GLASS ENVELOPE DEFINITION

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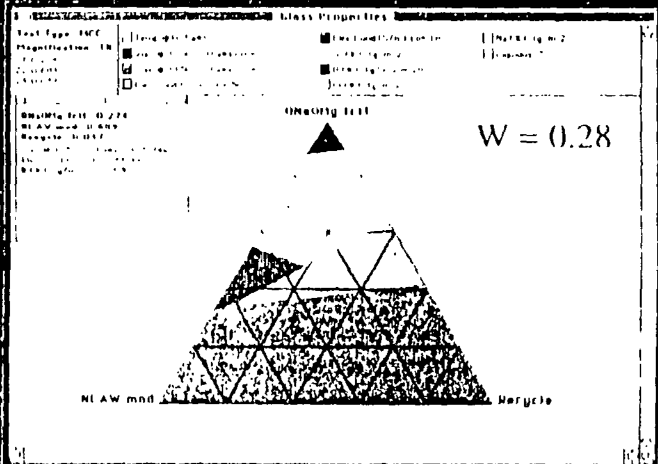
Presentation for
Nuclear Waste Technical Review Board
Tower Inn
Richland, WA
May 11-12, 1992

Pacific Northwest
Laboratory

Glass Envelope Definition



Glass Envelope Definition Objectives

- Provide validated and verified glass composition/property models for Hanford waste composition range to assure:
  - High quality, consistant product
  - HWVP process compatibility

Glass Property Requirements

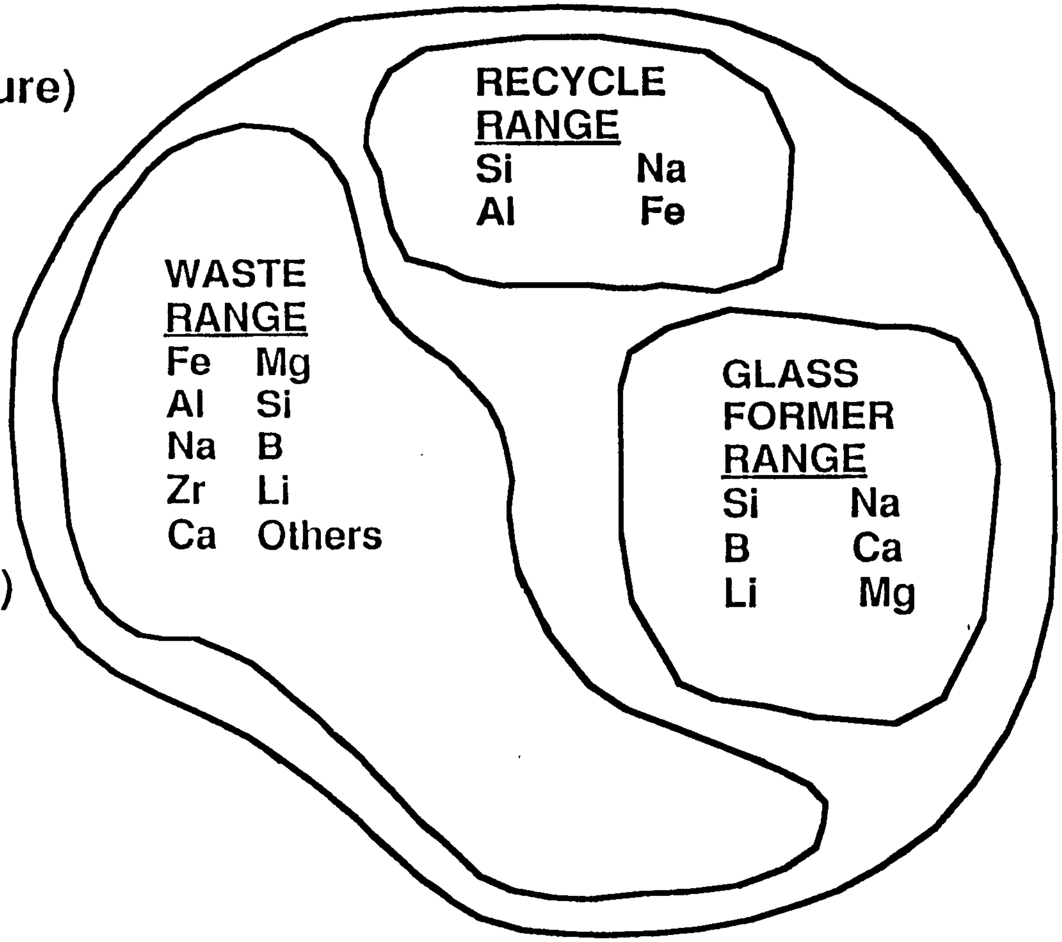
HWVP Glass Property	Acceptability Criteria
Processing	
Viscosity at 1150°C	2-10 Pa·s
Electrical conductivity at 1150°C	18-50 S/m
Liquidus temperature (excludes noble metals)	≤1050°C
Phase separation	No liquid-liquid melt phase separation
Processing characteristics	No melt foaming Acceptable melting rate
Waste Acceptance Preliminary Specifications - June 1991 Borosilicate Glass	
Composition (Chemical, crystalline, radiochemical)	Descriptive
Dissolution rate in deionized water	
PCT	≤EA glass (TBD)
(MCC-1 (28-day, SA/V = 10 m^{-1})	(≤1.0 g/m^2-day)
Glass transition temperature	Descriptive
Time/temperature/transition	Descriptiive
Devitrification during cooling	Cooled glass not exceed transition temperature

Waste Borosilicate Glass

Limited Solubility
(or Time/Temperature)

Immiscability
- $Ca_2(PO_4)_3$
- $(Na, Ca, etc.)_xSO_4$

Crystallinity
- Noble Metals
- $ZrSiO_2$
- Cr_2O_3 (Undissolved)
- $FeCr_2O_4$ (Spinels)
- CaF_2

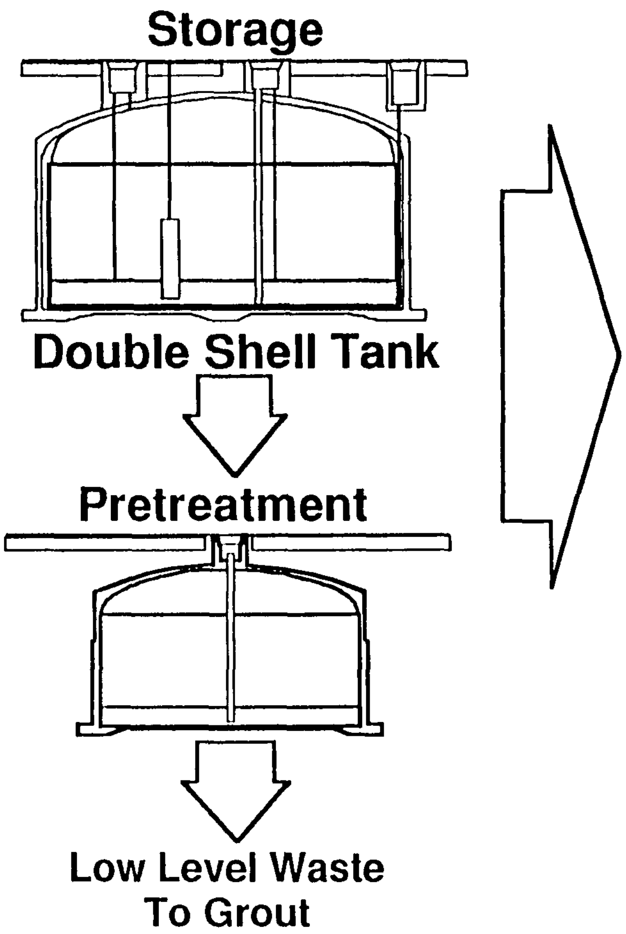


Acceptable Envelope

S9106102.14P

Glass Envelope Definition Approach

Waste Pretreatment and Characterization



- Scoping Studies
- Efficient Statistical Experimental Design for Mixture Modeling
- Testing
  - Waste Acceptance
  - Process
  - Replication
  - Other Glasses
- Testing Data Analyses (Modeling)
- Model Validation
- Modeling Application

