716	0.04542	-0.19149	-2.07R

R denotes an obs. with a large st. resid.

X denotes an obs. whose X value gives it large influence.

LNELEC = - 0.195 + 0.617 SIO2 + 1.55 B2O3 + 14.9 NA2O + 33.5 LI2O + 0.656 MGO + 0.939 AL2O3 + 0.984 ZRO2 - 92.2 NAXLI + 25.4 CAXFE + 18.1 BXFE + 26.9 MGXZR + 6.85 SIXOTH

121 cases used 1 cases contain missing values

Predictor	Coef	Stdev	t-ratio	p
Constant	-0.1947	0.4098	-0.48	0.636
SIO2	0.6168	0.4677	1.32	0.190
B2O3	1.5461	0.4013	3.85	0.000
NA2O	14.9441	0.6023	24.81	0.000
LI2O	33.525	1.211	27.67	0.000
MGO	0.6560	0.5893	1.11	0.268
AL2O3	0.9387	0.5177	1.81	0.073
ZRO2	0.9836	0.5791	1.70	0.092
NAXLI	-92.205	9.503	-9.70	0.000
CAXFE	25.352	7.063	3.59	0.000
BXFE	18.110	3.290	5.51	0.000
MGXZR	26.862	9.612	2.79	0.006
SIXOTH	6.8458	0.9860	6.94	0.000

s = 0.1077 R-sq = 96.9% R-sq(adj) = 96.5%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	12	38.8488	3.2374	279.06	0.000
Error	108	1.2529	0.0116		
Total	120	40.1017			

SOURCE	DF	SEQ SS
SIO2	1	2.2643
B2O3	1	7.3093
NA2O	1	3.5054
LI2O	1	23.6161
MGO	1	0.0318
AL2O3	1	0.1592
ZRO2	1	0.2519
NAXLI	1	1.0405
CAXFE	1	0.0111
BXFE	1	0.0542
MGXZR	1	0.0458
SIXOTH	1	0.5592

Unusual Observations

Obs.	SIO2	LNELEC	Fit	Stdev.Fit	Residual	St.Resid
1	0.480	2.92585	3.14805	0.01499	-0.22220	-2.08R
6	0.440	3.85630	3.64880	0.04491	0.20750	2.12R
7	0.570	1.92716	2.20363	0.04834	-0.27647	-2.87R
10	0.570	3.02578	2.48805	0.04583	0.53772	5.52R
12	0.420	4.18113	4.19687	0.07418	-0.01574	-0.20 X
18	0.421	4.18205	4.24372	0.07573	-0.06167	-0.81 X
52	0.439	1.93007	2.16271	0.04820	-0.23264	-2.42R

R denotes an obs. with a large st. resid.
X denotes an obs. whose X value gives it large influence.

LNELEC = 0.383 + 1.13 B2O3 + 14.5 NA2O + 33.4 LI2O - 94.3 NAXLI + 16.4 CAXFE + 14.2 BXFE + 27.9 MGXZR + 5.57 SIXOTH + 0.100 LIXZR

121 cases used 1 cases contain missing values

Predictor	Coef	Stdev	t-ratio	p
Constant	0.38257	0.01626	23.52	0.000
B2O3	1.13355	0.04340	26.12	0.000
NA2O	14.5157	0.0906	160.27	0.000
LI2O	33.4372	0.2158	154.93	0.000
NAXLI	-94.309	1.702	-55.41	0.000
CAXFE	16.3778	0.7669	21.36	0.000
BXFE	14.2337	0.4371	32.56	0.000
MGXZR	27.914	1.359	20.54	0.000
SIXOTH	5.5687	0.1224	45.51	0.000
LIXZR	0.099976	0.001748	57.21	0.000

s = 0.01956 R-sq = 99.9% R-sq(adj) = 99.9%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	9	40.0593	4.4510	11637.31	0.000
Error	111	0.0425	0.0004		
Total	120	40.1017			

SOURCE	DF	SEQ SS
B2O3	1	4.0591
NA2O	1	7.2225
LI2O	1	25.2515
NAXLI	1	0.7986
CAXFE	1	0.2932
BXFE	1	0.3175
MGXZR	1	0.0683
SIXOTH	1	0.7967
LIXZR	1	1.2517

Unusual Observations

Obs.	B2O3	LNELEC	Fit	Stdev.Fit	Residual	St.Resid
5	0.050	3.42556	3.47278	0.00571	-0.04722	-2.52R
9	0.196	2.12465	2.10517	0.00983	0.01948	1.15 X
10	0.085	3.02578	2.99463	0.01151	0.03114	1.97 X
12	0.176	4.18113	4.13114	0.01219	0.04999	3.27RX
17	0.050	3.35096	3.35212	0.01043	-0.00117	-0.07 X
18	0.050	4.18205	4.16025	0.01368	0.02180	1.56 X

86	0.113	3.59539	3.55510	0.00366	0.04029	2.10R
104	0.095	4.54425	4.58400	0.00667	-0.03974	-2.16R

3. Revised Final 2nd Order Modeling for PCT B

LNPCT = 2.77 - 7.95 SIO2 + 11.0 B2O3 + 18.1 NA2O + 20.7 LI2O + 11.3 CAO
- 39.4 MGO - 4.72 FE2O3 - 47.3 AL2O3 - 13.4 ZRO2 + 97.5 SIXMG
- 90.2 BXCA - 122 NAXCA + 127 ALXAL

Predictor	Coef	Stdev	t-ratio	p
Constant	2.769	1.616	1.71	0.089
SIO2	-7.946	1.939	-4.10	0.000
B2O3	11.041	1.966	5.62	0.000
NA2O	18.078	1.955	9.25	0.000
LI2O	20.681	2.807	7.37	0.000
CAO	11.337	5.624	2.02	0.046
MGO	-39.38	15.51	-2.54	0.012
FE2O3	-4.721	1.929	-2.45	0.016
AL2O3	-47.278	3.469	-13.63	0.000
ZRO2	-13.359	2.030	-6.58	0.000
SIXMG	97.52	30.29	3.22	0.002
BXCA	-90.15	29.71	-3.03	0.003
NAXCA	-121.87	34.36	-3.55	0.001
ALXAL	126.58	17.69	7.16	0.000

s = 0.5310 R-sq = 88.7% R-sq(adj) = 87.5%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	13	292.987	22.537	79.94	0.000
Error	133	37.497	0.282		
Total	146	330.484			

SOURCE	DF	SEQ SS
SIO2	1	5.320
B2O3	1	8.202
NA2O	1	57.966
LI2O	1	18.008
CAO	1	9.759
MGO	1	31.953
FE2O3	1	52.193
AL2O3	1	78.773
ZRO2	1	8.254
SIXMG	1	2.632
BXCA	1	2.461
NAXCA	1	3.024
ALXAL	1	14.441

Unusual Observations

Obs.	SIO2	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
2	0.550	-2.7181	-2.9619	0.2859	0.2438	0.54 X
5	0.570	-1.0356	-2.1751	0.1944	1.1394	2.31R
12	0.420	1.5394	2.0962	0.2846	-0.5567	-1.24 X
13	0.570	2.6442	3.7489	0.2415	-1.1047	-2.34R
45	0.570	2.2665	1.2132	0.2219	1.0533	2.18R
46	0.570	-1.7545	-1.1848	0.2844	-0.5696	-1.27 X
51	0.562	1.6378	0.4042	0.1980	1.2337	2.50R
53	0.519	1.8736	0.0414	0.1840	1.8323	3.68R
59	0.542	-0.7340	0.6355	0.2104	-1.3695	-2.81R
86	0.323	-1.1026	-1.5958	0.3626	0.4932	1.27 X

R denotes an obs. with a large st. resid.
X denotes an obs. whose X value gives it large influence.

LNPCT = - 5.18 SIO2 + 13.8 B2O3 + 20.8 NA2O + 23.5 LI2O + 14.1 CAO - 36.6 MGO - 1.95 FE2O3 - 44.5 AL2O3 - 10.6 ZRO2 + 2.77 OTHERS + 97.5 SIXMG - 90.2 BXCA - 122 NAXCA + 127 ALXAL

Predictor	Coef	Stdev	t-ratio	p
Noconstant				
SIO2	-5.1771	0.6187	-8.37	0.000
B2O3	13.810	1.139	12.12	0.000
NA2O	20.847	1.191	17.50	0.000
LI2O	23.450	2.188	10.72	0.000
CAO	14.107	5.562	2.54	0.012
MGO	-36.62	14.98	-2.44	0.016
FE2O3	-1.951	1.341	-1.46	0.148
AL2O3	-44.508	3.184	-13.98	0.000
ZRO2	-10.589	1.522	-6.96	0.000
OTHERS	2.771	1.616	1.71	0.089
SIXMG	97.53	30.29	3.22	0.002
BXCA	-90.15	29.71	-3.03	0.003
NAXCA	-121.87	34.36	-3.55	0.001
ALXAL	126.58	17.69	7.16	0.000

s = 0.5310

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	14	299.222	21.373	75.81	0.000
Error	133	37.496	0.282		
Total	147	336.718			

SOURCE	DF	SEQ SS
SIO2	1	5.065
B2O3	1	14.254
NA2O	1	40.586
LI2O	1	3.745
CAO	1	25.914
MGO	1	13.470
FE2O3	1	16.338
AL2O3	1	141.346
ZRO2	1	15.942
OTHERS	1	0.003
SIXMG	1	2.632
BXCA	1	2.462
NAXCA	1	3.024
ALXAL	1	14.441

Unusual Observations

Obs.	SIO2	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
2	0.550	-2.7181	-2.9619	0.2859	0.2438	0.54 X
5	0.570	-1.0356	-2.1752	0.1944	1.1395	2.31R
12	0.420	1.5394	2.0961	0.2846	-0.5566	-1.24 X
13	0.570	2.6442	3.7487	0.2415	-1.1045	-2.34R
45	0.570	2.2665	1.2134	0.2219	1.0532	2.18R
46	0.570	-1.7545	-1.1849	0.2844	-0.5695	-1.27 X
51	0.562	1.6378	0.4042	0.1980	1.2337	2.50R
53	0.519	1.8736	0.0413	0.1840	1.8324	3.68R
59	0.542	-0.7340	0.6354	0.2104	-1.3694	-2.81R
86	0.323	-1.1026	-1.5958	0.3626	0.4932	1.27 X

R denotes an obs. with a large st. resid.
X denotes an obs. whose X value gives it large influence.

LNPCT = - 0.11 - 5.13 SIO2 + 14.0 B2O3 + 21.0 NA2O + 24.1 LI2O + 13.3 CAO
- 36.8 MGO - 43.6 AL2O3 - 10.3 ZRO2 + 97.7 SIXMG - 87.1 BXCA
- 120 NAXCA + 123 ALXAL

Predictor	Coef	Stdev	t-ratio	p
Constant	-0.107	1.130	-0.10	0.924
SIO2	-5.128	1.589	-3.23	0.002
B2O3	14.011	1.576	8.89	0.000
NA2O	20.987	1.581	13.28	0.000
LI2O	24.098	2.480	9.72	0.000
CAO	13.313	5.668	2.35	0.020
MGO	-36.82	15.76	-2.34	0.021
AL2O3	-43.587	3.182	-13.70	0.000
ZRO2	-10.297	1.628	-6.33	0.000
SIXMG	97.74	30.85	3.17	0.002
BXCA	-87.12	30.23	-2.88	0.005
NAXCA	-120.33	34.99	-3.44	0.001
ALXAL	123.09	17.95	6.86	0.000

s = 0.5408 R-sq = 88.1% R-sq(adj) = 87.1%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	12	291.298	24.275	83.01	0.000
Error	134	39.186	0.292		
Total	146	330.484			

SOURCE	DF	SEQ SS
SIO2	1	5.320
B2O3	1	8.202
NA2O	1	57.966
LI2O	1	18.008
CAO	1	9.759
MGO	1	31.953
AL2O3	1	129.746
ZRO2	1	8.655
SIXMG	1	2.643
BXCA	1	2.327
NAXCA	1	2.972
ALXAL	1	13.747

Unusual Observations

Obs.	SIO2	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
2	0.550	-2.7181	-2.9657	0.2912	0.2476	0.54 X

13	0.570	2.6442	3.7565	0.2459	-1.1123	-2.31R
45	0.570	2.2665	0.9834	0.2047	1.2831	2.56R
46	0.570	-1.7545	-1.1930	0.2897	-0.5615	-1.23 X
51	0.562	1.6378	0.1726	0.1772	1.4652	2.87R
53	0.519	1.8736	0.2821	0.1584	1.5915	3.08R
59	0.542	-0.7340	0.8546	0.1940	-1.5886	-3.15R
61	0.515	0.1124	1.2230	0.1469	-1.1105	-2.13R
81	0.390	-0.2510	-0.5395	0.2812	0.2885	0.62 X
86	0.323	-1.1026	-1.5570	0.3689	0.4544	1.15 X

R denotes an obs. with a large st. resid.
X denotes an obs. whose X value gives it large influence.

