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Statistical Assessment of Bias and Random Uncertainties in WTP HLW CRV Mixing and Sampling

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ACCEPTED FOR
PROJECT USE
for W.L. Tamosaitis
5/27/04

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Test Specification: 24590-WTP-TSP-RT-02-007
Test Plan: TP-RPP-WTP-193, Rev. 1
Test Exceptions: 24590-WTP-TEF-RT-03-039
24590-WTP-TEF-RT-04-017
R&T Focus Area: Waste Form Qualification
Test Scoping Statements: B-61 and B-65

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Completeness of Testing

This report describes the results of work and testing related to Test Specification 24590-WTP-TSP-RT-02-007, Test Exceptions 24590-WTP-TEF-RT-03-039 and 24590-WTP-TEF-RT-04-017, and Test Plan TP-RPP-WTP-193, Rev. 1. The work and any associated testing followed the quality assurance requirements outlined in the Test Specification and Test Plan. The descriptions provided in this test report are an accurate account of both the conduct of the work and the data collected. Test plan results are reported. Also reported are any unusual or anomalous occurrences that are different from expected results. The test results and this report have been reviewed and verified.

Approved:

Gordon H. Beeman

Gordon H. Beeman, Manager
WTP R&T Support Project

5/24/04
Date

Summary

The immobilized high-level waste (IHLW) vitrification process of the River Protection Project-Waste Treatment and Immobilization Plant (RPP-WTP) will be subject to variation and several uncertainties. The compositions, compliance properties (i.e., Product Consistency Test [PCT], Toxicity Characteristic Leaching Procedure [TCLP], and waste loading), and process control properties (e.g., viscosity and one-percent crystallinity temperature [$T_{0.01}$]) of the IHLW melts and products will be subject to variation because the compositions of waste feeds will vary over time. The state of knowledge at any step of the IHLW process will be subject to sampling, chemical analysis, volume measurement, mixing, weighing, transfer, and other uncertainties. These uncertainties may be *systematic* and/or *random* in nature. The term *bias* is used rather than *systematic uncertainty* so that there is a clear difference in discussing *bias* versus *random uncertainty*.

The WTP compliance strategies for IHLW (Nelson 2003) associated with several Waste Acceptance Product Specifications (WAPS) (DOE-EM 1996) and Contract (DOE-ORP 2000) specifications are statistically based. That is, those compliance strategies account for variations and uncertainties in meeting requirements of the specifications. This report documents the work and results to assess the impacts on IHLW compliance and processing properties of bias and random uncertainty in mixing and sampling waste in the high-level waste (HLW) Concentrate Receipt Vessel (CRV). For this work, the impacts of HLW CRV mixing and sampling were studied jointly. That is, any bias in HLW CRV determinations could be due to mixing and/or sampling. Similarly, random uncertainty in HLW CRV determinations could be caused by mixing and/or sampling. Ideally, the effects (bias and random uncertainty) of mixing and sampling would have been studied separately. However, the work was completed in a short time at the request of the WTP Project, and so it was necessary to use compliance simulation software at its current stage of development, which did not provide for separately simulating CRV mixing and sampling effects (i.e., biases and random uncertainties).

Glass-optimization calculations were performed on actual waste sample data for three tank wastes (AZ-101, AZ-102, and C-106) to select the waste composition best suited for subsequent statistical evaluation. The waste composition chosen (associated with AZ-102) had the smallest acceptable glass compliance and processing envelope (i.e., the glass-composition space over which all processing and product quality properties are predicted to be acceptable with high confidence), ensuring that the subsequent statistical investigations would yield conservative results. Glass composition and property constraints based on glass compliance and processing conditions were used to optimize the glass formulation for the selected AZ-102 waste composition, where glass property-composition models were used to estimate the glass properties. Five specific glass formulations for the selected AZ-102 waste were chosen to provide a series of tradeoffs in meeting the most constraining properties, namely waste loading (WL) and temperature for 0.01 volume-fraction crystals ($T_{0.01}$). One of the five glass formulations with the optimal tradeoff between WL and $T_{0.01}$ was selected. These five glass compositions, including the selected optimal glass formulation, were then used in statistical simulation studies performed to assess the effects of HLW CRV mixing/sampling bias and random uncertainty, as well as other random uncertainties.

Three simulation studies were performed using software designed to simulate the CRV, glass-former chemical (GFC), and Melter Feed Preparation Vessel (MFPV) steps of the WTP IHLW process. Calculations were performed using the IHLW compliance strategy as well as the immobilized low-

activity waste (ILAW) compliance strategy applied to the IHLW situation[a]. In each of the three simulation studies, a computer experiment was performed in which several factors were varied according to the test matrix for that study. The factors that were varied in one or more of the test matrices included (1) HLW CRV mixing/sampling bias, (2) HLW CRV mixing/sampling random uncertainty, (3) other sources of random uncertainty affecting the CRV, GFCs, and MFPV,[b] (4) glass formulation, and (5) the number of samples from the CRV (IHLW and ILAW compliance strategies) and MFPV (IHLW compliance strategy). For each combination of factors in a computer experiment, a Monte Carlo simulation of 1000 runs was performed based on the specified values of random uncertainties for that combination of test factors. A given set of 1000 runs represented 1000 possible outcomes of producing a single HLW MFPV batch under that combination of test factors. Each of the 1000 simulation runs for a given combination of test factors resulted in a calculated glass composition and measures of uncertainty associated with each component of that composition. Using property-composition models and a waste-loading expression, values of several compliance properties (PCT, TCLP Cd release, waste loading) and processing properties ($T_{0.01}$, liquidus temperature, and viscosity) were calculated for each composition in each set of 1000 compositions. The sets of 1000 values of compliance and processing properties provided for quantifying the uncertainties in these properties for glass corresponding to a single HLW MFPV batch. Composition uncertainties (from the Monte Carlo runs) and property-composition model uncertainties were accounted for using 90% confidence intervals to assess whether compliance and processing conditions were satisfied.

The properties that most limited compliance and processability were WL and $T_{0.01}$. Figure S.1 shows the allowable ranges of HLW CRV mixing/sampling solids bias given three possible levels of CRV mixing/sampling random uncertainty (5, 15, and 25 %RSD[c]) for each of four situations. The four situations represent the combinations of using (1) the IHLW or ILAW compliance strategy, and (2) nominal levels of all other random uncertainties with 8 CRV and MFPV samples, or high levels of all other random uncertainties with 4 CRV and MFPV samples.

Figure S.1 shows that the range of allowable CRV mixing/sampling solids bias is larger with:

- smaller CRV mixing/sampling random uncertainties
- nominal values of all other random uncertainties as compared to higher values for these uncertainties
- the ILAW compliance strategy rather than the IHLW compliance strategy
- eight samples from the CRV (IHLW and ILAW strategies) and MFPV (IHLW strategy) rather than four samples.

In the worst case (bottom left plot in Figure S.1) with the IHLW strategy, high uncertainties for all other random uncertainties, and four CRV and MFPV samples, it is not possible to satisfy the WL and $T_{0.01}$ conditions with 90% confidence. In the best case (upper right plot in Figure S.1) with the ILAW strategy, nominal uncertainties for all other random uncertainties, and eight CRV samples, the "90% confidence"

(a) The IHLW strategy uses analyses of CRV and MFPV samples, in addition to other process measurements. The ILAW strategy uses analyses of CRV samples, measured masses of GFCs added to the MFPV, and other process measurements.
(b) These sources of uncertainty include CRV analytical, MFPV mixing/sampling, MFPV analytical, GFC composition, GFC masses added to MFPV, CRV volumes, and MFPV volumes.
(c) RSD = relative standard deviation; %RSD = percent RSD (the relative standard deviation multiplied by 100%).

allowable range of CRV mixing/sampling solids bias varies from roughly -4% to +6.5% for CRV mixing/sampling random uncertainty %RSD = 5 and from roughly -3% to +2% for CRV mixing/sampling random uncertainty %RSD = 25.

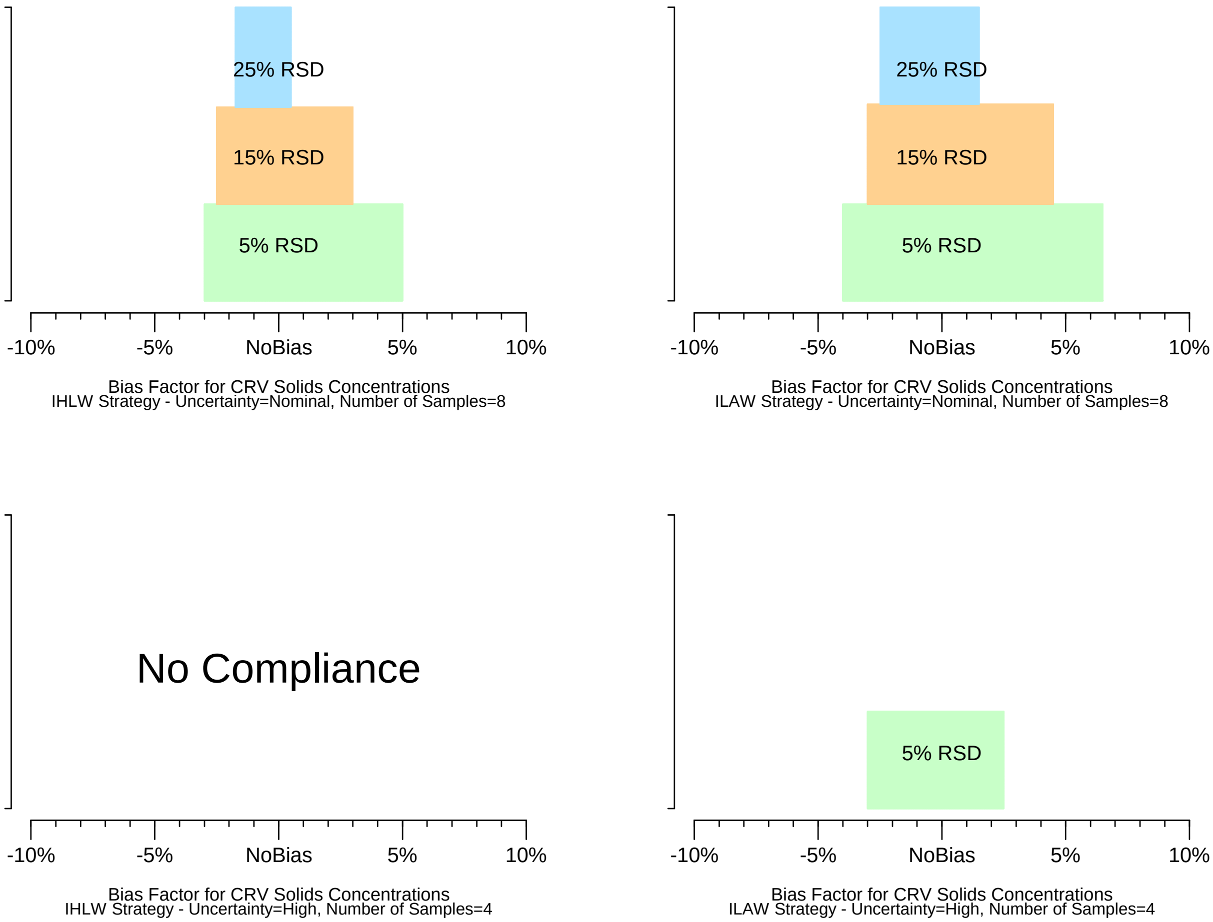

Figure S.1. Ranges of CRV Mixing/Sampling Bias that Allow Compliance and Processing Properties to be Satisfied with 90% Confidence. The dependence of the ranges on CRV mixing/sampling random uncertainty %RSD is shown.

Acronyms, Terms, and Abbreviations

a_i	Mass fraction of the i^{th} component in additive
$a_{P,i}$	Coefficient of the i^{th} component for the property P
ASTM	American Society for Testing and Materials
c_{Cd}	TCLP cadmium release concentration (mg/L)
CCI	combined confidence interval (see CL% CCI for definition)
CI	confidence interval (see CL% CI for definition)
CL	confidence level (in percent)
CL% CCI	CL% combined confidence interval—A confidence interval on the true mean value of a prediction made by a glass property-composition model for a given glass, which is formed by combining separate CL% confidence intervals that account for glass composition uncertainty and model uncertainty. The interval includes the true mean property value for a given glass composition with CL% confidence after accounting for glass composition and model uncertainties.
CL% CI	CL% confidence interval—An interval that includes the true mean value of a quantity with CL% confidence.
CL% LCI	CL% lower confidence interval—A one-sided lower confidence interval that includes the true mean value of a quantity with CL% confidence.
CL% LCCI	CL% lower combined confidence interval—A one-sided lower confidence interval on the true mean value of a prediction made by a glass property-composition model for a given glass, which is formed by combining separate CL% lower confidence intervals that account for glass composition uncertainty and model uncertainty. The interval includes the true mean property value for a given glass composition with CL% confidence after accounting for glass composition and model uncertainties.
CL% SCI	CL% simultaneous confidence interval—One of several confidence intervals on the true mean values of predictions made by a glass property-composition model for a set of glass compositions. All of the confidence intervals for the set of glass compositions simultaneously include the true mean property values for the glasses with CL% joint confidence after accounting for model uncertainty.
CL% SUCI	CL% simultaneous upper confidence interval— One of several upper confidence intervals on the true mean values of predictions made by a glass property-composition model for a set of glass compositions. All of the upper confidence intervals for the set of glass compositions simultaneously include the true mean

	property values for the glasses with CL% joint confidence after accounting for model uncertainty.
CL% UCI	CL% upper confidence interval—A one-sided upper confidence interval that includes the true mean value of a quantity with CL% confidence.
CL% UCCI	CL% upper combined confidence interval— A one-sided upper confidence interval for predictions made by a glass property-composition model, which is formed by combining separate CL% upper confidence intervals that account for glass composition uncertainty and model uncertainty. The interval includes the true, mean property value for a given glass composition with CL% confidence after accounting for glass composition and model uncertainties.
Compliance and processing envelope	The glass composition space over which all processing and product quality properties are predicted to be acceptable with high confidence.
CRV	Concentrate Receipt Vessel
DOE	U. S. Department of Energy
DOE-EM	U. S. DOE-Environmental Management
DOE-ORP	U.S. DOE-Office of River Protection
DWPF	Defense Waste Processing Facility
$f(P)$	Function (i.e., mathematical transformation) of a glass property P
GFC	glass-former chemical
G2	WTP Dynamic Flowsheet Model based on G2™ software
g_i	mass fraction of the i^{th} glass component
g_i^N	mass fraction of the i^{th} glass component normalized over N components
g	grams
g/L	grams per liter
g/m^2	grams per square meter
HBV	HLW Blend Vessel
HLW	high-level waste

IHLW	immobilized HLW
IHLW PCP	IHLW Product Compliance Plan
ILAW	immobilized low-activity waste
ILAW PCP	ILAW Product Compliance Plan
ITR	independent technical review
L	liters
LAW	low-activity waste
LCI	lower confidence interval (see CL% LCI for definition)
LCCI	lower combined confidence interval (see CL% LCCI for definition)
LOF	lack-of-fit
MFPV	Melter Feed Preparation Vessel
mg/L	milligrams per liter
N	Number of components in glass for which a property-composition model was fit.
n	Number of data points used to fit the parameters (coefficients) in a glass property-composition model.
NQA	nuclear quality assurance
90% CCI	90% combined confidence interval (see CL% CCI for definition)
90% CI	90% confidence interval (see CL% CI for definition)
90% LCCI	90% lower combined confidence interval (see CL% LCCI for definition)
90% LCI	90% lower confidence interval (see CL% LCI for definition)
90% SCI	90% simultaneous confidence interval (see CL% SCI for definition)
90% UCCI	90% upper combined confidence interval (see CL% UCCI for definition)
90% UCI	90% upper confidence interval (see CL% UCI for definition)

P	A glass property (e.g, PCT)
p	Number of fit parameters (coefficients) in a property-composition model.
PCT	Product Consistency Test
PNWD	Battelle—Pacific Northwest Division
QA	quality assurance
QARD	Quality Assurance and Requirements Document
R^2	Fraction of variation in a modeled property accounted for by the model.
R^2_A	Fraction of variation in a modeled property accounted for by the model, adjusted for the number of fitted coefficients in the model.
R&T	Research and Technology
RCRA	Resource Conservation and Recovery Act
RMSE	root mean squared error
RPP-WTP	River Protection Project-Waste Treatment and Immobilization Plant
RSD	relative standard deviation
%RSD	percent RSD (the relative standard deviation multiplied by 100%)
r_B	PCT normalized boron release (g/m^2)
r_{Li}	PCT normalized lithium release (g/m^2)
r_{Na}	PCT normalized sodium release (g/m^2)
s	Another notation for the RMSE of a fitted model.
SCI	simultaneous confidence interval (see CL% SCI for definition)
SD	standard deviation
SUCI	simultaneous upper confidence interval (see CL% SUCI for definition)
TCLP	Toxicity Characteristic Leaching Procedure
T	absolute temperature (K)

T_L	liquidus temperature (°C)
$T_{0.01}$	The temperature at which the volume fraction of crystals in glass is 0.01 (°C).
u	Uncertainty
UCI	upper confidence interval (see CL% UCI for definition)
UCCI	upper combined confidence interval (see CL% UCCI for definition)
Uncertainty	Lack of knowledge about a true, fixed state of affairs (e.g., analytical *uncertainty* in chemical analyses of a glass sample).
Variation	Real changes in a variable over time or space (for example, *variation* in glass composition within a waste type).
η_{1100}	viscosity at 1100°C (poise)
η_{1150}	viscosity at 1150°C (poise)
W	mass fraction of waste in glass
w_i	mass fraction of the i^{th} component in waste
WAPS	Waste Acceptance Product Specifications
Waste type	A quantity of waste feed to a vitrification facility that is relatively constant in composition.
WL	waste loading (expressed as a mass fraction or mass percent)
WTP	Waste Treatment and Immobilization Plant
WTPSP	Waste Treatment Plant Support Project
WVDP	West Valley Demonstration Project

Testing Summary

Objectives

The specific test objectives for the work in this report are listed and discussed as Items 1 to 4 in Table TS.1. These test objectives were determined in planning meetings with WTP R&T management and staff at the start of the work.

The specific test objectives for this work are related to three of the general test objectives from the applicable Test Plan (*Test Plan: Statistical Methods for Estimating Variations in HLW and LAW Waste Types*, TP-RPP-WTP-193, Rev. 1). These three general objectives are listed and discussed as Items 5 to 7 in Table TS.1.

Test Exceptions

Test exceptions 24590-WTP-TEF-RT-03-039 and 24590-WTP-TEF-RT-04-017 apply to the Test Specification and Test Plan for work under Technical Scoping Statements B-61 and B-65. However, these test exceptions relate to other scope changes and are unrelated to the work scope covered in this report.

Results and Performance Against Success Criteria

The success criteria and performance against those criteria are discussed in Table TS.2. The results of the work are summarized in the preceding Summary section, as well as Section 8 (Summary and Discussion) of the report.

Quality Requirements

Application of RPP-WTP Quality Assurance Requirements

PNWD implemented the RPP-WTP quality requirements by performing work in accordance with the PNWD Waste Treatment Plant Support Project quality assurance project plan (QAPjP) approved by the RPP-WTP Quality Assurance (QA) organization. This work was performed to the quality requirements of NQA-1-1989 Part I, Basic and Supplementary Requirements (ASTM 1989) and NQA-2a-1990, Part 2.7 (ASTM 1990). These quality requirements are implemented through PNWD's *Waste Treatment Plant Support Project (WTPSP) Quality Assurance Requirements and Description Manual*.

A matrix that cross-references the NQA-1 and 2a requirements with the PNWD's procedures for this work is given in Attachment 2 of the Test Plan (TP-RPP-WTP-193, Rev. 1, *Test Plan: Statistical Methods for Estimating Variations in HLW and LAW Waste Types*). The matrix includes justification for those requirements not implemented. For activities associated with HLW, the additional quality assurance requirements of DOE/RW-0333P, Rev. 13, *Quality Assurance Requirements and Description* (DOE-RW 2004) were also satisfied. A listing of the procedures implementing the DOE/RW-0333P quality assurance requirements is included in Attachment 1 of the Test Plan.

Conduct of Experimental and Analytical Work

No physical experiments, testing, or analytical work were conducted as part of the effort documented in this report. Only computer glass formulation calculations and statistical simulation “experiments” were performed, in accordance with the WTPSP procedure QA-RPP-WTP-1101 (*Scientific Investigations*) and other procedures. The glass formulation calculations were performed in accordance with WTPSP procedure QA-RPP-WTP-SCP (*Software Control*). The mass-balance-based equations implemented in the statistical simulation software underwent Independent Technical Reviews (ITRs) according to WTPSP procedure QA-RPP-WTP-604 (*Independent Technical Review*). The simulation software and its applications also satisfied the requirements of WTPSP procedure QA-RPP-WTP-SCP. Per this procedure, a software quality assurance package was prepared and received required WTPSP reviews and approvals (including an ITR under WTPSP procedure QA-RPP-WTP-604).

As stated in the Test Specification (24590-WTP-TSP-RT-02-007, Rev. 0, *Statistical Methods for Estimating Variations in HLW and LAW Waste Types*), BNI’s QAPjP, PL-24590-QA00001, is not applicable because the work was not performed in support of environmental/regulatory testing, and the results will not be used for such purposes.

Internal Data Verification and Validation

PNWD addressed internal verification and validation activities by conducting ITRs of the software quality assurance package and the final report in accordance with PNWD’s procedure QA-RPP-WTP-604. These reviews verify that the reported results are traceable, that inferences and conclusions are soundly based, and the reported work satisfies the Test Plan (TP-RPP-WTP-193, Rev. 1, *Test Plan: Statistical Methods for Estimating Variations in HLW and LAW Waste Types*) objectives. The QA-RPP-WTP-604 review procedure is part of PNWD's *WTPSP Quality Assurance Requirements and Description Manual*.

R&T Test Conditions

The test conditions applicable to this work are listed and discussed in Table TS.3. All test conditions were followed and no deviations were necessary.

Simulant Use

The work involved in this report was of a paper-study nature. No physical testing was performed, and thus no simulants were used.

Discrepancies and Follow-on Tests

There are no known discrepancies that remain unresolved.

Table TS.1. Summary of Objectives

Test Objective	Objective Met (Y/N)	Discussion
Specific Test Objectives for the Work in This Report		
1. Assess the impacts on IHLW compliance and processing properties (i.e., PCT, TCLP Cd release, waste loading, viscosity, liquidus temperature, and $T_{0.01}$) of mixing/sampling bias and random uncertainty in the HLW CRV.	Yes	The impacts on compliance and processing properties of HLW CRV mixing/sampling bias and random uncertainty were assessed using computer experiments. The factors varied in one or more of the computer experiments included (1) HLW CRV mixing/sampling bias, (2) HLW CRV mixing/sampling random uncertainty, (3) other sources of random uncertainty affecting the CRV, GFCs, and MFPV (listed in Section 3.2), (4) glass formulation, and (5) the number of samples from the CRV (IHLW and ILAW compliance strategies) and MFPV (IHLW compliance strategy). For each combination of factors varied in a computer experiment, a Monte Carlo simulation was performed to determine IHLW chemical composition and corresponding uncertainties. Property-composition models for PCT, TCLP Cd release, viscosity at 1100°C, liquidus temperature, and $T_{0.01}$ were applied to the simulated IHLW compositions to obtain simulated property values. The limiting waste loading expression was also calculated for the simulation runs. Confidence intervals were then calculated for each of the compliance and processing properties and compared to the compliance and processing limits. Analyses were performed to determine the bias range within which property conditions were satisfied and how process uncertainties and sample sizes affected the allowable bias ranges. A Monte Carlo simulation approach was required because of the complicated mathematical forms of mass-balance-based equations for the compliance quantities, which would make application of variance propagation methods difficult if not impossible. Because a single MFPV batch is simulated, statistical confidence intervals are the appropriate basis to account for uncertainty in assessing whether compliance and processing limits are satisfied.
2. Assess the ILAW compliance strategy (sampling and analyzing the CRV plus masses of GFCs added to the MFPV) as well as the IHLW compliance strategy (sampling and analyzing both the HLW CRV and MFPV).	Yes	The assessments were performed using the IHLW and ILAW compliance strategies. The ILAW strategy received inputs corresponding to wastes and glasses also assessed with the IHLW strategy. The range of acceptable HLW CRV mixing/sampling solids bias was dependent on the compliance strategy used, with the ILAW compliance strategy having less uncertainty and therefore wider allowable ranges of HLW CRV mixing/sampling solids bias.
3. Determine how large mixing/sampling bias and random uncertainty can be and still meet compliance and processability requirements.	Yes	The allowable range of HLW CRV mixing/sampling bias depends on several factors, including the compliance strategy (IHLW or ILAW), the HLW CRV mixing/sampling random uncertainty, the magnitudes of other random uncertainties (discussed in Section 3.2), and the number of CRV samples (IHLW and ILAW strategies) and MFPV samples (IHLW strategy). When using the IHLW strategy, four CRV and MFPV samples, and “high” levels for other random uncertainties, there was no range of HLW CRV mixing/sampling bias that allowed compliance and processing properties to be met, even with HLW CRV mixing/sampling random uncertainty as low as 5 %RSD. Switching to the ILAW strategy and keeping the levels of other factors the same allows a HLW CRV mixing/sampling bias range of -3% to +2% when the HLW CRV mixing/sampling random uncertainty is 5 %RSD. With eight MFPV and/or CRV samples and “nominal” levels of

Table TS.1. Summary of Objectives (cont.)

Test Objective	Objective Met (Y/N)	Discussion
3. (cont.)		other random uncertainties, allowable ranges of HLW CRV mixing/sampling bias are obtained for both IHLW and ILAW strategies and with HLW CRV mixing/sampling random uncertainty ranging from 5 to 25 %RSD. For example, with the ILAW strategy and HLW CRV mixing/sampling random uncertainty of 5 %RSD, the allowable range of HLW CRV mixing/sampling solids bias is -4% to +6.5%. The allowable range decreases to -3% to +2% when HLW CRV mixing/sampling random uncertainty is 25 %RSD. See Figure 8.1 and related text in Section 8 for additional description and discussion of the results.
4. Perform the assessments using glass compositions selected to consider tradeoffs in the most limiting compliance properties.	Yes	Waste compositions from the first three tanks to be processed by WTP (AY-102/C-106, AZ-101, and AZ-102) were considered using actual waste sample data and projected waste composition estimates (outputs from the WTP Dynamic Flowsheet Model based on G2™ software) for both washed and washed-plus-leached process assumptions. The waste composition estimates used in this assessment were not developed to demonstrate WTP performance or reflect WTP design requirements. It was found that the AZ-102 actual waste sample represented the most conservative case. Several "optimized" glass compositions based on the AZ-102 actual waste sample data were used in simulations.
General Test Objectives from Test Plan TP-RPP-WTP-193 Related to Work in This Report		
5. Project the expected variations in IHLW and ILAW chemical and radionuclide compositions resulting from variations and uncertainties in HLW and LAW waste feeds and the HLW and LAW vitrification processes.	No	The work documented in this report did "propagate" uncertainties in the IHLW process for selected waste feeds and corresponding glass compositions. However, because only uncertainties for a single MFPV for each waste/glass and not variations over multiple MFPV batches comprising a waste type, were assessed, quantifying the resulting variability in chemical and radionuclide composition was not a specific objective of the work. This objective will be satisfied by separate, future work scope that will address variations over multiple MFPV batches.
6. Develop methods to relate IHLW and ILAW composition variations to variations in glass properties (e.g., durability tests such as the PCT, VHT, and TCLP) through the use of property-composition models. These methods will be used to evaluate the sensitivity of PCT, VHT, and TCLP properties to variations in glass composition. These methods will also be used in separate work scope associated with TSSs B-68 and B-73 (Develop Qualified Glass Composition Regions for ILAW and IHLW) to demonstrate that expected variations in glass properties (such as PCT, VHT, and TCLP) for each HLW or LAW waste type will remain within associated specification limits.	Partially	The simulation software was modified to include the most recent property-composition models for predicting glass properties as a function of glass composition. Although only uncertainties affecting a single MFPV batch (and not variations over several MFPV batches corresponding to a waste type) are propagated by the simulation software, methods were developed to statistically compare uncertainties in glass property values for an MFPV batch to compliance and processing limits. Separate, future work scope in the Statistical Analysis Task will quantify variations in glass properties as functions of variations in glass composition over a waste type, as well as demonstrate expected glass property variations will remain within specification limits.