Glass Envelope Definition Empirical Models

- Fulcher's Equation
  - $\ln V = A + B/(T - T_o)$
    V - viscosity
    T - temperature
    A, B, T_o - coefficients

- Arrhenius Equation
  - $\ln E = A + B/T$
    E - electrical conductivity
    A, B - coefficients

Glass Envelope Definition Empirical Models (continued)

- **First-Order Model**

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

- **Second-Order Model**

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

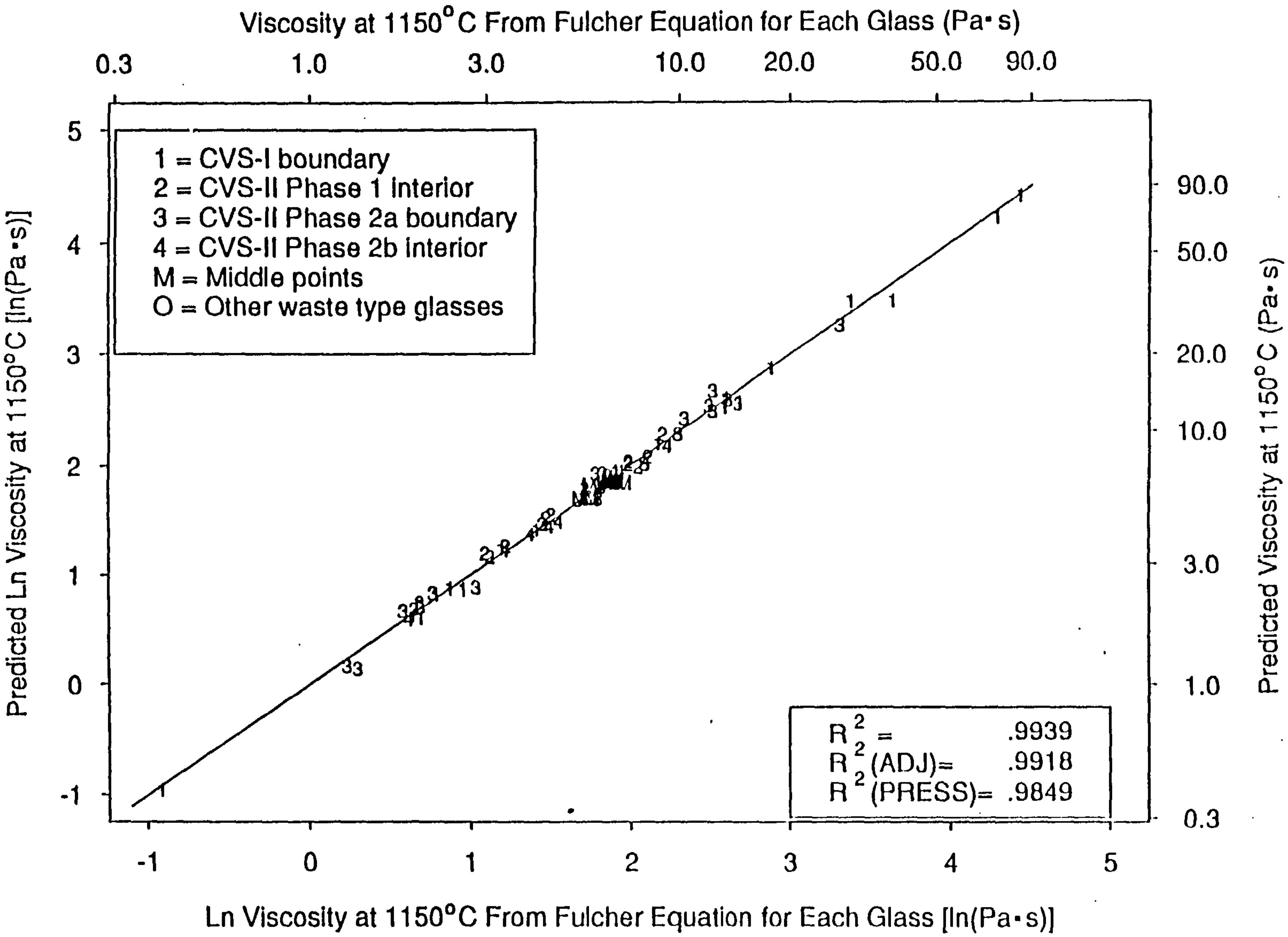
y - property or its mathematical transform

b_i and b_{ij} - coefficients

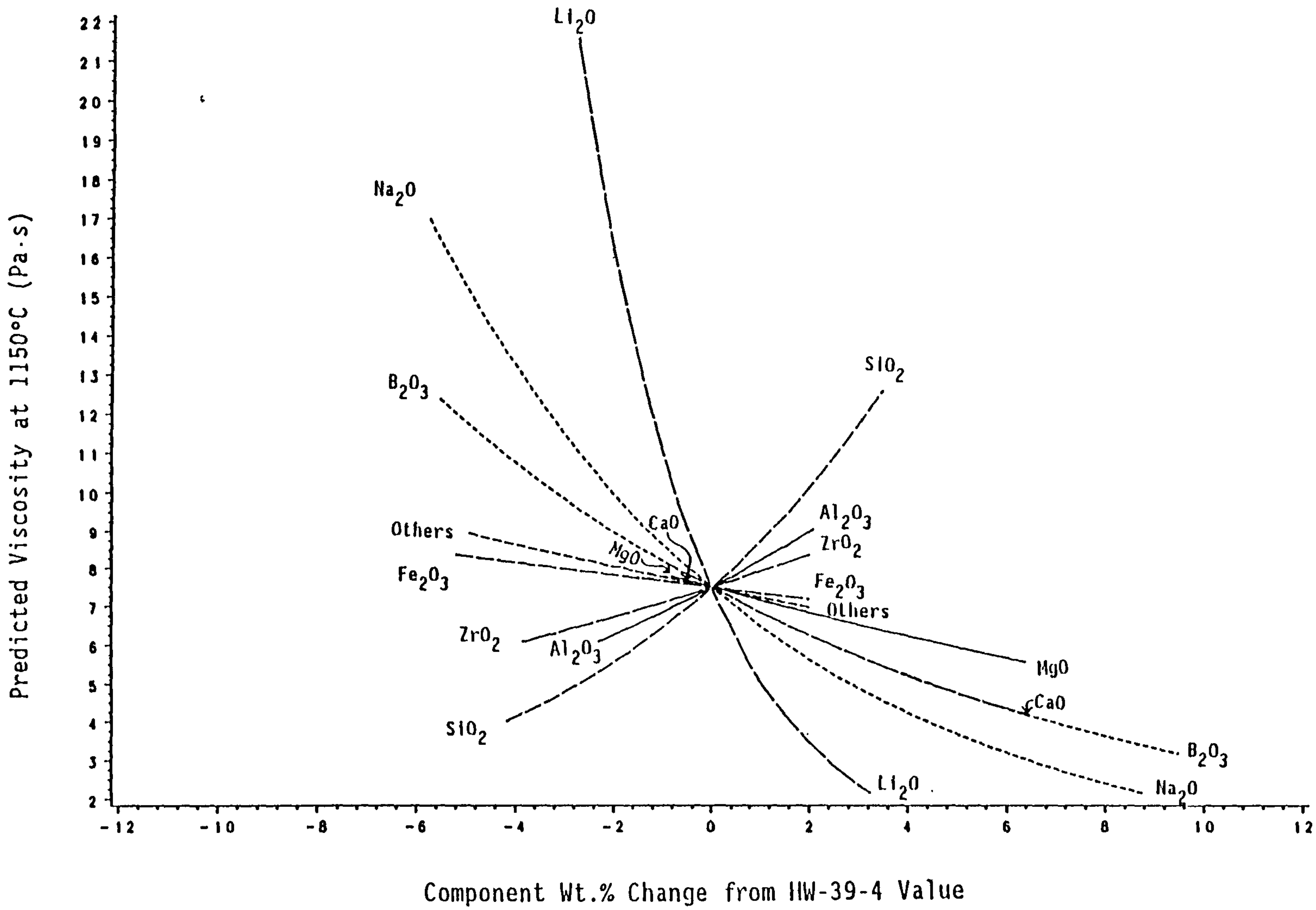
x_i - mass fractions of glass oxide components