LNPCT = - 5.27 SIO2 + 13.9 B2O3 + 20.9 NA2O + 24.0 LI2O + 13.3 CAO - 37.5 MGO - 43.6 AL2O3 - 10.4 ZRO2 + 99.0 SIXMG - 87.1 BXCA - 121 NAXCA + 123 ALXAL

Predictor	Coef	Stdev	t-ratio	p
Noconstant				
SIO2	-5.2717	0.5021	-10.50	0.000
B2O3	13.909	1.154	12.06	0.000
NA2O	20.890	1.204	17.35	0.000
LI2O	23.992	2.209	10.86	0.000
CAO	13.251	5.610	2.36	0.020
MGO	-37.54	13.81	-2.72	0.007
AL2O3	-43.629	3.139	-13.90	0.000
ZRO2	-10.362	1.475	-7.02	0.000
SIXMG	98.98	27.83	3.56	0.001
BXCA	-87.11	30.12	-2.89	0.004
NAXCA	-120.72	34.62	-3.49	0.001
ALXAL	123.09	17.89	6.88	0.000

s = 0.5388

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	12	297.530	24.794	85.41	0.000
Error	135	39.189	0.290		
Total	147	336.718			

SOURCE	DF	SEQ SS
SIO2	1	5.065
B2O3	1	14.254
NA2O	1	40.586
LI2O	1	3.745
CAO	1	25.914
MGO	1	13.470
AL2O3	1	157.277
ZRO2	1	14.581
SIXMG	1	3.557
BXCA	1	2.303
NAXCA	1	3.032
ALXAL	1	13.746

Unusual Observations

Obs.	SIO2	LNPCT	Fit	Stdev.Fit	Residual	St.Resid
2	0.550	-2.7181	-2.9688	0.2882	0.2507	0.55 X
13	0.570	2.6442	3.7426	0.1973	-1.0984	-2.19R

45	0.570	2.2665	0.9876	0.1992	1.2789	2.55R
51	0.562	1.6378	0.1714	0.1760	1.4664	2.88R
53	0.519	1.8736	0.2838	0.1569	1.5899	3.08R
59	0.542	-0.7340	0.8552	0.1932	-1.5892	-3.16R
61	0.515	0.1124	1.2271	0.1397	-1.1147	-2.14R
81	0.390	-0.2510	-0.5475	0.2676	0.2964	0.63 X
86	0.323	-1.1026	-1.5533	0.3655	0.4507	1.14 X

R denotes an obs. with a large st. resid.
X denotes an obs. whose X value gives it large influence.

4. Revised Final 2nd Order Modeling for MCC-1 B

LNMCC = 4.52 - 5.64 SIO2 + 10.9 B2O3 + 6.18 NA2O + 8.61 LI2O - 29.2 CAO
+ 2.61 MGO + 1.61 FE2O3 - 17.1 AL2O3 - 6.34 ZRO2 + 58.5 SIXCA
- 70.2 BXAL + 83.1 ALXAL

Predictor	Coef	Stdev	t-ratio	p
Constant	4.516	1.147	3.94	0.000
SIO2	-5.635	1.399	-4.03	0.000
B2O3	10.915	1.511	7.22	0.000
NA2O	6.183	1.317	4.70	0.000
LI2O	8.607	1.832	4.70	0.000
CAO	-29.239	8.081	-3.62	0.000
MGO	2.613	1.624	1.61	0.110
FE2O3	1.607	1.251	1.28	0.201
AL2O3	-17.063	2.575	-6.63	0.000
ZRO2	-6.335	1.328	-4.77	0.000
SIXCA	58.53	15.84	3.69	0.000
BXAL	-70.21	12.27	-5.72	0.000
ALXAL	83.08	12.39	6.70	0.000

s = 0.3296 R-sq = 79.4% R-sq(adj) = 77.4%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	12	52.0160	4.3347	39.90	0.000
Error	124	13.4699	0.1086		
Total	136	65.4859			

SOURCE	DF	SEQ SS
SIO2	1	6.5411
B2O3	1	1.4246
NA2O	1	4.2441
LI2O	1	0.9481
CAO	1	0.0355
MGO	1	0.8685
FE2O3	1	18.2358
AL2O3	1	10.5979
ZRO2	1	1.2884
SIXCA	1	1.0404
BXAL	1	1.9092
ALXAL	1	4.8823

Unusual Observations

Obs.	SIO2	LNMCC	Fit	Stdev.Fit	Residual	St.Resid

5	0.570	2.3974	2.1742	0.1809	0.2232	0.81 X
9	0.420	4.7747	4.9073	0.1809	-0.1326	-0.48 X
24	0.481	1.6134	2.5817	0.0808	-0.9683	-3.03R
32	0.473	3.2229	2.5706	0.0883	0.6523	2.05R
48	0.570	3.8506	2.9229	0.1344	0.9276	3.08R
50	0.420	2.6748	3.3320	0.1349	-0.6571	-2.19R
78	0.323	2.2664	2.2374	0.2358	0.0290	0.13 X
92	0.455	3.9035	3.2408	0.1163	0.6627	2.15R
95	0.507	3.8114	3.1310	0.1004	0.6804	2.17R
107	0.440	5.3774	4.4987	0.1055	0.8787	2.81R
108	0.440	4.4707	3.6550	0.0966	0.8158	2.59R
115	0.489	4.5082	3.7265	0.0687	0.7817	2.42R
126	0.482	4.5876	3.7990	0.0740	0.7886	2.46R

R denotes an obs. with a large st. resid.
X denotes an obs. whose X value gives it large influence.

LNMCC = 6.08 - 7.30 SIO2 + 9.20 B2O3 + 4.58 NA2O + 6.89 LI2O - 32.4 CAO
- 18.4 AL2O3 - 7.61 ZRO2 + 61.8 SIXCA - 68.2 BXAL + 82.2 ALXAL

Predictor	Coef	Stdev	t-ratio	p
Constant	6.0779	0.7096	8.57	0.000
SIO2	-7.301	1.034	-7.06	0.000
B2O3	9.199	1.151	7.99	0.000
NA2O	4.5813	0.9442	4.85	0.000
LI2O	6.885	1.544	4.46	0.000
CAO	-32.432	7.882	-4.11	0.000
AL2O3	-18.397	2.296	-8.01	0.000
ZRO2	-7.605	1.022	-7.44	0.000
SIXCA	61.82	15.74	3.93	0.000
BXAL	-68.22	12.26	-5.56	0.000
ALXAL	82.20	12.11	6.79	0.000

s = 0.3310 R-sq = 78.9% R-sq(adj) = 77.2%

Analysis of Variance

SOURCE	DF	SS	MS	F	p
Regression	10	51.6782	5.1678	47.16	0.000
Error	126	13.8077	0.1096		
Total	136	65.4859			

SOURCE	DF	SEQ SS
SIO2	1	6.5411
B2O3	1	1.4246
NA2O	1	4.2441
LI2O	1	0.9481
CAO	1	0.0355
AL2O3	1	26.6474
ZRO2	1	3.9559
SIXCA	1	1.0460
BXAL	1	1.7834
ALXAL	1	5.0521

Unusual Observations

Obs.	SIO2	LNMCC	Fit	Stdev.Fit	Residual	St.Resid
5	0.570	2.3974	2.1784	0.1816	0.2191	0.79 X
9	0.420	4.7747	4.8063	0.1698	-0.0316	-0.11 X
24	0.481	1.6134	2.6414	0.0713	-1.0280	-3.18R
48	0.570	3.8506	2.8912	0.1327	0.9593	3.16R
50	0.420	2.6748	3.3607	0.1146	-0.6859	-2.21R
78	0.323	2.2664	2.2012	0.2357	0.0652	0.28 X

82	0.460	2.4110	2.5319	0.1700	-0.1209	-0.43 X
95	0.507	3.8114	3.0663	0.0923	0.7451	2.34R
107	0.440	5.3774	4.5564	0.0997	0.8209	2.60R
108	0.440	4.4707	3.6223	0.0952	0.8485	2.68R
115	0.489	4.5082	3.6886	0.0639	0.8197	2.52R
126	0.482	4.5876	3.8119	0.0740	0.7757	2.40R

R denotes an obs. with a large st. resid.
X denotes an obs. whose X value gives it large influence.

APPENDIX I--R2 Calculations for Validation

This Appendix displays the R^2 calculations made on the validation sets for viscosity, PCT B, and MCC-1 B. Each table has calculations for the PNL 1st order model for that property (PNLL), PNL 2nd order model for that property (PNLN), Revised PNL 1st order model for that property (RevL), and Revised 2nd order model for that property (RevN).

1. R^2 Calculations for Viscosity Model Validation

Glass #	LNVISC	PNLL	PNLN	RevL	RevN
1	1.8245	1.8769	1.8646	1.9392	1.8601
2	1.8245	1.8969	1.9724	1.8915	1.9730
3	1.7066	1.7990	1.6995	1.7923	1.7006
4	1.4884	1.6604	1.6206	1.6627	1.6201
5	1.8050	1.8768	1.8938	1.8602	1.8969
6	1.7967	1.9314	1.8793	1.9898	1.8731
7	1.5476	1.5927	1.6879	1.5918	1.6891
8	1.8931	1.9272	1.7564	1.9511	1.7574
9	1.3712	1.5686	1.3218	1.5986	1.3219
10	1.8656	2.0159	1.8528	1.9929	1.8527
11	1.7422	1.9151	1.7226	1.9451	1.7205
12	1.9559	1.9998	1.8268	1.9554	1.8291
13	2.2214	2.0905	2.4672	2.0080	2.4726
14	1.8342	1.9998	1.8268	1.9554	1.8291
15	1.8116	1.9998	1.8268	1.9554	1.8291
16	1.9081	1.9998	1.8268	1.9554	1.8291
17	0.6152	0.6998	0.5525	0.8141	0.5384
18	0.1398	0.0102	0.0662	-0.0369	0.0714
19	0.9594	0.7235	1.1937	0.6263	1.1976
20	2.5572	2.3626	2.6339	2.2759	2.6366
21	2.2976	2.3617	2.2872	2.2955	2.2887
22	0.8671	0.9192	1.0292	0.9574	1.0163
23	2.1849	2.0868	2.1716	2.0178	2.1733
24	2.1041	2.0919	2.1031	2.0197	2.1104
25	2.1090	2.1083	2.0420	2.0579	2.0426
26	2.1939	2.1314	1.9988	2.0665	2.0009
27	2.8362	2.1263	2.2063	2.0695	2.2109
28	3.0978	2.1130	2.3847	2.0767	2.3873
29	2.3795	2.1334	2.1987	2.0761	2.2026
30	2.1401	2.0868	2.1716	2.0178	2.1733
31	2.0554	2.1083	2.0420	2.0579	2.0426
32	2.1599	2.1263	2.2063	2.0695	2.2109
33	2.2565	2.1130	2.3847	2.0767	2.3873
34	2.1587	2.1334	2.1987	2.0761	2.2026
35	0.1655	-0.0838	0.1509	-0.1509	0.1498
36	0.4383	0.2564	0.8946	0.2525	0.8919
37	3.3365	3.0201	3.1923	3.0056	3.1873
38	4.0476	3.0371	3.5622	3.0015	3.5672
39	4.1934	3.0269	3.4522	3.0275	3.4445
40	-0.3711	-0.6862	-0.2670	-0.6520	-0.2633

41	0.4574	0.1243	0.5117	0.0925	0.5207
42	-0.3011	-0.6962	-0.2265	-0.7010	-0.2250
43	0.1740	0.0801	0.5597	0.0105	0.5568
44	1.3913	0.9701	1.6230	0.9672	1.6200
45	3.3908	3.0452	3.1055	3.0390	3.1004
46	2.8893	2.7995	2.8371	2.7481	2.8314
47	1.2726	1.2298	1.5015	1.2048	1.5005
48	1.0225	1.3090	1.4465	1.2747	1.4383
49	1.2947	1.1541	1.3225	1.0550	1.3294
50	2.6610	2.5481	2.3643	2.5821	2.3719
51	0.0000	-0.0141	0.0349	0.0509	0.0337
52	-0.4463	-0.6205	-0.2739	-0.6402	-0.2747
53	-0.2107	-0.3280	-0.3674	-0.3654	-0.3664
54	0.4700	0.6614	0.5746	0.6139	0.5757
55	1.7138	1.9151	1.7226	1.9451	1.7205
56	1.9810	1.9998	1.8268	1.9554	1.8291
57	0.6419	0.7239	0.6919	0.6550	0.6878
58	2.1436	2.3214	2.2417	2.2776	2.2413
59	1.9242	2.1005	2.2296	2.0441	2.2288
60	0.4121	0.6614	0.5746	0.6139	0.5757