Table TS.1. Summary of Objectives (cont.)

Test Objective	Objective Met (Y/N)	Discussion
7. Develop methods to demonstrate that projected IHLW and ILAW composition variations for each HLW or LAW waste type will remain within composition specification limits (e.g., waste loading and radionuclide composition limits). This work will make use of compliance methods developed as part of the B-60/62/69/70 (Statistics for IHLW and ILAW Compliance) work scope.	Partially	This work developed and implemented methods for comparing HLW waste loading (and its uncertainty) for a single MFPV batch to associated specification limits. Separate, future work scope in the Statistical Analysis Task will develop and implement methods to demonstrate that radionuclide limits are met after accounting for uncertainties affecting each MFPV batch as well as variations over MFPV batches comprising a waste type. A recent baseline change request in the WTP compliance strategy and Statistical Analysis Task work scope, which is not yet reflected in the Test Plan, is that uncertainties and variations in waste loading will no longer be addressed.
CRV = Concentrate Receipt Vessel; GFC = glass-former chemical; HLW = high-level waste; IHLW = immobilized HLW; ILAW = immobilized LAW; LAW = low-activity waste; MFPV = Melter Feed Preparation Vessel; PCT = Product Consistency Test; TCLP = Toxicity Characteristic Leach Procedure; TSS = Technical Scoping Statement; VHT = Vapor Hydration Test; WTP = Waste Treatment and Immobilization Plant.		

Table TS.2. Summary of Success Criteria and Performance

Success Criterion	Discussion of Performance on Success Criterion
1. Complete work in accordance with quality assurance (QA) requirements	All work was completed in accordance with QA requirements for related work as described in Section 5 of the Test Plan (TP-RPP-WTP-193 Rev. 1, *Test Plan: Statistical Methods for Estimating Variations in HLW and LAW Waste Types*).
2. Issue a technical report describing the work performed and the results obtained.	This technical report assesses the consequences on IHLW compliance and processing properties of bias and random uncertainty in HLW CRV mixing/sampling. Subsequent reports will address other aspects of compliance-related work.
3. Determination by the WTP Project (through review of the technical report) that the investigations and results are satisfactory and appropriate regarding the objectives.	This technical report has completed the internal PNWD review and revision cycle as well as the WTP Project review and revision cycle. This technical report has been cleared by the WTP Project for project use. Approval for public release is also envisioned.
CRV = Concentrate Receipt Vessel; HLW = high-level waste; IHLW = immobilized HLW; PNWD = Battelle—Pacific Northwest Division; WTP = Waste Treatment and Immobilization Plant	

Table TS.3. Summary of R&T Test Conditions

R&T Test Condition	Discussion of Whether the Test Condition was Followed and Any Deviations if Necessary
1. Select an appropriate waste composition(s) and corresponding glass compositions to assess effects of HLW CRV mixing/sampling bias and random uncertainty.	Glass-optimization calculations were performed on actual waste sample data for three tank wastes (AZ-101, AZ-102, and C-106) to select the waste composition best suited for subsequent statistical evaluation. The waste composition chosen (associated with AZ-102) had the smallest acceptable glass compliance and processing envelope (i.e., glass composition space over which all processing and product quality properties are predicted to be acceptable with high confidence), ensuring that the subsequent statistical investigations would yield conservative results. Glass composition and property constraints based on glass compliance and processing conditions were used to optimize the glass formulation for the selected AZ-102 waste composition, where glass property-composition models were used to estimate the glass properties. Five specific glass formulations for the selected AZ-102 waste were chosen (the compositions are listed in Table 2.5) to provide a series of tradeoffs in meeting the most constraining properties, namely waste loading (WL) and temperature for 0.01 volume-fraction crystals ($T_{0.01}$). One of the five glass formulations with the optimal tradeoff between WL and $T_{0.01}$ was selected.
2. Adapt IHLW and ILAW CRV, GFC, and MFPV "single batch" simulation capabilities to assess the consequences on compliance and processing properties of HLW CRV mixing/sampling bias and random uncertainties.	Three simulation studies were performed to vary the levels of several factors and calculate the resulting compliance and processing properties. The primary factors were HLW CRV mixing/sampling solids bias (varied between -10% and +10%, relative) and HLW CRV mixing/sampling random uncertainty (varied between 1 and 25 %RSD). In each of the three studies, a 1000-run simulation was performed for a single IHLW MFPV batch corresponding to each combination of factor levels in a test matrix. Table 4.1 summarizes the test factors and their ranges for the three simulation studies, while the specific test matrices are given in Table 4.2, Table 4.9, and Table 4.11.
3. Perform assessments using the current IHLW compliance strategy and the ILAW compliance strategy applied to the IHLW situation.	The simulation software programs corresponding to the IHLW and ILAW compliance strategies were used in this work per the test condition. The simulation software for the ILAW compliance strategy was adapted to receive inputs for the HLW waste and glass compositions selected.
CRV = Concentrate Receipt Vessel; GFC = glass-former chemical; HLW = high-level waste; IHLW = immobilized HLW; ILAW = immobilized LAW; LAW = low-activity waste; MFPV = Melter Feed Preparation Vessel; %RSD = percent relative standard deviation; WTP = Waste Treatment and Immobilization Plant.	

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Contents

Figures

Tables

1.0 Introduction

Section 1.1 discusses the background for the work performed. Sections 1.2 and 1.3 summarize the objectives and purpose of the work. Section 1.4 provides a brief overview of the approach used to address the objectives. Section 1.5 discusses the quality assurance requirements and how they were met. Section 1.6 introduces the organization of the remainder of the report.

1.1 Background

Battelle—Pacific Northwest Division (PNWD) is contracted to Bechtel National Inc. (BNI) on the River Protection Project-Waste Treatment and Immobilization Plant (RPP-WTP) project to perform research and development activities. The purpose of the RPP-WTP project is to design, construct, and commission a plant to treat and immobilize high-level waste (HLW) and low-activity waste (LAW) stored in underground storage tanks at the Hanford Site.

The immobilized high-level waste (IHLW) vitrification process of the Waste Treatment and Immobilization Plant (WTP) will be subject to variation and several uncertainties. The IHLW compositions will be subject to variation because the compositions of high-level waste (HLW) feeds will vary over time. IHLW compositions will also be subject to uncertainty because the steps of the IHLW process will be subject to mixing, sampling, chemical analysis, volume measurement, weighing, transfer, and other uncertainties. Uncertainties in IHLW compositions translate into uncertainties in IHLW compliance properties (i.e., Product Consistency Test [PCT], Toxicity Characteristic Leaching Procedure [TCLP], and waste loading), and process-control properties (e.g., viscosity and the temperature at which the volume fraction of crystals in a glass melt is 0.01 [$T_{0.01}$]) of the IHLW melts and products.

The uncertainties inherent in the IHLW process may be *systematic* and/or *random* in nature. The term *bias* is used rather than *systematic uncertainty* so that there is a clear difference in discussing *bias* versus *random uncertainty*. It is important to understand the differences between random uncertainty and bias. Random uncertainty involves the random spread of data centered on the nominal or true value. There is no systematic cause for why multiple results would differ from the nominal or true value. For example, the variation in measurements from a uniformly mixed WTP HLW Concentrate Receipt Vessel (CRV) would constitute random uncertainty (see Figure 1.1a). Bias exists when there is a systematic cause for why multiple measurements differ from the nominal or true value. For example, if solids tend to be more prevalent in the bottom of a CRV due to nonuniform mixing, then there would be a bias in the amount of solids in the bottom versus the top of the vessel (see Figure 1.1b). Because uniform mixing and perfectly representative sampling of a CRV may be difficult to achieve completely, mixing and/or sampling biases may exist. In this work, analytical results were assumed to be unbiased and contain only random uncertainties.

The WTP compliance strategies for IHLW (Nelson 2003) associated with several Waste Acceptance Product Specifications (WAPS) (DOE-EM 1996) and Contract (DOE-ORP 2000) specifications are statistically based. That is, those compliance strategies account for variations and uncertainties in meeting requirements of the specifications.

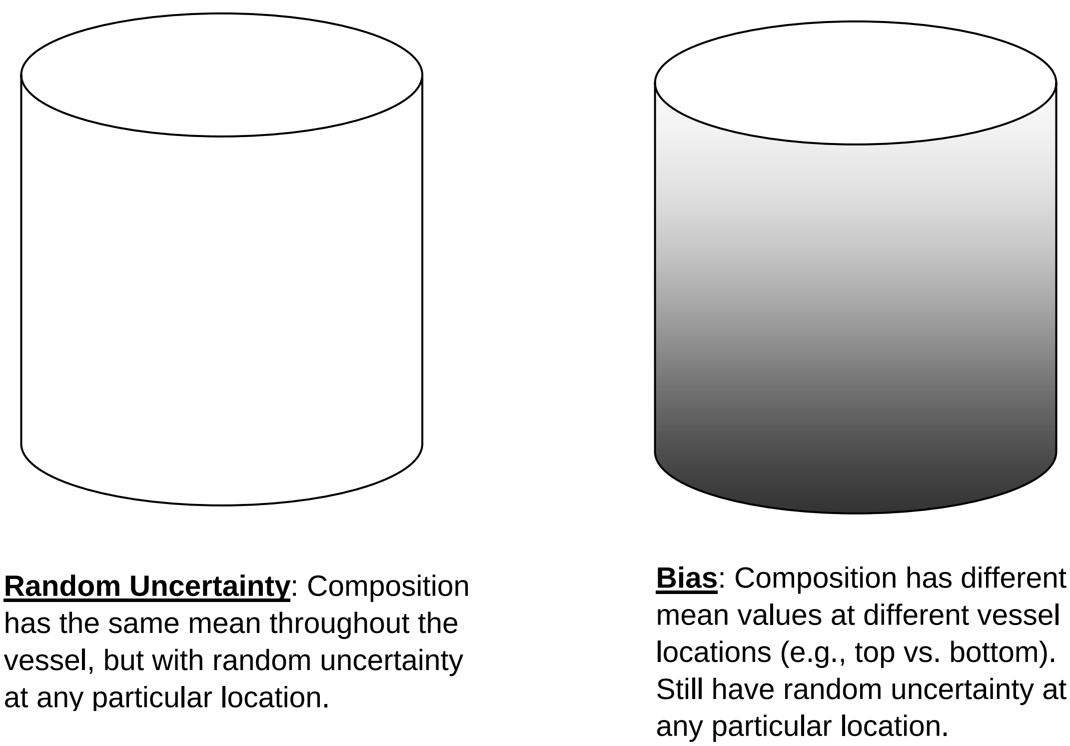

Figure 1.1. Illustration of Random Uncertainty Versus Bias

1.2 Objectives

The primary objectives of the work described in this report were to:

- Assess the impacts on IHLW compliance and processing properties (i.e., PCT, TCLP Cd release, waste loading, viscosity, liquidus temperature, and $T_{0.01}$) of mixing/sampling bias and random uncertainty in the HLW CRV.

- Determine how large mixing/sampling bias and random uncertainty can be and still meet compliance and processability requirements.

- Assess the ILAW compliance strategy (sampling and analyzing the CRV plus masses of GFCs added to the MFPV) as well as the IHLW compliance strategy (sampling and analyzing both the HLW CRV and MFPV).

- Perform the assessments using glass compositions selected to consider tradeoffs in the most limiting compliance properties. The waste composition estimates used in this assessment were not developed to demonstrate WTP performance or reflect WTP design requirements.

See Items 5 to 7 in Table TS.1 of the Testing Summary for a listing and discussion of the underlying general test plan objectives related to the preceding specific objectives.

1.3 Purpose

This report documents the work and results to statistically assess the impacts on IHLW compliance and processing properties of bias and random uncertainty in mixing/sampling waste from the HLW CRV. The impacts of other random uncertainties in the IHLW process, the number of process samples, and glass formulation were also investigated and are addressed in this report. The term “mixing/sampling” is used to denote that the effects (bias or random uncertainty) of mixing and sampling were considered jointly in this work. The reasons for this are described in a subsequent section of the report.

1.4 Approach

The approach followed to satisfy the objectives had both glass science and statistical aspects. The glass science aspect involved assessing HLW wastes to be processed by the WTP under the contract (DOE-ORP 2000), and selecting one (AZ-102) that would provide a conservative basis for the work. Five glass formulations were developed for this waste, forming a series of compromises between waste loading and $T_{0.01}$ (the temperature at which the volume fraction of crystals in glass is 0.01). These are the two most limiting glass property conditions among all compliance and processing conditions for IHLW. One of the five glasses providing the best compromise (given expected uncertainties) was selected for portions of the statistical investigation. The glass science aspects of the work, including the processing and compliance conditions considered, are discussed in detail in Section 2.

The statistical aspects of the approach involved conducting computer simulation experiments to assess the effects of HLW CRV mixing/sampling bias, CRV mixing/sampling random uncertainty, numbers of CRV and MFPV samples, other random uncertainties (discussed subsequently in Section 3.2), and using the IHLW versus the ILAW compliance strategy on satisfying processing and compliance conditions. For each combination of factors varied in the computer experiments, 1000 statistical simulations were performed using the values of random uncertainties for that combination. The 1000 simulations result in 1000 possible glass compositions corresponding to a single MFPV batch. Property-composition models were then used to calculate 1000 property values for each of the 1000 compositions for each combination of factors. The 1000 simulations for each combination of factors provided for quantifying the total composition-related uncertainty in each processing and compliance property considered. Statistical regression theory provided for quantifying the model uncertainties in predictions made with glass property-composition models. Sections 3 and 4 discuss in detail the statistical approach and test matrices used for the computer experiments.

Ultimately, glass composition and property-composition model uncertainties were combined in the form of 90% confidence intervals on glass processing and compliance properties, which were then graphically compared to the limiting values for these properties. The allowable ranges of HLW CRV mixing/sampling bias and random uncertainty were then read from the graphs. These results are discussed in detail in Sections 5, 6, and 7.

1.5 Quality Assurance

Section 1.5.1 discusses the application of RPP-WTP quality assurance (QA) requirements. Section 1.5.2 discusses the conduct of work. Section 1.5.3 discusses internal verification and validation.

1.5.1 Application of RPP-WTP Quality Assurance Requirements

PNWD implemented the RPP-WTP quality requirements by performing work in accordance with the PNWD Waste Treatment Plant Support Project quality assurance project plan (QAPjP) approved by the RPP-WTP QA organization. This work was performed to the quality requirements of NQA-1-1989 Part I, Basic and Supplementary Requirements (ASTM 1989) and NQA-2a-1990, Part 2.7 (ASTM 1990). These quality requirements are implemented through PNWD's *Waste Treatment Plant Support Project (WTPSP) Quality Assurance Requirements and Description Manual*.

A matrix that cross-references the NQA-1 and 2a requirements with the PNWD's procedures for this work is given in Attachment 2 of the Test Plan (TP-RPP-WTP-193, Rev. 1, *Test Plan: Statistical Methods for Estimating Variations in HLW and LAW Waste Types*). The matrix includes justification for those requirements not implemented. For activities associated with HLW, the additional quality assurance requirements of DOE/RW-0333P, Rev. 13, *Quality Assurance Requirements and Description* (DOE-RW 2004) were also satisfied. A listing of the procedures implementing the DOE/RW-0333P quality assurance requirements is included in Attachment 1 of the Test Plan.

1.5.2 Conduct of Experimental and Analytical Work

No physical experiments, testing, or analytical work were conducted as part of the effort documented in this report. Only computer glass formulation calculations and statistical simulation "experiments" were performed, in accordance with the WTPSP procedure QA-RPP-WTP-1101 (*Scientific Investigations*) and other procedures. The glass formulation calculations were performed in accordance with WTPSP procedure QA-RPP-WTP-SCP (*Software Control*). The mass-balance-based equations implemented in the statistical simulation software underwent Independent Technical Reviews (ITRs) according to WTPSP procedure QA-RPP-WTP-604 (*Independent Technical Review*). The simulation software and its applications also satisfied the requirements of WTPSP procedure QA-RPP-WTP-SCP. Per this procedure, a software quality assurance package was prepared and received required WTPSP reviews and approvals (including an ITR under WTPSP procedure QA-RPP-WTP-604).

As stated in the Test Specification (24590-WTP-TSP-RT-02-007, Rev. 0, *Statistical Methods for Estimating Variations in HLW and LAW Waste Types*), BNI's QAPjP, PL-24590-QA00001, is not applicable because no analytical data were generated, the work was not performed in support of environmental/regulatory testing, and the results will not be used for such purposes.

1.5.3 Internal Data Verification and Validation

PNWD addressed internal verification and validation activities by conducting ITRs of the software quality assurance package and the final report in accordance with PNWD's procedure QA-RPP-WTP-604. These reviews verify that the reported results are traceable, that inferences and conclusions are soundly based, and the reported work satisfies the Test Plan (TP-RPP-WTP-193, Rev. 1, *Test Plan:*

Statistical Methods for Estimating Variations in HLW and LAW Waste Types) objectives. The QA-RPP-WTP-604 review procedure is part of PNWD's *WTPSP Quality Assurance Requirements and Description Manual*.

1.6 Organization of the Remainder of the Report

Section 2 discusses the glass formulation optimization performed to select the glass formulations investigated in this work. Section 3 discusses the Monte Carlo simulation approach and computer experiments performed to assess the impacts on compliance and processing conditions of varying HLW CRV mixing/sampling bias and random uncertainty as well as other factors. Section 4 discusses the three simulation studies performed, including the test matrices and inputs used for the computer simulation experiments. Sections 5, 6, and 7 present and discuss the results from the three simulation studies. Section 8 summarizes and discusses the results. Section 9 lists the references cited in the report.

2.0 Glass-Formulation Optimization

This section describes the glass formulation optimization to select the waste composition best suited for statistical simulations and to calculate optimized glass compositions from the selected waste that have the best chance of satisfying the compliance conditions. The following subsections discuss (1) the waste compositions evaluated in this study, (2) glass property and composition constraints, (3) models used to estimate the glass properties, and (4) the method and results of glass-formation calculations.

2.1 Waste Compositions

Waste compositions used in the assessment include actual waste-sample data, as well as projected waste compositions in the CRV based on calculations with the WTP Dynamic Flowsheet Model (G2). Table 2.1 summarizes the compositions of three actual HLW samples used in this study. The composition of AZ-101 leached sludge is from Urie et al. (2002). The composition of AZ-102 was a modified version of that reported by Smith et al. (2001). The measured CdO concentration (on an oxide basis) in the sludge was 4.18 mass%, as reported by Smith et al. (2001). At this concentration, the TCLP response became a crucial issue for glass formulation. The current RPP-WTP Contract (DOE-ORP 2000) allows for lower waste loading to comply with Resource Conservation and Recovery Act (RCRA) regulations, which complicates the optimization approach. The WTP mass balance flowsheet and G2 models were evaluated to determine the maximum CdO concentration expected in any HLW batch, which was estimated to be 1.85 mass%. So, to avoid the unnecessary complication of TCLP response limitations, the CdO concentration in AZ-102 tank sludge was reduced to 1.85 mass% while keeping the relative proportions of all other components constant. The AY-102/C-106 composition was given by Porier et al. (2003). All these compositions are for pretreated (washed, leached, and washed in a Cells Unit Filter) HLW sludge.

The oxide compositions from G2 output were collected for CRV batches corresponding to HLW feeds from the first three HLW feed tanks (AY-102/C-106, AZ-101, and AZ-102). The data were generated from G2 runs MRQ-03-090 (for washed and leached) and MRQ-03-128 (for washed only). There were 34 washed-only HLW CRV batches and 29 washed-and-leached HLW CRV batches. Table 2.2 summarizes the composition ranges for these batches. Only the components with mass fraction 0.10 or higher at least in one waste batch were included in Table 2.2. However, the complete compositions were used in the calculations. The compositions from the G2 output (masses of ions and radionuclides in kg) were converted into mass fractions of oxides either to be consistent with the composition of actual waste samples, or to be used in the glass property-composition models (discussed in the next section). Then all waste-oxide compositions were normalized to sum to 1. Note that the waste composition estimates in Table 2.2 were not developed to demonstrate WTP performance or reflect WTP design requirements.

Table 2.1. Compositions (Mass Fractions)[(a)] of Actual Waste Samples

Oxide	AZ-101	AZ-102 Modified CdO[(b)]	AY-102/ C-106
Ag_2O	0.0012	0.0006	0.0020
Al_2O_3	0.2314	0.2357	0.1358
B_2O_3	0.0043	0.0006	0.0000
BaO	0.0021	0.0011	0.0014
BeO	0.0001	0.0001	0.0000
Bi_2O_3	0.0002	0.0000	0.0000
CaO	0.0134	0.0146	0.0103
CdO	0.0203	0.0185	0.0003
Ce_2O_3	0.0075	0.0017	0.0036
Cl	0.0018	0.0015	0.0000
CoO	0.0000	0.0002	0.0002
Cr_2O_3	0.0045	0.0028	0.0060
Cs_2O	0.0000	0.0003	0.0000
CuO	0.0009	0.0009	0.0009
F	0.0005	0.0004	0.0000
Fe_2O_3	0.3544	0.3725	0.3719
K_2O	0.0043	0.0008	0.0000
La_2O_3	0.0083	0.0092	0.0018
Li_2O	0.0003	0.0000	0.0016
MgO	0.0031	0.0037	0.0032
MnO	0.0104	0.0283	0.0584
MoO_3	0.0001	0.0000	0.0013
Na_2O	0.1084	0.0913	0.1561
Nd_2O_3	0.0061	0.0064	0.0000
NiO	0.0156	0.0235	0.0109
P_2O_5	0.0126	0.0142	0.0119
PbO	0.0023	0.0029	0.0132
PdO	0.0032	0.0000	0.0000
Rh_2O_3	0.0008	0.0000	0.0000
RuO_2	0.0024	0.0000	0.0000
SiO_2	0.0381	0.0195	0.1707
SnO_2	0.0000	0.0051	0.0189
SO_3	0.0000	0.0007	0.0000
SrO	0.0049	0.0457	0.0057
TiO_2	0.0004	0.0003	0.0008
UO_2	0.0277	0.0498	0.0117
V_2O_5	0.0000	0.0000	0.0005
Y_2O_3	0.0000	0.0005	0.0000
ZnO	0.0004	0.0013	0.0008
ZrO_2	0.1076	0.0451	0.0000
Total	1.0000	1.0000	1.0000

(a) The mass fractions in this table were rounded to four decimal places.
(b) The maximum CdO mass fraction of 0.0185 predicted by the G2 model was used instead of 0.0418 measured in the actual waste sample.

Table 2.2. Waste Oxide Composition (Mass Fraction)[(a)] Ranges from G2 Output for First Three Source Tanks[(b)]

Oxide	Washed and Leached		Washed Only	
	Min	Max	Min	Max
Al_2O_3	0.1655	0.1898	0.2091	0.3092
CdO	0.0004	0.0185	0.0003	0.0109
Cr_2O_3	0.0024	0.0033	0.0027	0.0044
Fe_2O_3	0.4280	0.4663	0.3269	0.3819
MnO	0.0122	0.0518	0.0097	0.0422
Na_2O	0.1268	0.1702	0.1598	0.2487
NiO	0.0074	0.0178	0.0043	0.0131
SiO_2	0.0007	0.0145	0.0007	0.0239
SrO	0.0007	0.0013	0.0005	0.0011
UO_2	0.0101	0.0291	0.0084	0.0211
ZrO_2	0.0001	0.0991	0.0001	0.0651
Ag_2O	0.0001	0.0013	0.0001	0.0010
B_2O_3	0.0004	0.0038	0.0003	0.0027
BaO	0.0026	0.0031	0.0019	0.0025
CaO	0.0100	0.0251	0.0077	0.0212
Ce_2O_3	0.0040	0.0066	0.0029	0.0054
Cs_2O	0.0000	0.0011	0.0000	0.0009
F	0.0005	0.0047	0.0005	0.0033
K_2O	0.0047	0.0104	0.0051	0.0103
La_2O_3	0.0048	0.0135	0.0039	0.0095
Li_2O	0.0003	0.0032	0.0003	0.0019
MgO	0.0068	0.0144	0.0056	0.0110
Nd_2O_3	0.0040	0.0100	0.0033	0.0072
P_2O_5	0.0017	0.0041	0.0037	0.0069
PbO	0.0095	0.0340	0.0083	0.0277
Pr_6O_{11}	0.0012	0.0018	0.0008	0.0013
RuO_2	0.0004	0.0019	0.0003	0.0016
SO_3	0.0005	0.0039	0.0011	0.0125
ThO_2	0.0009	0.0021	0.0006	0.0018
WO_3	0.0001	0.0010	0.0001	0.0008
ZnO	0.0006	0.0015	0.0004	0.0011

(a) The mass fractions in this table were rounded to four decimal places.
(b) Waste tanks AZ-101, AZ-102, and AY-102/C-106.

2.2 Compliance and Processing Conditions

The RPP-WTP compliance strategy for meeting WAPS (DOE-EM 1996) and Contract (DOE-ORP 2000) specifications for IHLW is discussed by Nelson (2003). In addition to satisfying applicable compliance conditions, IHLW produced by the RPP-WTP must also satisfy several processing conditions. The following paragraphs describe each of the compliance and processing conditions considered in selecting optimized glass formulations.[a] In cases where uncertainties in the compliance or process variables are to be accounted for in the WTP HLW compliance and process control strategies, they were accounted for in developing optimized glass formulations. For such cases, the type of statistical interval used to quantify the uncertainty in model predictions of compliance or processing properties is noted in the discussion. The types of statistical intervals are discussed further in Section 2.3.

2.2.1 Compliance Conditions

Three compliance conditions were factored into the glass composition optimization. These conditions are briefly described in the following paragraphs.

IHLW produced by the RPP-WTP must satisfy limits on PCT (ASTM 1998) normalized releases of boron (r_B), lithium (r_{Li}), and sodium (r_{Na}). The PCT normalized releases must remain below the prescribed limits of 8.35 g/m^2 for r_B, 4.79 g/m^2 for r_{Li}, and 6.68 g/m^2 for r_{Na} (Jantzen et al. 1993). The uncertainty for models relating the natural logarithm of PCT normalized releases to HLW glass composition was calculated using 95% simultaneous confidence intervals (SCIs) (see Section 2.3).