Overview of Glasses Tested So Far

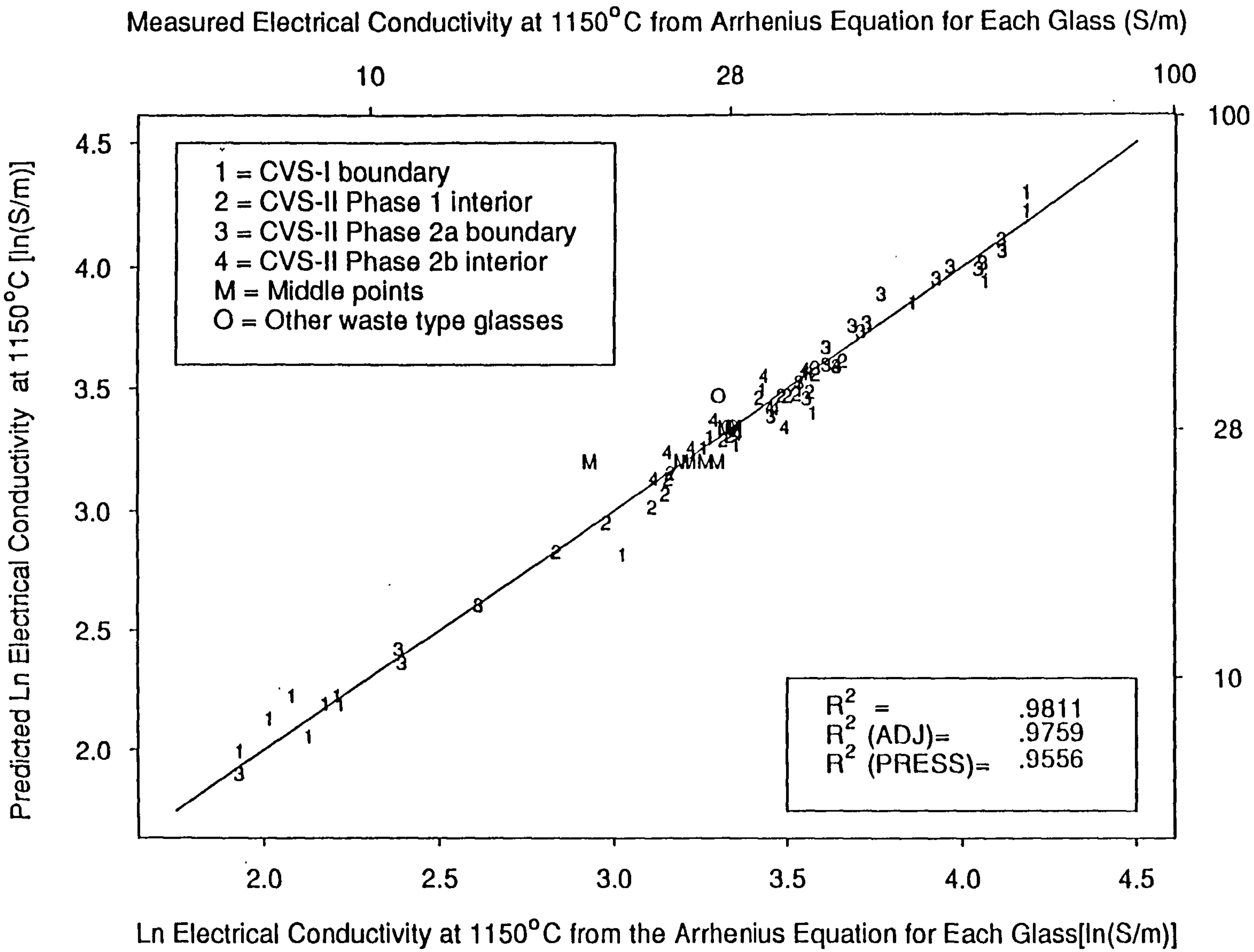
- Glasses selected from study region intended to be somewhat larger than region of glasses with acceptable properties
- 81 glasses tested so far: 23 in CVS-I, 19 in CVS-II Phase 1, 39 in CVS-II Phase 2 (73 distinct and 8 replicates)
- 42 glasses on boundary, 25 on interior, and 14 in the "center" of study region
- 3 glasses with NCRW-, PFP-, and CC-based "Others" mixes and 2 glasses with UO_2



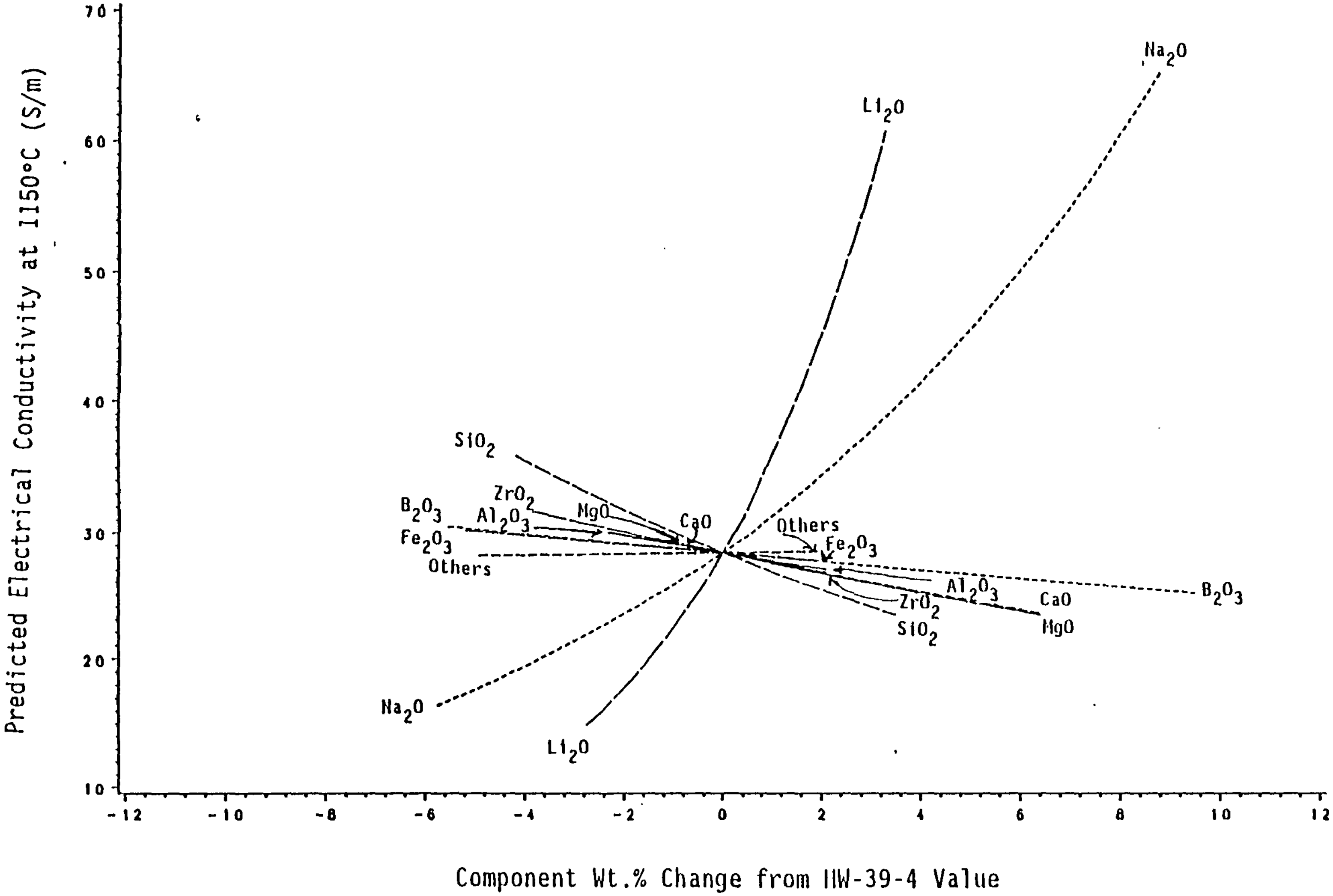
Predicted Viscosity at 1150°C from the Second-Order Mixture Model #1 (from Table 7.6) Versus Predicted Viscosity at 1150°C From the Fulcher Equation for Each Glass (from Table B.2)