SST	56.2165	50.6991	55.6690	50.7187
SSE	5.5820	3.1429	6.1650	3.1279
R2	0.900706	0.938008	0.889256	0.938328

2. R^2 Calculations for PCT Model Validation

Glass #	LNPCT	PNLL	PNLN	RevL	RevN
1	-0.58519	3.553373	2.858979	2.729748	3.040806
2	-0.58519	0.10606	-0.32572	0.678327	-0.15952
3	-1.19073	-0.23459	-0.421	-0.43006	-0.36267
4	1.015593	0.791013	0.742093	1.096156	0.785122
5	0.294161	0.791013	0.742093	1.096156	0.785122
6	0.349952	0.791013	0.742093	1.096156	0.785122
7	0.151862	0.791013	0.742093	1.096156	0.785122
8	-0.25103	-0.6668	-0.78025	-1.41937	-0.71299
9	0.464363	0.124757	0.057796	0.178435	0.120343
10	0.484892	0.612487	0.457644	0.997168	0.458513
11	-1.50508	-2.31426	-1.21571	-1.85207	-1.03939
12	0.001998	0.125298	-0.79034	0.489773	-0.70152
13	-1.10262	-2.11743	-1.82163	-2.53514	-1.28016
14	-0.97022	0.121344	-0.16634	0.601643	-0.04706
15	-1.09362	0.211779	0.025208	0.583327	0.089778
16	-1.56065	-1.08761	-0.90548	-0.79553	-0.8448
17	-0.66943	-2.54995	0.26867	-2.26256	0.496132
18	-1.17766	-1.99837	-0.75933	-1.68497	-0.58848
19	-1.48722	-0.75576	-1.08487	-0.44785	-0.97677
20	-1.16475	-2.36896	-0.50864	-2.06969	-0.30353
21	-0.88916	0.121344	-0.16634	0.601643	-0.04706
22	-1.56065	-1.08761	-0.90548	-0.79553	-0.8448
23	-1.41059	-1.99837	-0.75933	-1.68497	-0.58848
24	-1.48722	-0.75576	-1.08487	-0.44785	-0.97677
25	-1.28013	-2.36896	-0.50864	-2.06969	-0.30353
26	2.699413	1.817917	1.566234	2.051004	1.616159
27	2.252554	1.871621	2.172152	1.757635	2.181156
28	-0.06828	0.357775	0.343484	0.564456	0.367302
29	-0.29571	0.284423	0.241745	0.702237	0.322299
30	-0.26919	0.078427	-0.02391	0.210267	-0.01254
31	2.810186	2.853867	2.921952	2.544252	2.918684
32	3.78419	3.018336	3.182684	3.01914	3.156592
33	3.545471	2.700569	2.477654	2.547694	2.575284
34	2.522524	1.776451	1.976492	2.010955	1.958506
35	-0.78526	-1.10111	0.485336	-1.2205	0.603899
36	-2.16282	-2.75812	-1.47627	-2.70754	-1.30222
37	-1.72597	-0.97061	-1.04023	-0.69867	-1.04566
38	-1.17766	-1.23968	-1.27625	-1.2091	-1.27391
39	0.539996	1.093721	0.82256	1.215031	0.872553
40	1.718651	1.247376	1.030628	1.809233	1.098329
41	2.156634	1.584721	1.799393	1.497755	1.808687
42	2.922624	2.424814	2.385601	1.954335	2.3866
43	2.58226	2.571583	2.857681	2.579681	2.869222
44	1.403643	1.664245	0.996553	1.635113	1.064954
45	2.300182	1.823981	1.70746	1.999649	1.68218
46	-0.70725	-0.16593	-0.54472	-0.31266	-0.56665
47	0.360468	0.791013	0.742093	1.096156	0.785122
48	1.508512	0.448495	1.587855	0.623683	1.501371

49	-1.46102	-0.19054	-0.43047	0.155904	-0.40014
50	-1.12086	-0.15507	-0.35004	0.294702	-0.23948
51	2.156865	1.823981	1.70746	1.999649	1.68218
52	0.982827	0.803986	0.752497	1.113926	0.796856
53	1.803853	1.86811	2.030627	1.782078	2.002916
54	1.713438	1.529365	1.634274	1.570294	1.627962
55	1.52388	1.188423	1.22466	1.35549	1.239997
56	0.501381	0.508852	0.381959	0.927934	0.448902
57	-0.23826	0.221528	0.097031	0.606057	0.171816
58	0.762673	1.273614	1.287463	1.523383	1.305321
59	1.741693	1.801878	1.897352	1.98443	1.886033
60	-1.15836	-0.20234	-0.41191	0.220947	-0.32131
61	1.81401	1.40816	1.459775	1.649476	1.473706
62	2.667228	2.213225	2.4113	2.363764	2.385603
63	-0.49102	0.294194	0.218551	0.668982	0.260048
64	1.962346	1.21886	1.186767	1.476375	1.233498
65	2.241348	1.404839	1.38238	1.639063	1.430876
66	1.102604	0.67796	0.591168	0.927921	0.630582
67	0.463734	0.73038	0.637775	1.135093	0.690775
68	1.289233	0.907873	0.898378	1.086619	0.930989
69	1.33579	1.45441	1.722831	1.782714	1.799896
70	-1.23443	0.048513	-0.17926	0.336773	-0.15641
71	-1.61445	-1.35944	-1.35474	-1.11001	-1.31914
72	-1.64507	-2.76489	-1.79811	-2.5549	-1.68399
73	0.387301	0.791013	0.742093	1.096156	0.785122
74	1.716856	2.206408	2.417074	1.994032	2.36917

SST	159.8244	113.8844	148.2088	106.3678
SSE	51.7474739	36.50055046	58.79853	40.74295
R2	0.676223	0.679495	0.603272	0.616962

3. R^2 Calculations for MCC Model Validation

Glass #	LNMCC	PNLL	PNLN	RevL	RevN
1	2.846652	2.809514	2.912986	2.778885	3.074898
2	2.726545	2.809514	2.912986	2.778885	3.074898
3	2.576422	2.755997	2.799758	2.833037	2.72724
4	2.482821	3.093292	2.914329	3.161294	2.838604
5	2.804572	2.712111	2.652787	2.740234	2.762632
6	2.388304	1.493969	2.212096	1.52354	2.573857
7	2.51689	3.055544	3.100573	3.016255	3.170113
8	2.26644	3.008643	2.825114	3.114345	3.102681
9	2.510818	2.310789	2.235019	2.273795	2.437945
10	2.241241	2.417167	2.414775	2.446213	2.595097
11	2.463428	2.07429	2.180998	2.069729	2.312509
12	2.410991	1.706027	2.771732	1.758863	3.314673
13	2.357073	1.657402	2.189889	1.661818	2.583843
14	2.290513	1.864347	1.872506	1.797061	2.1201
15	2.447551	1.610329	2.382081	1.634838	2.823485
16	2.484907	2.310789	2.235019	2.273795	2.437945
17	2.463428	2.07429	2.180998	2.069729	2.312509
18	1.893865	1.657402	2.189889	1.661818	2.583843
19	2.290513	1.864347	1.872506	1.797061	2.1201
20	2.154085	1.610329	2.382081	1.634838	2.823485
21	3.278276	3.636682	3.601676	3.673037	3.491442
22	3.903487	2.897615	2.903366	2.926518	2.929044
23	3.470412	2.803939	3.04916	2.766103	3.292783
24	3.470412	2.684474	3.037393	2.594314	3.328909
25	3.811429	2.881871	3.067325	2.880697	3.093317
26	4.67451	3.618621	3.744786	3.645962	3.628267
27	3.61604	3.535347	3.746161	3.515289	3.89199
28	3.401531	3.391185	3.297936	3.477328	3.102894
29	2.91723	1.981568	2.954418	2.037258	3.179799
30	2.116858	1.628928	2.463546	1.633315	2.740723
31	2.245486	2.222148	2.06979	2.244403	2.063925
32	2.209373	2.294976	2.141818	2.366759	1.959034
33	3.649099	3.613027	3.551663	3.665379	3.373178
34	3.372112	3.21026	3.522556	3.195279	3.747993
35	3.788951	2.881187	3.312846	2.77171	3.797819
36	4.459161	3.323589	3.716342	3.33027	3.795854
37	5.37736	3.656802	3.980748	3.670428	3.951353
38	4.470724	3.680421	3.505406	3.732712	3.401846
39	3.89508	3.467627	3.494135	3.485621	3.470468
40	2.528126	2.716282	2.553134	2.72501	2.435863
41	2.556452	2.809514	2.912986	2.778885	3.074898
42	3.415758	3.000118	3.075248	3.069878	3.093569
43	2.634762	2.545066	2.450034	2.522511	2.455031
44	2.647946	2.421669	2.389195	2.400824	2.437734
45	4.508219	3.467627	3.494135	3.485621	3.470468
46	2.956887	2.80959	2.919739	2.777448	3.091913
47	3.968573	3.485655	3.609299	3.526186	3.437145
48	3.432922	3.270103	3.392707	3.287464	3.328356

49	3.120998	3.054507	3.172463	3.048728	3.217038
50	2.593013	2.622011	2.723067	2.569708	2.994099
51	2.528924	2.422555	2.364802	2.376042	2.561863
52	3.123334	3.122192	3.374339	3.10166	3.52583
53	4.509056	3.471687	3.890865	3.464091	4.019948
54	2.315304	2.371342	2.485202	2.309087	2.734547
55	3.257019	3.073945	3.182674	3.059875	3.307191
56	4.587607	3.423429	3.530194	3.433358	3.592004
57	2.546864	2.623974	2.713169	2.567605	2.934038
58	3.012147	2.960298	3.086819	2.947994	3.218857
59	3.381131	3.027645	3.162223	3.024138	3.276829
60	2.984064	2.864317	2.968311	2.835308	3.077813
61	2.994882	2.779236	2.884891	2.745585	3.071057
62	3.014848	2.853312	2.970008	2.823356	3.122203
63	4.037298	3.040782	3.427157	2.999544	3.736486
64	2.602838	2.54173	2.457973	2.520176	2.516966
65	2.313525	2.041937	1.961748	2.040147	1.945244
66	2.230229	1.542637	1.940557	1.560508	2.023198
67	2.750343	2.809514	2.912986	2.778885	3.074898
SST	24.63421	19.89193	25.17666	17.70036	
SSE	22.03451	12.76023	22.32954	15.24397	
R2	0.105532	0.358522	0.113086	0.138776	

APPENDIX J--Classification of Waste Glasses

Table 1 displays the set of 113 glasses to be classified as glass/non-glass by each statistical model. Tables 2-6 show the actual classifications. In each table, there are four columns that determine if one of the four properties is violated for a property given that the property value is physically MEASURED. Then a fifth column displays the overall classification of the waste form. Five more columns are then dedicated to determining if the particular statistical model classifies the waste form as a glass/non-glass. The last column of Tables 2-6 determines if there is a difference between the actual measurement and the model's prediction.

1. Set of Glasses To Be Classified

Glass #	SIO2	B2O3	NA2O	LI2O	CAO	MGO	FE2O3	AL2O3	ZRO2	OTHERS
1	0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407
2	0.55	0.05	0.05	0.07	0.1	0	0.02	0.15	0	0.01
3	0.42	0.2	0.05	0.07	0	0.08	0.02	0.14	0.01	0.01
4	0.57	0.05	0.07	0.07	0	0	0.15	0.08	0	0.01
5	0.57	0.05	0.0964	0.01	0.1	0	0.0336	0	0.13	0.01
6	0.5363	0.05	0.0837	0.01	0	0.08	0.15	0	0.08	0.01
7	0.57	0.0851	0.0949	0.01	0	0	0.02	0.12	0	0.1
8	0.42	0.1549	0.0751	0.01	0.1	0	0.02	0.14	0	0.08
9	0.42	0.1764	0.0736	0.07	0.1	0	0.15	0	0	0.01
10	0.42	0.2	0.1862	0.01	0	0	0.02	0.0238	0.13	0.01
11	0.4327	0.05	0.1873	0.01	0	0.08	0.0858	0.1442	0	0.01
12	0.4545	0.05	0.1455	0.01	0.1	0	0.14	0	0	0.1
13	0.4214	0.05	0.1186	0.07	0.02	0.08	0.02	0	0.13	0.09
14	0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407
15	0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407
16	0.5363	0.05	0.0837	0.01	0	0.08	0.15	0	0.08	0.01
17	0.5153	0.0956	0.1052	0.0375	0.0289	0.0084	0.1179	0.0456	0.0063	0.0393
18	0.5226	0.0874	0.07	0.06	0	0.05	0.04	0.08	0.01	0.08
19	0.5017	0.07	0.0883	0.06	0.07	0	0.045	0.11	0.03	0.025
20	0.4645	0.132	0.07	0.0435	0.07	0.01	0.045	0.1032	0.0368	0.025
21	0.56	0.1095	0.07	0.0536	0.07	0	0.04	0.0619	0.01	0.025
22	0.4751	0.159	0.101	0.02	0.0348	0	0.04	0.08	0.01	0.08
23	0.5373	0.07	0.07	0.0382	0.07	0.0046	0.12	0.0159	0.01	0.0641
24	0.4814	0.17	0.07	0.0591	0.0094	0	0.04	0.0953	0.01	0.0648
25	0.5115	0.07	0.0985	0.06	0	0.05	0.114	0.061	0.01	0.025
26	0.5431	0.0944	0.0924	0.06	0	0	0.0712	0.0138	0.1	0.025
27	0.4694	0.17	0.1306	0.02	0	0	0.0669	0.1043	0.01	0.0288
28	0.4915	0.0751	0.0833	0.06	0.07	0.01	0.04	0.01	0.0935	0.0665
29	0.4683	0.17	0.07	0.0466	0.07	0.01	0.04	0.0901	0.01	0.025
30	0.4937	0.07	0.1692	0.0225	0.03	0.05	0.04	0.0896	0.01	0.025
31	0.46	0.1313	0.0802	0.0486	0.05	0.02	0.04	0.0243	0.1	0.0457
32	0.4729	0.07	0.17	0.0214	0.0601	0	0.04	0.0756	0.01	0.08
33	0.5353	0.1053	0.1125	0.0375	0.0083	0.0084	0.0719	0.0231	0.0385	0.0592
34	0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407
35	0.5353	0.1053	0.1125	0.0375	0.0083	0.0084	0.0719	0.0231	0.0385	0.0592