To be compliant, IHLW produced by the RPP-WTP must have TCLP releases below the proposed delisting limits (Cook and Blumenkranz 2003). For the wastes evaluated in this study, cadmium (Cd) is the only RCRA constituent present in high enough concentrations to be of concern (Kot et al. 2003). The proposed delisting limit for the TCLP Cd release, c_{Cd}, is 0.48 mg/L. The uncertainty in the model relating ln(c_{Cd}) to glass composition was calculated using a 90% confidence interval (CI) (see Section 2.3), as specified by Cook and Blumenkranz (2003).

Compliance for waste loading (WL) is based on the constraints in Table TS-1.1 of the WTP Contract (DOE-ORP 2000). These constraints specify the minimum fraction of a component or sum of components in glass that must be from the waste for at least one such component or sum of components. Waste-loading compliance is achieved if the *WL factor* is above 1 for at least one component or sum of components. For a given glass formulation, the WL factor is defined as the fraction of a component or sum of components in glass from the waste, relative to (that is, divided by) the corresponding TS-1.1 limit value. Hence, to satisfy a given WL limit from Table TS-1.1 of the WTP Contract (DOE-ORP 2000), the WL factor must be greater than one. According to the WTP Project compliance strategy for waste loading, composition uncertainty need not be accounted for in demonstrating waste-loading compliance.[b] However, this decision was made after a substantial portion of the work in this report (which accounted for composition uncertainties in WL) was completed. It was decided to present the results of accounting for waste-loading uncertainty in this report so that the WTP Project would have those results for informational purposes.

(a) Many property and composition conditions/constraints are typically applied to the development of waste glass compositions. Only those key conditions/constraints critical to determining if a glass can be fabricated with uncertain and varying compositions were applied in this study.
(b) Note that this decision is not reflected in the current WTP IHLW compliance strategy (Nelson 2003), but it will be reflected therein the next time that document is revised.

2.2.2 Processing Conditions

Two processing conditions were factored into the glass composition optimization. These conditions are briefly described in the following paragraphs.

The processing condition for crystals in the WTP HLW melter is based on $T_{0.01}$, defined as the temperature at which the equilibrium volume fraction of crystals in glass is 0.01 (on a quenched glass basis). The condition is that $T_{0.01}$ should remain below the limit of 950˚C. This condition is imposed to avoid the accumulation of crystals in the melter, which may disrupt the power distribution in the melter or the ability to pour glass from the melter. According to the WTP HLW melter design basis document (Clarke 2003), the melter should be able to continually operate with a glass melt that has a liquidus temperature (T_L) of less than or equal to 950°C.[a] In the design basis document, T_L is not defined, rather it refers to the System Description (Peters and Casassa 2003). That document states that T_L is defined by Kot et al. (2001), in which T_L is defined as the temperature at which up to one volume percent of slow settling crystals exist in equilibrium with the melt. This is effectively the same as $T_{0.01}$, used in this study.

The model uncertainty for $T_{0.01}$ was calculated using 90% SCIs (see Section 2.3). Although not used as a processing condition for glass composition optimization, the T_L of glass (defined here as the highest temperature at which crystals exist at equilibrium with the melt) is a similar processing property that was calculated and considered as part of the work. In summary, the condition $T_{0.01} \leq 950°C$ has been used in WTP melter design and testing and was used in this study. Meanwhile, T_L (a related property), was calculated but not used as a formulation condition.

For the glass-optimization work discussed in this report, viscosity at 1150˚C (η_{1150}) was restricted to be between 25 and 60 poise. Also, viscosity at 1100˚C (η_{1100}) was restricted to be between 10 and 150 poise. The uncertainties for the models relating $\ln(\eta_{1150})$ and $\ln(\eta_{1100})$ to HLW glass composition were calculated using a 90% CI (see Section 2.3).

2.3 Glass-Composition and Property Constraints

Several glass-composition and property constraints were assumed for the glass formulation optimization. Constraints were primarily lower and/or upper limits on single components, sums of components, and glass-property estimates from property-composition models. The property-composition models used to optimize glass formulation include:

- models for PCT normalized releases of boron, lithium, and sodium (r_B, r_{Li}, r_{Na}) vs. composition from Piepel and Cooley (2003)
- model relating viscosity (η) to temperature and composition from Gan et al. (2004)
- model relating TCLP Cd release concentration (c_{Cd}) to composition from Kot et al. (2003)
- model relating temperature at 1% crystals ($T_{0.01}$) to composition from Vienna et al. (2003).

(a) The minimum melt cavity temperature was estimated to 961°C during idling and normal operation. However, temperatures as low as 826°C were estimated in the pour region of the melter for periods of up to 473 minutes during normal operation.

A model for T_L from Vienna et al. (2003) was also considered, but not restricted in optimizing glass formulations.

The models for spinel phase-field $T_{0.01}$ and T_L, as well as PCT $\ln(r_B)$, $\ln(r_{Li})$, and $\ln(r_{Na})$, had the typical first-order mixture model form:

$$f(P) = \sum_{i=1}^{N} a_{P,i} g_i^N \tag{2.1}$$

where

$$g_i^N = \frac{g_i}{\sum_{i=1}^{N} g_i} \quad \text{where} \quad \sum_{i=1}^{N} g_i^N = 1 \tag{2.2}$$

and $f(P)$ = function of property P
$a_{P,i}$ = i^{th} component coefficient for the property P
g_i = mass fraction of i^{th} component in glass
N = number of components in glass for which the model was fit (dependent on property P)
g_i^N = normalized mass fraction of i^{th} model component.

In Equation 2.1, $f(T_{0.01}) = T_{0.01}$, and $f(r_i) = \ln(r_i)$ for i = B, Li, and Na.

The model used to estimate TCLP $\ln(c_{Cd})$ had the form:

$$ln(c_{Cd}) = \sum_{i=1}^{N} a_{cCd,i} g_i^N + b_1 \, ln(g_{CdO}) \tag{2.3}$$

where $a_{cCd,i}$ is the coefficient of the i^{th} normalized oxide component (g_i^N), and b_1 is the coefficient of the natural logarithm of unnormalized CdO (g_{CdO}) in the HLW glass.

The model for viscosity as a function of temperature and composition was given as:

$$ln(\eta_T) = \frac{1}{T^2} \sum_i a_{\eta,i} g_i + b_0 \tag{2.4}$$

where T = absolute temperature
$a_{\eta,i}$ = i^{th} component coefficient
g_i = unnormalized mass fraction of the i^{th} component in glass
b_0 = a constant coefficient.

Note that the summation is over components i selected to appear in the model.

Table 2.3 lists the coefficients and goodness-of-fit statistics (R^2, R^2_A, and s) for the models used based on Equations (2.1), (2.3), and (2.4). R^2 is the fraction of variation in a modeled response property

Table 2.3. Summary of Model Coefficients Used to Estimate Constrained Glass Properties

Component	$a_{\eta,i}$ η in poise	$a_{T0.01,i}$ $T_{0.01}$ in °C	$a_{TL,I}$ [(a)] T_L in °C	PCT $a_{rB,i}$ r in g/m^2	PCT $a_{rLi,I}$ r in g/m^2	PCT $a_{rNa,i}$ r in g/m^2	TCLP $a_{cCd,i}$ c in mg/L
Al_2O_3	37891514.9	3391.671	2831.304	-10.1923	-7.7581	-9.8577	0.3234
B_2O_3	-2159757.3	378.066	755.683	5.5843	3.2707	2.4722	8.6749
BaO	---[(b)]	---	---	---	16.4840	---	---
CaO	---	---	---	-12.3992	-17.2629	-6.8451	---
CdO	15321023.8	---	6240.569	---	---	---	21.6666
Cr_2O_3	75211455.7	27121.869	25944.901	---	---	---	---
F	---	---	5337.415	---	---	---	---
Fe_2O_3	6194895.3	3637.894	2759.090	-1.9050	-4.6857	-2.6664	1.0137
K_2O	---	---	-1211.097	---	120.4309	---	---
Li_2O	-60583987.6	-2655.938	-2019.216	10.9736	11.5538	11.7138	9.4055
MgO	---	---	2233.803	---	-25.1557	---	---
MnO	2628377.0	2852.645	1862.042	---	---	---	6.4471
Na_2O	-10331075.2	-1786.463	-827.133	12.9950	10.7807	16.8788	10.1264
NiO	19582478.7	13169.614	9316.218	---	---	---	---
P_2O_5	---	---	-3949.229	---	---	---	---
Sb_2O_3	-140193402.2	---	---	---	---	---	---
SeO_2	162438842.9	---	---	---	---	---	---
SiO_2	26918300.2	393.836	862.703	-4.4708	-3.0641	-4.8793	-0.9421
SrO	-8115167.1	-479.834	---		-3.3994	-11.1662	6.6293
ThO_2	---	---	1766.893	-124.0320		-115.9263	-0.5965
TiO_2	---	---	---	---	-44.3963	---	---
Tl_2O_3	12149218.8	---	---	---	---	---	---
UO_2	---	---	---	---	4.1184	---	8.776
U_3O_8	---	---	2270.202	---	---	---	---
ZnO	---	---	---	---	-10.4650	---	14.3107
ZrO_2	21982480.7	4056.761	2122.182	---	-7.7551	---	0.6811
b_0	-2.42258	---	---	---	---	---	---
b_1	---	---	---	---	---	---	0.9085
Observations (n)	240	41	160	42	41	44	101
Parameters (p)	16	11	17	8	15	9	14
R^2	0.961	0.869	0.892	0.854	0.907	0.877	0.981
Adjusted R^2	0.958	0.825	0.880	0.795	0.819	0.820	0.978
s	0.2790	53.492	32.183	0.4310	0.3156	0.4114	0.2049

(a) The T_L model was not used for glass formulation calculations but was used in the statistical simulation studies discussed in Sections 3 through 6.
(b) Denotes that this term was not included in the model.

[i.e., $f(P)$] accounted for by the model and can take values from 0 to 1. R^2_A is the fraction of variation in a modeled response property, adjusted for the number of fitted coefficients in the model. Finally, s is the root mean squared error (RMSE) of prediction errors, calculated from the data used to fit a model by (1) taking the sum-of-squares of differences in measured and predicted $f(P)$ values, (2) dividing by the model degrees-of-freedom, $n - p$, where n is the number of data points used to fit the p coefficients in the model, and (3) taking the square root. If the model does not have a statistically significant lack-of-fit (LOF), then s = RMSE is an estimate of the experimental error standard deviation in fabricating glasses and measuring $f(P)$.

Two types of model-uncertainty measures were used, both of which are uncertainties on the mean property response [i.e., $f(P)$] for composition $\boldsymbol{x}$. The first model-uncertainty measure is for the mean $f(P)$ on a single composition $\boldsymbol{x}$, based on a CL% CI:

$$u_{CL\%\,CI} = t_{CL,n-p}\, s\sqrt{\boldsymbol{x}'\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}\boldsymbol{x}}\ . \tag{2.5}$$

The second model uncertainty measure is for the mean $f(P)$ values corresponding to any set of compositions $\boldsymbol{x}$, based on a CL% SCI [(a)]:

$$u_{CL\%\,SCI} = s\sqrt{p\,F_{CL,p,n-p}\ \boldsymbol{x}'\left(\boldsymbol{X}'\boldsymbol{X}\right)^{-1}\boldsymbol{x}} \tag{2.6}$$

In Equations (2.5) and (2.6),

$u_{CL\%\,CI}$ = uncertainty of a model prediction at composition $\boldsymbol{x}$ corresponding to the width of an upper CL% confidence interval on the mean transformed property $f(P)$

$u_{CL\%\,SCI}$ = uncertainty of a model prediction at composition $\boldsymbol{x}$ corresponding to the width of an upper CL% simultaneous confidence interval on the mean transformed property $f(P)$ values for any set of compositions $\boldsymbol{x}$

CL = confidence level in percent (e.g., 90% or 95%)

$t_{CL,n-p}$ = CL^{th} percentile of a t-distribution with $n - p$ degrees-of-freedom (df) at the given confidence level

$F_{CL,p,n-p}$ = CL^{th} percentile of an F-distribution with p numerator df and $n - p$ denominator df at the given confidence level

s = root mean square error

p = number of fit parameters in the model

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

$\boldsymbol{x}$ = composition vector of the glass for which the property is being predicted

$\boldsymbol{X}$ = matrix of glass compositions used to fit the model

$'$ = a matrix or vector transpose

"-1" superscript = a matrix inverse.

In general, uncertainties based on SCIs are larger than uncertainties based on single CIs because an SCI provides the desired confidence level for the application of a model to any number of compositions,

---

(a) Based on the statistical theory, the set can contain an infinite number of compositions and provide the stated simultaneous confidence about the mean $f(P)$ values for all such compositions.

whereas a CI only provides the desired confidence for a single composition at a time. Hence, CIs are narrower than SCIs. However, there is a higher probability of one or more CIs not containing the mean $f(P)$ as the number of CIs for different $\boldsymbol{x}$ compositions increases.

Table 2.4 summarizes the constraints used for glass-optimization calculations, including their lower and upper limits and purposes. Note that only $T_{0.01}$ (and not T_L) was constrained for the glass-formulation optimization. The glass-property constraints account for model uncertainties in determining the acceptable boundaries, as discussed in Section 2.2. Out of the 25 waste-loading constraints given in Table TS-1.1 of the WTP Contract (DOE-ORP 2000), the four that are relevant to the current evaluation[(a)] are given in Table 2.4.

Table 2.4. Glass-Composition and Property Constraints Used for Glass-Formulation Optimization

Constraints	Lower Limit	Upper Limit	Purpose
Glass Property Constraints			
$T_{0.01} + u$ (90% SCI), °C	---[(a)]	950	Melter processability
η (at 1150°C) - u (90% CI), poise	25	---	
η (at 1150°C) + u (90% CI), poise	---	60	
η (at 1100°C) - u (90% CI), poise	10	---	
η (at 1100°C) + u (90% CI), poise	---	150	
TCLP $c_{Cd} + u$ (90% CI), mg/L	---	0.48	Delisting
PCT $r_B + u$ (95% SCI), g/m^2	---	8.35	Waste acceptance
PCT $r_{Li} + u$ (95% SCI), g/m^2	---	4.79	
PCT $r_{Na} + u$ (95% SCI), g/m^2	---	6.68	
Waste Loading Constraints (minimum mass fraction from waste for at least one constraint)			
Fe_2O_3	0.125	---	TS-1.1 WL factor = 1 (only the active constraints are listed)
Al_2O_3	0.11	---	
$Fe_2O_3 + Al_2O_3 + ZrO_2$	0.21	---	
$Al_2O_3 + ZrO_2$	0.14	---	
Single-Component Constraints (in mass fraction)			
Al_2O_3	0.03	---	Model validity (only the active constraints are listed)
B_2O_3	0.05	---	
CdO	---	0.016	
Fe_2O_3	---	0.14	
Li_2O	---	0.05	
Na_2O	0.05	0.15	
SiO_2	0.35	0.53	
ZnO	0.02	---	
(a) --- denotes that no limit was imposed.			

(a) For the possible glass compositions corresponding to the waste compositions in this evaluation, only 4 of the 25 waste loading conditions have any chance of being violated.

The property-composition models, as empirical relationships, are only valid over fixed component concentration ranges. Model validity constraints were added to ensure that the glass composition did not deviate from the ranges of model validity. Although there are some differences in the validity ranges between models, one set of the single-component ranges that are common for all the property models was used for the simplicity of glass-optimization calculations. Only single-component concentration constraints were used to define the model-validity range, although, in some cases, multi-component constraints were used to develop the glass-property data used for model fitting. Table 2.4 also lists these single-component constraints for model validity.

2.4 Glass Formulation Calculations

The glass composition is calculated from a mass balance:

$$g_i = W\, w_i + (1 - W)\, a_i \tag{2.7}$$

where g_i = mass fraction of the i^{th} component in glass
W = mass fraction of waste in glass (simply called "waste loading")
w_i = mass fraction of the i^{th} component in waste
a_i = mass fraction of the i^{th} component in additives.

The initial optimization calculation involves finding the maximum W for each waste while satisfying all the constraints listed in Table 2.4. The W is always limited by more than one constraint after one of the Table TS-1.1 constraints is met. Stated in another way, other constraints must be satisfied in addition to satisfying one of the Table TS-1.1 limits for there to be an acceptable composition. For example, if one of the property constraints was met for a particular waste, the additive composition would be adjusted until at least one additional constraint was met, including model-validity constraints. For a glass limited by a single-component concentration constraint for components that come from waste, a unique optimum composition cannot be obtained.

The initial optimization process revealed that the $T_{0.01}$ constraint is the most limiting property for all wastes in this study, accompanied by one or more single-component constraints (i.e., within single-component constraints). The maximum WL factor[a] at $T_{0.01} + u$ = 950°C represents one of the primary compliance and processing envelope boundaries. The resulting maximum WL factor values for three waste compositions are shown at the $T_{0.01} + u$ = 950°C axis in Figure 2.1.

The second step was to calculate the value of $T_{0.01} + u$ at WL factor = 1 for each of the three wastes considered. The resulting $T_{0.01} + u$ values are plotted on the WL factor = 1 axis in Figure 2.1. Then, finally, the WL-factor values were calculated for varied values of $T_{0.01} + u$ to define the extent of the glass compliance and processing envelope for each waste composition. Figure 2.1 shows that the WL factor increases as the $T_{0.01} + u$ value increases and reaches a maximum value at $T_{0.01} + u$ = 950°C for AZ-101 and AZ-102. However, for AY-102/C-106 waste, the WL factor reaches the maximum value before the $T_{0.01} + u$ reaches 950°C because the concentration of Fe_2O_3 in glass reaches the single-component

(a) See Section 2.2.1 for a definition of WL factor.

constraint (model-validity constraint) starting at $T_{0.01} + u = 864°C$. Figure 2.1 shows that, among three actual waste samples used in this study, AZ-102 represents the bounding case (i.e., it has the smallest acceptable glass compliance and processing envelope).

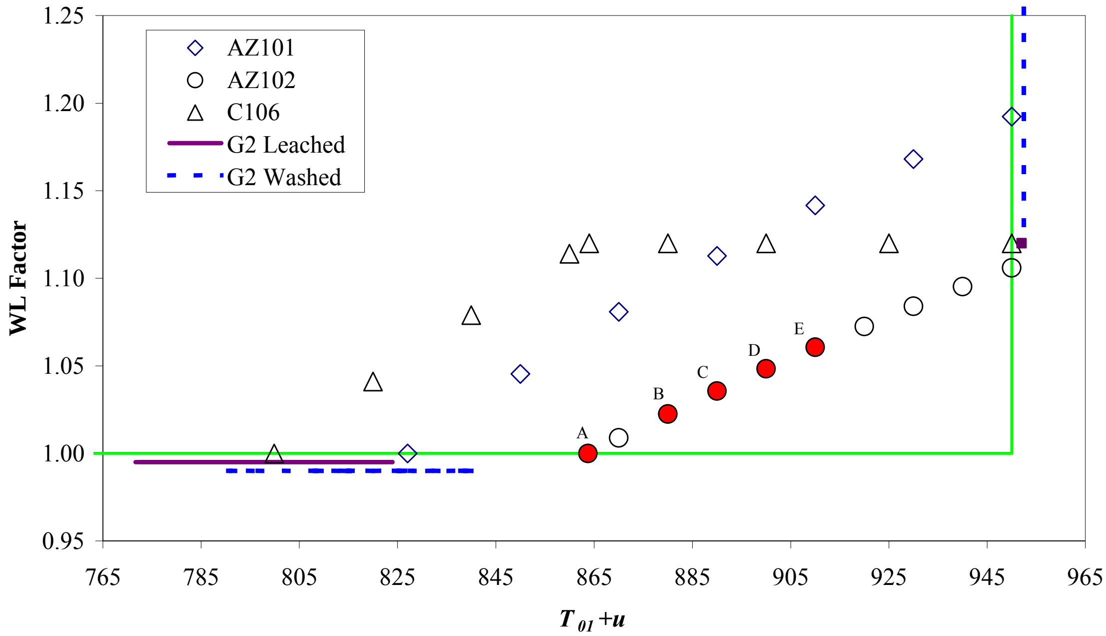

Figure 2.1. Plot of WL Factor Versus $T_{0.01} + u$ for Three Actual Waste Compositions and G2 Output Compositions Leached and Washed

The glass-optimization for G2 compositions was performed to check if there are any potential waste compositions that have smaller compliance and processing envelopes than AZ-102. The maximum WL factors at $T_{0.01} + u = 950°C$ and the $T_{0.01} + u$ values at WL factor = 1 were calculated for all the 34 washed-only HLW CRV batches and the 29 washed-and-leached HLW CRV batches. Figure 2.1 shows the results using bars representing: (1) the range of WL factor values at $T_{0.01} + u = 950°C$ and (2) the range of $T_{0.01} + u$ values at WL factor = 1. The WL factor at $T_{0.01} + u = 950°C$ for leached HLW CRV batches is constant at 1.12 (i.e., no range and thus only a filled square rather than a bar is shown in Figure 2.1) because it reached the model-validity constraint for Fe_2O_3 as in the AY-102/C-106 waste case above. Figure 2.1 shows that the AZ-102 case is bounding and, therefore, was used for detailed statistical evaluation.

2.5 Glass Formulations Selected for Assessment

To help identify the appropriate level of mixing and sampling uncertainties in the HLW CRV, specific glasses were selected from the boundary of the AZ-102 actual waste-sample processing window displayed in Figure 2.1. Because composition uncertainties would cause the properties to cross constraint boundaries, glasses away from the two limiting axes were selected. It was further assumed that the composition uncertainties would be more significant for the $T_{0.01}$ property than for the WL factor, so the glasses closer to the WL factor = 1 axis were selected. In other words, in Figure 2.1, glasses near the center or to the left of the center of AZ-102 glasses would allow for the largest possible composition uncertainty and bias before failing a constraint. The five selected formulations were labeled “A”, “B”, “C”, “D”, and “E”, as shown in Figure 2.1. The compositions of these five glass formulations are listed in Table 2.5.

Table 2.5. Compositions (Mass Fractions)[(a)] of Five AZ-102 Glass Formulations Selected for Investigation in the Statistical Simulations

Oxide	AZ-102 Glass Formulations[(b)]				
	A	B	C	D	E
Ag_2O	0.000180	0.000185	0.000187	0.000189	0.000191
Al_2O_3	0.076137	0.077839	0.078833	0.079790	0.080716
B_2O_3	0.062215	0.060577	0.059480	0.058373	0.057258
BaO	0.000368	0.000376	0.000381	0.000385	0.000390
BeO	0.000030	0.000030	0.000031	0.000031	0.000031
CaO	0.004737	0.004842	0.004904	0.004964	0.005021
CdO	0.005929	0.006063	0.006141	0.006217	0.006290
Ce_2O_3	0.000551	0.000563	0.000570	0.000578	0.000584
Cl	0.000527	0.000538	0.000545	0.000551	0.000558
CoO	0.000059	0.000060	0.000061	0.000062	0.000063
Cr_2O_3	0.000919	0.000939	0.000952	0.000963	0.000975
Cs_2O	0.000098	0.000101	0.000102	0.000103	0.000104
CuO	0.000282	0.000289	0.000292	0.000296	0.000299
F	0.000121	0.000124	0.000126	0.000127	0.000129
Fe_2O_3	0.119434	0.122136	0.123713	0.125232	0.126702
K_2O	0.000259	0.000265	0.000269	0.000272	0.000275
La_2O_3	0.002950	0.003017	0.003056	0.003094	0.003130
Li_2O	0.038791	0.039621	0.040224	0.040881	0.041586
MgO	0.001228	0.001255	0.001270	0.001285	0.001299
MnO	0.009064	0.009269	0.009389	0.009505	0.009616
Na_2O	0.150000	0.150000	0.150000	0.150001	0.150001
Nd_2O_3	0.002058	0.002104	0.002131	0.002158	0.002183
NiO	0.007532	0.007702	0.007802	0.007898	0.007990
P_2O_5	0.004565	0.004668	0.004729	0.004787	0.004843
PbO	0.000925	0.000946	0.000959	0.000970	0.000982
SiO_2	0.443812	0.438192	0.434935	0.431770	0.428682
SnO_2	0.000255	0.000260	0.000264	0.000267	0.000270
SO_3	0.001624	0.001661	0.001683	0.001703	0.001723
SrO	0.014656	0.014988	0.015182	0.015369	0.015549
TiO_2	0.000136	0.000137	0.000138	0.000139	0.000140
UO_2	0.015966	0.016327	0.016538	0.016742	0.016938
Y_2O_3	0.000151	0.000154	0.000156	0.000158	0.000160
ZnO	0.020000	0.020000	0.020000	0.020000	0.020001
ZrO_2	0.014440	0.014767	0.014957	0.015141	0.015319
Total	1.000000	1.000000	1.000000	1.000000	1.000000

(a) The mass fractions in this table were rounded to six decimal places.
(b) Only waste loading and GFC compositions change from glasses A to E. The waste constituents are in the same relative proportions for all five glasses.

3.0 Simulation of Glass Compositions and Properties

The impacts on compliance and processing properties of HLW CRV mixing/sampling bias and random uncertainty were assessed using computer experiments. A *computer experiment* is similar to a *physical experiment* in that several factors are varied to assess the impacts on one or more response variables of interest. However, a computer experiment is performed using software calculations rather than physically performing experiments and measuring response variables. In this case, software was used to simulate the IHLW vitrification process from the CRV to the Melter Feed Preparation Vessel (MFPV), with glass compositions that would be made from the MFPV contents being the result. Section 3.1 provides an overview discussion of the simulation approach.

The simulation software implemented the mass-balance-based equations from the IHLW and immobilized low-activity waste (ILAW) compliance strategies currently planned for use by the WTP. The mass-balance-based equations calculate the chemical composition (as mass fractions) of the HLW glass that would be made from the MFPV contents. Section 3.2 provides an overview of the calculation approaches based on the two compliance strategies and explains why the equations from the ILAW compliance strategy were investigated along with the equations from the IHLW compliance strategy.

After the simulation software calculated glass compositions corresponding to MFPV contents, values of compliance and processing properties were calculated using models or equations. Section 3.3 discusses the glass properties calculated for simulated glass compositions as part of this work.

3.1 Overview of the Computer Experiment and Simulation Approach

Computer experiments were performed to assess the impact of HLW mixing/sampling bias and random uncertainty, as well as several other factors, on the ability to meet compliance and processing conditions. The computer experiments varied the magnitudes of several factors:

- Glass composition (the five compositions based on AZ-102 waste as discussed in Section 2)
- CRV mixing/sampling bias
- CRV mixing/sampling random uncertainty
- Other random uncertainties relevant to the IHLW or ILAW compliance strategy (see Section 3.2)
- The numbers of samples (with one chemical analysis per sample) for each CRV batch (IHLW and ILAW compliance strategies) and MFPV batch (IHLW compliance strategy).