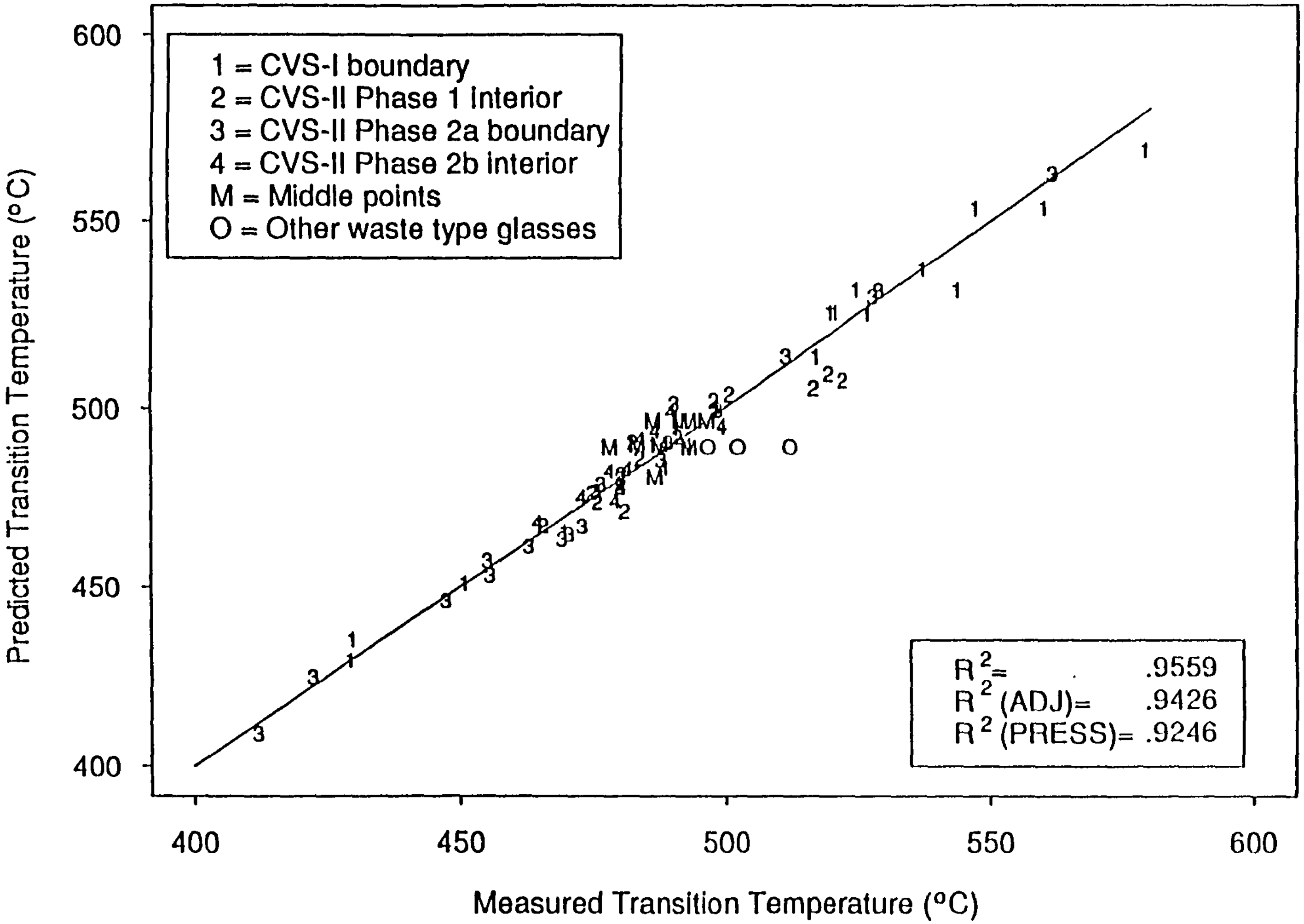
Predicted Component Effects on Viscosity at 1150°C Relative to the HW-39-4 Composition



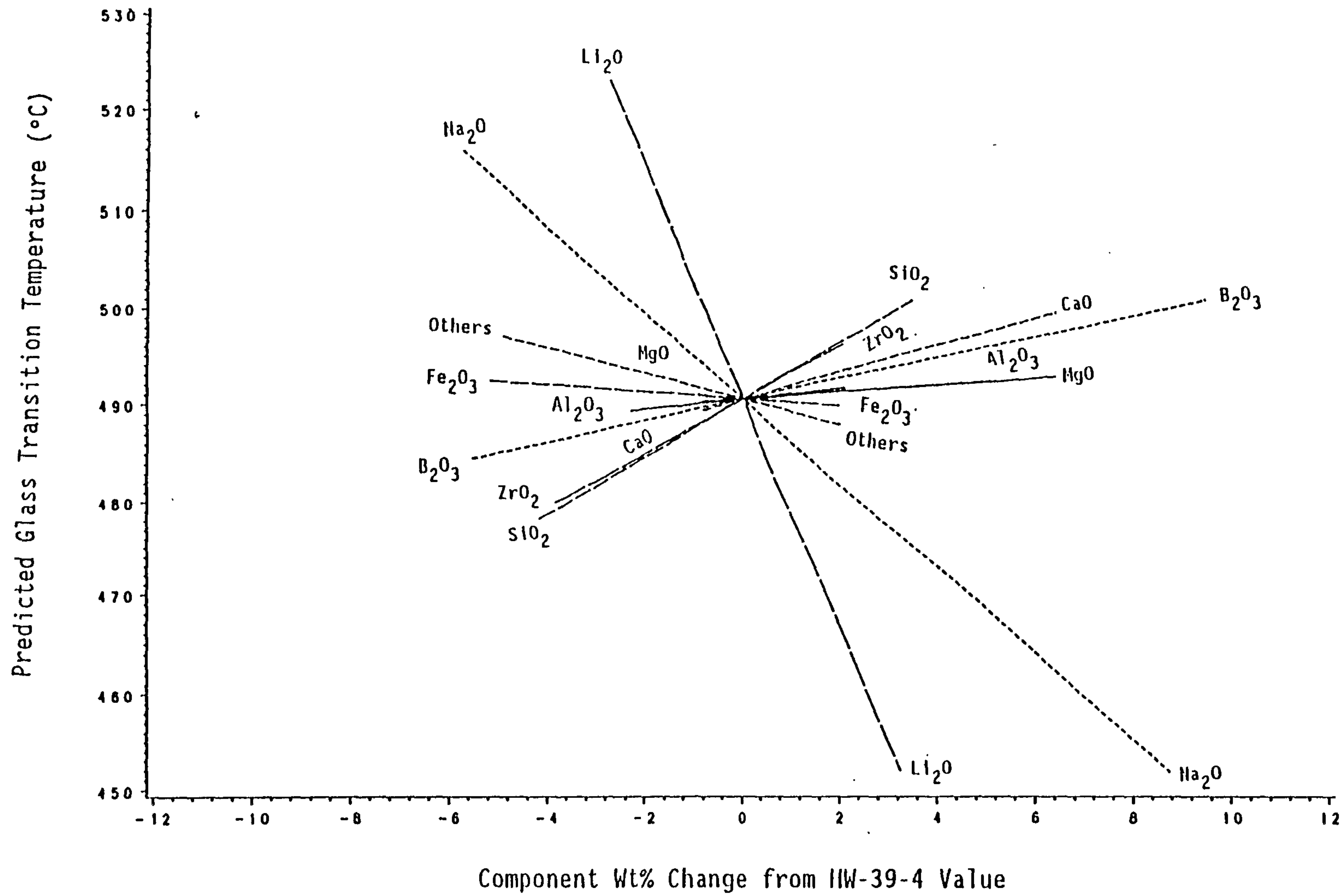
Predicted Electricial Conductivity at 1150°C from the Second-Order Mixture Model #1 (from Table 8.4) Versus Predicted Electrical Conductivity at 1150°C from the Arrhenius Equation for Each Glass (from Table C.2)