36	0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596
37	0.57	0.05	0.1031	0.0669	0	0	0.06	0.01	0.13	0.01
38	0.57	0.1314	0.05	0.07	0	0.08	0.02	0.0686	0	0.01
39	0.57	0.05	0.0735	0.07	0	0.08	0.02	0.0365	0	0.1
40	0.57	0.0522	0.2	0.01	0.08	0	0.02	0.0578	0	0.01
41	0.4464	0.2	0.0736	0.07	0	0	0.02	0.0961	0	0.0939
42	0.5059	0.05	0.0841	0.07	0.08	0	0.15	0.0033	0	0.0567
43	0.4431	0.2	0.0512	0.07	0.08	0	0.02	0.0257	0.1	0.01
44	0.5463	0.05	0.2	0.0155	0	0.08	0.02	0.0782	0	0.01
45	0.5619	0.05	0.2	0.0126	0	0	0.02	0.0555	0	0.1
46	0.4391	0.2	0.0675	0.01	0.08	0	0.02	0	0.0834	0.1
47	0.519	0.2	0.0832	0.01	0	0	0.132	0.0458	0	0.01
48	0.57	0.1843	0.05	0.0331	0.08	0	0.02	0.0526	0	0.01
49	0.5445	0.05	0.2	0.0428	0	0	0.02	0.0027	0.13	0.01
50	0.42	0.0544	0.2	0.0364	0	0.08	0.02	0.0892	0	0.1
51	0.42	0.1743	0.2	0.0369	0	0	0.02	0.1388	0	0.01
52	0.42	0.05	0.2	0.0428	0.08	0	0.0632	0.134	0	0.01
53	0.5421	0.05	0.0891	0.07	0.08	0	0.15	0.0088	0	0.01
54	0.57	0.0839	0.1061	0.07	0	0	0.02	0.14	0	0.01
55	0.5147	0.1109	0.1044	0.01	0	0.08	0.1428	0.0272	0	0.01
56	0.4838	0.05	0.1362	0.07	0	0.08	0.0742	0.0258	0.07	0.01
57	0.504	0.0639	0.15	0.0421	0.02	0.05	0.02	0.1	0.02	0.03
58	0.5325	0.0694	0.0781	0.07	0.05	0.02	0.03	0.1	0.02	0.03
59	0.5675	0.05	0.0625	0.07	0.032	0.038	0.1	0.03	0.02	0.03
60	0.507	0.1477	0.05	0.0653	0.02	0.03	0.03	0.05	0.07	0.03
61	0.57	0.1078	0.05	0.0699	0.05	0.02	0.02	0.0623	0.02	0.03
62	0.5299	0.1106	0.05	0.0595	0.02	0.05	0.0308	0.0592	0.02	0.07
63	0.5264	0.1259	0.0577	0.07	0.02	0.02	0.02	0.0746	0.02	0.0654
64	0.5294	0.05	0.1277	0.0429	0.05	0.02	0.02	0.04	0.05	0.07
65	0.47	0.1442	0.0968	0.039	0.05	0.02	0.02	0.0854	0.02	0.0546
66	0.5073	0.1357	0.0957	0.0413	0.02	0.02	0.0515	0.0785	0.02	0.03
67	0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407
68	0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596
69	0.6	0.0817	0.045	0.0788	0.0008	0.0009	0.072	0.0233	0.0385	0.059
70	0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596
71	0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596
72	0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596
73	0.39	0.2	0.05	0.07	0.02	0.08	0.02	0.15	0.01	0.01
74	0.438	0.1718	0.1268	0.0727	0.0375	0.0005	0.02	0.115	0.0075	0.0102
75	0.5281	0.0876	0.1725	0.0743	0.0063	0.0005	0.02	0.0925	0.0075	0.0107
76	0.5281	0.0664	0.12	0.073	0	0	0.02	0.1625	0.0175	0.0125
77	0.5579	0.1765	0.1125	0.0156	0.05	0.0005	0.02	0.05	0.0075	0.0095
78	0.3232	0.1717	0.19	0.0051	0.1	0	0.02	0.18	0	0.01
79	0.5697	0.0509	0.0925	0.0642	0.0025	0.0008	0.0812	0.0288	0.0431	0.0663
80	0.5344	0.1128	0.086	0.0697	0.0007	0.0004	0.0013	0.0196	0.1548	0.0203
81	0.5175	0.0917	0.1211	0.0523	0.0097	0.0061	0.0388	0.118	0.0026	0.0422
82	0.4596	0.1587	0.1086	0.0583	0.0024	0.0001	0.0004	0.2043	0	0.0076
83	0.504	0.1355	0.0797	0.0696	0.0007	0.0002	0.0046	0.164	0.0001	0.0416
84	0.566	0.0781	0.0664	0,0713	0.0079	0.0032	0.0334	0.0816	0.0005	0.0916
85	0.4854	0.1418	0.0812	0.0691	0.0008	0.0008	0.008	0.1819	0.0005	0.0305
86	0.5697	0.0509	0.0925	0.0642	0.0025	0.0008	0.0812	0.0288	0.0431	0.0663

87	0.5175	0.0917	0.1211	0.0523	0.0097	0.0061	0.0388	0.118	0.0026	0.0422
88	0.504	0.1355	0.0797	0.0696	0.0007	0.0002	0.0046	0.164	0.0001	0.0416
89	0.566	0.0781	0.0664	0.0713	0.0079	0.0032	0.0334	0.0816	0.0005	0.0916
90	0.4854	0.1418	0.0812	0.0691	0.0008	0.0008	0.008	0.1819	0.0005	0.0305
91	0.5018	0.06	0.18	0.0632	0.04	0.005	0.105	0.02	0.005	0.02
92	0.455	0.06	0.18	0.07	0.005	0.005	0.005	0.02	0.11	0.09
93	0.56	0.16	0.05	0.0254	0.005	0.04	0.0699	0.02	0.0497	0.02
94	0.5479	0.16	0.05	0.0121	0.005	0.005	0.105	0.02	0.005	0.09
95	0.5074	0.16	0.05	0.0176	0.005	0.04	0.105	0.02	0.075	0.02
96	0.49	0.0951	0.18	0.0699	0.04	0.005	0.005	0.02	0.005	0.09
97	0.455	0.06	0.18	0.07	0.005	0.005	0.105	0.02	0.08	0.02
98	0.44	0.06	0.18	0.07	0.005	0.02	0.005	0.17	0.005	0.045
99	0.4764	0.06	0.18	0.0136	0.04	0.005	0.005	0.17	0.005	0.045
100	0.4983	0.08	0.18	0.018	0.0137	0.005	0.025	0.0987	0.0613	0.02
101	0.4597	0.06	0.1403	0.07	0.04	0.005	0.025	0.105	0.075	0.02
102	0.44	0.1171	0.18	0.01	0.04	0.005	0.105	0.02	0.0629	0.02
103	0.56	0.16	0.0542	0.07	0.005	0.005	0.1008	0.02	0.005	0.02
104	0.56	0.16	0.105	0.01	0.005	0.04	0.005	0.02	0.005	0.09
105	0.44	0.16	0.1	0.07	0.005	0.04	0.005	0.02	0.07	0.09
106	0.44	0.1337	0.1279	0.07	0.0098	0.005	0.0986	0.02	0.005	0.09
107	0.44	0.16	0.18	0.0526	0.04	0.005	0.0271	0.0703	0.005	0.02
108	0.4895	0.1112	0.1671	0.0428	0.0113	0.0166	0.0897	0.0367	0.0041	0.031
109	0.4801	0.1142	0.1003	0.0376	0.0275	0.0363	0.0568	0.0636	0.0429	0.0407
110	0.5328	0.1048	0.1129	0.0373	0.0082	0.0084	0.0733	0.0235	0.0392	0.0596
111	0.42	0.1743	0.2	0.0369	0	0	0.02	0.1388	0	0.01
112	0.5203	0.0969	0.098	0.0356	0.0097	0.0077	0.1019	0.0523	0.0199	0.0577
113	0.5329	0.074	0.0626	0.0596	0.0035	0.0012	0.1229	0.0286	0.0443	0.0704

2. Classification Tables for PNL 1st Order Models

Glass #	ActViol VISC	Act Viol ELEC	Act Viol PCT	Act Viol MCC	PNL 1st Viol VISC	PNL 1st Viol ELEC	PNL 1st Viol PCT	PNL 1st Viol MCC	Act Glass	PRED GLASS	DIFFER
1	1	1	1	1	1	1	1	1	1	1	0
2	0	1	1	1	0	1	1	1	0	0	0
3	1	1	1	1	1	1	1	1	1	1	0
4	0	1	1	1	0	1	1	1	0	0	0
5	0	0	1	1	0	1	1	1	0	0	0
6	0	0	1	1	0	1	1	1	0	0	0
7	0	1	1	1	0	1	1	1	0	0	0
8	0	0	1	1	0	1	1	1	0	0	0
9	0	1	1	0	0	1	1	0	0	0	0
10	1	1	0	0	1	1	1	0	0	0	0
11	0	1	1	1	0	1	1	1	0	0	0
12	1	1	1	0	1	1	1	0	0	0	0
13	0	1	0	1	0	1	1	1	0	0	0
14	1	1	1	1	1	1	1	1	1	1	0
15	1	1	1	1	1	1	1	1	1	1	0
16	0	0	1	1	0	1	1	1	0	0	0
17	1	1	1	1	1	1	1	1	1	1	0
18	1	1	1	1	1	1	1	1	1	1	0
19	1	1	1	1	1	1	1	1	1	1	0
20	1	1	1	1	1	1	1	1	1	1	0
21	1	1	1	1	1	1	1	1	1	1	0
22	1	1	1	1	1	1	1	1	1	1	0
23	1	1	1	1	1	1	1	1	1	1	0
24	1	1	1	1	1	1	1	1	1	1	0
25	1	1	1	1	1	1	1	1	1	1	0
26	1	1	1	1	1	1	1	1	1	1	0
27	1	1	1	1	1	1	1	1	1	1	0
28	1	1	1	1	1	1	1	1	1	1	0
29	1	1	1	1	1	1	1	1	1	1	0
30	1	1	1	1	1	1	1	1	1	1	0
31	1	1	1	1	1	1	1	1	1	1	0
32	1	1	1	1	1	1	1	1	1	1	0
33	1	1	1	1	1	1	1	1	1	1	0
34	1	1	1	1	1	1	1	1	1	1	0
35	1	1	1	1	1	1	1	1	1	1	0
36	1	1	1	1	1	1	1	1	1	1	0
37	0	1	1	1	0	1	1	1	0	0	0
38	1	1	1	1	1	1	1	1	1	1	0
39	1	1	0	1	1	1	1	1	0	1	1
40	1	1	1	1	1	1	1	1	1	1	0
41	0	1	1	1	0	1	1	1	0	0	0
42	0	1	1	0	0	1	1	0	0	0	0
43	0	1	1	0	0	1	1	0	0	0	0
44	0	1	1	1	0	1	1	1	0	0	0
45	0	1	1	1	0	1	1	1	0	0	0
46	1	0	1	0	1	1	1	0	0	0	0

47	0	1	1	1	0	1	1	0	0	0	0
48	0	1	1	0	1	1	1	1	0	1	1
49	1	1	0	1	1	1	1	1	0	1	1
50	1	1	1	1	1	1	1	1	1	1	0
51	0	1	1	0	1	1	1	0	0	0	0
52	1	1	1	1	1	1	1	1	1	1	0
53	0	1	1	1	0	1	1	1	0	0	0
54	0	1	1	1	0	1	1	1	0	0	0
55	0	1	1	1	0	1	1	1	0	0	0
56	0	1	0	1	1	1	1	1	0	1	1
57	1	1	1	1	1	1	1	1	1	1	0
58	1	1	1	1	1	1	1	1	1	1	0
59	1	1	1	1	1	1	1	1	1	1	0
60	1	1	1	1	1	1	1	1	1	1	0
61	1	1	1	1	1	1	1	1	1	1	0
62	1	1	1	1	1	1	1	1	1	1	0
63	1	1	1	1	1	1	1	1	1	1	0
64	1	1	1	1	1	1	1	1	1	1	0
65	1	1	1	1	1	1	1	1	1	1	0
66	1	1	1	1	1	1	1	1	1	1	0
67	1	1	1	1	1	1	1	1	1	1	0
68	1	1	1	1	1	1	1	1	1	1	0
69	1	1	1	1	1	1	1	1	1	1	0
70	1	1	1	1	1	1	1	1	1	1	0
71	1	1	1	1	1	1	1	1	1	1	0
72	1	1	1	1	1	1	1	1	1	1	0
73	0	1	1	1	1	1	1	1	0	1	1
74	0	1	1	1	0	1	1	1	0	0	0
75	1	1	1	1	1	1	1	1	1	1	0
76	0	1	1	1	0	1	1	1	0	0	0
77	1	1	1	1	0	1	1	1	1	0	1
78	1	1	1	1	1	1	1	1	1	1	0
79	1	1	1	1	1	1	1	1	1	1	0
80	1	1	1	1	1	1	1	1	1	1	0
81	1	1	1	1	1	1	1	1	1	1	0
82	1	1	1	1	1	1	1	1	1	1	0
83	0	1	1	1	1	1	1	1	0	1	1
84	0	1	1	1	1	1	1	1	0	1	1
85	0	1	1	1	1	1	1	1	0	1	1
86	1	1	1	1	1	1	1	1	1	1	0
87	1	1	1	1	1	1	1	1	1	1	0
88	1	1	1	1	1	1	1	1	1	1	0
89	1	1	1	1	1	1	1	1	1	1	0
90	1	1	1	1	1	1	1	1	1	1	0
91	0	1	0	1	0	1	1	0	0	0	0
92	0	1	0	0	0	0	1	1	0	0	0
93	0	0	1	0	0	1	1	1	0	0	0
94	0	1	1	0	0	0	1	1	0	0	0
95	0	0	1	0	0	0	1	1	0	0	0
96	0	1	0	0	0	0	0	0	0	0	0
97	0	1	0	0	0	0	1	0	0	0	0