For each combination of factors varied in a computer experiment, a Monte Carlo simulation was performed to determine IHLW chemical composition and corresponding uncertainties. Property-composition models for PCT, TCLP Cd release, viscosity at 1100°C, T_L, and $T_{0.01}$ were applied to the simulated IHLW compositions to obtain simulated property values. CIs were then calculated for each of the compliance and processing properties and compared to the compliance and processing limits. Analyses were performed to determine the ranges of CRV mixing/sampling bias and random uncertainty within which compliance and processing limits were met and how process uncertainties and sample sizes affected these ranges.

A Monte Carlo simulation approach was required because of the complicated mathematical forms of mass-balance-based equations for calculating the composition of glass that would be made from an HLW

MFPV batch. With complicated mathematical equations, variance propagation methods are difficult if not impossible to apply. Hence, Monte Carlo methods were used. A flowchart explaining the Monte Carlo simulation approach is shown in Figure 3.1. Because a single MFPV batch is simulated, statistical confidence intervals are the appropriate basis for quantifying uncertainties in calculated glass compositions and in compliance and processing properties calculated from the glass compositions. The specific types of confidence intervals used in this work are described in the subsections of Section 3.3.

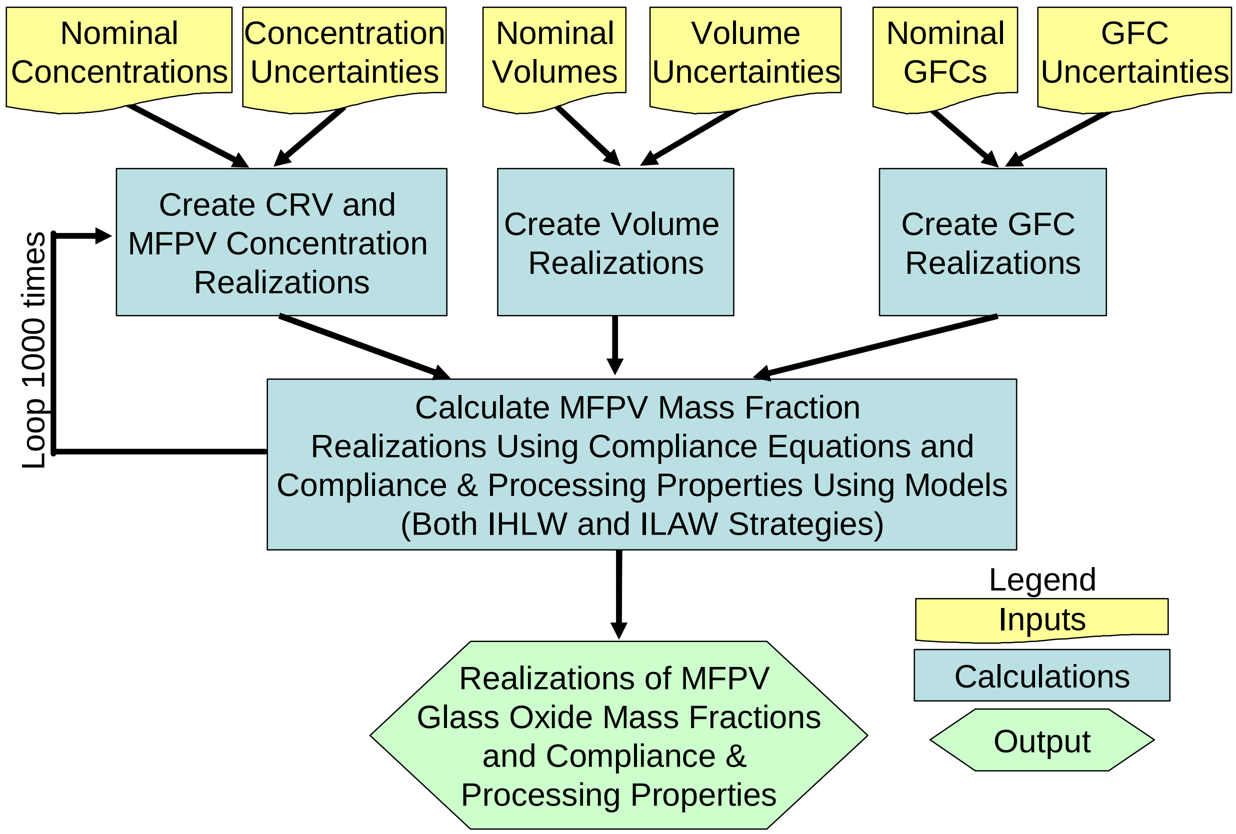

Figure 3.1. Flowchart of the Monte Carlo Simulation Approach

The Monte Carlo simulations start with nominal values of all variables appearing in the mass-balance-based equations for calculating IHLW chemical composition. These variables are the ones that would be measured during the WTP HLW vitrification process, according to the IHLW or ILAW compliance strategy being followed. Nominal values of all these variables were obtained for each of the five glass compositions discussed in Section 2.5. The simulations then introduce random uncertainties into the equations for IHLW chemical composition. The magnitudes of the random uncertainties used are based on previous knowledge or past history. Some of these random uncertainties are documented in an interim report by Heredia-Langner et al. (2003) while others are documented for the first time in this report (see Section 4). Nominal uncertainties and higher uncertainties (usually 2× the nominal uncertainties) were used to bound the expected range for the uncertainties. Using “nominal” and “high” uncertainties also provided for assessing the effects of different magnitudes of uncertainties on compliance and processing properties. Each set of random uncertainties is simulated 1000 times to obtain a distribution of glass compositions (mass fractions) corresponding to a single MFPV batch. The simulated glass compositions (mass fractions) are then used to calculate compliance and processing properties so that there are 1000 simulated values for each of these properties also. This simulation process provides for calculating and understanding the total uncertainty in the glass composition as well as compliance and processing properties and thus for understanding the confidence that compliance and processing conditions will be satisfied.

Some simulation runs were made with biases in the HLW CRV nominal compositions, corresponding to biases that might result from incomplete mixing of CRV batches and/or biased sampling of CRV batches. The manner in which biases were handled is discussed in Section 4.

3.2 IHLW and ILAW Calculation Strategies

Glass compositions (mass fractions) that would be made from HLW MFPV contents were calculated using two different approaches for each simulation. The first approach used the IHLW compliance strategy. The second approach used the ILAW compliance strategy applied to the IHLW process. Each strategy is now discussed in turn.

3.2.1 Calculations for the IHLW Strategy

The sampling locations and other measurements to be taken based on the WTP IHLW compliance strategy are discussed in the *IHLW Product Compliance Plan* (IHLW PCP) (Nelson 2003). The equations for calculating glass compositions (mass fractions) corresponding to the contents of an HLW MFPV batch, using the IHLW compliance strategy, are from the working document *Compliance Equations for IHLW Chemical Composition*, Rev. A.6. That working document will be incorporated in an appendix of technical report WTP-RPT-072, *Interim Report: Statistical Aspects of WTP IHLW and ILAW Compliance*, which is currently being written and will be issued later in 2004.

The equations for calculating chemical composition are based on chemical analyses of HLW CRV samples and MFPV samples after the glass-former chemicals (GFCs) have been added. The IHLW compliance strategy does not use the direct measurements of masses of GFCs before they are added to the MFPV. Because the masses of GFCs must be estimated from analyses of samples under the IHLW compliance strategy using complicated calculations (in the previously mentioned working document), it is expected that this strategy will have larger uncertainty than the ILAW compliance strategy.

Several other random uncertainties (in addition to HLW CRV mixing/sampling random uncertainty) affect the calculation of compliance and processing properties according to the IHLW compliance strategy. These include:

- CRV analytical
- CRV volume before a transfer to the MFPV
- CRV volume after a transfer to the MFPV
- Oxide compositions of each GFC
- MFPV mixing/sampling

- MFPV analytical
- MFPV volume before a transfer from the CRV
- MFPV volume after a transfer from the CRV
- MFPV volume after addition of GFCs

For work summarized in this report, it was assumed that only random uncertainties and not bias affected these other factors. Specific values of these random uncertainties used in this work are presented in Section 4.

3.2.2 Calculations for the ILAW Strategy

The sampling locations and other measurements to be taken based on the WTP ILAW compliance strategy are discussed in the *ILAW Product Compliance Plan* (ILAW PCP) (Nelson et al. 2003). The ILAW PCP nominally addresses the strategy for complying with ILAW specifications in the WTP Contract (DOE-ORP 2000). The equations for calculating glass compositions (mass fractions) corresponding to the contents of an HLW MFPV batch, using the ILAW compliance strategy, are from the working document *Compliance Equations for ILAW Chemical Composition*, Rev. B.4. That working document will be incorporated in an appendix of technical report WTP-RPT-072, *Interim Report: Statistical Aspects of WTP IHLW and ILAW Compliance*, which is currently being written and will be issued later in 2004.

The ILAW compliance strategy calculates glass compositions that would be made from HLW MFPV contents based on analyses of CRV samples, certified compositions of GFCs, and measured masses of individual GFCs added to the MFPV. The HLW MFPV is not sampled and analyzed under the ILAW compliance strategy. The ILAW strategy is expected to yield glass compositions (and thus compliance and processing properties calculated from the glass compositions) with smaller uncertainties than the IHLW strategy. The ILAW strategy was investigated in this work, along with the IHLW strategy, to provide input to future decisions regarding possible changes to the IHLW compliance strategy.

Several other random uncertainties (in addition to HLW CRV mixing/sampling random uncertainty) affect the calculation of compliance and processing properties according to the ILAW compliance strategy. These include:

- CRV analytical
- CRV volume before a transfer to the MFPV
- CRV volume after a transfer to the MFPV
- MFPV volume before a transfer from the CRV
- MFPV volume after a transfer from the CRV
- Oxide composition of each GFC
- Mass of each GFC added to MFPV

For work summarized in this report, it was assumed that only random uncertainties and not bias affected these other factors. Specific values of these random uncertainties used in this work are presented in Section 4.

3.3 Compliance and Processing Properties

The following subsections describe (1) the compliance and processing properties and (2) the specific types of statistical confidence intervals used to quantify uncertainties in the properties, which were used to assess whether compliance and processing limits were satisfied for compositions resulting from the simulations performed. It was decided to use 90% confidence levels in this work, based on our judgment that 90% is the minimum defensible confidence for demonstrating that a compliance or processing property satisfies its specified limit. The use of 90% confidence should not be taken as an indication that this is the preferred or recommended confidence level for meeting all compliance and processing requirements. There is precedent at other HLW vitrification plants in the United States (e.g., DWPF and WVDP) that 95% confidence be used for some or all compliance and processing properties. In fact, that is why 95% SCIs were used to quantify PCT model uncertainty in the glass formulation optimization work (see Section 2.2.1 and Table 2.5). Note that it is not a discrepancy or error that 95% confidence was used to address PCT model uncertainty for glass formulation selection in Section 2, but that 90% confidence was used to address all uncertainties in the computer simulation experiments. The glass formulation selection and computer simulation experiments were separate aspects of the work.

When demonstrating that compliance properties are satisfied during WTP operations, it is recommended that the WTP report the confidence level actually achieved (e.g., 99.9% confidence) rather than to just report satisfying a compliance criterion at a pre-set confidence level such as 90% or 95%. Reporting the actual confidence level achieved allows for making a much stronger statement about having satisfied the compliance conditions.

3.3.1 Product Consistency Test (PCT)

PCT is a compliance property for WTP IHLW, as discussed in Section 2.2.1. PCT normalized releases of B, Li, and Na were calculated for glass compositions (mass fractions) resulting from the simulations using the models presented previously in Table 2.3. As discussed previously, the PCT normalized releases must remain below the prescribed limits to be compliant. These limits are 8.35 g/m^2 for B, 4.78 g/m^2 for Li, and 6.67 g/m^2 for Na.

To assess compliance, 90% upper combined confidence intervals (90% UCCIs) were calculated for comparison to the PCT limits. The UCCIs were calculated by adding to the nominal PCT value from the simulation the model uncertainty and the composition uncertainty. The model uncertainty was calculated using the 90% SUCI uncertainty formula in Equation (2.6). The composition uncertainty was based on the 90th percentile from the simulation results, which provides an empirical 90% UCI. The 90% confidence levels were chosen as the minimum defensible (as discussed in Section 3.3) for demonstrating compliance with the PCT limits. The fact that the Defense Waste Processing Facility (DWPF) and West Valley Demonstration Project (WVDP) have used 95% confidence levels for demonstrating PCT compliance suggests that such higher confidence levels may be preferred in future work and during WTP IHLW production. Figure 3.2 illustrates the 90% UCCI concept for PCT.

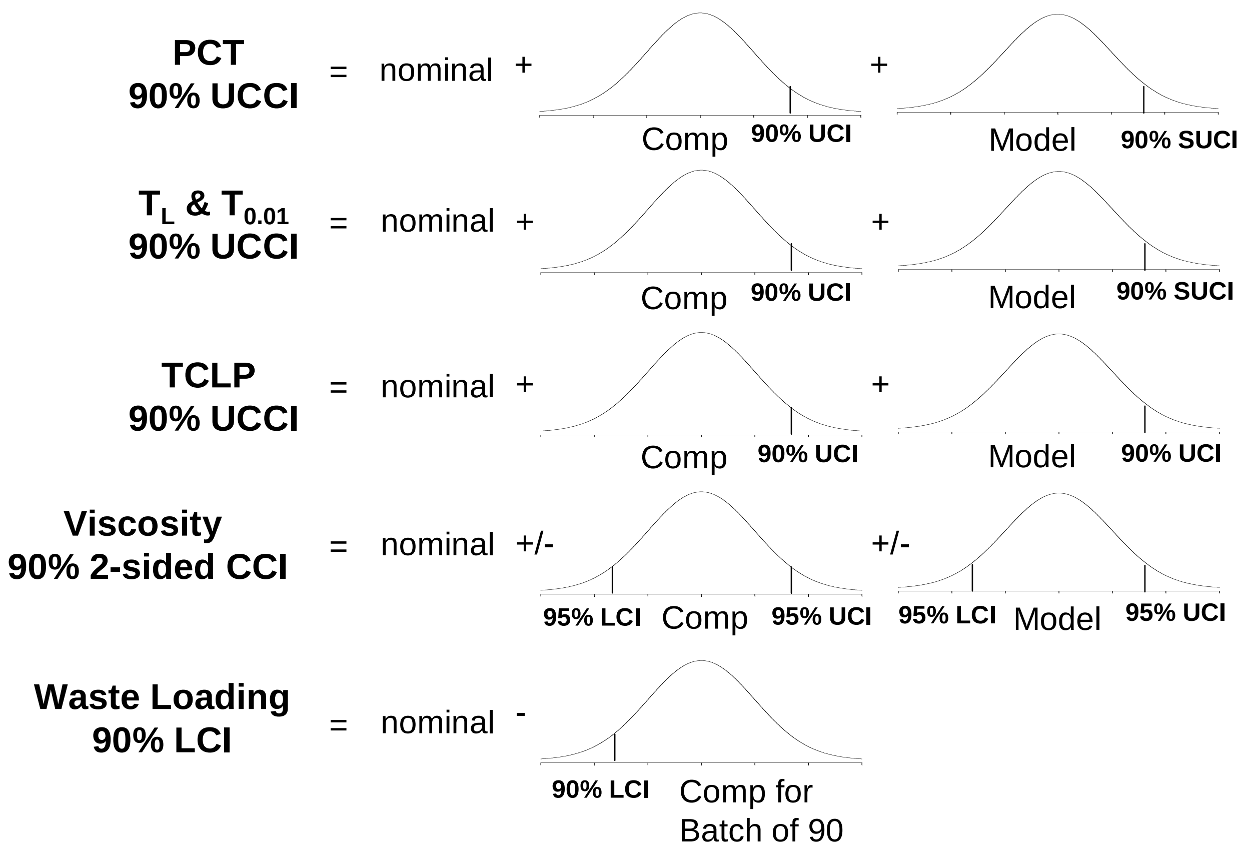

Figure 3.2. Illustrations of Statistical Intervals Used with Each Property

3.3.2 Liquidus Temperature

T_L is a processing property for WTP IHLW, as discussed in Section 2.2.2. T_L (°C) values were calculated for glass compositions (mass fractions) resulting from the simulations using the T_L model presented previously in Table 2.3. T_L values must remain below the limit of 950°C to satisfy the current WTP design-basis processing constraint. However, the WTP Project is considering a switch to a 950°C limit on $T_{0.01}$, with no limit on T_L (as discussed in Section 2.2.2). Hence, it was decided to calculate T_L and $T_{0.01}$ values and their uncertainties as part of the work summarized in this report.

90% UCCI values were calculated for comparison to the T_L processing limit. The 90% UCCIs were calculated by adding the nominal T_L value from the simulation to the model uncertainty and the composition uncertainty. The model uncertainty was calculated using the 90% SCI uncertainty formula in Equation (2.6). The composition uncertainty was based on the 90th percentile from the simulation results, which provides an empirical 90% UCI. Figure 3.2 illustrates the 90% UCCI concept for T_L.

3.3.3 Temperature for One Volume Percent of Crystals in the Glass ($T_{0.01}$)

$T_{0.01}$ (°C) is a processing property for WTP IHLW, as discussed in Section 2.2.2. $T_{0.01}$ values were calculated for glass compositions (mass fractions) resulting from the simulations using the model presented previously in Table 2.3. The WTP Project is considering a processing constraint that would require $T_{0.01}$ values to remain below a limit of 950°C.

90% UCCI values were calculated for comparison to the $T_{0.01}$ processing limit. 90% UCCIs were calculated by adding to the nominal $T_{0.01}$ value from the simulation the model uncertainty and the composition uncertainty (both expressed in property units of °C). The model uncertainty was calculated using the 90% SCI uncertainty formula in Equation (2.6). The composition uncertainty was based on the 90^{th} percentile from the simulation results, which provides an empirical 90% UCI. Figure 3.2 illustrates the 90% UCCI concept for $T_{0.01}$.

3.3.4 Waste Loading (WL)

WL is a compliance property for WTP IHLW, as discussed in Section 2.2.1. WL values were calculated for glass compositions (mass fractions) resulting from the simulations using the compliance equations given in the working document *Compliance Equations for IHLW Waste Loading*, Rev. A. That working document will be incorporated in an appendix of technical report WTP-RPT-072, *Interim Report: Statistical Aspects of WTP IHLW and ILAW Compliance*, which is currently being written and will be issued later in 2004. WL is expressed as the mass percent of an oxide or group of oxides in the waste. Although there are many waste-loading conditions as discussed in Section 2.2.1, the waste loading requirement is satisfied if any one of the conditions is met. For AZ-102 glasses, the applicable waste-loading condition is on $Al_2O_3 + Fe_2O_3 + ZrO_2$. The limit for this condition is 21%, meaning that the sum of the mass-percent oxides must be at or above the limit to be in compliance.

To assess compliance, 90% lower confidence intervals (LCIs)[a] were calculated for comparison to the WL limit. The 90% LCIs were calculated by subtracting from the nominal WL value for a given glass the composition uncertainty in WL (i.e., the uncertainty in $Al_2O_3 + Fe_2O_3 + ZrO_2$) as determined from the simulation. The composition uncertainty in WL for a single MFPV batch was obtained as the 10^{th} percentile from the simulation results, which provides an empirical 90% LCI. Figure 3.2 illustrates the 90% LCI concept for WL. However, the WTP IHLW compliance strategy (Nelson 2003) calls for demonstrating that the average WL over glass corresponding to a waste type satisfies the compliance conditions. For purposes of this work, the variation in WL over the MFPV batches corresponding to an HLW waste type was assumed to be equal to three times the uncertainty for a given MFPV batch. Further, it was assumed that a waste type for purposes of WL compliance would be a whole waste tank (e.g., AZ-102). The WTP Project has estimated that an HLW tank will yield four to six HLW Blend Vessels (HBVs). For this work, five HBVs per HLW tank were assumed. Then, with nine CRV batches per HBV and two MFPV batches per CRV batch, an HLW tank (waste type) would yield $5 \times 9 \times 2 = 90$ MFPV batches. Thus, the composition uncertainty for the average WL over 90 MFPV batches was used.

(a) The term "90% lower confidence interval" rather than "90% lower combined confidence interval" was used because only composition uncertainty is applicable, given that there is no model (or model uncertainty) for waste loading.

As discussed previously in Section 2.2.1, the WTP Project has decided to revise the compliance strategy for waste loading so that it does not involve accounting for composition uncertainty in demonstrating waste-loading compliance. This decision was made after a substantial portion of the work in this report (which accounted for composition uncertainties in WL) was completed. Also, this WTP Project decision has not yet been incorporated in a revision of the IHLW PCP (Nelson 2003). Hence, it was decided to present the results of accounting for WL uncertainty in this report so that the WTP Project would have those results for informational purposes. Some results are also presented without accounting for WL uncertainty.

3.3.5 3.3.5 TCLP Cd Release Concentration

TCLP Cd release concentration (mg/L) is a compliance property for WTP IHLW, as discussed in Section 2.2.1. TCLP Cd releases were calculated for glass compositions (mass fractions) resulting from the simulations using the model presented previously in Table 2.3. TCLP Cd release concentrations must remain below the limit of 0.48 mg/L to be compliant.

To assess compliance, 90% UCCIs were calculated for comparison to the TCLP Cd release limit. The 90% UCCIs were calculated by adding to the nominal TCLP Cd release concentration from the simulation the model uncertainty and the composition uncertainty. The model uncertainty was calculated using the formula associated with a 90% UCI as given in Equation (2.5). A 90% UCI rather than a 90% simultaneous UCI (90% SUCI) was used in keeping with a decision in the data quality objectives report for delisting (Cook and Blumenkranz 2003). The composition uncertainty was based on the 90th percentile from the simulation results, which provides an empirical 90% UCI. Figure 3.2 illustrates the 90% UCCI concept for TCLP Cd release.

3.3.6 Viscosity at 1100°C

Viscosity at 1100°C (poise) is a processing property for the WTP IHLW, as discussed in Section 2.2.2. Viscosity at 1100°C values were calculated for glass compositions (mass fractions) resulting from the simulations using the viscosity model presented previously in Equation (2.4) with coefficients in Table 2.3. Viscosity at 1100°C values should remain between the limits of 10 and 150 poise for IHLW to be processable.

Two-sided 90% combined confidence intervals (CCIs) consisting of 95% lower combined confidence intervals (LCCIs) and UCCIs for viscosity at 1100°C were calculated for comparison to the viscosity processability limits. Two-sided 90% CCIs were calculated by adding and subtracting the model uncertainty and the composition uncertainty from the nominal viscosity value for each simulation. The model uncertainty was calculated as two-sided 90% CIs (i.e., 95% LCIs and UCIs) using the formula given in Equation (2.5). The composition uncertainty was based on the 5th and 95th percentiles from the simulation results, which provide an empirical two-sided 90% CI. Figure 3.2 illustrates the 90% two-sided CCI concept for viscosity at 1100°C.

4.0 Experimental Designs and Inputs for the Simulation Studies

Three simulation studies were conducted to assess the impact of HLW CRV mixing/sampling bias and/or random uncertainty, as well as other factors, on the ability to satisfy IHLW compliance and processing conditions. The main differences in the three simulation studies are summarized in Table 4.1. Details of the experimental designs (test matrices) and inputs for each of the three simulation studies are presented in Sections 4.1, 4.2, and 4.3.

Table 4.1. Overview of Three Simulation Studies to Assess the Impacts of HLW CRV Mixing/Sampling Bias and Random Uncertainty

Factors Varied in Simulation Study	**Levels of Factors for Each Simulation Study**		
	1	**2**	**3**
Compliance strategy	IHLW, ILAW	IHLW, ILAW	IHLW, ILAW
Glass formulations (#)	5	1	1
Mixing/sampling random (%RSD)	1, 5, 10, 15	5, 10	5, 15, 25
Other uncertainties[(a)]	Nominal, High	Nominal High	Nominal
CRV/MPFV Samples (#)	4, 8	8 4	8
Mixing/sampling solids bias (% relative)	(b)	-10, -5, 0, +5, +10	-10, -5, 0, +5, +10
Number factor combinations studied	160	20	30

(a) Other random uncertainties corresponding to the IHLW and ILAW compliance strategies are discussed in Section 3.2. The values of "nominal" and "high" uncertainties for each are discussed in Sections 4.1 to 4.3.
(b) Not varied in this study.

4.1 Simulation Study #1 to Assess CRV Mixing/Sampling Random Uncertainty

Section 4.1.1 presents the experimental design (test matrix) used in the computer experiment simulation to assess the effects of CRV mixing/sampling random uncertainties and other factors on satisfying compliance and processing conditions. Section 4.1.2 presents the inputs used for this simulation study. Subsequently in this report, this simulation study is referred to as Simulation Study #1.

4.1.1 Experimental Design for Simulation Study #1 to Assess CRV Mixing/Sampling Random Uncertainty

An experimental design (test matrix) was created to assess the effects of the following factors on satisfying compliance and processing conditions:

- All five glass formulations (A, B, C, D, and E as discussed in Section 2.5)

- Four levels of CRV mixing/sampling random uncertainty quantified in terms of percent relative standard deviation (%RSD[a])
- Nominal and high levels of other uncertainties (see Section 3.2)
- Either four or eight CRV (IHLW and ILAW compliance strategies) and MFPV (IHLW compliance strategy) samples with one analysis per sample.[b]

The test matrix for Simulation Study #1 is listed in Table 4.2 and contains a total of $5 \times 4 \times 2 \times 2 = 80$ combinations of the four factors studied. The "Other Uncertainties" column in Table 4.2 includes the following separate sources of random uncertainty: CRV analytical, MFPV mixing/sampling, MFPV analytical, GFC composition, GFC masses added to MFPV, CRV volumes, and MFPV volumes. Based on previous work, it was decided to only investigate one analysis per sample within the CRV and MFPV and only one volume measurement for a given volume determination. Each of the 80 test cases consisted of a simulation with 1000 runs, creating a distribution of MFPV glass compositions (mass fractions) for each test case. These 1000 glass compositions for each test case were then used to calculate 1000 values of each of the compliance and processing properties. From these sets of 1000 values, measures of total composition-related uncertainty for a single MFPV batch were calculated, as discussed in Section 3.3.

The test matrix in Table 4.2 was run in each of two separate simulations, one with the IHLW compliance strategy, and one with the ILAW compliance strategy, as discussed previously in Section 3.2.

4.1.2 Inputs for Simulation Study #1 to Assess CRV Mixing/Sampling Random Uncertainty

Inputs associated with process samples, analyses, and measurements according to the IHLW and ILAW compliance strategies were necessary to perform the simulations for each of the five glass compositions associated with AZ-102 (see Section 2.5 and Table 2.5). These inputs describe both nominal values and uncertainties necessary to simulate the IHLW process from the CRV to the MFPV and calculate MFPV glass compositions using the mass-fraction equations corresponding to the compliance strategy used (IHLW or ILAW). Table 4.3 lists the CRV nominal elemental concentrations for AZ-102 and the MFPV nominal elemental concentrations corresponding to each of the five glass compositions (A, B, C, D, and E).

Table 4.4 gives simulation inputs for the HLW CRV analytical uncertainties, MFPV analytical uncertainties, and MFPV mixing/sampling uncertainties. Each of these uncertainties is given as a %RSD. The "nominal" and "high" uncertainties listed in Table 4.4 were provided by representatives of the WTP analytical laboratory group, who considered analytical uncertainties from Tables 5.5 and 5.7 of Heredia-Langner et al. (2003), as well as professional judgment. Heredia-Langner et al. (2003) reported that no data were available on HLW MFPV sampling and analytical uncertainties. Hence, the estimates of those uncertainties provided by the WTP analytical laboratory group in Table 4.4 are new. Finally, it is noted

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(a) %RSD = percent RSD (the relative standard deviation multiplied by 100%).