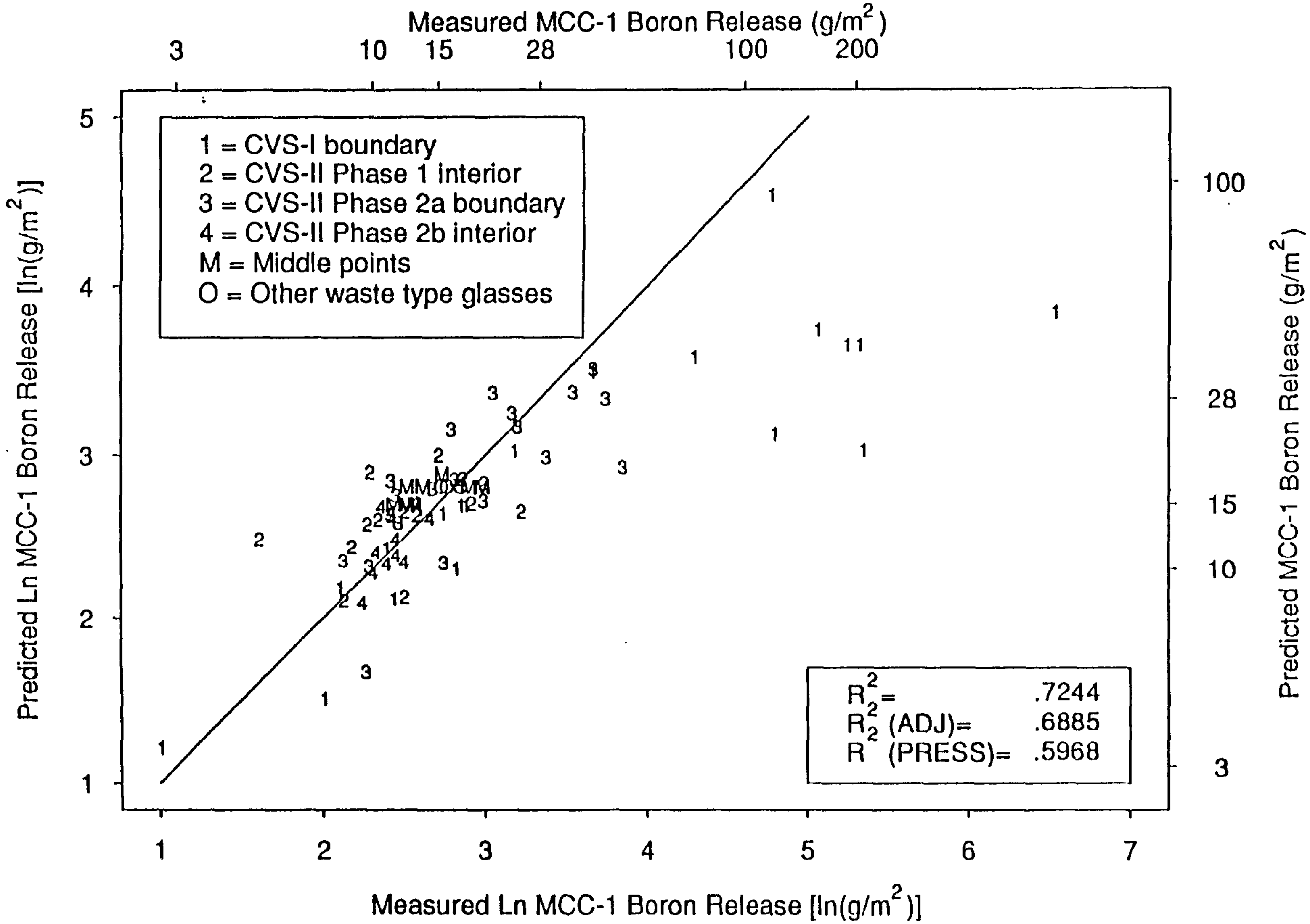
Predicted Component Effects on Electrical Conductivity at 1150°C Relative to the HW-39-4 Composition



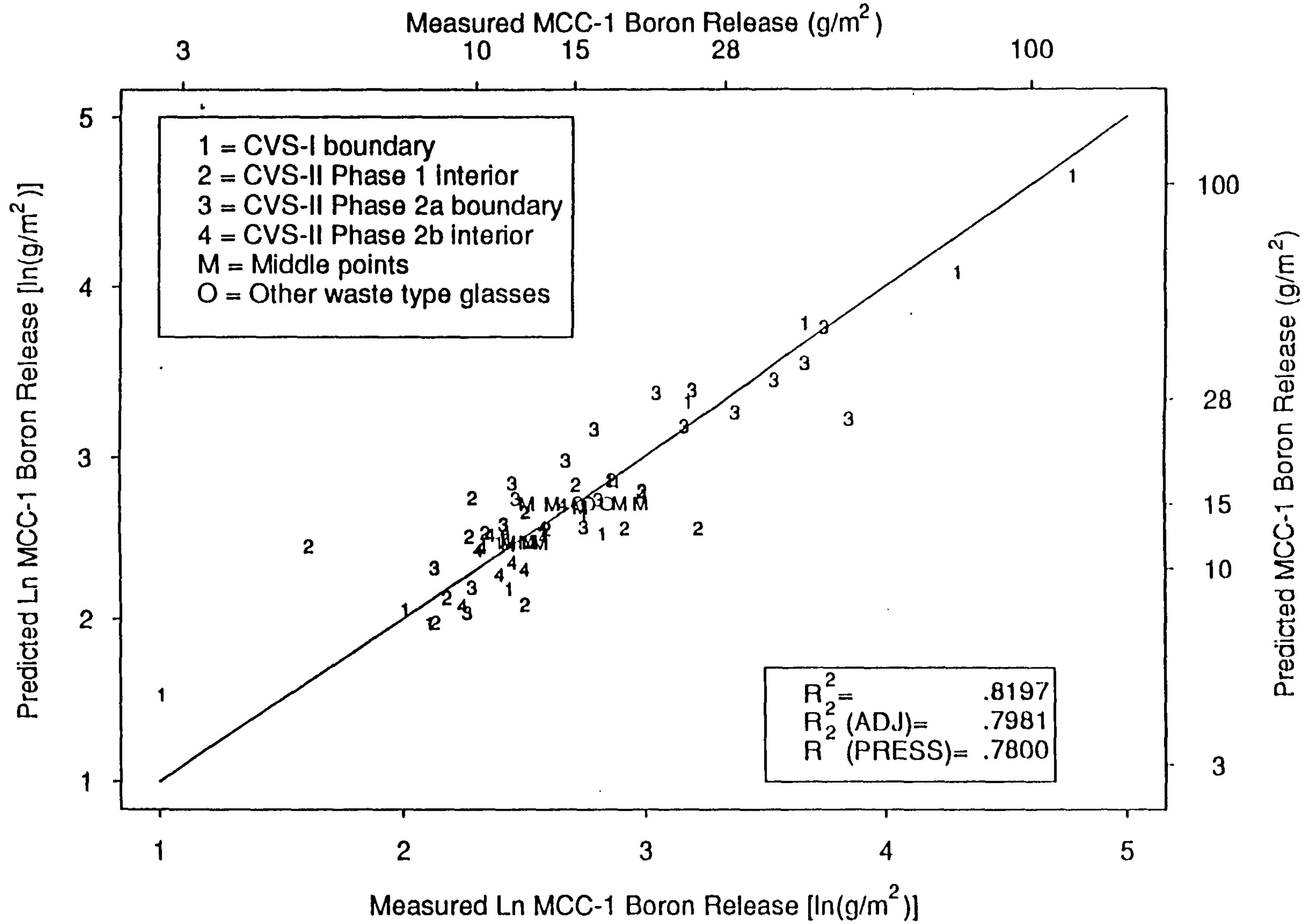
Predicted Versus Measured Glass Transition Temperature Values
for the Second-Order Mixture Model #1 (from Table 9.3)