98	1	1	1	1	1	1	1	1	1	1	0
99	0	1	1	1	0	1	1	1	0	0	0
100	0	1	1	1	0	1	1	1	0	0	0
101	1	1	1	1	1	1	1	1	1	1	0
102	1	1	1	0	1	1	1	0	0	0	0
103	1	1	1	0	1	1	1	0	0	0	0
104	0	1	0	0	0	1	1	1	0	0	0
105	0	1	0	0	0	1	0	0	0	0	0
106	0	1	0	0	0	1	0	0	0	0	0
107	0	1	1	0	0	1	0	0	0	0	0
108	0	1	0	0	1	1	1	0	0	0	0
109	1	1	1	1	1	1	1	1	1	1	0
110	1	1	1	1	1	1	1	1	1	1	0
111	0	1	1	0	1	1	1	0	0	0	0
112	1	1	1	1	0	1	1	1	1	0	1
113	1	1	1	1	1	1	1	1	1	1	0

3. Classification Tables for PNL 2nd Order Models

Glass #	ActViol VISC	Act Viol ELEC	Act Viol PCT	Act Viol MCC	PNL 2nd Viol VISC	PNL 2nd Viol ELEC	PNL 2nd Viol PCT	PNL 2nd Viol MCC	Act Glass	PRED GLASS	DIFFER
1	1	1	1	1	1	1	1	1	1	1	0
2	0	1	1	1	0	1	1	1	0	0	0
3	1	1	1	1	1	1	1	1	1	1	0
4	0	1	1	1	0	1	1	1	0	0	0
5	0	0	1	1	0	0	1	1	0	0	0
6	0	0	1	1	0	0	1	1	0	0	0
7	0	1	1	1	0	1	1	1	0	0	0
8	0	0	1	1	0	0	1	1	0	0	0
9	0	1	1	0	0	1	1	0	0	0	0
10	1	1	0	0	1	1	0	0	0	0	0
11	0	1	1	1	0	1	1	1	0	0	0
12	1	1	1	0	1	1	1	0	0	0	0
13	0	1	0	1	0	1	1	0	0	0	0
14	1	1	1	1	1	1	1	1	1	1	0
15	1	1	1	1	1	1	1	1	1	1	0
16	0	0	1	1	0	0	1	1	0	0	0
17	1	1	1	1	1	1	1	1	1	1	0
18	1	1	1	1	1	1	1	1	1	1	0
19	1	1	1	1	1	1	1	1	1	1	0
20	1	1	1	1	1	1	1	1	1	1	0
21	1	1	1	1	1	1	1	1	1	1	0
22	1	1	1	1	1	1	1	1	1	1	0
23	1	1	1	1	1	1	1	1	1	1	0
24	1	1	1	1	1	1	1	1	1	1	0
25	1	1	1	1	1	1	1	1	1	1	0
26	1	1	1	1	1	1	1	1	1	1	0
27	1	1	1	1	1	1	1	1	1	1	0
28	1	1	1	1	1	1	1	1	1	1	0
29	1	1	1	1	1	1	1	1	1	1	0
30	1	1	1	1	1	1	1	1	1	1	0
31	1	1	1	1	1	1	1	1	1	1	0
32	1	1	1	1	1	1	1	1	1	1	0
33	1	1	1	1	1	1	1	1	1	1	0
34	1	1	1	1	1	1	1	1	1	1	0
35	1	1	1	1	1	1	1	1	1	1	0
36	1	1	1	1	1	1	1	1	1	1	0
37	0	1	1	1	0	1	1	1	0	0	0
38	1	1	1	1	1	1	1	1	1	1	0
39	1	1	0	1	1	1	1	1	0	1	1
40	1	1	1	1	0	1	1	1	1	0	1
41	0	1	1	1	0	1	1	1	0	0	0
42	0	1	1	0	0	1	1	0	0	0	0
43	0	1	1	0	0	1	1	0	0	0	0
44	0	1	1	1	0	1	1	1	0	0	0
45	0	1	1	1	0	1	1	1	0	0	0

46	1	0	1	0	1	0	1	0	0	0	0
47	0	1	1	1	0	1	1	0	0	0	0
48	0	1	1	0	0	1	1	1	0	0	0
49	1	1	0	1	1	1	1	1	0	1	1
50	1	1	1	1	1	1	1	1	1	1	0
51	0	1	1	0	0	1	1	1	0	0	0
52	1	1	1	1	1	1	1	1	1	1	0
53	0	1	1	1	0	1	1	0	0	0	0
54	0	1	1	1	0	1	1	1	0	0	0
55	0	1	1	1	0	1	1	0	0	0	0
56	0	1	0	1	0	1	1	1	0	0	0
57	1	1	1	1	1	1	1	1	1	1	0
58	1	1	1	1	1	1	1	1	1	1	0
59	1	1	1	1	1	1	1	1	1	1	0
60	1	1	1	1	1	1	1	1	1	1	0
61	1	1	1	1	1	1	1	1	1	1	0
62	1	1	1	1	1	1	1	1	1	1	0
63	1	1	1	1	1	1	1	1	1	1	0
64	1	1	1	1	1	1	1	1	1	1	0
65	1	1	1	1	1	1	1	1	1	1	0
66	1	1	1	1	1	1	1	1	1	1	0
67	1	1	1	1	1	1	1	1	1	1	0
68	1	1	1	1	1	1	1	1	1	1	0
69	1	1	1	1	0	1	1	1	1	0	1
70	1	1	1	1	1	1	1	1	1	1	0
71	1	1	1	1	1	1	1	1	1	1	0
72	1	1	1	1	1	1	1	1	1	1	0
73	0	1	1	1	0	1	1	1	0	0	0
74	0	1	1	1	0	1	1	1	0	0	0
75	1	1	1	1	1	1	1	1	1	1	0
76	0	1	1	1	0	1	1	1	0	0	0
77	1	1	1	1	0	1	1	1	1	0	1
78	1	1	1	1	1	1	1	1	1	1	0
79	1	1	1	1	1	1	1	1	1	1	0
80	1	1	1	1	1	1	1	1	1	1	0
81	1	1	1	1	1	1	1	1	1	1	0
82	1	1	1	1	1	1	1	1	1	1	0
83	0	1	1	1	1	1	1	1	0	1	1
84	0	1	1	1	0	1	1	1	0	0	0
85	0	1	1	1	1	1	1	1	0	1	1
86	1	1	1	1	1	1	1	1	1	1	0
87	1	1	1	1	1	1	1	1	1	1	0
88	1	1	1	1	1	1	1	1	1	1	0
89	1	1	1	1	0	1	1	1	1	0	1
90	1	1	1	1	1	1	1	1	1	1	0
91	0	1	0	1	0	1	1	0	0	0	0
92	0	1	0	0	1	1	1	1	0	1	1
93	0	0	1	0	0	1	1	1	0	0	0
94	0	1	1	0	0	0	1	1	0	0	0
95	0	0	1	0	0	0	1	1	0	0	0
96	0	1	0	0	0	1	0	0	0	0	0

97	0	1	0	0	0	1	1	0	0	0	0
98	1	1	1	1	1	1	1	1	1	1	0
99	0	1	1	1	0	1	1	1	0	0	0
100	0	1	1	1	0	1	1	1	0	0	0
101	1	1	1	1	1	1	1	1	1	1	0
102	1	1	1	0	1	1	1	0	0	0	0
103	1	1	1	0	1	1	1	0	0	0	0
104	0	1	0	0	0	1	1	0	0	0	0
105	0	1	0	0	0	1	0	0	0	0	0
106	0	1	0	0	0	1	0	0	0	0	0
107	0	1	1	0	0	1	1	0	0	0	0
108	0	1	0	0	0	1	1	0	0	0	0
109	1	1	1	1	1	1	1	1	1	1	0
110	1	1	1	1	1	1	1	1	1	1	0
111	0	1	1	0	0	1	1	1	0	0	0
112	1	1	1	1	1	1	1	1	1	1	0
113	1	1	1	1	1	1	1	1	1	1	0

4. Classification Tables for Revised 1st Order Models

Glass #	Act VISC	Act ELEC	Act PCT	Act MCC	R 1st VISC	R 1st ELEC	R 1st PCT	R 1st MCC	Act Glass	PRED GLASS	DIFFER
1	1	1	1	1	1	1	1	1	1	1	0
2	0	1	1	1	0	1	1	1	0	0	0
3	1	1	1	1	1	1	1	1	1	1	0
4	0	1	1	1	0	1	1	1	0	0	0
5	0	0	1	1	0	1	1	1	0	0	0
6	0	0	1	1	0	1	1	1	0	0	0
7	0	1	1	1	0	1	1	1	0	0	0
8	0	0	1	1	0	1	1	1	0	0	0
9	0	1	1	0	0	1	1	0	0	0	0
10	1	1	0	0	1	1	0	0	0	0	0
11	0	1	1	1	0	1	1	1	0	0	0
12	1	1	1	0	1	1	1	0	0	0	0
13	0	1	0	1	0	1	1	1	0	0	0
14	1	1	1	1	1	1	1	1	1	1	0
15	1	1	1	1	1	1	1	1	1	1	0
16	0	0	1	1	0	1	1	1	0	0	0
17	1	1	1	1	1	1	1	1	1	1	0
18	1	1	1	1	1	1	1	1	1	1	0
19	1	1	1	1	1	1	1	1	1	1	0
20	1	1	1	1	1	1	1	1	1	1	0
21	1	1	1	1	1	1	1	1	1	1	0
22	1	1	1	1	1	1	1	1	1	1	0
23	1	1	1	1	1	1	1	1	1	1	0
24	1	1	1	1	1	1	1	1	1	1	0
25	1	1	1	1	1	1	1	1	1	1	0
26	1	1	1	1	1	1	1	1	1	1	0
27	1	1	1	1	1	1	1	1	1	1	0
28	1	1	1	1	1	1	1	1	1	1	0
29	1	1	1	1	1	1	1	1	1	1	0
30	1	1	1	1	1	1	1	1	1	1	0
31	1	1	1	1	1	1	1	1	1	1	0
32	1	1	1	1	1	1	1	1	1	1	0
33	1	1	1	1	1	1	1	1	1	1	0
34	1	1	1	1	1	1	1	1	1	1	0
35	1	1	1	1	1	1	1	1	1	1	0
36	1	1	1	1	1	1	1	1	1	1	0
37	0	1	1	1	0	1	1	1	0	0	0
38	1	1	1	1	1	1	1	1	1	1	0
39	1	1	0	1	1	1	1	1	0	1	1
40	1	1	1	1	1	1	1	1	1	1	0
41	0	1	1	1	0	1	1	0	0	0	0
42	0	1	1	0	0	1	1	0	0	0	0
43	0	1	1	0	0	1	1	0	0	0	0
44	0	1	1	1	0	1	1	1	0	0	0
45	0	1	1	1	0	1	1	1	0	0	0
46	1	0	1	0	1	1	1	0	0	0	0
47	0	1	1	1	0	1	1	1	0	0	0