(b) The CRV and MFPV samples were assumed to be taken from the designed sampling locations in each vessel with the designed sampling methods, although the specifics of these locations and methods are not important, as only the mixing/sampling uncertainty values used had impact on the results. The multiple samples are assumed to be taken over time as the vessels are mixed and before transfer operations between vessels.

Table 4.2. Simulation Study #1 Test Matrix to Assess HLW CRV Mixing/Sampling Random Uncertainties

Test Case	Glass Formulation	CRV Mixing/ Sampling %RSD	Other[(a)] Uncertainties	CRV/MFPV # Samples	Test Case	Glass Formulation	CRV Mixing/ Sampling %RSD	Other[(a)] Uncertainties	CRV / MFPV # Samples
1	A	1	Nominal	4	41	C	1	High	4
2	A	1	Nominal	8	42	C	1	High	8
3	A	5	Nominal	4	43	C	5	High	4
4	A	5	Nominal	8	44	C	5	High	8
5	A	10	Nominal	4	45	C	10	High	4
6	A	10	Nominal	8	46	C	10	High	8
7	A	15	Nominal	4	47	C	15	High	4
8	A	15	Nominal	8	48	C	15	High	8
9	A	1	High	4	49	D	1	Nominal	4
10	A	1	High	8	50	D	1	Nominal	8
11	A	5	High	4	51	D	5	Nominal	4
12	A	5	High	8	52	D	5	Nominal	8
13	A	10	High	4	53	D	10	Nominal	4
14	A	10	High	8	54	D	10	Nominal	8
15	A	15	High	4	55	D	15	Nominal	4
16	A	15	High	8	56	D	15	Nominal	8
17	B	1	Nominal	4	57	D	1	High	4
18	B	1	Nominal	8	58	D	1	High	8
19	B	5	Nominal	4	59	D	5	High	4
20	B	5	Nominal	8	60	D	5	High	8
21	B	10	Nominal	4	61	D	10	High	4
22	B	10	Nominal	8	62	D	10	High	8
23	B	15	Nominal	4	63	D	15	High	4
24	B	15	Nominal	8	64	D	15	High	8
25	B	1	High	4	65	E	1	Nominal	4
26	B	1	High	8	66	E	1	Nominal	8
27	B	5	High	4	67	E	5	Nominal	4
28	B	5	High	8	68	E	5	Nominal	8
29	B	10	High	4	69	E	10	Nominal	4
30	B	10	High	8	70	E	10	Nominal	8
31	B	15	High	4	71	E	15	Nominal	4
32	B	15	High	8	72	E	15	Nominal	8
33	C	1	Nominal	4	73	E	1	High	4
34	C	1	Nominal	8	74	E	1	High	8
35	C	5	Nominal	4	75	E	5	High	4
36	C	5	Nominal	8	76	E	5	High	8
37	C	10	Nominal	4	77	E	10	High	4
38	C	10	Nominal	8	78	E	10	High	8
39	C	15	Nominal	4	79	E	15	High	4
40	C	15	Nominal	8	80	E	15	High	8

(a) The "other uncertainties" are identified for each of the IHLW and ILAW compliance strategies in Section 3.3. The nominal and high values of these uncertainties are listed in subsequent tables of Section 4.

Table 4.3. AZ-102 CRV and MFPV Nominal Elemental Concentrations for the Five Glass Compositions

Element	CRV Concentrations (mg/L)	MFPV Concentrations (mg/L) for Glass				
		A	B	C	D	E
Ag	87.564	73.306	73.688	73.905	74.111	74.305
Al	20828.910	17579.210	17665.780	17715.140	17761.670	17805.720
B	31.867	8429.440	8067.545	7843.5130	7625.102	7411.944
Ba	171.549	143.616	144.364	144.790	145.192	145.573
Be	5.546	4.643	4.667	4.681	4.694	4.706
Bi	0	0	0	0	0	0
Ca	1747.778	1476.871	1484.082	1488.193	1492.069	1495.738
Cd	2703.627	2264.146	2275.921	2282.633	2288.962	2294.956
Ce	245.027	205.129	206.198	206.807	207.381	207.925
Cl	253.101	229.993	230.887	231.418	231.930	232.425
Co	24.210	20.268	20.373	20.434	20.490	20.544
Cr	324.113	274.218	275.643	276.463	277.243	277.986
Cs	48.392	40.512	40.723	40.843	40.957	41.064
Cu	117.491	98.360	98.872	99.164	99.439	99.700
F	63.275	52.972	53.248	53.405	53.554	53.694
Fe	43499.630	36443.380	36632.250	36739.910	36841.420	36937.560
Hg	0	0	0	0	0	0
K	112.154	93.892	94.381	94.660	94.923	95.171
La	1310.925	1097.467	1103.183	1106.441	1109.514	1112.423
Li	0	7861.943	7893.055	7934.394	7988.182	8052.625
Mg	369.197	323.165	324.439	325.174	325.870	326.533
Mn	3658.081	3062.437	3078.387	3087.479	3096.052	3104.171
Mo	0	0	0	0	0	0
Na	11311.560	48546.270	47718.290	47248.720	46804.440	46382.160
Nd	919.302	769.612	773.621	775.906	778.060	780.101
Ni	3084.077	2581.898	2595.345	2603.010	2610.238	2617.083
P	1038.160	869.117	873.644	876.224	878.657	880.961
Pb	447.690	374.793	376.745	377.858	378.907	379.901
Pd	0	0	0	0	0	0
Pr	0	0	0	0	0	0
Rh	0	0	0	0	0	0
Ru	0	0	0	0	0	0
Se	0	0	0	0	0	0
Si	1522.818	90503.270	87833.06	86322.240	84888.100	83520.680
S	43.835	44.538	44.703	44.815	44.930	45.049
Sn	666.785	558.213	561.120	562.777	564.340	565.820
Sr	6458.220	5406.630	5434.791	5450.841	5465.977	5480.310
Ta	0	0	0	0	0	0
Th	0	0	0	0	0	0
Ti	28.702	35.505	35.286	35.162	35.045	34.932
U	7333.920	6139.740	6171.719	6189.945	6207.134	6223.411
V	0	0	0	0	0	0
Y	61.945	51.859	52.129	52.283	52.428	52.565
Zn	170.371	7010.069	6890.540	6822.736	6758.607	6697.685
Zr	5570.609	4663.548	4687.838	4701.683	4714.738	4727.102

Table 4.4. Uncertainties in CRV and MFPV Elemental Concentrations

Element	CRV Analytical %RSD		MFPV Mixing/ Sampling %RSD		MFPV Analytical %RSD	
	Nominal	High[(a)]	Nominal	High	Nominal	High[(a)]
Ag	50	50	5	15	50	50
Al	5	10	5	15	5	10
B	50	50	5	15	5	10
Ba	15	30	5	15	15	30
Be	50	50	1	5	50	50
Bi	N/A[(b)]	N/A	N/A	N/A	N/A	N/A
Ca	10	20	5	15	10	20
Cd	5	10	5	15	5	10
Ce	50	50	5	15	50	50
Cl	5	10	1	5	10	20
Co	50	50	5	15	50	50
Cr	10	20	5	15	10	20
Cs	15	30	1	5	15	30
Cu	20	40	5	15	20	40
F	10	20	1	5	10	20
Fe	5	10	5	15	5	10
Hg	N/A	N/A	N/A	N/A	N/A	N/A
K	50	50	1	5	50	50
La	10	20	5	15	10	20
Li	50	50	1	5	10	20
Mg	50	50	5	15	50	50
Mn	5	10	5	15	5	10
Mo	N/A	N/A	N/A	N/A	N/A	N/A
Na	5	10	1	5	5	10
Nd	7[(c)]	14	5	15	10	20
Ni	5	10	5	15	5	10
P	10	20	5	15	10	20
Pb	50	50	5	15	50	50
Pd	N/A	N/A	N/A	N/A	N/A	N/A
Pr	N/A	N/A	N/A	N/A	N/A	N/A
Rh	N/A	N/A	N/A	N/A	N/A	N/A
Ru	N/A	N/A	N/A	N/A	N/A	N/A
Se	N/A	N/A	N/A	N/A	N/A	N/A
Si	50	50	5	15	5	10
S	50	50	1	5	50	50
Sn	10	20	5	15	10	20
Sr	5	10	5	15	5	10
Ta	N/A	N/A	N/A	N/A	N/A	N/A
Th	N/A	N/A	N/A	N/A	N/A	N/A
Ti	50	50	5	15	50	50
U	10	20	5	15	10	20
V	N/A	N/A	N/A	N/A	N/A	N/A
Y	50	50	5	15	50	50
Zn	10	20	5	15	10	20
Zr	5	10	5	15	5	10

(a) "High" case is two times the "Nominal" case, with the exception that when the "Nominal" case is 50 %RSD, the "High" case is also 50 %RSD.
(b) N/A denotes "not applicable, because these elements had zero nominal concentrations in Table 4.3.
(c) Although no other element had 7 %RSD, this value for Nd is the one provided by WTP analytical laboratory experts.

that the high values of analytical uncertainties specified in Table 4.4 are sometimes smaller and sometimes larger than the "required precisions" specified in Table D.3 of Kaiser et al. (2003). Table D.3 of that document specifies required precision of ≤ 20 %RSD for non-radionuclides and some radionuclides measured in units of μg/mL, and < 15 %RSD for radionuclides measured in units of μCi/mL. Kaiser et al. (2003) note that their Table D.3 is based on results from Patello et al. (1999) as well as professional judgment. However, Tables 7.1 and 7.2 of Patello et al. (1999) show required precisions of < 15 %RSD for most nonradionuclides and radionuclides. Hence, the many differences are presumably associated with professional judgment. It should also be noted that the results of Kaiser et al. (2003) and Patello et al. (1999) are intended as generally applicable to many wastes. On the other hand, the %RSDs in Table 4.4 are based on recent estimates by the WTP analytical laboratory group for the CRV and MFPV compositions specific to the AZ-102 waste composition addressed in this work.

Table 4.5 gives the nominal compositions (in oxide mass fractions) and uncertainty intervals for each of the GFCs. The "Nominal" columns of Table 4.5 list the GFC compositions, while the "Case Ranges" columns list nominal and high ranges around the nominal values for GFC composition uncertainty. These nominal compositions and ranges were used to define triangular distributions for the Monte Carlo treatment of GFC uncertainties. Table 4.5 is derived from Table 5.14 of Heredia-Langner et al. (2003), which contained information for 13 GFCs. Glasses made from AZ-102 waste are expected to only use 5 of the possible 13 GFCs, so the other 8 GFCs are not shown in Table 4.5. Note that the sum of the mass fractions of GFC components sum to less than 1.0 when the GFCs contain moisture or other volatile components that will not be incorporated into the glass. Possible uncertainties or variations in moisture contents of GFCs were not directly varied in any of the simulation studies performed. However, the uncertainties in GFC components represented in Table 4.5 provided for indirectly assessing the uncertainty in moisture content as well as other aspects of GFC compositions.

Table 4.6 lists the amounts of GFCs that would need to be added to the AZ-102 CRV waste to yield each of the five glass formulations. These amounts are given in grams of GFCs per liter of CRV waste. Note that these inputs are only applicable to the ILAW strategy.

Table 4.7 lists the nominal volumes for the CRV and MFPV tanks, before and after adding the waste and GFCs, as well as the corresponding uncertainties (expressed as standard deviations). The nominal values were obtained by converting from gallons to liters the nominal values in Table 5.12 of Heredia-Langner et al. (2003). The "Nominal Uncertainty Case" volume standard deviations (SDs) in Table 4.7 were obtained by converting the SDs from Table 5.12 of Heredia-Langner et al. (2003) from gallons to liters, and then dividing by three. The reason for this is as follows. Heredia-Langner et al. (2003) obtained estimates for vessel level determination uncertainty ranging from 0.5 inch to 1.5 inch. Hence, they decided to use 0.5 inch as the SD, so that three SDs would correspond to the 1.5-inch estimate. However, discussion with WTP R&T staff at the start of this work led to the decision that the WTP design basis of 0.5-inch uncertainty in vessel level determination should be treated as three times the SD rather than the SD. Thus, the 0.5-inch SD in vessel level determination was translated to volume uncertainties in liters, leading to the values in the "Nominal Uncertainty Case" column of Table 4.7. The "High Uncertainty Case" volume SDs in Table 4.7 are two times the nominal SD values.

The uncertainties listed in Table 4.4 to Table 4.7 are the ones referred to as "other uncertainties" in Section 3.2, Section 4.1.1, and subsequently in this report.

Table 4.5. Mass Fractions and Uncertainty Ranges of Oxides in Each GFC

Oxide	Silica		Zincite		Borax		Sodium Carbonate		Lithium Carbonate	
	Nominal	**Case Ranges[(a)]**	**Nominal**	**Case Ranges[(a)]**	**Nominal**	**Case Ranges[(a)]**	**Nominal**	**Case Ranges[(a)]**	**Nominal**	**Case Ranges[(a)]**
Al_2O_3	0.00135	0.0004 – 0.0040 0 – 0.0067	0	---	0	---	0	---	0	---
B_2O_3	0	---	0	---	0.3750	0.3690 – 0.3820 0.3630 – 0.3890	0	---	0	---
CaO	0.00008	0 – 0.0002 0 – 0.0003	0	---	0	---	0	0 – 0.0001 0 – 0.0002	0	0 – 0.0220 0 – 0.0439
CdO	0	---	0.0001	0 – 0.0002 0 – 0.0003	0	---	0	---	0	---
Cl	0	---	0	---	0	0 – 0.0007 0 – 0.0014	0.0002	---	0.0001	---
Cr_2O_3	0	---	0	---	0	---	0	0 – 0.0006 0 – 0.0010	0.0001	0 – 0.0002 0 – 0.0002
Fe_2O_3	0.00016	0.00003 – 0.000373 0 – 0.000426	0	0 – 0.0001 0 – 0.0001	0	0 – 0.0001 0 – 0.0001	0	0 – 0.0001 0 – 0.0001	0	0 – 0.0001 0 – 0.0001
K_2O	0	0 – 0.0002 0 – 0.0004	0	---	0	---	0	---	0	0 – 0.0001 0 – 0.0001
Li_2O	0	---	0	---	0	---	0	---	0.4020	0.4000 – 0.4044 0.3980 – 0.4068
MgO	0.00008	0 – 0.0001 0 – 0.0001	0	---	0	---	0	0 – 0.0001 0 – 0.0002	0.0001	0 – 0.0002 0 – 0.0002
MnO	0	---	0	0 – 0.0001 0 – 0.0001	0	---	0	---	0	---
Na_2O	0.00019	0 – 0.0002 0 – 0.0002	0	---	0.1670	0.1640 – 0.1700 0.1610 – 0.1730	0.5837	0.5848 – 0.5831 0.5825 – 0.5859	0.0008	0 – 0.0011 0 – 0.0014
NiO	0	---	0	---	0	---	0	---	0	---
P_2O_5	0	---	0	---	0	---	0	---	0	---
PbO	0	---	0	0 – 0.0001 0 – 0.0001	0	---	0	---	0	---
SiO_2	0.9970	0.9920 – 0.9990 0.9870 – 1.0000	0	---	0	---	0	---	0	---
SO_3	0	---	0	---	0	0 – 0.0005 0 – 0.0010	0.0001	0 – 0.0002 0 – 0.0003	0.0003	0 – 0.0004 0 – 0.0005
TiO_2	0.00008	0 – 0.00045 0 – 0.0009	0	---	0	---	0	---	0	---
UO_2	0	---	0	---	0	---	0	---	0	---
V_2O_5	0	---	0	---	0	---	0	---	0	---
ZnO	0	---	0.9990	0.9930 – 0.9999 0.9870 – 1.0000	0	---	0	---	0	---
ZrO_2	0	---	0	---	0	---	0	---	0	---
Total	0.99894[(b)]	0.9925 – 1.0046 0.9870 – 1.0091	0.9991	0.9931 – 1.0004 0.9870 – 1.0006	0.5420	0.5330 – 0.5533 0.5240 – 0.5645	0.5842	0.5832 – 0.5859 0.5825 – 0.5877	0.4027	0.4001 – 0.4541 0.3980 – 0.4532

(a) Top range is "Nominal" uncertainty case, and bottom range is "High" case.
(b) Total mass fractions less than one indicate GFCs that contain water or other volatile components that will not be present in the glass.

Table 4.6. Masses of GFCs per Liter of HLW Waste for Glasses A to E and Corresponding %RSDs[a]

GFC[b]	AZ-102 Glass A (g/L)	AZ-102 Glass B (g/L)	AZ-102 Glass C (g/L)	AZ-102 Glass D (g/L)	AZ-102 Glass E (g/L)	%RSD "Nominal" Uncertainty Case	%RSD "High" Uncertainty Case
Silica	228.704	220.693	216.193	211.949	207.928	0.67	1.33
Zincite	10.220	9.989	9.859	9.737	9.622	0.67	1.33
Borax	86.182	82.041	79.520	77.083	74.724	0.67	1.33
Sodium Carbonate	82.989	81.210	80.263	79.391	78.584	0.67	1.33
Lithium Carbonate	50.285	50.222	50.337	50.538	50.812	0.67	1.33

(a) These inputs are only applicable for the ILAW compliance strategy.
(b) The compositions of these GFCs are listed in the "nominal" columns of Table 4.5.

Table 4.7. Nominal HLW CRV and MFPV Volumes and Associated Uncertainties

IHLW Process Stage	Nominal Volume (L)	Volume Standard Deviations (L)	
		"Nominal" Uncertainty Case	"High" Uncertainty Case[a]
CRV Before Transfer to MFPV	43,854	56.29	112.58
CRV After Transfer to MFPV	26,819.6	56.29	112.58
MFPV Before Transfer from CRV	6113.06	37.38	74.76
MFPV After Transfer from CRV	23,147.8	37.38	74.76
MFPV After CRV Transfer and GFCs Added	26,932.83	37.38	74.76

(a) The "high" standard deviations are two times the "nominal" SDs.

4.2 Simulation Study #2 to Assess CRV Mixing/Sampling Bias

After the optimal glass formulation (Glass C) was selected based on Simulation Study #1 described in Section 4.1, HLW mixing/sampling bias and random uncertainty were then studied using the optimal glass formulation. Section 4.2.1 presents the experimental design (test matrix) used in the computer experiment simulation to assess the effects of CRV mixing/sampling bias and random uncertainties and other factors on satisfying compliance and processing conditions. Section 4.2.2 presents the inputs used for this simulation study. Subsequently in this report, this second simulation study is referred to as Simulation Study #2. The reasons why Glass C was selected as the optimal formulation from Glasses A to E is discussed subsequently in Section 5.7.

4.2.1 Experimental Design for Simulation Study #2 to Assess CRV Mixing/Sampling Bias

An experimental design (test matrix) was created to assess the effects of five different bias amounts, including no bias, in the HLW CRV nominal elemental concentrations. The CRV biases were specified as the "% solids" bias in elements expected to be insoluble (i.e., solids) in the HLW CRV. These bias levels were -10% solids bias, -5% solids bias, no solids bias, +5% solids bias, and +10% solids bias. The "no solids bias" case was the same case as the "C" glass-formulation case in the simulation discussed in Section 4.1. The biases in soluble elements resulting from the biases in insoluble elements were calculated to yield new starting CRV and MFPV elemental concentrations for each of the five bias cases based on Glass C. Table 4.8 displays the resulting nominal glass compositions corresponding to each of the bias situations.

The test matrix for Simulation Study #2 is listed in Table 4.9. It was run in each of two separate simulations, one with the IHLW compliance strategy, and one with the ILAW compliance strategy, as discussed previously in Section 3.2. In addition to varying the HLW CRV bias, the test matrix also jointly varied the levels of CRV mixing/sampling random uncertainty (%RSD), nominal and high levels of other random uncertainties (%RSDs), and either four or eight CRV samples (IHLW and ILAW compliance strategies) and MFPV samples (IHLW compliance strategy). Note that the last three factors were varied together and not separately. For this simulation study, a CRV mixing/sampling random uncertainty of 5 %RSD was always combined with nominal levels of other random uncertainties and with eight MFPV and/or CRV samples. Similarly, CRV mixing/sampling random uncertainty of 10 %RSD was always combined with high levels of other random uncertainties and with four MFPV and/or CRV samples. The listing of the test cases in Table 4.9 clarifies this topic.

The "Other Uncertainties" column in Table 4.9 includes the following separate sources of random uncertainty: CRV analytical, MFPV mixing/sampling, MFPV analytical, GFC composition, GFC masses added to MFPV, CRV volumes, and MFPV volumes. Based on previous work, it was decided to only investigate one analysis per sample within the CRV and MFPV and only one volume measurement for a given volume determination. Each of the 10 test cases consisted of a simulation with 1000 runs, creating a distribution of MFPV glass compositions (mass fractions) for each test case. These 1000 glass compositions for each test case were then used to calculate 1000 values of each of the compliance and processing properties. From these sets of 1000 values, measures of total composition-related uncertainty for a single MFPV batch were calculated, as discussed in Section 3.3.

Table 4.8. Nominal Glass Compositions (Mass Fractions) Resulting from Applying CRV Mixing/Sampling Solids Biases to AZ-102 Glass Formulation C

Oxide	Biased[a] Versions of AZ-102 Glass Formulation C				
	C – 10% Bias	C – 5% Bias	C	C + 5% Bias	C + 10% Bias
Ag_2O	0.000173	0.000180	0.000187	0.000194	0.000200
Al_2O_3	0.073096	0.076006	0.078833	0.081580	0.084251
B_2O_3	0.061230	0.060342	0.059480	0.058642	0.057828
BaO	0.000395	0.000388	0.000381	0.000374	0.000367
BeO	0.000028	0.000029	0.000031	0.000032	0.000033
CaO	0.005089	0.004995	0.004904	0.004816	0.004730
CdO	0.005690	0.005919	0.006141	0.006357	0.006568
Ce_2O_3	0.000529	0.000550	0.000570	0.000591	0.000610
Cl	0.000565	0.000555	0.000545	0.000535	0.000526
CoO	0.000057	0.000059	0.000061	0.000063	0.000065
Cr_2O_3	0.000883	0.000918	0.000952	0.000985	0.001017
Cs_2O	0.000106	0.000104	0.000102	0.000100	0.000098
CuO	0.000271	0.000282	0.000292	0.000303	0.000313
F	0.000131	0.000128	0.000126	0.000124	0.000121
Fe_2O_3	0.114622	0.119233	0.123713	0.128066	0.132299
K_2O	0.000279	0.000274	0.000269	0.000264	0.000259
La_2O_3	0.002831	0.002945	0.003056	0.003164	0.003268
Li_2O	0.041406	0.040806	0.040224	0.039658	0.039108
MgO	0.001317	0.001293	0.001270	0.001247	0.001225
MnO	0.008699	0.009049	0.009389	0.009720	0.010041
Na_2O	0.154660	0.152296	0.150000	0.147769	0.145600
Nd_2O_3	0.001975	0.002054	0.002131	0.002207	0.002280
NiO	0.007228	0.007519	0.007802	0.008076	0.008344
P_2O_5	0.004907	0.004816	0.004729	0.004643	0.004560
PbO	0.000888	0.000924	0.000959	0.000992	0.001025
SiO_2	0.447049	0.440904	0.434935	0.429134	0.423493
SnO_2	0.001559	0.001622	0.001683	0.001742	0.001800
SO_3	0.000273	0.000268	0.000264	0.000259	0.000255
SrO	0.014065	0.014632	0.015182	0.015717	0.016237
TiO_2	0.000132	0.000135	0.000138	0.000141	0.000144
UO_2	0.015322	0.015939	0.016538	0.017121	0.017687
Y_2O_3	0.000145	0.000151	0.000156	0.000162	0.000167
ZnO	0.020545	0.020269	0.020000	0.019740	0.019486
ZrO_2	0.013857	0.014415	0.014957	0.015484	0.015997
Total	1.000000	1.000000	1.000000	1.000000	1.000000

(a) The -10%, -5%, +5%, and +10% biases were applied to the elemental concentrations of insoluble (solids) constituents in the HLW CRV. Appropriate offsetting biases were applied to elemental concentrations of soluble constituents in the HLW CRV. Corresponding biases were applied to elemental concentrations in the MFPV for the IHLW compliance strategy where MFPV samples are used. This table lists the nominal glass compositions (mass fractions) resulting from applying these biases. The mass fractions have been rounded to six decimal places in this table.

Table 4.9. Simulation Study #2 Test Matrix to Assess HLW CRV Mixing/Sampling Bias

Test Case	Solids Bias	CRV Mixing/ Sampling Random Uncertainty (%RSD)	Other[(a)] Uncertainties	CRV/MFPV # Samples
1	-10% bias	5	"Nominal" Case	8
2	-10% bias	10	"High" Case	4
3	-5% bias	5	"Nominal" Case	8
4	-5% bias	10	"High" Case	4
5	no bias	5	"Nominal" Case	8
6	no bias	10	"High" Case	4
7	+5% bias	5	"Nominal" Case	8
8	+5% bias	10	"High" Case	4
9	+10% bias	5	"Nominal" Case	8
10	+10% bias	10	"High" Case	4

(a) The "other uncertainties" are identified for each of the IHLW and ILAW compliance strategies in Section 3.3. The nominal and high values of these uncertainties are listed in preceding tables of Section 4.

4.2.2 Inputs for Simulation Study #2 to Assess CRV Mixing/Sampling Bias

The biases included in Simulation Study #2 affected the nominal CRV and MFPV concentrations. The CRV concentrations changed according to the amount of bias included in insoluble components and the offsetting biases included in soluble components. Corresponding changes were made to the MFPV nominal concentrations for the biased cases. The no-bias case used the same CRV and MFPV nominal concentrations that were used for Glass C in the simulation study discussed in Section 4.1. Table 4.10 gives the different CRV and MFPV concentration values used in this simulation study.

Other simulation inputs remained the same as those used in Simulation Study #1 discussed in Section 4.1. Specifically, the CRV and MFPV analytical random uncertainties and the MFPV mixing/sampling random uncertainty values are given in Table 4.4. The GFC nominal mass fractions and associated uncertainty ranges are found in Table 4.5. Table 4.6 shows the amounts of GFCs added to the waste in this study (the "Glass C" column) and the corresponding uncertainties. The nominal volume amounts and uncertainties are found in Table 4.7.