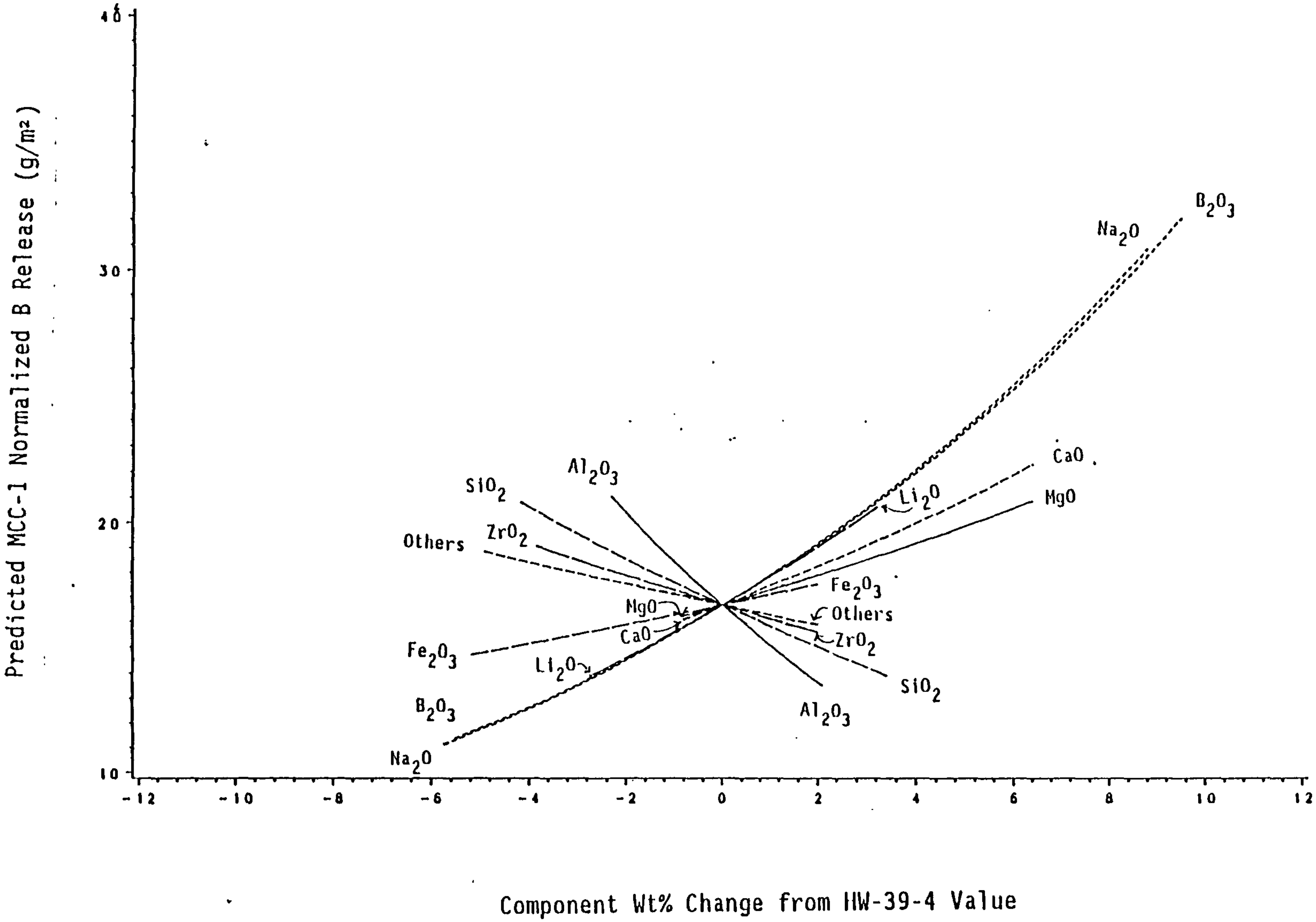
Predicted Component Effects on Glass Transition Temperature
Relative to the HW-39-4 Composition



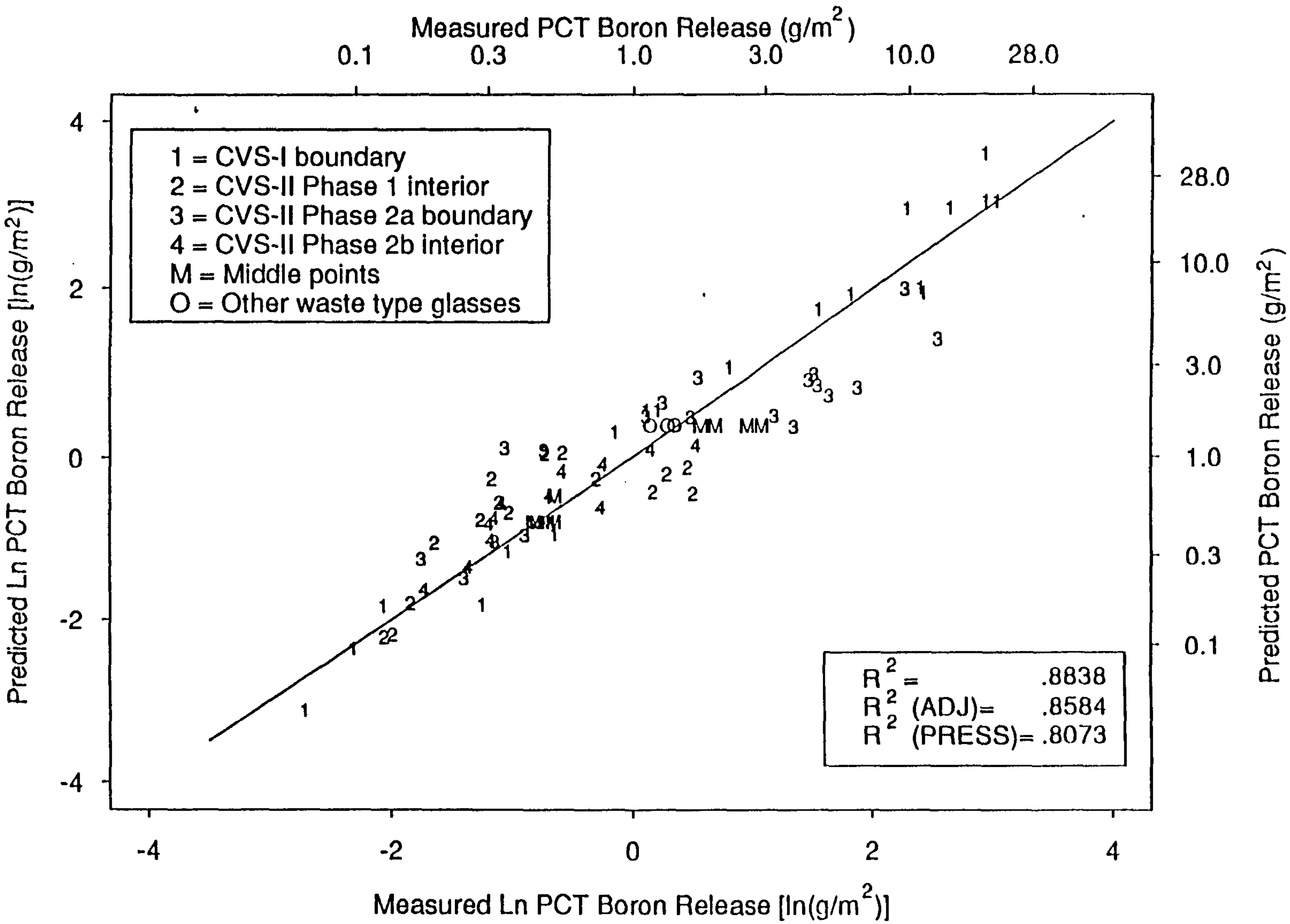
Predicted Versus Measured MCC-1 B Release for the First-Order Mixture Model Fitted to the Full Data Set (from Table 12.2)