48	0	1	1	0	1	1	1	1	0	1	1
49	1	1	0	1	1	1	1	1	0	1	1
50	1	1	1	1	1	1	1	1	1	1	0
51	0	1	1	0	1	1	1	1	0	1	1
52	1	1	1	1	1	1	1	1	1	1	0
53	0	1	1	1	0	1	1	1	0	0	0
54	0	1	1	1	0	1	1	1	0	0	0
55	0	1	1	1	0	1	1	1	0	0	0
56	0	1	0	1	1	1	1	1	0	1	1
57	1	1	1	1	1	1	1	1	1	1	0
58	1	1	1	1	1	1	1	1	1	1	0
59	1	1	1	1	1	1	1	1	1	1	0
60	1	1	1	1	1	1	1	1	1	1	0
61	1	1	1	1	1	1	1	1	1	1	0
62	1	1	1	1	1	1	1	1	1	1	0
63	1	1	1	1	1	1	1	1	1	1	0
64	1	1	1	1	1	1	1	1	1	1	0
65	1	1	1	1	1	1	1	1	1	1	0
66	1	1	1	1	1	1	1	1	1	1	0
67	1	1	1	1	1	1	1	1	1	1	0
68	1	1	1	1	1	1	1	1	1	1	0
69	1	1	1	1	1	1	1	1	1	1	0
70	1	1	1	1	1	1	1	1	1	1	0
71	1	1	1	1	1	1	1	1	1	1	0
72	1	1	1	1	1	1	1	1	1	1	0
73	0	1	1	1	1	1	1	1	0	1	1
74	0	1	1	1	0	1	1	1	0	0	0
75	1	1	1	1	1	1	1	1	1	1	0
76	0	1	1	1	0	1	1	1	0	0	0
77	1	1	1	1	0	1	1	1	1	0	1
78	1	1	1	1	1	1	1	1	1	1	0
79	1	1	1	1	1	1	1	1	1	1	0
80	1	1	1	1	1	1	1	1	1	1	0
81	1	1	1	1	1	1	1	1	1	1	0
82	1	1	1	1	1	1	1	1	1	1	0
83	0	1	1	1	1	1	1	1	0	1	1
84	0	1	1	1	1	1	1	1	0	1	1
85	0	1	1	1	1	1	1	1	0	1	1
86	1	1	1	1	1	1	1	1	1	1	0
87	1	1	1	1	1	1	1	1	1	1	0
88	1	1	1	1	1	1	1	1	1	1	0
89	1	1	1	1	1	1	1	1	1	1	0
90	1	1	1	1	1	1	1	1	1	1	0
91	0	1	0	1	0	1	0	0	0	0	0
92	0	1	0	0	0	1	1	0	0	0	0
93	0	0	1	0	0	1	1	1	0	0	0
94	0	1	1	0	0	0	1	1	0	0	0
95	0	0	1	0	0	0	1	1	0	0	0
96	0	1	0	0	0	0	0	0	0	0	0
97	0	1	0	0	0	0	1	0	0	0	0
98	1	1	1	1	1	1	1	1	1	1	0

99	0	1	1	1	0	1	1	1	0	0	0
100	0	1	1	1	0	1	1	1	0	0	0
101	1	1	1	1	1	1	1	1	1	1	0
102	1	1	1	0	1	1	1	0	0	0	0
103	1	1	1	0	1	1	1	0	0	0	0
104	0	1	0	0	0	1	1	1	0	0	0
105	0	1	0	0	0	1	0	0	0	0	0
106	0	1	0	0	0	1	0	0	0	0	0
107	0	1	1	0	0	1	0	0	0	0	0
108	0	1	0	0	1	1	1	0	0	0	0
109	1	1	1	1	1	1	1	1	1	1	0
110	1	1	1	1	1	1	1	1	1	1	0
111	0	1	1	0	1	1	1	1	0	1	1
112	1	1	1	1	0	1	1	1	1	0	1
113	1	1	1	1	1	1	1	1	1	1	0

5. Classification Tables for Combs 2nd Order Models

Glass #	Act VISC	Act ELEC	Act PCT	Act MCC	R 2nd VISC	R 2nd ELEC	R 2nd PCT	R 2nd MCC	Act Glass	PRED GLASS	DIFFER
1	1	1	1	1	1	1	1	1	1	1	0
2	0	1	1	1	0	1	1	1	0	0	0
3	1	1	1	1	1	1	1	1	1	1	0
4	0	1	1	1	0	1	1	1	0	0	0
5	0	0	1	1	0	0	1	1	0	0	0
6	0	0	1	1	0	0	1	1	0	0	0
7	0	1	1	1	0	1	1	1	0	0	0
8	0	0	1	1	0	0	1	1	0	0	0
9	0	1	1	0	0	1	0	0	0	0	0
10	1	1	0	0	1	1	0	0	0	0	0
11	0	1	1	1	0	1	1	1	0	0	0
12	1	1	1	0	1	1	1	0	0	0	0
13	0	1	0	1	0	1	1	0	0	0	0
14	1	1	1	1	1	1	1	1	1	1	0
15	1	1	1	1	1	1	1	1	1	1	0
16	0	0	1	1	0	0	1	1	0	0	0
17	1	1	1	1	1	1	1	1	1	1	0
18	1	1	1	1	1	1	1	1	1	1	0
19	1	1	1	1	1	1	1	1	1	1	0
20	1	1	1	1	1	1	1	1	1	1	0
21	1	1	1	1	1	1	1	1	1	1	0
22	1	1	1	1	1	1	1	1	1	1	0
23	1	1	1	1	1	1	1	1	1	1	0
24	1	1	1	1	1	1	1	1	1	1	0
25	1	1	1	1	1	1	1	1	1	1	0
26	1	1	1	1	1	1	1	1	1	1	0
27	1	1	1	1	1	1	1	1	1	1	0
28	1	1	1	1	1	1	1	1	1	1	0
29	1	1	1	1	1	1	1	1	1	1	0
30	1	1	1	1	1	1	1	1	1	1	0
31	1	1	1	1	1	1	1	1	1	1	0
32	1	1	1	1	1	1	1	1	1	1	0
33	1	1	1	1	1	1	1	1	1	1	0
34	1	1	1	1	1	1	1	1	1	1	0
35	1	1	1	1	1	1	1	1	1	1	0
36	1	1	1	1	1	1	1	1	1	1	0
37	0	1	1	1	0	1	1	1	0	0	0
38	1	1	1	1	1	1	1	1	1	1	0
39	1	1	0	1	1	1	1	1	0	1	1
40	1	1	1	1	0	1	1	1	1	0	1
41	0	1	1	1	0	1	1	1	0	0	0
42	0	1	1	0	0	1	1	0	0	0	0
43	0	1	1	0	0	1	1	0	0	0	0
44	0	1	1	1	0	1	1	1	0	0	0
45	0	1	1	1	0	1	1	1	0	0	0
46	1	0	1	0	1	0	1	0	0	0	0
47	0	1	1	1	0	1	1	1	0	0	0

48	0	1	1	0	1	1	1	1	0	1	1
49	1	1	0	1	1	1	1	1	0	1	1
50	1	1	1	1	1	1	1	0	1	0	1
51	0	1	1	0	0	1	1	1	0	0	0
52	1	1	1	1	1	1	1	1	1	1	0
53	0	1	1	1	0	1	1	0	0	0	0
54	0	1	1	1	0	1	1	1	0	0	0
55	0	1	1	1	0	1	1	1	0	0	0
56	0	1	0	1	0	1	1	1	0	0	0
57	1	1	1	1	1	1	1	1	1	1	0
58	1	1	1	1	1	1	1	1	1	1	0
59	1	1	1	1	1	1	1	1	1	1	0
60	1	1	1	1	1	1	1	1	1	1	0
61	1	1	1	1	1	1	1	1	1	1	0
62	1	1	1	1	1	1	1	1	1	1	0
63	1	1	1	1	1	1	1	1	1	1	0
64	1	1	1	1	1	1	1	1	1	1	0
65	1	1	1	1	1	1	1	1	1	1	0
66	1	1	1	1	1	1	1	1	1	1	0
67	1	1	1	1	1	1	1	1	1	1	0
68	1	1	1	1	1	1	1	1	1	1	0
69	1	1	1	1	0	1	1	1	1	0	1
70	1	1	1	1	1	1	1	1	1	1	0
71	1	1	1	1	1	1	1	1	1	1	0
72	1	1	1	1	1	1	1	1	1	1	0
73	0	1	1	1	0	1	1	1	0	0	0
74	0	1	1	1	0	1	1	1	0	0	0
75	1	1	1	1	1	1	1	1	1	1	0
76	0	1	1	1	0	1	1	1	0	0	0
77	1	1	1	1	1	1	1	1	1	1	0
78	1	1	1	1	1	1	1	1	1	1	0
79	1	1	1	1	1	1	1	1	1	1	0
80	1	1	1	1	1	1	1	1	1	1	0
81	1	1	1	1	1	1	1	1	1	1	0
82	1	1	1	1	1	1	1	1	1	1	0
83	0	1	1	1	1	1	1	1	0	1	1
84	0	1	1	1	0	1	1	1	0	0	0
85	0	1	1	1	1	1	1	1	0	1	1
86	1	1	1	1	1	1	1	1	1	1	0
87	1	1	1	1	1	1	1	1	1	1	0
88	1	1	1	1	1	1	1	1	1	1	0
89	1	1	1	1	0	1	1	1	1	0	1
90	1	1	1	1	1	1	1	1	1	1	0
91	0	1	0	1	0	1	1	0	0	0	0
92	0	1	0	0	1	1	1	0	0	0	0
93	0	0	1	0	0	0	1	1	0	0	0
94	0	1	1	0	0	0	1	1	0	0	0
95	0	0	1	0	0	0	1	1	0	0	0
96	0	1	0	0	0	1	0	0	0	0	0
97	0	1	0	0	0	1	0	0	0	0	0
98	1	1	1	1	1	1	1	1	1	1	0

99	0	1	1	1	0	1	1	1	0	0	0
100	0	1	1	1	0	1	1	1	0	0	0
101	1	1	1	1	1	1	1	1	1	1	0
102	1	1	1	0	1	1	1	0	0	0	0
103	1	1	1	0	1	1	1	0	0	0	0
104	0	1	0	0	0	1	1	0	0	0	0
105	0	1	0	0	0	1	0	0	0	0	0
106	0	1	0	0	0	1	0	0	0	0	0
107	0	1	1	0	0	1	1	0	0	0	0
108	0	1	0	0	0	1	1	0	0	0	0
109	1	1	1	1	1	1	1	1	1	1	0
110	1	1	1	1	1	1	1	1	1	1	0
111	0	1	1	0	0	1	1	1	0	0	0
112	1	1	1	1	1	1	1	1	1	1	0
113	1	1	1	1	1	1	1	1	1	1	0

6. Classification Tables for NN/Combs ELEC Models

Glass #	Act VISC	Act ELEC	Act PCT	Act MCC	NN VISC	R 2nd ELEC	NN PCT	NN MCC	Act Glass	PRED GLASS	DIFFER
1	1	1	1	1	1	1	1	1	1	1	0
2	0	1	1	1	0	1	1	1	0	0	0
3	1	1	1	1	1	1	1	1	1	1	0
4	0	1	1	1	0	1	1	1	0	0	0
5	0	0	1	1	0	0	1	1	0	0	0
6	0	0	1	1	0	0	1	1	0	0	0
7	0	1	1	1	0	1	1	1	0	0	0
8	0	0	1	1	0	0	1	1	0	0	0
9	0	1	1	0	0	1	1	0	0	0	0
10	1	1	0	0	1	1	1	0	0	0	0
11	0	1	1	1	0	1	1	1	0	0	0
12	1	1	1	0	1	1	1	0	0	0	0
13	0	1	0	1	0	1	0	1	0	0	0
14	1	1	1	1	1	1	1	1	1	1	0
15	1	1	1	1	1	1	1	1	1	1	0
16	0	0	1	1	0	0	1	1	0	0	0
17	1	1	1	1	1	1	1	1	1	1	0
18	1	1	1	1	1	1	1	1	1	1	0
19	1	1	1	1	1	1	1	1	1	1	0
20	1	1	1	1	1	1	1	1	1	1	0
21	1	1	1	1	1	1	1	1	1	1	0
22	1	1	1	1	1	1	1	1	1	1	0
23	1	1	1	1	1	1	1	1	1	1	0
24	1	1	1	1	1	1	1	1	1	1	0
25	1	1	1	1	1	1	1	1	1	1	0
26	1	1	1	1	1	1	1	1	1	1	0
27	1	1	1	1	1	1	1	1	1	1	0
28	1	1	1	1	1	1	1	1	1	1	0
29	1	1	1	1	1	1	1	1	1	1	0
30	1	1	1	1	1	1	1	1	1	1	0
31	1	1	1	1	1	1	1	1	1	1	0
32	1	1	1	1	1	1	1	1	1	1	0
33	1	1	1	1	1	1	1	1	1	1	0
34	1	1	1	1	1	1	1	1	1	1	0
35	1	1	1	1	1	1	1	1	1	1	0
36	1	1	1	1	1	1	1	1	1	1	0
37	0	1	1	1	0	1	1	1	0	0	0
38	1	1	1	1	1	1	1	1	1	1	0
39	1	1	0	1	1	1	1	1	0	1	1
40	1	1	1	1	1	1	1	1	1	1	0
41	0	1	1	1	0	1	1	1	0	0	0
42	0	1	1	0	0	1	1	0	0	0	0
43	0	1	1	0	0	1	1	0	0	0	0
44	0	1	1	1	0	1	1	1	0	0	0
45	0	1	1	1	0	1	1	1	0	0	0
46	1	0	1	0	1	0	1	0	0	0	0