Table 4.10. Element Concentrations of Pre-Treated Waste in the CRV and Waste Plus GFCs in the MFPV for All Five Bias Levels

Element	Solid ? (a)	-10% Solids Bias		-5% Solids Bias		No Bias		+5% Solids Bias		+10% Solids Bias	
		CRV Conc. (mg/L)	MFPV Conc. (mg/L)	CRV Conc. (mg/L)	MFPV Conc. (mg/L)	CRV Conc. (mg/L)	MFPV Conc. (mg/L)	CRV Conc. (mg/L)	MFPV Conc. (mg/L)	CRV Conc. (mg/L)	MFPV Conc. (mg/L)
Ag	Y	78.81	66.51	83.19	70.21	87.56	73.91	91.94	77.60	96.32	81.30
Al	Y	18746.02	15952.45	19787.47	16831.45	20828.91	17710.45	21870.36	18589.44	22911.81	19468.44
B	N	32.12	7843.73	32.00	7843.62	31.87	7843.51	31.74	7843.40	31.61	7843.30
Ba	N	172.93	145.96	172.24	145.37	171.55	144.79	170.86	144.21	170.17	143.62
Be	Y	4.99	4.21	5.27	4.45	5.55	4.68	5.82	4.91	6.10	5.15
Bi	---	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ca	N	1761.86	1497.91	1754.82	1491.97	1747.78	1486.02	1740.73	1480.08	1733.69	1474.13
Cd	Y	2433.26	2054.08	2568.45	2168.17	2703.63	2282.27	2838.81	2396.36	2973.99	2510.46
Ce	Y	220.52	186.13	232.78	196.47	245.03	206.81	257.28	217.15	269.53	227.49
Cl	N	255.14	231.92	254.12	231.06	253.10	230.20	252.08	229.34	251.06	228.48
Co	Y	21.79	18.39	23.00	19.41	24.21	20.43	25.42	21.46	26.63	22.48
Cr	Y	291.70	246.20	307.91	259.88	324.11	273.56	340.32	287.23	356.52	300.91
Cs	N	48.78	41.17	48.59	41.01	48.39	40.84	48.20	40.68	48.00	40.51
Cu	Y	105.74	89.25	111.62	94.21	117.49	99.16	123.37	104.12	129.24	109.08
F	N	63.79	53.84	63.53	53.62	63.28	53.41	63.02	53.19	62.77	52.97
Fe	Y	39149.67	33075.47	41324.65	34911.19	43499.63	36746.91	45674.61	38582.63	47849.59	40418.35
Hg	---	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K	N	113.06	95.42	112.61	95.04	112.15	94.66	111.70	94.28	111.25	93.90
La	Y	1179.83	995.80	1245.38	1051.12	1310.92	1106.44	1376.47	1161.76	1442.02	1217.09
Li	---	0.00	7933.03	0.00	7933.03	0.00	7933.03	0.00	7933.03	0.00	7933.03
Mg	N	372.17	348.42	370.68	347.17	369.20	345.91	367.71	344.66	366.22	343.40
Mn	Y	3292.27	2778.73	3475.18	2933.10	3658.08	3087.48	3840.98	3241.85	4023.89	3396.23
Mo	---	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Na	N	11402.73	47299.26	11357.14	47260.78	11311.56	47222.31	11265.97	47183.83	11220.39	47145.36
Nd	Y	827.37	698.32	873.34	737.11	919.30	775.91	965.27	814.70	1011.23	853.50
Ni	Y	2775.67	2342.71	2929.87	2472.86	3084.08	2603.01	3238.28	2733.16	3392.48	2863.31
P	N	1046.53	883.29	1042.34	879.75	1038.16	876.22	1033.98	872.69	1029.79	869.16
Pb	Y	402.92	340.15	425.31	359.04	447.69	377.94	470.07	396.83	492.46	415.72
Pd	---	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pr	---	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Rh	---	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ru	---	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Se	---	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Si	Y	1370.54	86193.71	1446.68	86257.97	1522.82	86322.24	1598.96	86386.50	1675.10	86450.76
S	N	44.19	39.41	44.01	39.26	43.83	39.11	43.66	38.96	43.48	38.81
Sn	Y	600.11	506.50	633.45	534.64	666.79	562.78	700.12	590.92	733.46	619.05
Sr	Y	5812.40	4905.76	6135.31	5178.30	6458.22	5450.84	6781.13	5723.38	7104.04	5995.92
Ta	---	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Th	---	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ti	Y	25.83	30.56	27.27	31.77	28.70	32.99	30.14	34.20	31.57	35.41
U	Y	6600.53	5570.95	6967.22	5880.45	7333.92	6189.95	7700.62	6499.44	8067.31	6808.94
V	---	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Y	Y	55.75	47.05	58.85	49.67	61.95	52.28	65.04	54.90	68.14	57.51
Zn	Y	153.33	6807.93	161.85	6815.12	170.37	6822.31	178.89	6829.50	187.41	6836.69
Zr	Y	5013.55	4231.51	5292.08	4466.60	5570.61	4701.68	5849.14	4936.77	6127.67	5171.85

(a) Elements marked with "Y" were treated as solid components, while elements marked with an "N" were treated as liquid components when applying the specified bias in percent solids. Elements marked "---" were not present in the CRV.

4.3 Simulation Study #3 to Assess CRV Mixing/Sampling Bias and Random Uncertainty

A third simulation study (referred to as Simulation Study #3) was performed for Glass C to jointly investigate the effects of HLW CRV mixing/sampling bias and random uncertainty on satisfying the compliance and processing conditions. CRV mixing/sampling random uncertainty was tested at %RSD = 5%, 15%, and 25% for each of the five levels of CRV mixing/sampling bias studied previously (-10% solids, -5% solids, no bias, +5% solids, and +10% solids). Both the IHLW and ILAW calculation strategies were investigated. The other random uncertainties were held constant at the "nominal uncertainty" case, and the number of CRV samples (IHLW and ILAW compliance strategy) and MFPV samples (IHLW compliance strategy) was held constant at eight samples. The test matrix corresponding to Simulation Study #3 is listed in Table 4.11. Note that Test Cases # 1 to 5 in Table 4.11 are the same as Test Cases # 1, 3, 5, 7, and 9 in Table 4.9.

The main differences between Simulation Studies #2 and #3 were that:

- different amounts of HLW CRV mixing/sampling random uncertainty were investigated for Study #2 (5 and 10 %RSD) and for Study #3 (5, 15, and 25 %RSD)
- the "other uncertainties" and "numbers of CRV and MFPV samples" were varied at two combinations for Study #2 (nominal and 8, high and 4), whereas these factors were held constant at nominal uncertainties and 8 samples for Study #3.

Hence, Simulation Study #2 provided for investigating the individual and interactive effects of the "other uncertainties/number of CRV and MFPV samples" factor with the "CRV mixing/sampling bias" and "CRV mixing/sampling random uncertainty" factors. However, the effects of the "CRV mixing/sampling random uncertainty" factor were only investigated over the 5 to 10 %RSD range. On the other hand, Simulation Study #3 investigated only the individual and interactive effects of the "CRV mixing/sampling bias" and "CRV mixing/sampling random uncertainty" factors, where the effects of the latter factor were investigated over a wider range of uncertainties (5, 15, and 25% RSD).

The inputs for Simulation Study #3 are the same as listed previously in Table 4.4 through Table 4.6 (Glass C and uncertainties), Table 4.7, and Table 4.10.

Table 4.11. Simulation Study #3 Test Matrix to Assess HLW CRV Mixing/Sampling Bias and Random Uncertainty

Test Case	Solids Bias	CRV Mixing/ Sampling Random Uncertainty (%RSD)	Other[(a)] Uncertainties	CRV / MFPV # Samples
1	-10% bias	5	"Nominal" Case	8
2	-5% bias	5	"Nominal" Case	8
3	no bias	5	"Nominal" Case	8
4	+5% bias	5	"Nominal" Case	8
5	+10% bias	5	"Nominal" Case	8
6	-10% bias	15	"Nominal" Case	8
7	-5% bias	15	"Nominal" Case	8
8	no bias	15	"Nominal" Case	8
9	+5% bias	15	"Nominal" Case	8
10	+10% bias	15	"Nominal" Case	8
11	-10% bias	25	"Nominal" Case	8
12	-5% bias	25	"Nominal" Case	8
13	no bias	25	"Nominal" Case	8
14	+5% bias	25	"Nominal" Case	8
15	+10% bias	25	"Nominal" Case	8

(a) The "other uncertainties" are identified for each of the IHLW and ILAW compliance strategies in Section 3.3. The nominal and high values of these uncertainties are listed in preceding tables of Section 4.

5.0 Results of Simulation Study #1 to Assess CRV Mixing/Sampling Random Uncertainty and Other Factors

The WTP IHLW compliance strategy is statistically based for several IHLW specifications. Simulations were performed that emulated the IHLW process for the purpose of assessing the effects of several factors on the probability of satisfying compliance and processing conditions. As discussed in Section 4.1, the focus of the first simulation (henceforth referred to as Simulation Study #1 in this section) was to assess the impact of HLW CRV mixing/sampling random uncertainties on satisfying compliance and processing properties. However, this simulation also studied the effects of the five AZ-102 glass formulations and how low and high levels of random uncertainties affected meeting compliance and processing limits. The optimal glass formulation was determined by finding which formulation has the best chance of satisfying the compliance and processing conditions under the varying uncertainty conditions.

Results are shown graphically in figures that are discussed in the following subsections for the various compliance and processing conditions. Each set of plots contains lines that represent the appropriate 90% combined confidence intervals (90% CCIs), (as discussed in Section 3.3) for each glass formulation. For viscosity at 1100°C, two-sided 90% CCIs (i.e., one-sided 95% LCCIs and UCCIs) are plotted. For waste loading, only a 90% LCI is plotted. All other criteria used only a 90% UCCI. Graphical results for the simulation studies using both the ILAW and IHLW calculation strategies are presented. The 90% CCIs are consistently tighter (smaller) when using the ILAW strategy. Tighter 90% CCIs represent a better chance of complying with a given compliance or processing condition. As expected, the ILAW strategy consistently resulted in tighter 90% CCIs because of the reduced uncertainty associated with using direct measurements of GFC mass additions rather than having to estimate those masses using samples and analyses of the MFPV.

The plots also include a comparison of the high uncertainty cases (including four CRV and MFPV samples) and the nominal uncertainty cases (including eight CRV and MFPV samples). As expected, the 90% CCIs are consistently tighter for the cases using the nominal uncertainty and eight samples.

5.1 PCT Results for Simulation Study #1

All 90% UCCIs (calculated as described in Section 3.3.1) for PCT normalized boron, lithium, and sodium releases were well below the corresponding compliance limits, regardless of the calculation strategy (IHLW or ILAW), and the magnitudes of the other factors varied per the test matrix in Table 4.2. Because of this, Figure 5.1 only shows the largest 90% UCCIs, which were produced using the IHLW strategy, four CRV and MFPV samples, and high levels of uncertainties. As can be seen in Figure 5.1, neither the AZ-102 glass compositions A to E (see Table 2.5) nor the magnitude of HLW CRV mixing/sampling random uncertainty have much impact on the PCT 90% UCCIs.

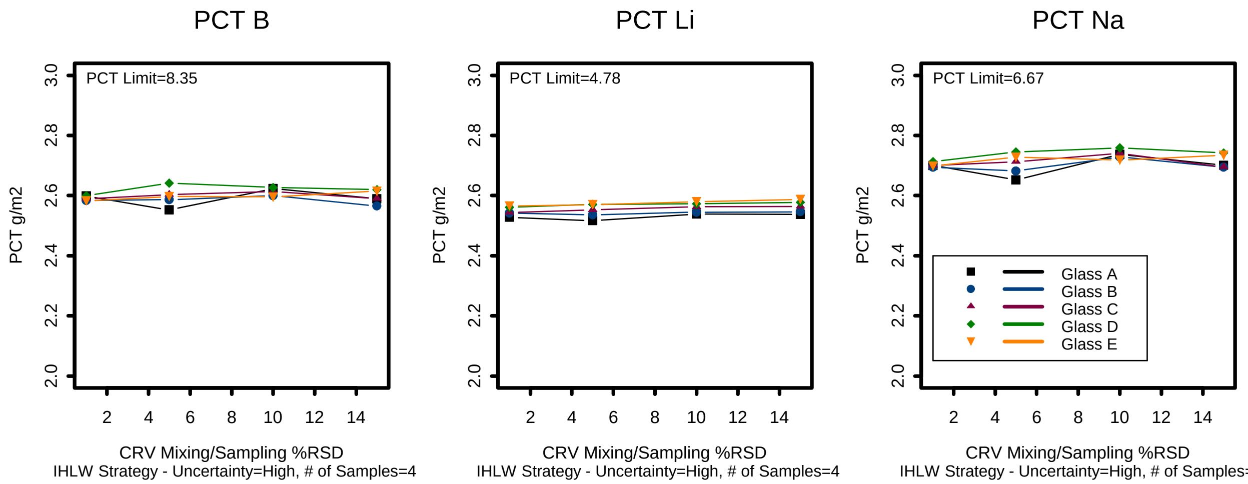

Figure 5.1. PCT Plots Showing 90% UCCIs as a Function of HLW CRV Mixing/Sampling Random Uncertainty %RSD for Each Glass Formulation

5.2 Liquidus Temperature Results for Simulation Study #1

Figure 5.2 shows the 90% UCCIs (calculated as described in Section 3.3.2) for T_L as a function of HLW CRV mixing/sampling random uncertainty %RSD for each glass formulation. Plots are separated according to the high and nominal uncertainty cases as well as IHLW and ILAW strategies. In each case, the 90% UCCIs for T_L are above (i.e., violate) the acceptable processing limit of 950°C. Although not shown in Figure 5.2, even the nominal predicted T_L values for Glasses A to E (i.e., model predictions without composition or model uncertainty added) violate the 950°C limit. This is so because only $T_{0.01}$, and not T_L, was restricted to be below 950°C in formulating Glasses A to E (as discussed in Section 2.3). These results demonstrate that $T_L \leq 950$°C is a much stricter processability criterion than is $T_{0.01} \leq 950$°C. While some glasses may satisfy both criteria, in general there will be many glasses that satisfy the $T_{0.01} \leq 950$°C condition but not the $T_L \leq 950$°C condition.

5.3 $T_{0.01}$ Results for Simulation Study #1

The $T_{0.01}$ values calculated for the nominal compositions of Glasses A to E were very close to the $T_{0.01}$ limit. Hence, the simulations with reduced variability and more samples did better at satisfying the $T_{0.01}$ processability limit than those with higher variability and less samples. Figure 5.3 plots the 90% UCCIs (calculated as described in Section 3.3.3) for $T_{0.01}$ as a function of HLW CRV mixing/sampling random uncertainty %RSD for each glass formulation. Those simulations that had lower uncertainties applied, as well as eight CRV (IHLW and ILAW strategies) and MFPV (IHLW strategy) samples were below the $T_{0.01}$ limit, and therefore, compliant. For most of the glass formulations, the $T_{0.01}$ 90% UCCIs struggled with satisfying the 950°C limit when using the IHLW strategy, the higher uncertainties, and only four CRV and MFPV samples. The 90% UCCIs for $T_{0.01}$ slightly increased as the CRV mixing/sampling random uncertainty (in %RSD) increased. . For each increase of 1 %RSD, there was generally a 1°C to 2°C increase in the $T_{0.01}$ 90% UCCI.

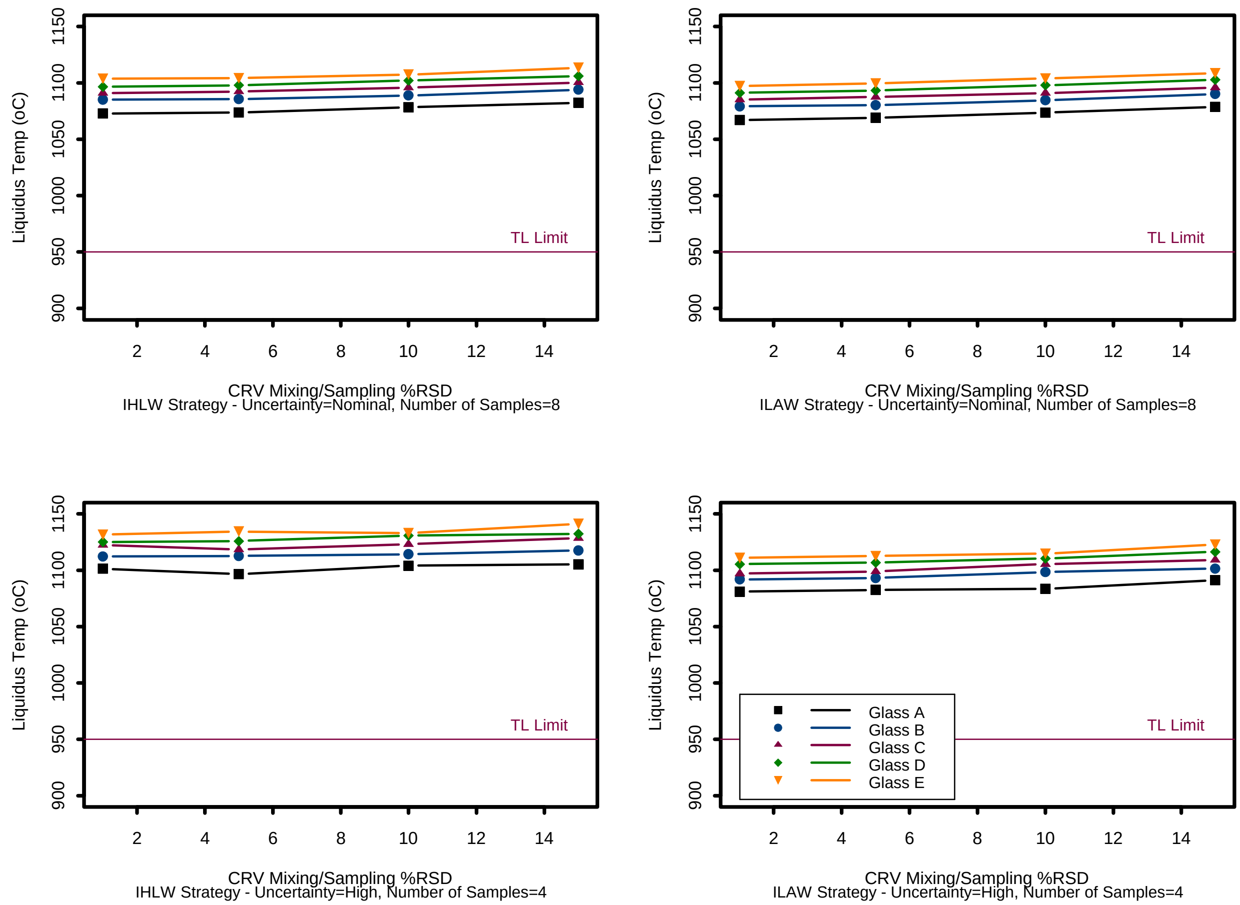

Figure 5.2. T_L Plots Showing 90% UCCIs as a Function of HLW CRV Mixing/Sampling Random Uncertainty %RSD for Each Glass Formulation

The results in Figure 5.3 for Glasses A to E are as expected based on Figure 2.1. That is, because Glass E was closest to the 950°C limit for $T_{0.01}$ in Figure 2.1, it has the highest 90% UCCIs in Figure 5.3. Because glasses D, C, B, and A were progressively farther from the 950°C limit in Figure 2.1, their 90% UCCIs are also progressively farther from the limit.

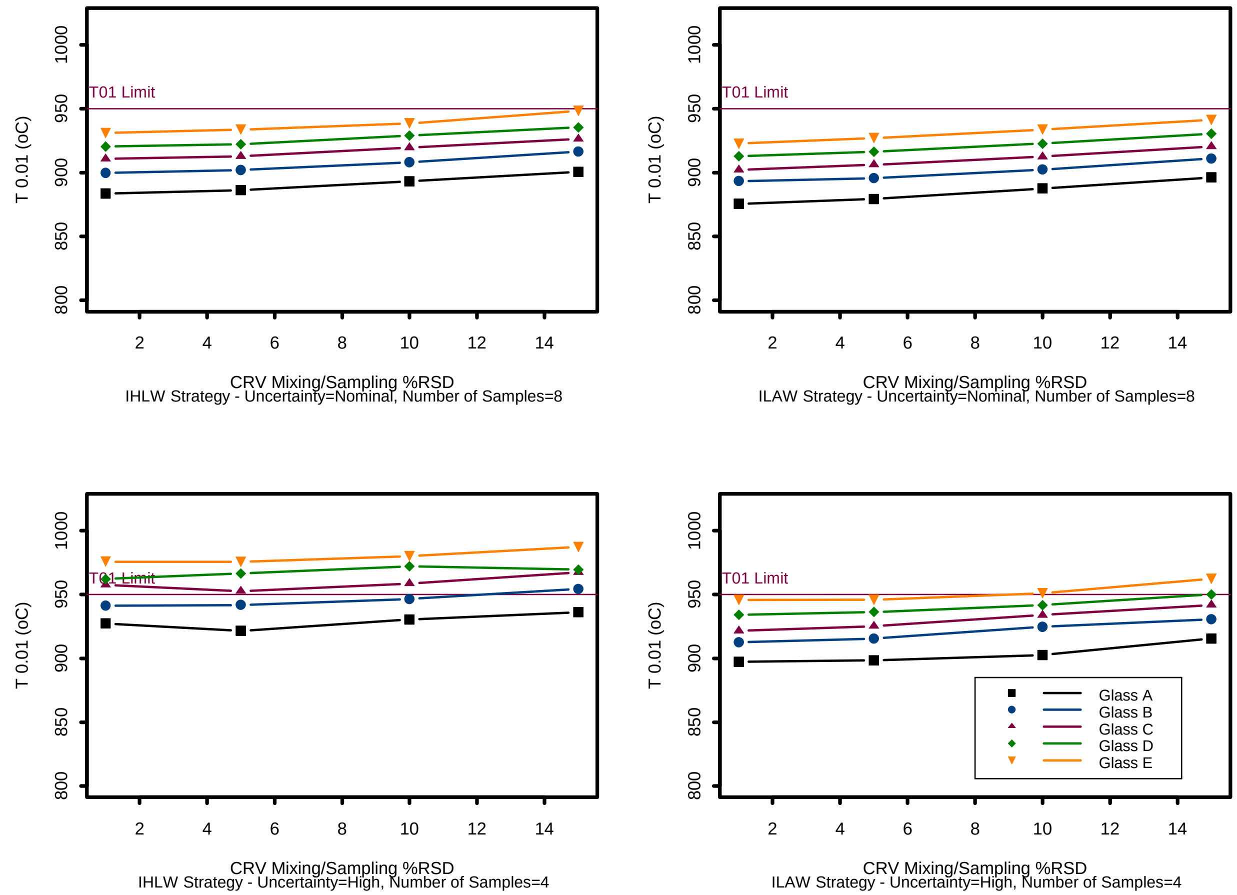

Figure 5.3. $T_{0.01}$ **Plots Showing 90% UCCIs as a Function of HLW CRV Mixing/Sampling Random Uncertainty %RSD for Each Glass Formulation**

5.4 Waste Loading Results for Simulation Study #1

Figure 5.4 shows the waste loading 90% LCIs (calculated as described in Section 3.3.4) as a function of HLW CRV mixing/sampling random uncertainty %RSD for each of the glass formulations. There are many waste-loading criteria, any one of which can be met to demonstrate compliance. The waste-loading criterion met by AZ-102 Glasses A to E was $Al_2O_3 + Fe_2O_3 + ZrO_2$. The condition for this criterion is that the waste-loading percentage should be above 21%. As shown in Figure 2.1 and Table 2.5, Glass A was formulated with a nominal $Al_2O_3 + Fe_2O_3 + ZrO_2 = 21\%$. A few of the glass compositions using high uncertainty and four samples had 90% LCIs that did not meet the WL limit. Only Glass A had 90% LCI values not meeting the WL limit for simulations using nominal uncertainties and eight samples. There was a slight decrease in waste-loading percentage as HLW CRV mixing/sampling random uncertainty %RSD increased. Generally, this amounted to a decrease of about 0.25% in waste loading when the %RSD increased from 1% to 15%.

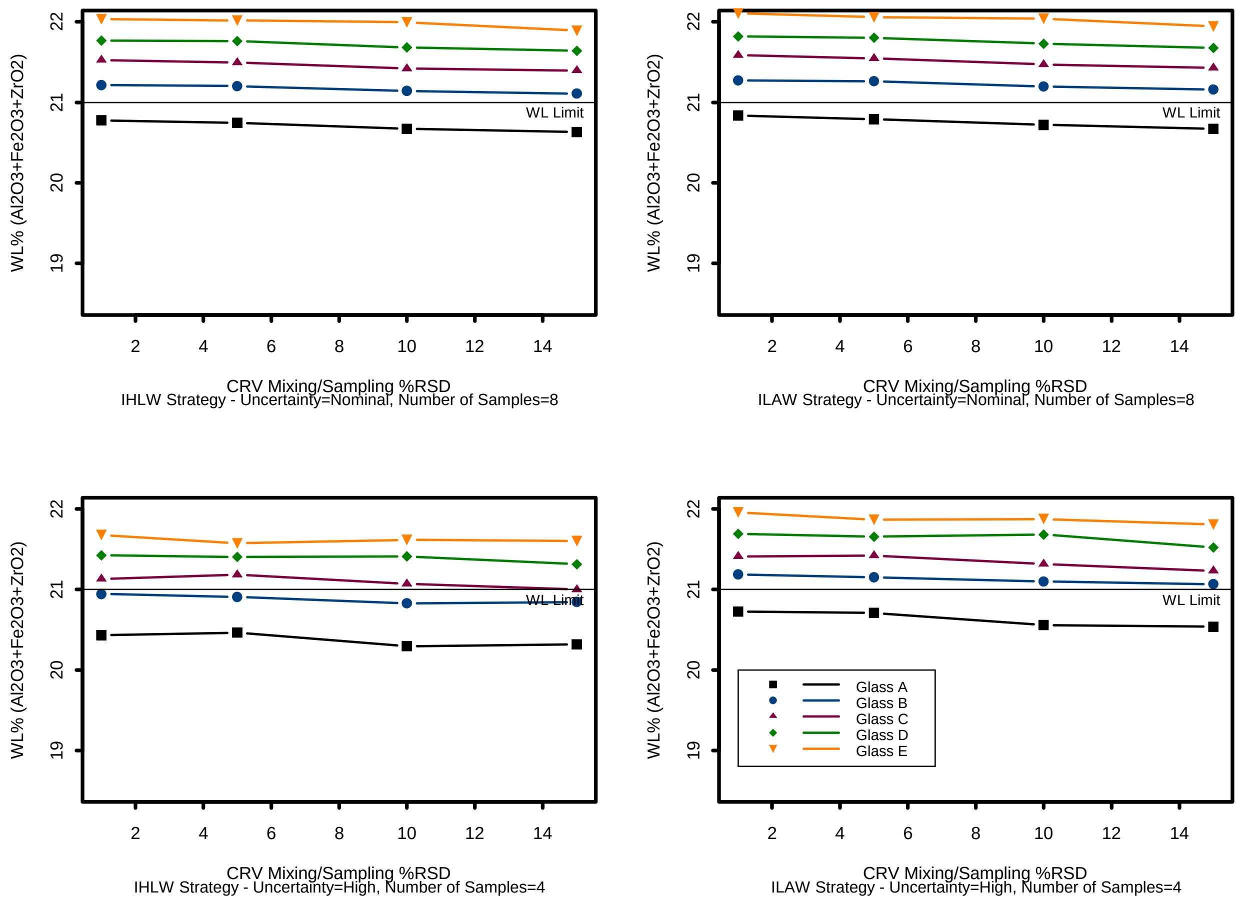

Figure 5.4. Waste-Loading Plots Showing 90% LCIs as a Function of HLW CRV Mixing/Sampling Random Uncertainty %RSD for Each Glass Formulation

5.5 TCLP Cd Release Results for Simulation Study #1

Figure 5.5 shows TCLP Cd release (mg/L) 90% UCCI values (calculated as described in Section 3.3.5) as a function of CRV mixing/sampling random uncertainty %RSD for each of the glass formulations. All these values were well below the compliance limit of 0.48 mg/L, resulting in TCLP compliance under any of the factor combinations investigated in this simulation study.[a]

(a) It should be noted that the CdO concentration of glass was maintained within the TCLP response-composition model validity range (i.e., ≤ 1.6 mass%) and that the CdO concentration from the analyzed pretreated AZ-102 HLW was adjusted downward for the purpose of this evaluation (see Section 2.1).