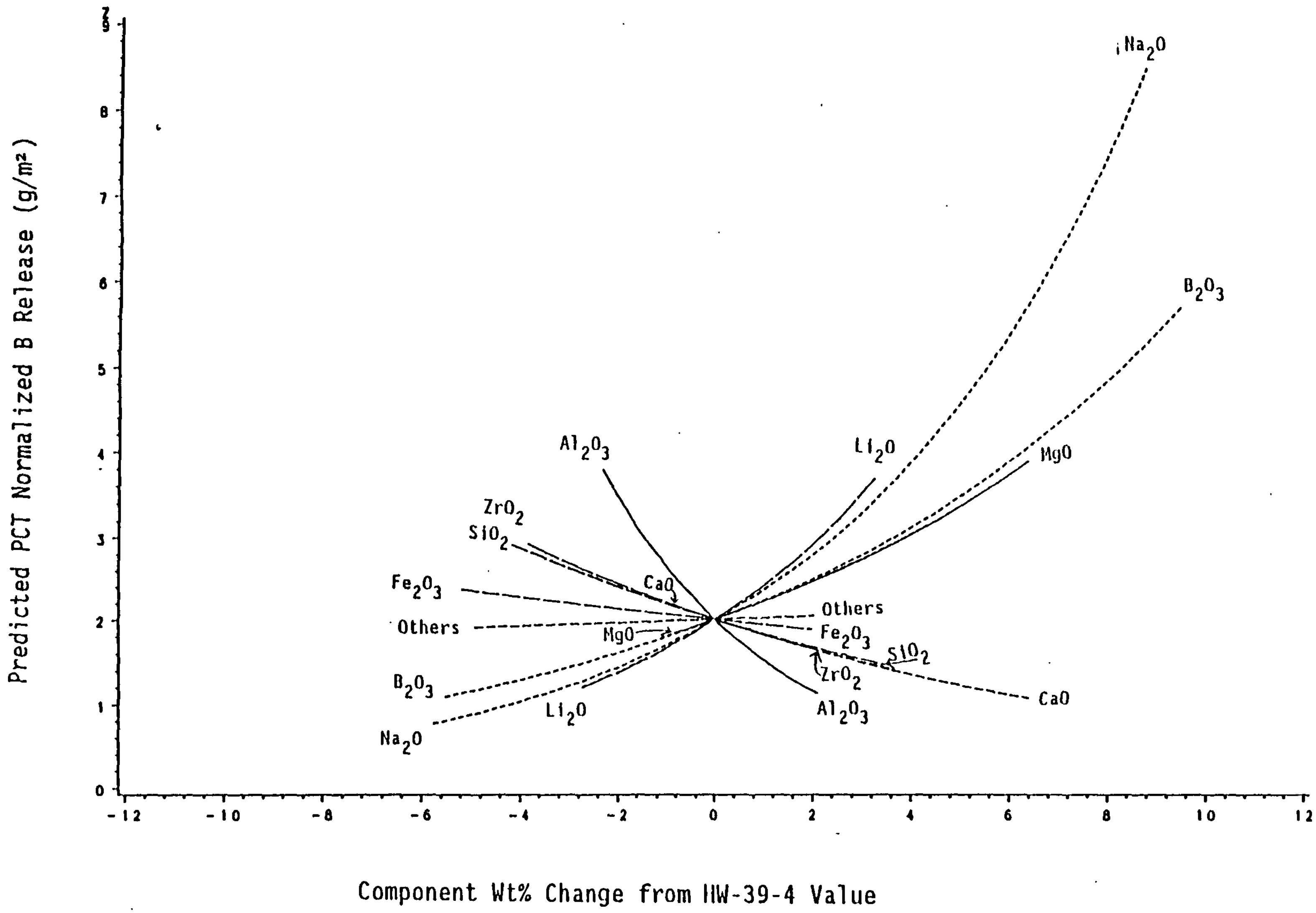
Predicted Versus Measured MCC-1 B Release for the Second-Order Mixture Model Fitted #1 to the Reduced Data Set (from Table 12.4)



Predicted Component Effects on MCC-1 Normalized B Release (Based on First-Order Mixture Model Fitted to The Reduced Data Set, N=73 Means) Relative to the HW-39-4 Composition

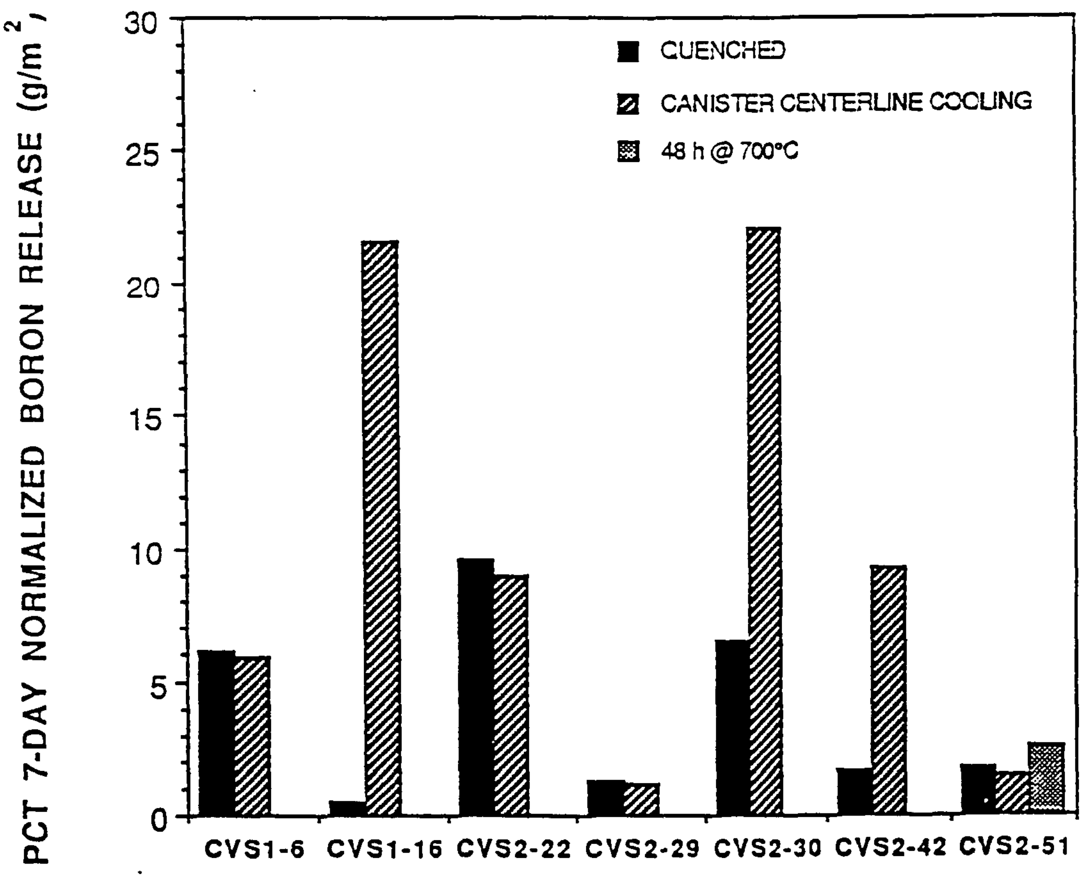


Predicted Versus Measured PCT B Release for the Second-Order Mixture Model #1 (from Table 12.11)