47	0	1	1	1	0	1	1	1	0	0	0
48	0	1	1	0	0	1	1	0	0	0	0
49	1	1	0	1	1	1	1	1	0	1	1
50	1	1	1	1	1	1	1	1	1	1	0
51	0	1	1	0	0	1	1	0	0	0	0
52	1	1	1	1	1	1	1	1	1	1	0
53	0	1	1	1	0	1	1	1	0	0	0
54	0	1	1	1	0	1	1	1	0	0	0
55	0	1	1	1	0	1	1	1	0	0	0
56	0	1	0	1	0	1	0	1	0	0	0
57	1	1	1	1	1	1	1	1	1	1	0
58	1	1	1	1	1	1	1	1	1	1	0
59	1	1	1	1	1	1	1	1	1	1	0
60	1	1	1	1	1	1	1	1	1	1	0
61	1	1	1	1	1	1	1	1	1	1	0
62	1	1	1	1	1	1	1	1	1	1	0
63	1	1	1	1	1	1	1	1	1	1	0
64	1	1	1	1	1	1	1	1	1	1	0
65	1	1	1	1	1	1	1	1	1	1	0
66	1	1	1	1	1	1	1	1	1	1	0
67	1	1	1	1	1	1	1	1	1	1	0
68	1	1	1	1	1	1	1	1	1	1	0
69	1	1	1	1	1	1	1	1	1	1	0
70	1	1	1	1	1	1	1	1	1	1	0
71	1	1	1	1	1	1	1	1	1	1	0
72	1	1	1	1	1	1	1	1	1	1	0
73	0	1	1	1	0	1	1	1	0	0	0
74	0	1	1	1	0	1	1	1	0	0	0
75	1	1	1	1	1	1	1	1	1	1	0
76	0	1	1	1	0	1	1	1	0	0	0
77	1	1	1	1	1	1	1	1	1	1	0
78	1	1	1	1	1	1	1	1	1	1	0
79	1	1	1	1	1	1	1	1	1	1	0
80	1	1	1	1	1	1	1	1	1	1	0
81	1	1	1	1	1	1	1	1	1	1	0
82	1	1	1	1	1	1	1	1	1	1	0
83	0	1	1	1	0	1	1	1	0	0	0
84	0	1	1	1	0	1	1	1	0	0	0
85	0	1	1	1	0	1	1	1	0	0	0
86	1	1	1	1	1	1	1	1	1	1	0
87	1	1	1	1	1	1	1	1	1	1	0
88	1	1	1	1	0	1	1	1	1	0	1
89	1	1	1	1	0	1	1	1	1	0	1
90	1	1	1	1	0	1	1	1	1	0	1
91	0	1	0	1	0	1	0	1	0	0	0
92	0	1	0	0	0	1	1	0	0	0	0
93	0	0	1	0	0	0	1	0	0	0	0
94	0	1	1	0	0	0	1	0	0	0	0
95	0	0	1	0	0	0	1	0	0	0	0
96	0	1	0	0	0	1	0	0	0	0	0
97	0	1	0	0	0	1	0	0	0	0	0

98	1	1	1	1	1	1	1	1	1	1	0
99	0	1	1	1	0	1	1	1	0	0	0
100	0	1	1	1	0	1	1	1	0	0	0
101	1	1	1	1	1	1	1	1	1	1	0
102	1	1	1	0	1	1	1	0	0	0	0
103	1	1	1	0	1	1	1	0	0	0	0
104	0	1	0	0	0	1	0	0	0	0	0
105	0	1	0	0	0	1	0	0	0	0	0
106	0	1	0	0	0	1	0	0	0	0	0
107	0	1	1	0	0	1	1	0	0	0	0
108	0	1	0	0	0	1	0	0	0	0	0
109	1	1	1	1	1	1	1	1	1	1	0
110	1	1	1	1	1	1	1	1	1	1	0
111	0	1	1	0	0	1	1	0	0	0	0
112	1	1	1	1	0	1	1	1	1	0	1
113	1	1	1	1	1	1	1	1	1	1	0

APPENDIX K--Neural Network Hidden and Output Layer Weights

This Appendix displays the hidden layer weights and output layer weights for each neural network model. These weights are used to calculate predicted property values for the constraints of the neural network NLP.

A paragraph is included that describes how these weights are extracted from SNNAP.

1. Spreadsheet of NN Weights for Viscosity

a. Hidden Layer

Hidden Node	Input Node 1	2	3	4	5	6	7	8	9	10	bias
1	-0.0016	0.043045	-0.07237	-0.06956	-0.03889	0.030404	-0.01909	0.007561	0.068668	0.030328	-0.26663
2	-0.034	0.185582	-0.41124	0.464455	-0.13165	0.419068	0.423362	-0.04554	0.029228	-0.79274	-0.22928
3	0.050392	-0.01416	-0.02937	0.057311	-0.03105	0.006153	-0.13667	0.055368	0.012284	-0.08236	-0.18924
4	0.027706	-0.08797	-0.02184	0.120132	-0.02238	0.04681	-0.12831	0.1316	-0.13866	0.02519	-0.31243
5	-0.02983	-0.35556	0.797347	0.30638	0.20495	0.581285	-0.96557	-0.13487	0.099185	-0.16516	-0.69528
6	-0.13959	0.098758	0.151678	0.02082	0.001084	0.005641	-0.05719	-0.1534	0.03984	-0.01767	-0.16013
7	0.021367	-0.02965	-0.13161	0.010222	0.037423	0.049512	-0.12466	0.130443	-0.11252	0.084164	-0.31248
8	0.090443	-0.01378	-0.00735	0.017884	0.066279	0.073677	-0.12517	0.16247	-0.02325	-0.00858	-0.2116
9	0.052911	-0.00453	-0.02547	0.082929	0.147516	0.033317	-0.06658	0.149727	0.025005	-0.00026	-0.20033
10	1.110895	0.305538	-0.4173	-0.73715	-0.24323	-0.30954	-0.62565	0.309382	0.053292	-0.53592	0.275241
11	-0.18755	0.246714	0.114599	0.312339	0.138339	0.033843	0.013363	-0.22059	-0.02194	-0.27421	-0.08629
12	-0.06893	0.007477	0.357956	0.167644	0.043579	0.097786	0.086886	-0.26188	-0.02026	-0.00732	-0.12786
13	0.235217	0.960401	-0.07529	0.039553	0.746256	-0.43404	-1.12391	-0.04058	-0.17564	-0.4919	-0.0106
14	0.324482	0.072588	-0.59778	-1.19275	-0.1662	0.699244	0.727072	0.358233	0.229253	-1.03069	-2.29023
15	0.093547	0.036964	-0.16167	-0.22193	0.076424	-0.05275	-0.01958	0.050314	0.205831	-0.00351	-0.45024
16	-0.04678	-0.03821	0.212138	-0.13775	-0.12072	-0.07894	0.09795	-0.04962	0.106409	0.069939	-0.19416
17	0.280329	-0.0345	-0.14425	-0.18053	-0.05515	0.092795	-0.08784	0.173135	0.167816	-0.00947	-0.26275
18	0.167094	0.134257	-0.28045	-0.31169	-0.0184	-0.28619	-0.0406	0.324994	0.108651	-0.0981	-0.42304
19	-0.25825	-0.11715	-0.30094	-0.75792	-0.02834	-0.6451	0.164723	1.195709	0.095988	-0.18351	0.406891
20	0.326789	0.612589	-0.52154	-0.04206	0.01735	-0.09012	-0.39951	-0.33882	0.391356	-0.13149	-0.12911
21	0.508955	-0.65604	-0.06743	-0.4145	-0.01614	-0.04035	-0.24866	0.274802	0.109164	0.368612	-0.68448
22	0.083853	-0.11295	-1.24997	-1.40719	-0.40185	0.033724	-0.40759	1.304017	0.913646	0.931617	-1.91824
23	0.394276	-0.1932	-0.15666	-0.37022	-0.11966	-0.39508	-0.0373	0.333823	-0.13812	0.180211	-0.46206
24	0.037923	0.058738	0.052979	0.081378	0.101642	-0.07365	-0.07192	-0.04487	-0.00167	-0.05458	-0.14546
25	0.048681	-0.19928	-0.03044	-0.16863	0.024774	0.065576	0.004168	-0.05399	0.15672	-0.04255	-0.23109
26	0.128467	-0.16903	-0.17257	-0.05813	0.041316	-0.0131	-0.11383	0.110454	-0.08029	0.071728	-0.22593
27	0.009831	0.651083	0.623645	0.029401	-0.12586	0.809677	-1.12287	-0.69692	-0.10762	0.31028	-0.24675
28	0.150269	0.00478	-0.1114	-0.1856	0.023495	-0.15022	-0.00949	0.185916	0.05162	-0.05706	-0.34265
29	1.098796	-0.10059	-0.6674	-0.09446	-0.19825	0.242163	-0.03648	-0.6199	0.470757	-0.35986	-0.60837
30	0.177535	-0.20698	-0.21724	-0.20629	-0.14031	-0.01867	-0.08271	0.303998	-0.14056	0.128639	-0.28847
31	0.066641	0.036044	-0.11696	-0.03649	-0.04135	0.004828	-0.09266	-0.03382	-0.04908	-0.11663	-0.22107
32	-0.1156	0.127155	-0.00431	-0.01151	0.063265	-0.08223	-0.18546	-0.04116	-0.11424	-0.0366	-0.25382
33	0.012933	0.182962	-0.26089	-0.19094	0.12667	-0.15753	-0.01052	0.062477	0.058856	-0.06819	-0.4667
34	-0.04626	0.080859	-0.02623	0.028235	0.090417	0.089603	-0.00096	0.043387	-0.06874	0.000105	-0.13084
35	-0.02502	0.079702	0.138335	0.035672	-0.00163	0.073787	-0.03612	-0.15945	-0.0775	-0.09138	-0.22915

b. Output Layer--wt from hidden node I to output node

1	2	3	4	5	6	7	8	9	10
-0.03063	-0.65283	0.042615	0.15686	1.08501	-0.16989	0.13712	0.071737	0.076551	1.098515
			1	3					
11	12	13	14	15	16	17	18	19	20
-0.26494	-0.33456	-1.00748	1.53423	0.074969	-0.33317	0.110877	0.22384	1.050316	0.615628
21	22	23	24	25	26	27	28	29	30
0.484152	1.397268	0.365283	-0.03255	-0.12285	0.150066	-0.93194	0.035986	0.768905	0.267874
31	32	33	34	35	bias				
0.022862	-0.04966	0.193499	0.016658	-0.11815	-0.20744				

2. Spreadsheet of NN Weights for PCT

Hidden Node	Input Node 1	2	3	4	5	6	7	8	9	10	bias
1	0.035302	-0.15184	-0.22611	-0.27628	-0.12714	-0.02152	-0.12997	0.45578	-0.00961	-0.11777	0.007351
2	0.185074	0.213204	-0.07246	-0.15998	0.22961	-0.10181	0.009275	-0.0147	-0.04205	-0.29543	-0.24503
3	-0.01156	-0.08122	0.036804	0.139756	-0.10089	-0.07734	-0.07902	-0.06066	0.014429	0.128527	-0.2095
4	-0.01652	0.016856	-0.07898	-0.00092	-0.00895	0.051266	-0.03565	0.071754	0.093716	-0.01563	-0.26522
5	-0.38838	-0.00906	0.138566	0.188798	0.045422	-0.03549	0.013744	-0.11398	0.11692	0.218495	-0.16436
6	0.455706	0.142578	-0.33845	-0.27634	0.150203	-0.04739	-0.02806	0.325225	-0.13964	-0.60973	-0.10812
7	-0.20006	-0.3809	0.247764	0.174788	-0.085	0.160526	-0.05419	0.137381	0.116784	0.352565	-0.20213
8	-0.02604	0.193626	0.086715	-0.16679	0.210622	0.01078	-0.10012	-0.02205	-0.17843	-0.10994	-0.16186
9	0.126399	-0.07419	-0.01117	-0.08831	-0.03493	-0.09203	-0.04204	0.037317	0.067607	0.047325	-0.2558
10	-0.39067	1.58286	2.081791	0.494184	-0.95243	1.401137	-0.15688	-2.66637	-0.71743	0.141492	-0.17997
11	-0.03682	-0.01972	-0.01229	-0.04325	-0.00468	-0.02263	-0.08567	-0.04983	-0.0891	-0.0675	-0.19471
12	-0.03043	-0.0467	-0.02467	0.084022	0.032101	-0.12749	0.057278	0.035485	0.044829	0.0221	-0.27648
13	-0.04889	0.012453	0.115957	-0.21619	0.043805	0.070165	-0.03738	0.009229	-0.07779	-0.07332	-0.30041
14	-0.14707	0.104867	-0.00404	-0.06014	-0.00914	-0.19493	0.015586	0.078167	0.150939	0.174139	-0.15118
15	0.222465	-0.07017	-0.02643	-0.2109	-0.07703	0.066935	-0.14661	0.242116	-0.02992	-0.10156	-0.231
16	-0.5209	-1.16993	-1.32892	-0.51921	1.362588	0.774172	0.33924	0.656426	0.901507	0.531806	1.557255
17	-0.11509	0.104543	0.048724	0.073425	-0.03387	-0.18524	0.024581	-0.07975	0.081217	0.138019	-0.1456
18	0.155964	0.266138	-0.13145	-0.29238	0.175123	-0.23925	0.040557	-0.08926	-0.04716	-0.40348	-0.29222
19	0.131292	0.08447	0.009355	-0.09751	0.045043	0.085037	-0.02904	0.084724	0.047325	-0.18474	-0.27864
20	-0.12495	0.103669	0.192599	-0.10974	0.257203	0.085321	-0.1425	-0.1045	-0.16506	-0.10029	-0.22342
21	-0.81636	-0.28933	-0.62712	-0.01561	0.505243	-0.44245	-1.05143	2.079795	0.465518	-0.08106	0.958363
22	0.936408	-0.06297	-0.12987	0.131703	-0.31592	0.247248	-0.10305	0.050601	-0.26719	-1.05039	-0.37991
23	-0.05945	0.529423	0.655306	0.304478	-0.67413	-0.60356	-0.62756	0.629553	-0.3359	-0.74615	-0.06635
24	0.084112	-0.0296	-0.14753	-0.33246	0.051596	0.178757	-0.15928	0.104232	-0.008	-0.15601	-0.05426
25	-0.16803	0.421936	0.364225	0.214605	-0.12741	-0.10994	-0.15771	-0.10951	-0.00949	0.014454	-0.37287
26	-0.20082	0.17204	0.162475	0.037939	0.036038	-0.05799	0.017141	0.043275	0.106123	-0.01797	-0.2441
27	-0.04054	0.000613	0.03914	-0.0617	-0.11748	-0.04105	0.057714	0.108244	0.013049	0.012323	-0.25528
28	0.08091	-0.04686	-0.06595	-0.0474	-0.06491	0.071205	-0.04561	-0.00437	-0.08136	0.025056	-0.21274
29	-0.25077	0.017263	-0.03846	0.093846	0.001982	-0.26173	0.078651	0.129728	0.171293	0.17387	-0.1958
30	0.104699	0.055277	-0.08581	-0.27494	0.136598	0.081061	0.001672	0.0882	0.038754	-0.04502	-0.09041
31	0.032054	0.065166	-0.01443	-0.0781	0.194474	-0.02114	-0.03036	-0.0373	0.007734	-0.09295	-0.15412
32	-0.05684	-0.15814	-0.18026	-0.22855	0.131014	0.003588	-0.19628	0.695142	0.058675	-0.24638	0.117243
33	0.646236	0.172487	0.314346	0.783874	1.112659	1.262713	-0.66883	-2.2751	-0.01311	0.397517	-2.05428
34	-0.94359	0.754	0.024892	0.614339	0.750264	-0.1837	0.67007	-0.39755	-0.15696	-0.53072	-0.10549
35	-0.35321	0.776008	0.332089	0.243547	-0.37445	-0.04653	-0.17199	-0.26812	0.116695	-0.57231	-0.55291