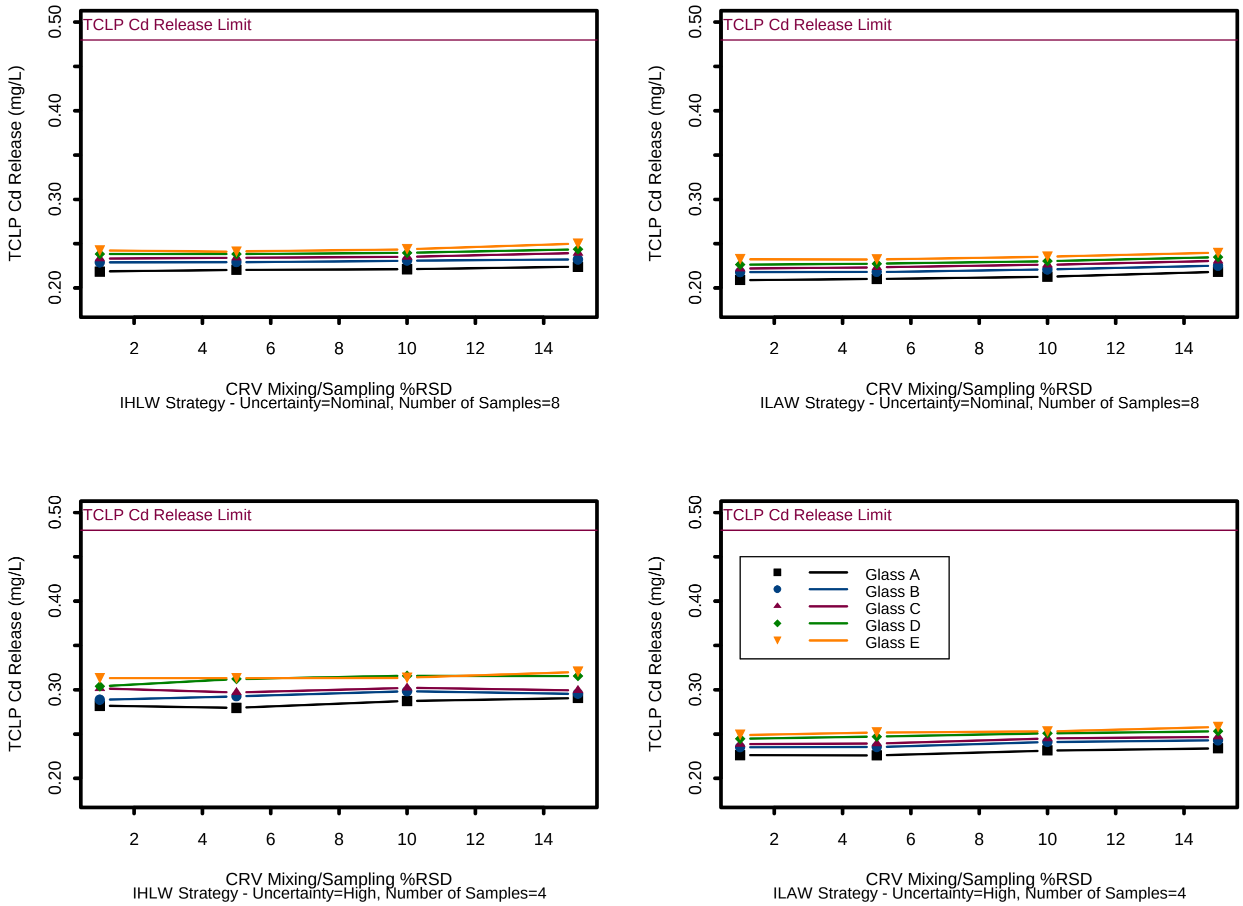

Figure 5.5. TCLP Cd Release Plots Showing 90% UCCIs as a Function of HLW CRV Mixing/Sampling Random Uncertainty %RSD for Each Glass Formulation

5.6 Viscosity at 1100°C Results for Simulation Study #1

HLW glass is considered processable when the viscosity at 1100°C (η_{1100}) is between 10 and 150 poise. Because of this, two-sided 90% CCIs (i.e., one-sided 95% LCCIs and UCCIs) were calculated as discussed in Section 3.3.6. Figure 5.6 shows these two-sided 90% CCIs as functions of HLW CRV mixing/sampling random uncertainty %RSD for each of the glass formulations. The processability limits are also plotted for comparison purposes. Both the IHLW and ILAW strategies were plotted as well as low uncertainties and high uncertainties. All cases had two-sided 90% CCIs within the η_{1100} processability limits. However, the lower limit was approached with high uncertainties, four samples, and the IHLW strategy.

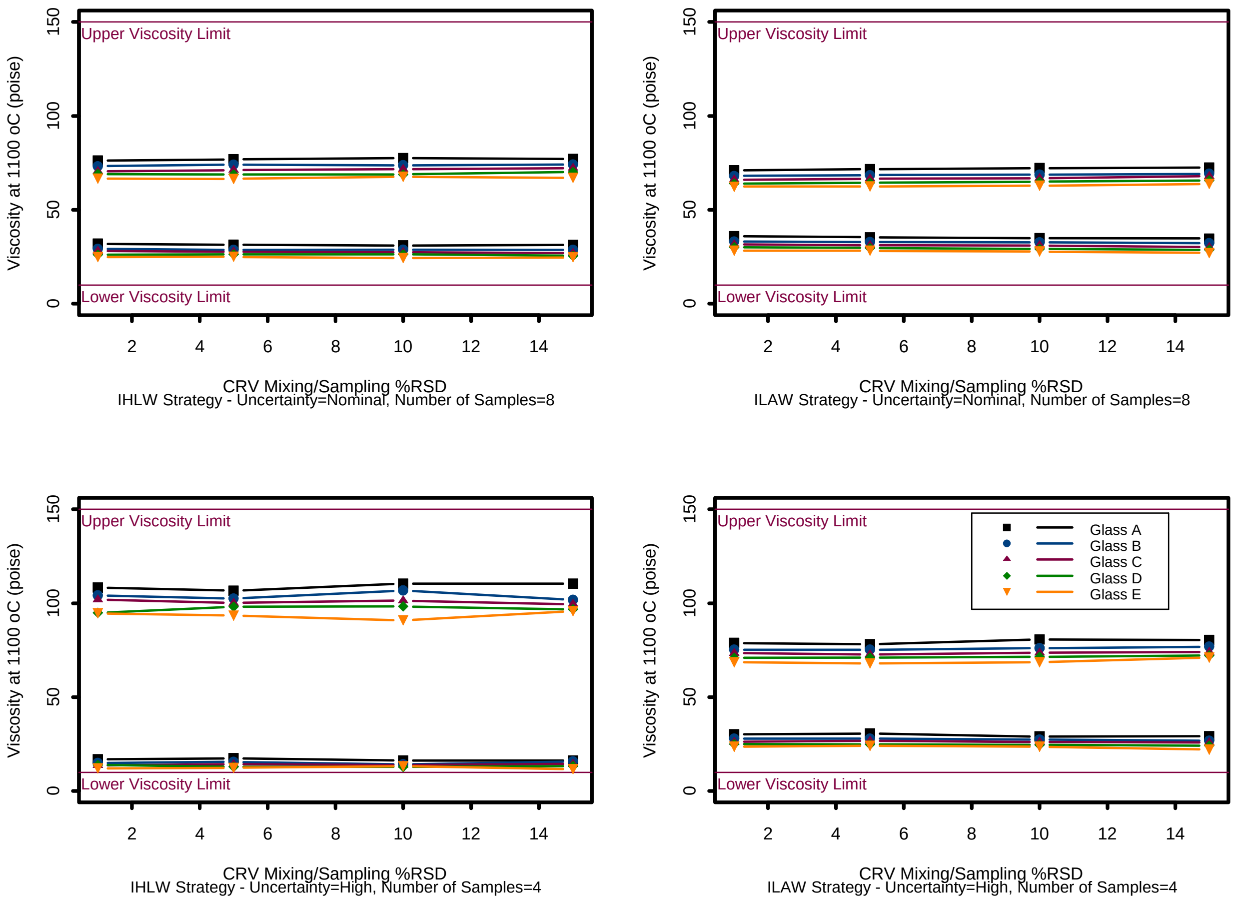

Figure 5.6. Viscosity at 1100°C Plots Showing Two-Sided 90% CCIs as Functions of HLW CRV Mixing/Sampling Random Uncertainty %RSD for Each Glass Formulation

5.7 Optimal Glass Formulation Considering Results for All Compliance and Processing Properties

Glass C from the AZ-102 series (see Section 2.5) was selected as the most appropriate composition for detailed simulations. This glass was formulated to have a $T_{0.01}+u$ of 890°C and a WL factor of 1.04. This glass is within the acceptable glass envelope roughly 30% of the way between the border of the WL limit and the $T_{0.01}+u$ border (see Figure 2.1). A glass formulation closer to the WL limit was selected because the effect of composition uncertainty is greater for meeting the $T_{0.01}+u$ constraint than it is for meeting the WL constraint. Glass C was expected to yield the largest tolerance to composition uncertainties of any of the AZ-102 series glasses, and thus was selected as the optimal glass for subsequent investigations.

6.0 Results of Simulation Study #2 to Assess CRV Mixing/Sampling Bias and Other Factors

Simulation Study #2 focused on investigating the effects of HLW CRV mixing/sampling bias on satisfying compliance and processing conditions when using Glass C, the optimal glass formulation for AZ-102 waste (as discussed in Section 5.7). It also investigated the effects of HLW CRV mixing/sampling random uncertainty, as well as the other uncertainties in the IHLW vitrification process (see Section 3.2). See Section 4.2 for discussion of Simulation Study #2 and the specific test matrix used.

Results are shown graphically in figures that are discussed in the following subsections for the various compliance and processing conditions. Each set of plots contains lines that represent the appropriate 90% CCIs (as discussed in Section 3.3) for each glass formulation. Each set of plots contains results using the IHLW and ILAW strategies. The 90% CCIs are consistently tighter (smaller) when using the ILAW strategy. Tighter 90% CCIs represent a better chance of satisfying the given condition. The 90% CCIs for the IHLW strategy are wider because the GFC masses added to the MFPV must be estimated from MFPV sample, analysis, and other measurement information. This leads to larger uncertainties.

The plots also include a comparison of the high uncertainty cases (with four CRV and MFPV samples) and the nominal uncertainty cases (with eight CRV and MFPV samples). As expected, the 90% CCIs are consistently tighter when using the nominal uncertainty cases and eight samples.

Prior to presenting and discussing the results in subsequent subsections, it is worthwhile noting that the effects of HLW CRV mixing/sampling solids bias on compliance and processing properties will depend on the expressions used to calculate those properties. Waste loading is calculated as Al_2O_3 + Fe_2O_3 + ZrO_2 in mass percent. Per Table 4.10, Al, Fe, and Zr were all treated as solids in the CRV. Hence, a positive solids bias will increase the WL, while a negative solids bias will decrease WL. The remaining properties assessed in this work (PCT, T_L, $T_{0.01}$, TCLP Cd release, and viscosity at 1100ºC) all are calculated using property-composition models. Hence, how negative and positive solids biases affect those properties depends on the signs and magnitudes of the coefficients of the property-composition models used to predict the properties. It is possible that a particular property might be minimally affected by solids bias because of "cancellation" of the effects of solids and liquid components resulting from the signs and magnitudes of model coefficients. The property-composition model coefficients are listed in Table 2.3.

6.1 PCT Results for Simulation Study #2

Figure 6.1 shows plots of the Simulation Study #2 results for PCT normalized releases of boron, lithium, and sodium. Each plot contains lines corresponding to "Nominal PCT", "Nominal PCT + Comp. Unc.", and "Nominal PCT + Comp.Unc. + Model.Unc." results as functions of HLW CRV mixing/sampling solids bias. All three types of results are for the nominal compositions of the "no-bias" Glass C formulation and the various "biased Glass C formulations" listed in Table 4.8. The "Nominal PCT" results are predictions from applying the PCT-composition models from Table 2.3 to the nominal glass compositions in Table 4.8. The "Nominal PCT + Comp. Unc." results consist of the model

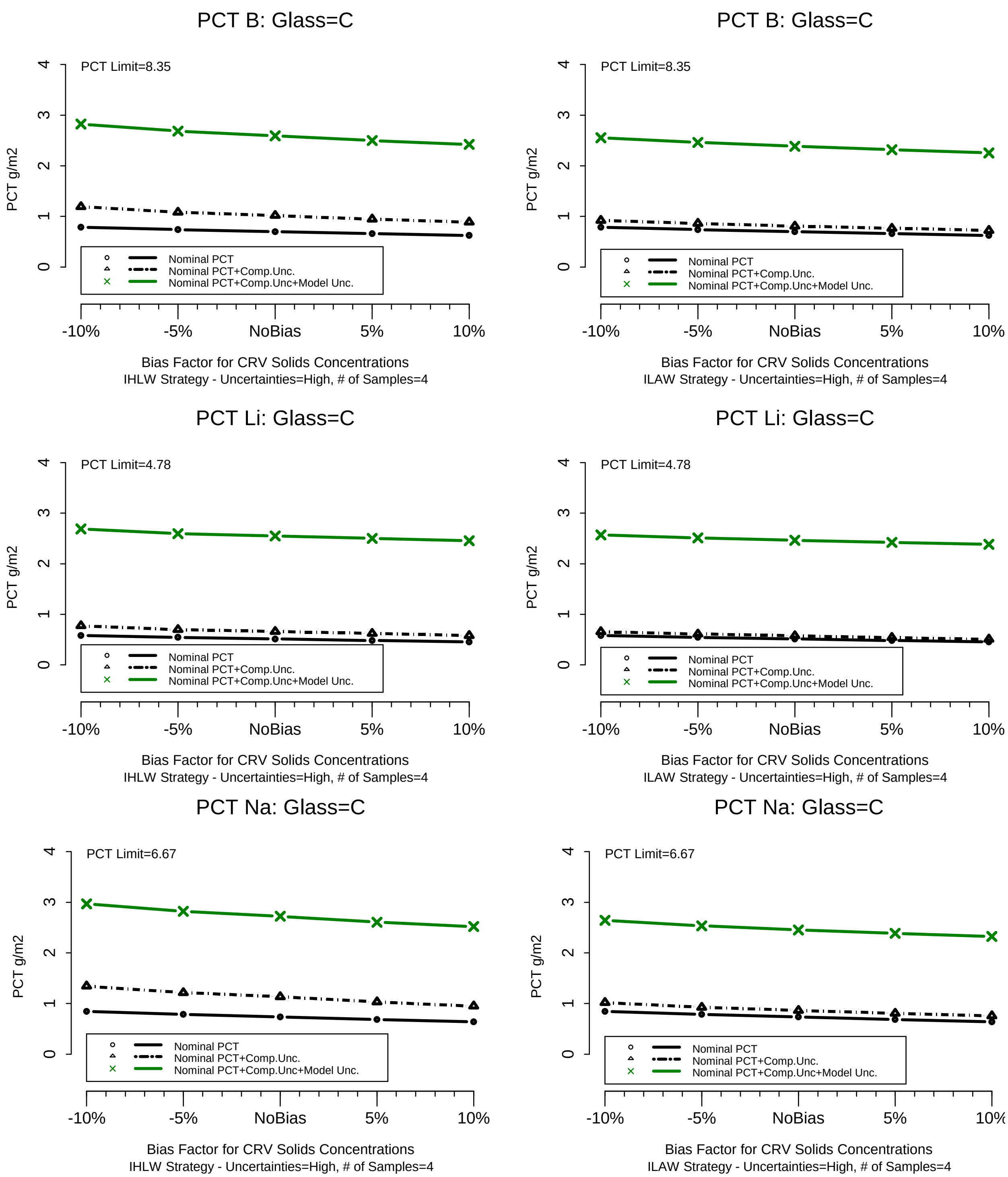

Figure 6.1. PCT Nominal and 90% UCCI Results as a Function of HLW CRV Mixing/Sampling Bias

predictions for these nominal compositions plus composition uncertainties. As discussed in Section 3.3.1, these results are the 90th percentiles of the distributions of PCT results (normalized B, Li, or Na releases) obtained by applying the PCT B, Li, and Na models to the 1000 glass compositions from a simulation run. These results, expressed in PCT normalized release units (g/m^2), capture only the composition uncertainty associated with a single MFPV batch. The "Nominal PCT + Comp.Unc. + Model.Unc." results add to the "Nominal PCT" results both composition uncertainty as just discussed as well as uncertainty in the PCT-composition models. As also discussed in Section 3.3.1, the model uncertainty was calculated using 90% SUCIs. The 90% UCCIs are represented by the "Nominal PCT + Comp.Unc. + Model.Unc." results in Figure 6.1. The 90% UCCI results of this type were previously displayed in Figure 5.1 for each of the Glasses A to E.

Figure 6.1 displays two plots for each of PCT B, Li, and Na, corresponding to the IHLW and ILAW calculation strategies. Only results for the CRV mixing/sampling random uncertainty = 10 %RSD, high levels of other random uncertainties, four CRV samples (IHLW and ILAW strategies), and four MFPV samples (IHLW strategy) are shown. Combinations of CRV mixing/sampling random uncertainty = 5 %RSD, low levels of other random uncertainties, and eight CRV samples (IHLW and ILAW strategies) and eight MFPV samples (IHLW strategy) yielded results even farther below the compliance limits. Hence, it was decided not to display plots of those results.

It is clear from the plots in Figure 6.1 that uncertainty due to the PCT models is much larger than the composition uncertainty. This observation requires some additional explanation. First, the composition uncertainty corresponds to the uncertainty in the glass that would be made from a single MFPV batch, which is what the simulation software addresses. Variations in glass composition resulting from batch-to-batch variations in MFPV composition over an HLW waste type are not included in the composition uncertainties shown in Figure 6.1. Second, the model uncertainties displayed in Figure 6.1 are based on SCIs, which are generally much wider than single CIs (see Section 2.3). Because property-composition models (such as the PCT-composition models) will be used many times during WTP production, it is appropriate to use SCIs to limit the probability of the CIs not containing the true results. Still, the use of SCIs to quantify PCT-composition model uncertainties is only part of the explanation for the large model uncertainty. The PCT-composition models used are preliminary ones that perform relatively well, but still are subject to significant lack-of-fit (i.e., more uncertainty than can be accounted for by experimental and testing uncertainties). Despite the composition uncertainties and relatively large model uncertainties, the PCT 90% UCCIs are still well below the compliance limits for normalized B, Li, and Na releases.

In summary, all 90% UCCIs (calculated as described in Section 3.3.1) for PCT normalized boron, lithium, and sodium releases were well below the corresponding compliance limits, regardless of the calculation strategy (IHLW or ILAW), the level of CRV mixing/sampling solids bias (-10%, -5%, 0%, +5%, +10%), the level of CRV mixing/sampling random uncertainty (5 and 10 %RSD, and the numbers of CRV and MFPV samples (four or eight). The 90% UCCIs are so far below the limiting values that it was necessary to print the limiting values on the plots rather than show them as horizontal lines.

6.2 Liquidus Temperature Results for Simulation Study #2

Figure 6.2 shows plots of the Simulation Study #2 results for T_L. Each plot contains lines corresponding to “Nominal TL”[(a)] and “Nominal TL + Comp.Unc. + Model.Unc.” results as a function of HLW CRV mixing/sampling solids bias. Both types of results are for the nominal compositions of the “no-bias” Glass C formulation and the various “biased Glass C formulations” listed in Table 4.8. The “Nominal TL” results are predictions from applying the T_L-composition model from Table 2.3 to the nominal glass compositions listed in Table 4.8. The “Nominal TL + Comp. Unc. + Model Unc.” results consist of adding composition uncertainties and model uncertainties to the model predictions for the nominal compositions. As discussed in Section 3.3.2, the composition uncertainty results are the 90th percentiles of the distributions of T_L results obtained by applying the T_L-composition model to the 1000 glass compositions from a simulation run. As also discussed in Section 3.3.2, the model uncertainty was calculated using 90% SUCIs. The 90% UCCIs are represented by the “Nominal TL + Comp.Unc. + Model.Unc.” results in Figure 6.2. The 90% UCCI results of this type were previously displayed in Figure 5.2 for each of the Glasses A to E.

Figure 6.2 shows T_L nominal values and 90% UCCIs for the IHLW and ILAW strategies as well as nominal and high uncertainty cases. The “nominal uncertainty case” included CRV mixing/sampling random uncertainty = 5 %RSD, nominal values of other random uncertainties, and eight CRV (IHLW and ILAW strategies) and eight MFPV samples (IHLW strategy). The “high uncertainty case” included CRV mixing/sampling random uncertainty = 10 %RSD, high values of other random uncertainties, and four CRV (IHLW and ILAW strategies) and four MFPV samples (IHLW strategy). All T_L results (both the nominal values and the 90% UCCIs) were above, and hence violate, the 950°C limit. This is so because only $T_{0.01}$, and not T_L, was restricted to be below 950°C in formulating Glasses A to E (as discussed in Section 2.3). These results demonstrate that $T_L \leq 950°C$ is a much stricter processability criterion than is $T_{0.01} \leq 950°C$. While some glasses may satisfy both criteria, in general there will be many glasses that satisfy the $T_{0.01} \leq 950°C$ condition but not the $T_L \leq 950°C$ condition. Figure 6.2 also shows that bias has a significant effect on T_L. For each increase in solids bias of 1%, there is an increase in the T_L 90% UCCI of between 6°C and 8°C.

Figure 6.2 also shows that increasing the sample size and obtaining nominal uncertainties greatly reduces the 90% UCCI, especially for the IHLW strategy. The difference between the 90% UCCI and the nominal T_L is almost 150°C for the high uncertainty and 4 sample cases as compared to a difference of 100°C for the nominal uncertainty and 8 sample cases.

(a) Note that “TL” denotes T_L, but is referred to in this way to match the figure legend, where subscripting was not available.

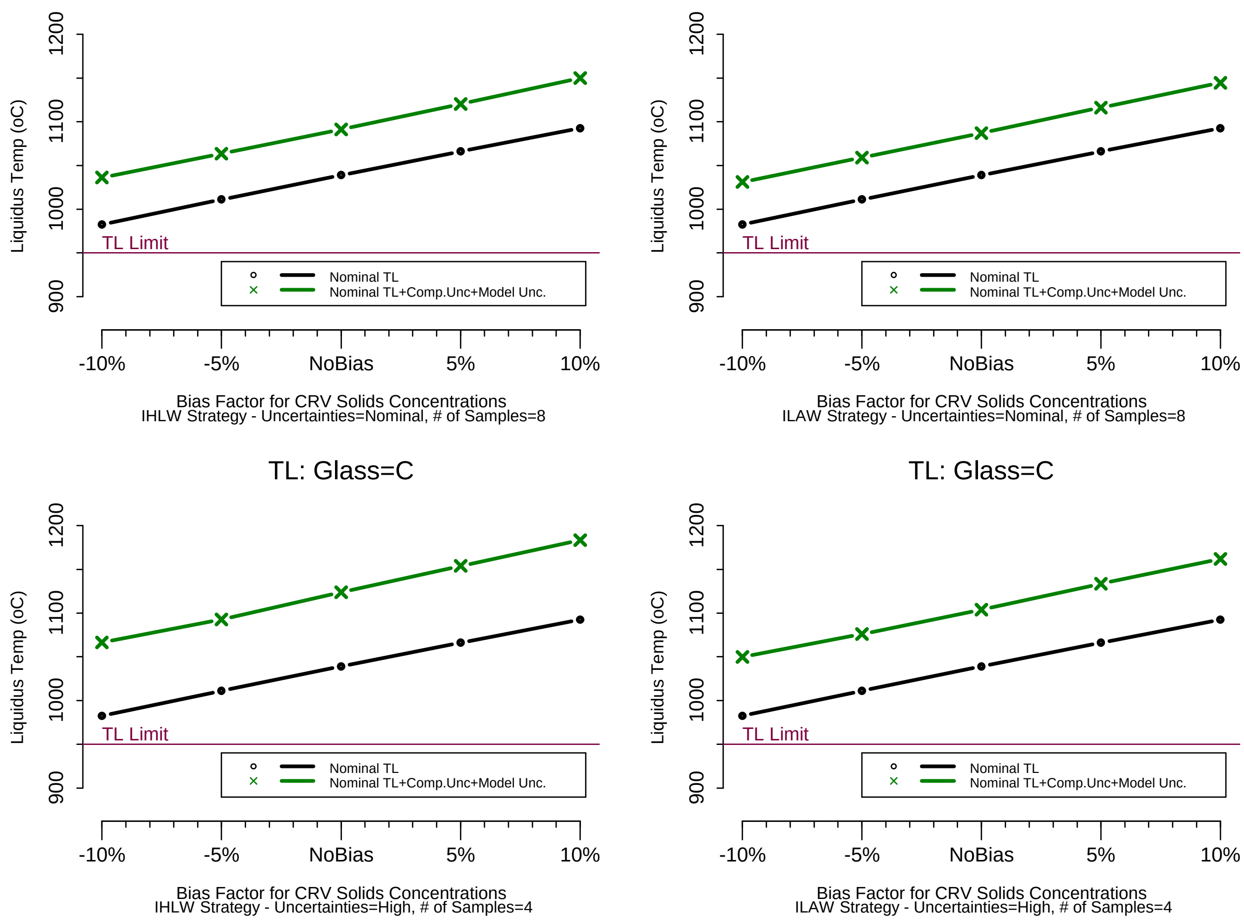

Figure 6.2. T_L Nominal and 90% UCCI Results as a Function of HLW CRV Mixing/Sampling Bias

6.3 $T_{0.01}$ Results for Simulation Study #2

Figure 6.3 shows plots of the Simulation Study #2 results for $T_{0.01}$. Each plot contains lines corresponding to "Nominal T01"[(a)] and "Nominal T01 + Comp.Unc. + Model.Unc." results as a function of HLW CRV mixing/sampling solids bias. Both types of results are for the nominal compositions of the "no-bias" Glass C formulation and the various "biased Glass C formulations" listed in Table 4.8. The "Nominal T01" results are predictions from applying the $T_{0.01}$-composition model from Table 2.3 to the nominal glass compositions listed in Table 4.8. The "Nominal T01 + Comp. Unc. + Model Unc." results consist of adding composition uncertainties and model uncertainties to the model predictions for the nominal compositions. As discussed in Section 3.3.3, the composition uncertainty results are the 90th percentiles of the distributions of $T_{0.01}$ results obtained by applying the $T_{0.01}$-composition model to the 1000 glass compositions from a simulation run. As also discussed in Section 3.3.3, the model uncertainty

(a) Note that "T01" denotes $T_{0.01}$, but is referred to in this way to match the figure legend, where subscripting was not available.