Predicted Component Effects on PCT Normalized B Release (Based on First-Order Mixture Model Fitted to the Full Data Set, N=79 Means) Relative to the HW-39-4 Composition

Comparison of Quenched and Cooled Glass Durability



Ternary Waste Envelope Assessment Tool (TWEAT)

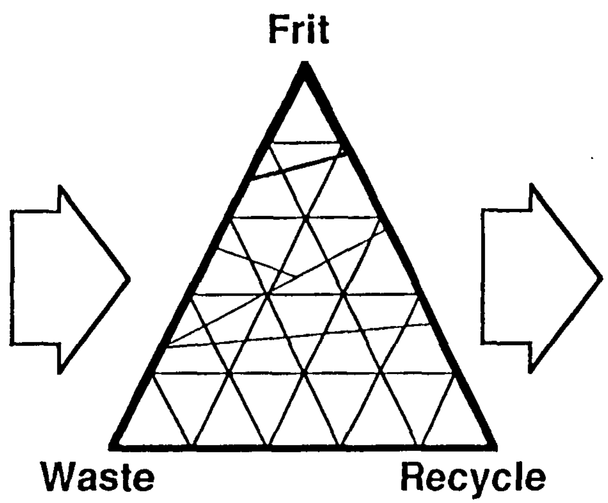
Current Capability

Uses Linear Property Models

INPUT

- Composition
  - Waste (10 Components)
  - Frit (10 Components)
  - Recycle (10 Components)
- Constraint Properties
  - Viscosity
  - Electrical Conductivity
  - Durability
  - (Liquidus Temperature)

DISPLAYS



INFORMATION

- Acceptable Composition Envelope
  - Waste
  - Frit
  - Recycle
- Specific Glass Composition Properties
- Displays Constraints

TWEAT Run Summary

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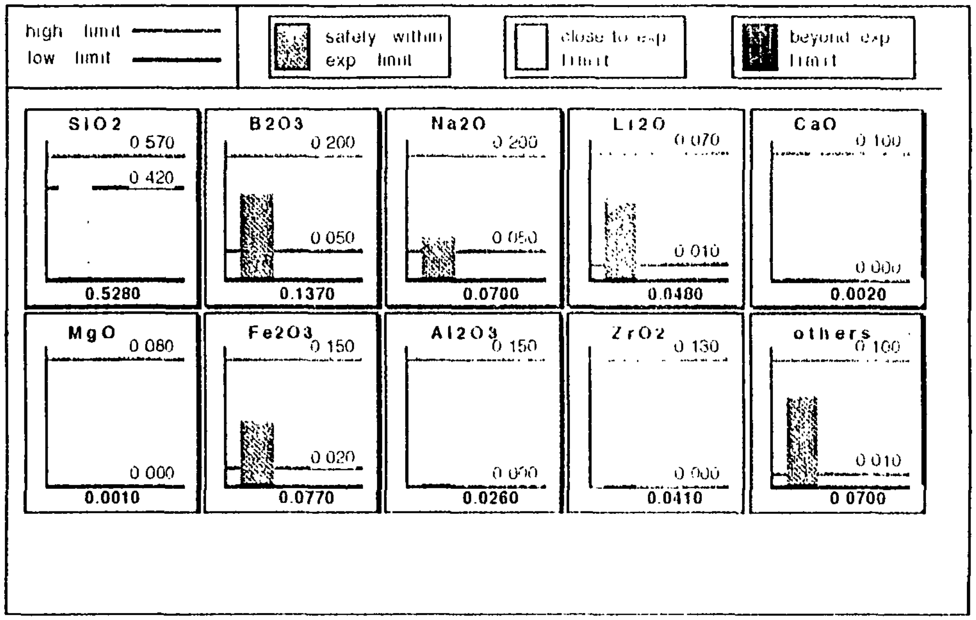
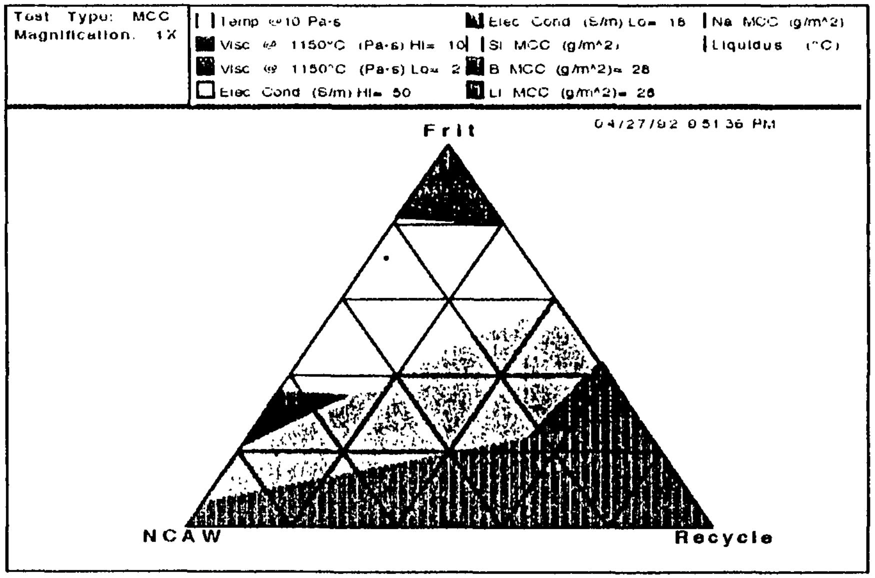
Weight Fraction Oxides

Comp.	Frit	NCAW	Recycle	Glass	Outside exp bndry
SiO_2	0.7356	0.0040	0.4367	0.5280	No
B_2O_3	0.1963	0.0001	0.0000	0.1370	No
Na_2O	0.0000	0.2142	0.4253	0.0700	No
Li_2O	0.0681	0.0000	0.0000	0.0480	No
CaO	0.0000	0.0079	0.0030	0.0020	No
MgO	0.0000	0.0020	0.0032	0.0010	No
Fe_2O_3	0.0000	0.2821	0.0107	0.0770	No
Al_2O_3	0.0000	0.0904	0.0410	0.0260	No
ZrO_2	0.0000	0.1511	0.0000	0.0410	No
others	0.0000	0.2482	0.0801	0.0700	No
sum	1.0000	1.0000	1.0000	1.0000	
vertex fraction	0.7000	0.2727	0.0273		





Data at Selected Point

Waste Loading (g/g glass)	0.2727
Recycle Loading (g/g glass)	0.0273
Frit Required (g/g glass)	0.7000
Temperature @ 10 Pa•s (°C)	
Viscosity @ 1150 °C (Pa•S)	6.985
Electrical Conductivity (S/m)	25.072
Si	
B	15.304
Li	14.537
Na	
Liquidus (°C)	

Waste Simulant and Glass Property Models Validation

Approach

Test Data/Property Models Correlation

Property Models

- Glass Envelope Studies
- Laboratory Simulant Slurry Studies

HWVP Process

Laboratory-Scale
- Radioactive
- Simulant

Bench-Scale
- Radioactive
- Simulant

Pilot-Scale
- Simulant

Validated Models for HWVP

- Design
- Feed Processability
- Operations
- Permitting
- Safety
- Waste Form Qualification

Summary

- **Current Results Indicate that:**

  Empirical Modeling based on statistical experimental testing appears to adequately predict glass properties

  Melt electrical conductivity
  Melt viscosity
  Glass transition temperature
  Glass durability

  based on composition

Summary (continued)

- Investigation of glass temperature history effects on some glass properties such as durability is planned

- The approach appears viable to define a glass envelope for HWVP operation when supplemented with melter testing and redox modeling