b. Output Layer--wt from hidden node I to output node

1	2	3	4	5	6	7	8	9	10
0.146372	-0.26336	0.137265	0.077453	0.068985	-0.35836	0.37308	-0.27781	0.136515	1.685482
11	12	13	14	15	16	17	18	19	20
-0.03186	0.104607	-0.13241	0.141278	0.042165	-1.34952	0.082881	-0.3565	-0.05199	-0.34845
21	22	23	24	25	26	27	28	29	30
-1.3915	-0.87123	0.920359	-0.05917	-0.11745	-0.04791	0.111872	0.06028	0.213698	-0.03047
31	32	33	34	35	bias				
-0.12195	-0.00357	2.333948	0.863901	0.429925	0.09425				

3. Spreadsheet of NN Weights for MCC

Hidden Node	Input Node 1	2	3	4	5	6	7	8	9	10	bias
1	-0.25697	-0.08956	0.50101	-0.30732	0.153468	0.237438	-0.19955	0.071305	-0.20317	-0.02518	-0.56464
2	0.147596	0.047658	0.108092	-0.25436	0.228946	-0.13507	0.7216	-0.24854	-0.50097	-0.52867	-0.1713
3	-0.06815	0.284566	0.412812	0.289055	0.16876	-0.23177	-0.18427	-0.53201	-0.05272	0.095307	-0.75203
4	-0.20763	0.058358	0.386027	-0.08269	0.250971	0.035651	-0.03957	0.065552	0.066451	-0.1138	-0.61855
5	0.802981	2.180977	0.738231	-0.55415	0.343137	0.431733	0.074078	-2.33253	-1.41398	-0.33221	-2.97201
6	-0.06395	-0.16894	0.251068	0.338232	0.026701	0.090112	-0.1035	-0.07415	-0.10347	-0.11811	-0.6343
7	-0.02179	0.292996	0.411444	0.258044	0.304978	-0.22756	-0.28554	-0.5453	-0.03677	0.072808	-0.73128
8	-0.22396	0.070467	0.354832	-0.05887	-0.01576	0.047473	-0.10869	0.069424	-0.11475	-0.24615	-0.54103
9	-1.34574	-0.18224	0.511715	-0.6516	-0.26586	0.362178	0.747896	0.869781	-0.22571	0.16155	-1.00658
10	-0.12828	0.033463	0.285681	0.17272	0.037341	0.111977	0.121204	0.048697	-0.02007	-0.35536	-0.63995
11	0.118002	-0.10053	0.230612	0.053411	0.368573	-0.09516	0.140155	-0.22752	-0.02875	-0.14462	-0.44576
12	-0.06556	-0.02396	0.196156	-0.07569	0.274899	0.02826	-0.12383	-0.04951	-0.01558	-0.28564	-0.51198
13	-0.69895	0.017711	1.507572	-0.34447	0.265247	0.154931	-0.12182	-0.12386	-0.08297	-0.78512	-0.67531
14	-0.80136	-0.38599	1.178177	-0.25066	0.69594	-0.01656	-0.48013	-0.17228	0.37465	-0.05774	-0.51347
15	0.157878	-0.74523	0.779935	0.346521	0.274205	0.628914	-0.34176	-0.21389	-0.16506	-0.38748	-1.02949
16	-0.07218	0.461163	0.463209	-0.36176	-0.64486	0.163882	-0.17935	0.539141	-0.596	-0.16188	-0.80542
17	-0.07043	-0.10434	0.180405	-0.02353	0.276633	-0.04392	-0.08672	0.034002	-0.02271	-0.26989	-0.51558
18	-0.3708	0.193059	2.207142	0.443713	-0.82106	0.548607	-1.21511	-0.43992	-0.94725	0.398841	-2.25333
19	-0.16432	-0.09332	0.321368	0.186438	0.22568	-0.01443	-0.17149	-0.01491	0.079026	-0.02072	-0.58114
20	-0.06089	-0.24409	0.33094	-0.10608	0.448384	-0.05028	-0.08055	0.271527	0.002479	-0.43233	-0.34507
21	-0.15683	-0.05892	0.143746	0.011529	0.039094	-0.09506	0.062129	-0.21449	-0.02603	-0.1238	-0.62418
22	0.157281	-1.34722	1.454541	1.152132	0.227814	0.946377	-0.8153	-0.20275	-0.95988	0.288275	0.044773
23	-0.08141	-0.27994	0.676558	-0.51454	0.112589	0.547958	-0.39809	-0.05344	-0.17332	0.024519	-0.85244
24	0.096033	-0.49132	0.43379	0.447816	0.043401	-0.03318	-0.52433	-0.05948	0.000297	-0.10288	-0.91478
25	-0.06911	0.007105	0.285143	-0.14527	0.364526	-0.03323	-0.30431	0.162405	0.024833	-0.4179	-0.53906
26	-0.38684	-0.36674	-0.28848	0.604447	-1.34114	0.0197	0.224318	0.126117	1.818512	0.176822	1.476715
27	-0.55377	0.405297	0.285617	-0.01149	0.792881	0.130623	0.145984	-1.36864	0.778558	0.570934	-0.67294
28	-0.20536	-0.05112	0.267596	-0.02919	0.39725	-0.01717	-0.15052	0.301678	-0.10126	-0.2948	-0.46388
29	-0.20916	-0.16067	0.374761	-0.22289	0.558435	-0.0119	-0.33447	0.678705	-0.10571	-0.60712	-0.50466
30	-0.40206	-0.28281	0.463522	0.106518	-0.18735	-0.04946	0.171237	0.282189	0.01766	-0.16007	-0.56698
31	-0.07205	0.014196	0.168044	0.008218	0.223047	-0.12112	-0.10311	-0.28714	-0.00616	-0.15351	-0.52333
32	-0.37334	0.035047	0.269073	0.023681	0.234762	0.066529	0.087218	-0.0367	0.02449	-0.4028	-0.64572
33	-0.16451	-0.02046	0.305497	-0.22737	0.445883	-0.02877	-0.43276	0.344299	-0.03858	-0.53503	-0.57749
34	-0.46855	-0.33833	0.241372	0.510312	0.325309	-0.39875	-0.13242	0.011898	0.262377	-0.02183	-0.73457
35	-0.35884	-0.12185	0.589688	-0.29524	0.193872	-0.12248	-0.40655	0.166594	0.056932	0.126291	-0.60836

b. Output Layer--wt from hidden node I to output node

1	2	3	4	5	6	7	8	9	10
-0.31732	0.593869	0.555732	-0.05493	1.653657	-0.14322	0.608999	-0.11585	1.523363	-0.14013
11	12	13	14	15	16	17	18	19	20
0.321084	0.15398 4	-0.9675	-0.87472	-0.92601	-1.0809	0.174892	2.035383	-0.07978	0.380733
21	22	23	24	25	26	27	28	29	30
0.168219	1.29841 4	-0.69242	-0.66227	0.345934	1.245485	1.42322	0.284222	0.69748	0.317505
31	32	33	34	35	bias				
0.280807	-0.20867	0.537707	-0.51458	-0.40429	-0.11806				

4. Example of Spreadsheet Code for NN/Combs ELEC NLP

SIO2I	B2O3I	NA2OI	LI2OI	CAOI	MGOI	FE2O3I	AL2O3I	ZRO2I	OTHERSI
48.95	11.12	16.71	4.28	1.13	1.66	8.97	3.67	0.41	3.1
SIO2A	B2O3A	NA2OA	LI2OA	CAOA	MGOA	NA2CO3A	H3BO3A	BORAX	TOTAL
8.1061379657	0	0	0	3.598541245	0	0	0	0	=SUM(A3:J3)+SUM(A5:I5)
C1	C2	C3	C4	C5	C6	C7	C8	C9	
0.0497	0.0435	0.3392	1.378	0.02998	0.0473	0.01608	0.01868	0.01002	
SIO2	B2O3	NA2O	LI2O	CAO	MGO	FE2O3	AL2O3	ZRO2	OTHERS
=(A3+A5)/J5	=(B3+2*I5+0.5*H5)/J5	=(C3+I5+G5)/J5	=(D3+D5)/J5	=(E3+E5)/J5	=(F3+F5)/J5	=G3/J5	=H3/J5	=I3/J5	0.0407
OBJ FN		ELEC	LNVISC	VISC	LNPCT	PCT	LNMCC	MCC	
=A7*A5+B7*B5+C7*C5+D7*D5+E7*E5+F7*F5+G7*G5+H7*H5+I7*I5		=EXP(0.38257+1.13355*B9+14.5157*C9+3.4372*D9-94.309*C9*D9+16.3778*E9*G9+14.2337*B9*G9+27.914*F9*I9+5.5687*A9*J9+0.099976*D9*I9)	='C:\EXCEL\THESIS\WVISC.XLS'!$R$4	=EXP(D12)	='C:\EXCEL\THESIS\WPCT.XLS'!$R$4	=EXP(F12)	='C:\EXCEL\THESIS\WMCC.XLS'!$R$4	=EXP(H12)	

How to Extract Weights from SNNAP:

1. Go to Network menu of SNNAP.
2. Click on "Text Save."
3. Save the file to a file name such as weights.txt.
4. Open the file in MicroSoft Excel as a space-delimited file. Eliminate all excess spaces between column cells.
5. Identify the hidden layer weights in the middle of the file. Eliminate all rows above these.
6. Identify the output layer weights towards the bottom of the file. Eliminate all rows below them and all rows between the output layer weights and the hidden layer weights.
7. The hidden layer and output layer weights are now extracted.

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13. ABSTRACT *(Maximum 200 words)*

This thesis describes the development of a methodology to minimize the cost of vitrifying nuclear waste. Pacific Northwest Laboratory (PNL) regression models are used as baseline equations for modeling glass properties such as viscosity, electrical conductivity, and two types of durability. Revised PNL regression models are developed that eliminate insignificant variables from the original models. The Revised PNL regression model for electrical conductivity is shown to better predict electrical conductivity than the original PNL regression model. Neural networks are developed for viscosity and the two types of durability, PCT-B and MCC-1 B. The neural network models are shown to outperform every PNL and Revised PNL regression model in terms of predicting property values for viscosity, PCT-B, and MCC-1 B. The combined Neural Network/Revised PNL 2nd order electrical conductivity models are shown to be the best classifiers of nuclear waste glass, i.e. they have the highest probability of classifying a vitrified waste form as glass when it actually did produce glass in the laboratory. Finally, five nonlinear programs are developed with constraints containing 1) the PNL original 1st order models, 2) the PNL original 2nd order models, 3) the Revised PNL 1st order models, 4) the Revised PNL 2nd order models, and 5) the Neural Network/Revised PNL 2nd order electrical conductivity models. The Neural Network/Revised PNL 2nd order electrical conductivity nonlinear program is shown to minimize the total expected cost of vitrifying nuclear waste glass. This nonlinear program allows DOE to minimize its risk and cost of high-level nuclear waste vitrification.

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