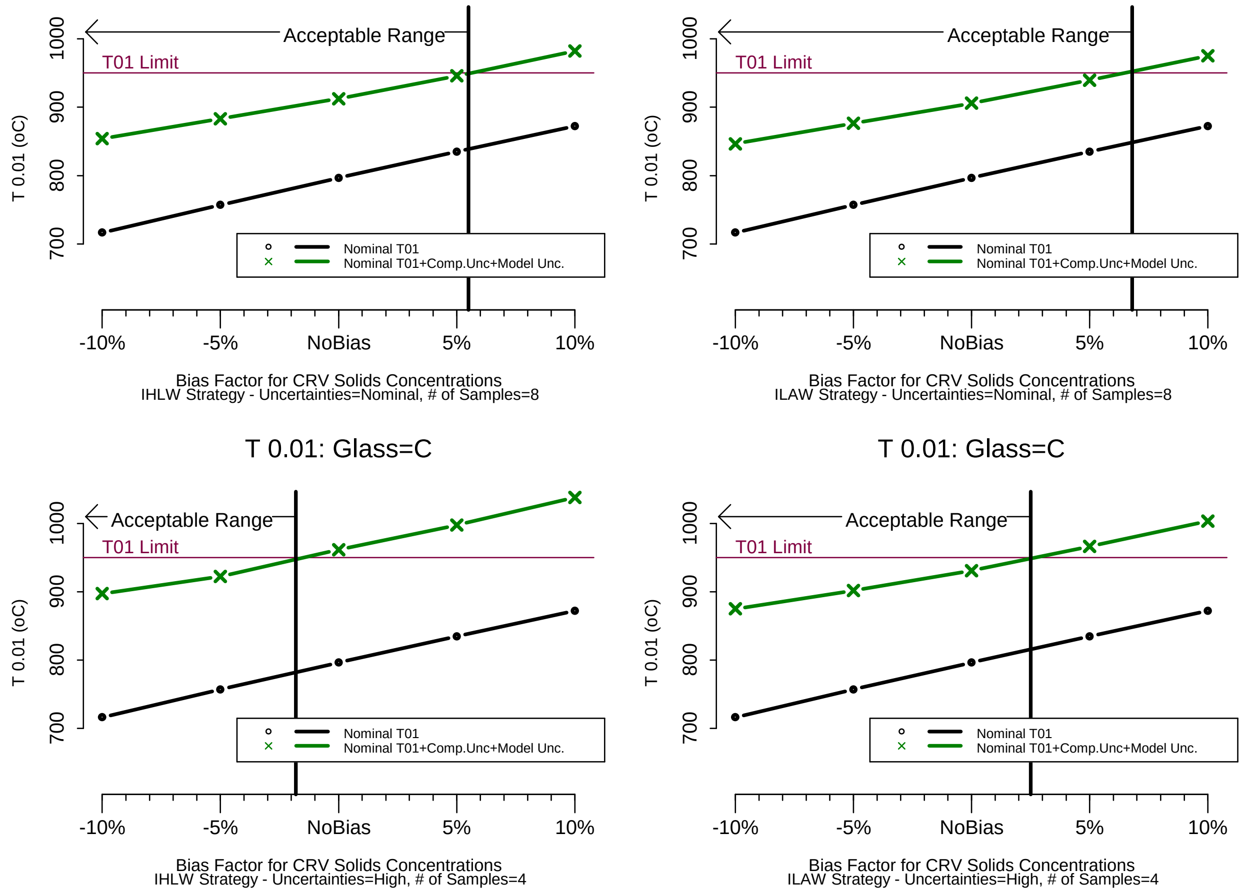

Figure 6.3. $T_{0.01}$ Nominal and 90% UCCI Results as a Function of HLW CRV Mixing/Sampling Bias. The acceptable range of bias for each situation is marked with an arrow.

was calculated using 90% SUCIs. The 90% UCCIs are represented by the "Nominal PCT + Comp.Unc. + Model.Unc." results in Figure 6.3. The 90% UCCI results of this type were previously displayed in Figure 5.3 for each of the Glasses A to E.

The results in Figure 6.3 show that satisfying the $T_{0.01} \leq 950°C$ processability condition was dependent upon the amount of CRV mixing/sampling bias, the type of strategy used in the calculations (ILAW or IHLW), and uncertainty level (nominal or high). The "nominal uncertainty" case represents HLW CRV mixing/sampling random uncertainty = 5 %RSD, nominal levels of other random uncertainties, and eight CRV (IHLW and ILAW strategies) and eight MFPV (IHLW strategy) samples with one chemical analysis per sample. The "high uncertainty" case represents HLW CRV mixing/sampling random uncertainty = 10 %RSD, high levels of other random uncertainties, and four CRV (IHLW and ILAW strategies) and four MFPV (IHLW strategy) samples with one chemical analysis per sample. Figure 6.3 shows when the processability constraint is and is not satisfied for four combinations of these factors. In each plot of Figure 6.3, the range of HLW CRV mixing/sampling bias values that allows the 90% UCCI (Nominal T01 + Comp.Unc + Model.Unc) to be less than the 950°C limit is identified as the "Acceptable Range". Figure 6.3 also shows that bias has a significant effect on

$T_{0.01}$. For each increase in solids bias of 1%, there is an increase in the $T_{0.01}$ 90% UCCI of between 6°C and 9°C.

For the IHLW strategy with nominal uncertainty case (Figure 6.3, top left plot), the 90% UCCIs on $T_{0.01}$ meet the 950°C limit when the CRV mixing/sampling solids bias is +5.5% or less. When the IHLW strategy is combined with the high uncertainty case (bottom left plot), the limit is satisfied only when the HLW CRV mixing/sampling solids bias is -2% or less. For the ILAW strategy, the acceptable ranges of HLW CRV mixing/sampling bias widen somewhat compared to the IHLW strategy. For the nominal uncertainty case (top right plot), the 90% UCCIs meet the 950°C limit when the HLW CRV mixing/sampling solids bias is +7% or less. For the high uncertainty case (bottom right plot), the limit is satisfied when the HLW CRV mixing/sampling solids bias is +2.5% or less.

6.4 Waste Loading Results for Simulation Study #2

Figure 6.4 shows plots of the Simulation Study #2 results for WL = $Al_2O_3 + Fe_2O_3 + ZrO_2$, which must be greater than 21% for Glass C and its biased variations (see Table 4.8) to be compliant. Each plot contains lines corresponding to “Nominal WL” and “Nominal WL - Avg.Unc.” results as a function of HLW CRV mixing/sampling solids bias. Both types of results are for the nominal compositions of the “no-bias” Glass C formulation and the various “biased Glass C formulations” listed in Table 4.8. The “Nominal WL” results (for $Al_2O_3 + Fe_2O_3 + ZrO_2$) are calculated from the nominal glass compositions listed in Table 4.8. The “Nominal WL - Avg.Unc.” results consist of the nominal WL values for the nominal compositions minus composition uncertainties averaged over 90 MFPV batches as discussed in Section 3.3.4. The average composition uncertainty results (referred to as 90% LCIs)[a] are the 10th percentiles of the distributions of 1000 WL results corresponding to the 1000 glass compositions from a simulation run. The 90% LCIs are represented by the “Nominal WL - Avg.Unc.” results in Figure 6.4. The 90% LCI results of this type were previously displayed in Figure 5.4 for each of the Glasses A to E.

The results in Figure 6.4 show that satisfying the WL ≥ 21% compliance condition was dependent upon the amount of HLW CRV mixing/sampling bias, the type of strategy used in the calculations (ILAW or IHLW), and uncertainty level (nominal or high). The “nominal uncertainty” case represents HLW CRV mixing/sampling random uncertainty = 5 %RSD, nominal levels of other random uncertainties, and eight CRV (IHLW and ILAW strategies) and eight MFPV (IHLW strategy) samples with one chemical analysis per sample. The “high uncertainty” case represents HLW CRV mixing/sampling random uncertainty = 10 %RSD, high levels of other random uncertainties, and four CRV (IHLW and ILAW strategies) and four MFPV (IHLW strategy) samples with one chemical analysis per sample. Figure 6.4 shows when the WL compliance constraint is and is not satisfied for four combinations of these factors. In each plot of Figure 6.4, the range of HLW CRV mixing/sampling bias values that allow the 90% LCI (Nominal WL - Avg.Unc.) to be greater than or equal to the 21% limit is identified on each plot as the “Acceptable Range”. Figure 6.4 also shows that bias has a significant effect on WL. For each increase in solids bias of 1%, there is an increase in the WL 90% UCCI of approximately 0.15% ($Al_2O_3 + Fe_2O_3 + ZrO_2$).

(a) A LCI (lower confidence interval) is appropriate rather than LCCI (lower combined confidence interval), because for waste loading, there is no model uncertainty to combine with composition uncertainty.

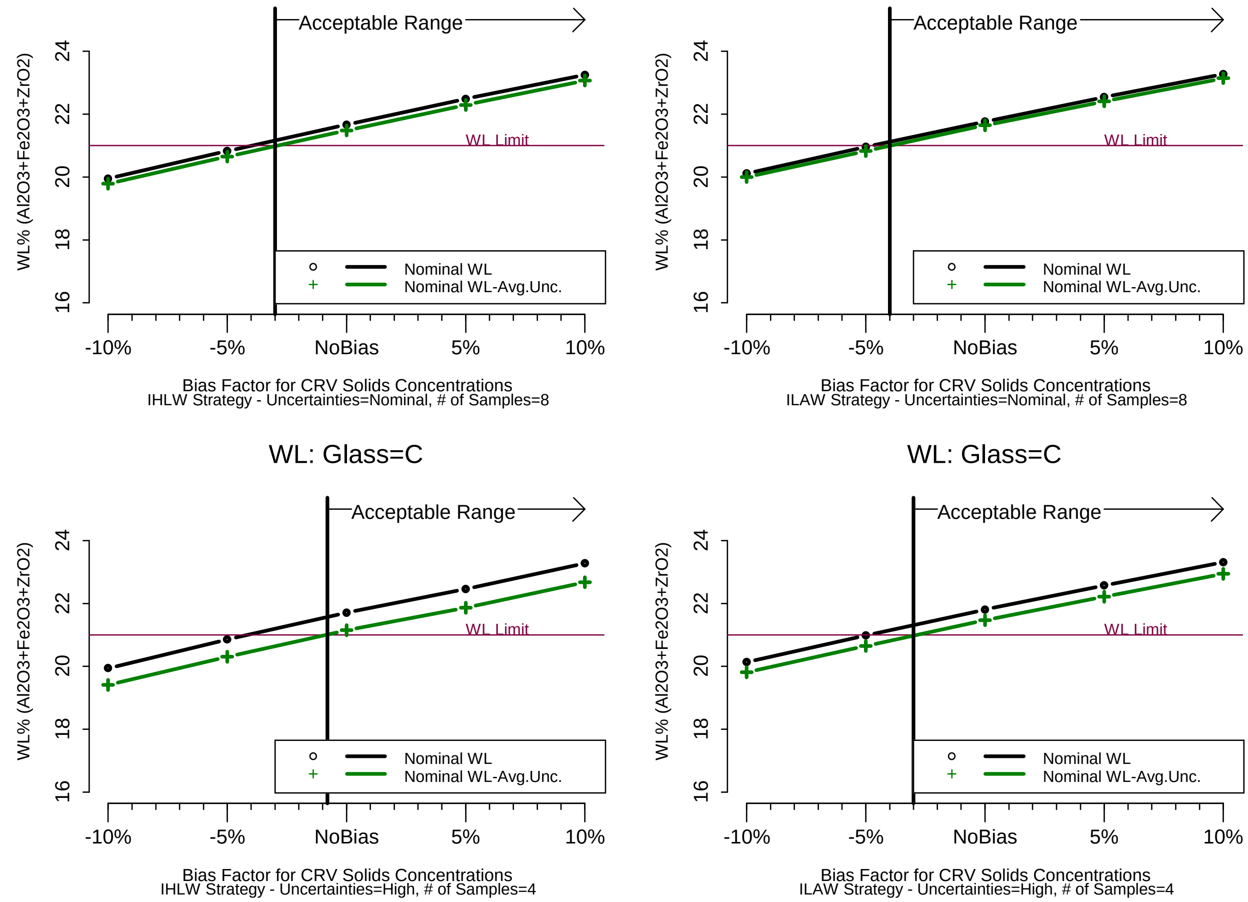

Figure 6.4. Waste Loading Nominal and 90% LCI Results as a Function of HLW CRV Mixing/Sampling Bias. The acceptable range of bias for each situation is marked with an arrow.

Figure 6.4 also illustrates that increasing the sample size and obtaining nominal uncertainties greatly reduces the 90% LCI. The difference between the 90% LCI and the nominal WL is almost 1 WL% for the high uncertainty and 4 sample cases, compared to a difference of approximately 0.1 WL% for the nominal uncertainty and 8 sample cases.

For the IHLW strategy with the nominal-uncertainty case (Figure 6.4, top left plot), the 90% LCIs on WL meet the 21% limit when the CRV mixing/sampling solids bias is -3% or greater. When the IHLW strategy is combined with the high-uncertainty case (bottom left plot), the limit is satisfied only when the HLW CRV mixing/sampling solids bias is -1% or greater. For the ILAW strategy, the acceptable ranges of HLW CRV mixing/sampling bias widen somewhat compared to the IHLW strategy. For the ILAW strategy and nominal uncertainty case (top right plot), the 90% LCIs for WL meet the 21% limit when the HLW CRV mixing/sampling solids bias is -4% or greater. For the ILAW strategy and the high uncertainty case (bottom right plot), the WL limit is satisfied when the HLW CRV mixing/sampling solids bias is -3% or greater.

6.5 TCLP Cd Release Results for Simulation Study #2

Figure 6.5 shows plots of the Simulation Study #2 results for TCLP Cd release (mg/L). Each plot contains lines corresponding to "Nominal TCLP" and "Nominal TCLP + Comp.Unc. + Model.Unc." results as a function of HLW CRV mixing/sampling solids bias. Both types of results are for the nominal compositions of the "no-bias" Glass C formulation and the various "biased Glass C formulations" listed in Table 4.8. The "Nominal TCLP" results are predictions from applying the TCLP Cd release-composition model from Table 2.3 to the nominal glass compositions listed in Table 4.8. The "Nominal TCLP + Comp. Unc. + Model Unc." results consist of composition uncertainties and model uncertainties added to the model predictions for the nominal compositions. As discussed in Section 3.3.5, the composition uncertainty results are the 90th percentiles of the distributions of TCLP Cd release concentrations obtained by applying the TCLP Cd release-composition model to the 1000 glass compositions from a simulation run. As also discussed in Section 3.3.5, the model uncertainty was calculated using 90% (single, not simultaneous) UCIs. The 90% UCCIs are represented by the "Nominal TCLP + Comp.Unc. + Model.Unc." results in Figure 6.5. The 90% UCCI results of this type were previously displayed in Figure 5.5 for each of the Glasses A to E.

The results in Figure 6.5 show that satisfying the TCLP Cd release = 0.48 mg/L compliance criterion was not dependent upon the amount of HLW CRV mixing/sampling bias, the type of strategy used in the calculations (ILAW or IHLW), or the uncertainty level (nominal or high). The "nominal uncertainty" case represents HLW CRV mixing/sampling random uncertainty = 5 %RSD, nominal levels of other random uncertainties, and eight CRV (IHLW and ILAW strategies) and eight MFPV (IHLW strategy) samples with one chemical analysis per sample. The "high uncertainty" case represents HLW CRV mixing/sampling random uncertainty = 10 %RSD, high levels of other random uncertainties, and four CRV (IHLW and ILAW strategies) and four MFPV (IHLW strategy) samples with one chemical analysis per sample. In each of the four cases shown in Figure 6.5, the 90% UCCI (Nominal TCLP + Comp.Unc. + Model.Unc.) was well below the TCLP Cd release limit. Figure 6.5 also shows that bias does not have a significant effect on TCLP Cd release. The slopes of the 90% UCCI for TCLP Cd release are between 0.001 and 0.002 mg/L for each 1% increase in bias. These plots indicate that HLW CRV mixing/sampling solids biases from -10% to +10% for each of the testing conditions still allow compliance with the TCLP Cd release limit.

Figure 6.5 also illustrates that increasing the sample size and obtaining nominal uncertainties greatly reduces the 90% UCCI, especially for the IHLW strategy. The difference between the 90% UCCI and the nominal TCLP is over twice the size for the high uncertainties and 4 samples (0.12 mg/l) compared to the nominal uncertainties and 8 samples (0.05 mg/L).

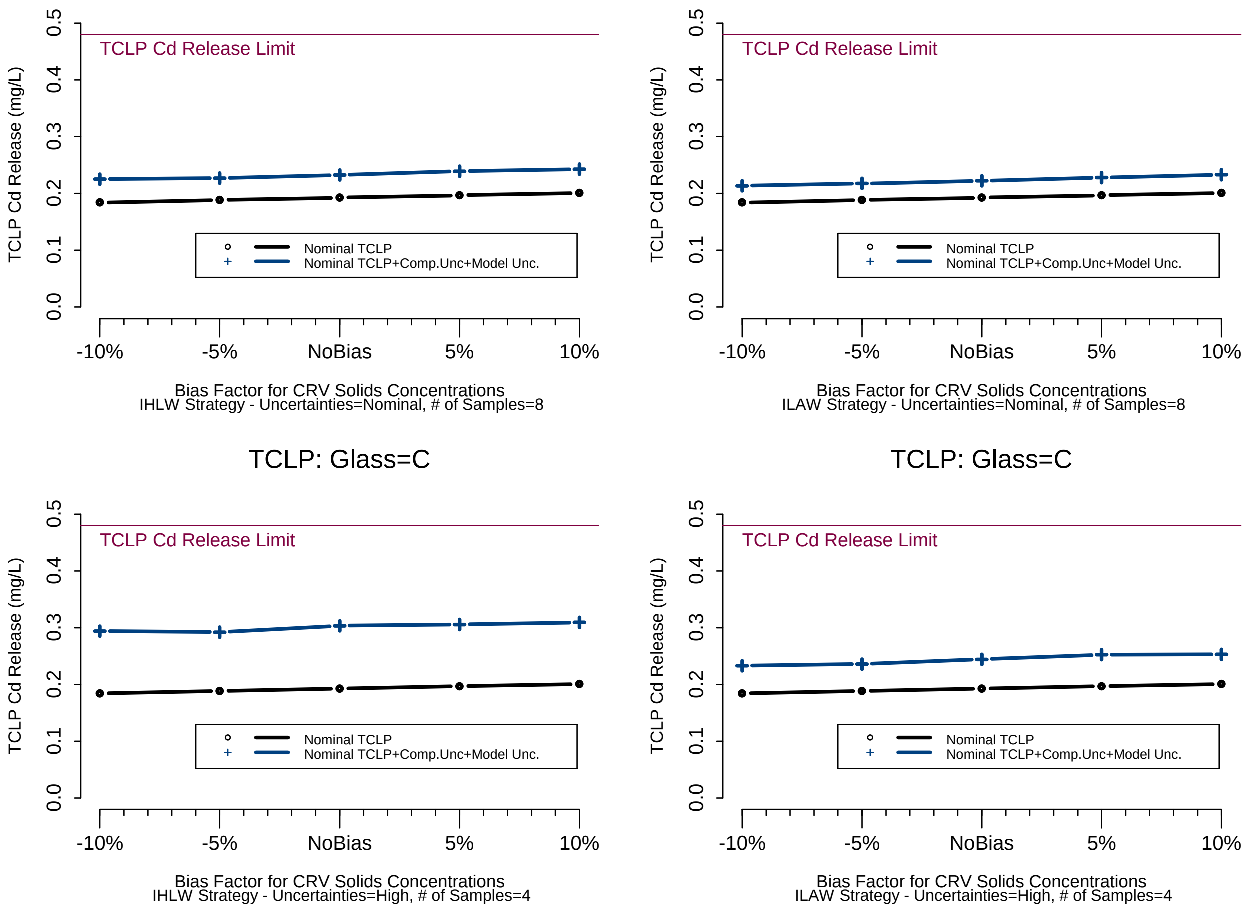

Figure 6.5. TCLP Cd Release Nominal and 90% UCCI Results as a Function of HLW CRV Mixing/Sampling Bias

6.6 Viscosity at 1100°C Results for Simulation Study #2

Figure 6.6 shows plots of the Simulation Study #2 results for viscosity at 1100°C (η_{1100}, poise). Each plot contains lines corresponding to "Nominal Visc", "Nominal Visc - Comp.Unc. - Model.Unc.", and "Nominal Visc + Comp.Unc. + Model.Unc.". Each of these results is shown as a function of HLW CRV mixing/sampling solids bias in Figure 6.6. All three types of results are for the nominal compositions of the "no-bias" Glass C formulation and the various "biased Glass C formulations" listed in Table 4.8. The "Nominal Visc" results are predictions from applying the η_{1100}-composition model with coefficients in Table 2.3 to the nominal glass compositions listed in Table 4.8. The "Nominal Visc - Comp. Unc. - Model Unc." and "Nominal Visc + Comp. Unc. + Model Unc." results consist of the model predictions for the nominal compositions minus and plus, respectively, composition uncertainties and model uncertainties. As discussed in Section 3.3.6, the composition uncertainty results are two-sided 90% empirical CIs (i.e., lower and upper 95th percentiles) of the distributions of η_{1100} (poise) values obtained by applying the η_{1100}--composition model to the 1000 glass compositions from a simulation run. As also discussed in Section 3.3.6, the model uncertainty was calculated using two-sided 90% (single, not simultaneous) CIs (i.e., one-sided 95% LCIs and UCIs). The two-sided 90% CCIs (i.e., one-sided 95%

LCCIs and UCCIs) are represented by the “Nominal Visc - Comp. Unc. - Model Unc.” and “Nominal TCLP + Comp.Unc. + Model.Unc.” results in Figure 6.6.

Figure 6.6 shows the nominal values and two-sided 90% CCIs on η_{1100} under the same strategies and uncertainties as the other compliance and processability criteria studied in Simulation Study #2. In each case, the two-sided 90% CCIs were well between the η_{1100} limits of 10 to 150 poise. This indicates that under each of the solid biases tested and for each of the testing conditions, Glass C would satisfy the viscosity processability limits. Figure 6.6 shows that HLW CRV mixing/sampling solids bias has only a slight effect on viscosity.

Figure 6.6 also illustrates that increasing the sample size and obtaining nominal uncertainties greatly reduces the two-sided 90% CCIs, especially for the IHLW strategy. The width of the interval for the high uncertainty and 4 sample cases was nearly 75 poise as compared to an interval width of 30 poise for the nominal uncertainty and 8 sample cases.

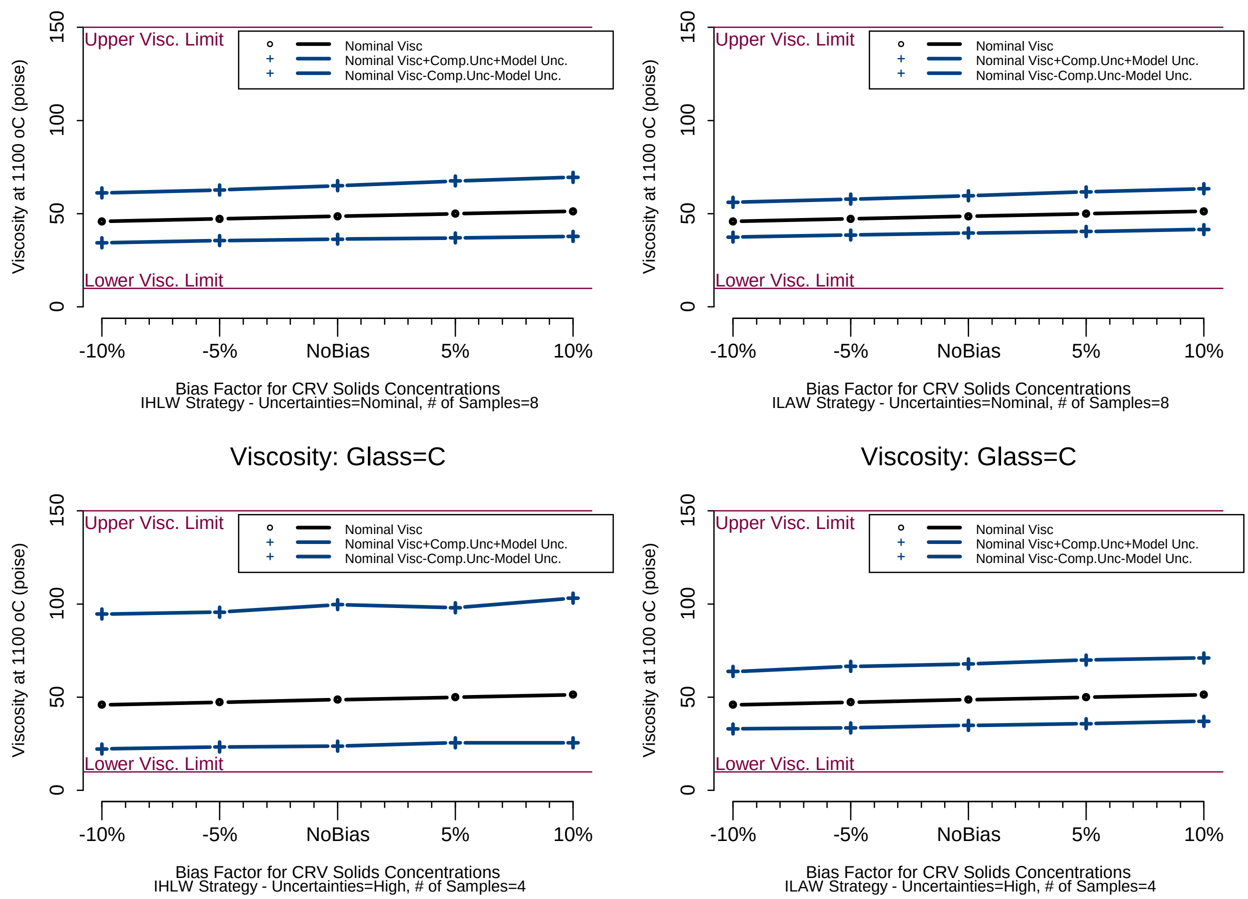

Figure 6.6. Viscosity at 1100°C Nominal and Two-Sided 90% CCI Results as Functions of HLW CRV Mixing/Sampling Bias

7.0 Results of Simulation Study #3 to Assess CRV Mixing/Sampling Bias and Random Uncertainties

Simulation Study #3 focused on assessing the joint effects of HLW CRV mixing/sampling bias and random uncertainty. HLW CRV mixing/sampling solids biases was tested at -10%, -5%, 0% (no bias), +5%, and +10%. HLW CRV mixing/sampling random uncertainty was tested at %RSD values of 5%, 15%, and 25%, which was a wider range of uncertainties than assessed in Simulation Study #2. All 5 × 3 = 15 combinations of these two factors were studied, as shown in the test matrix listed previously in Table 4.11. Both the IHLW and ILAW calculation strategies were investigated. The other random uncertainties were at the nominal case and the number of CRV (IHLW and ILAW strategies) and MFPV (IHLW strategy) samples was set to eight.

Prior to presenting and discussing the results, it is worthwhile noting that the effects of HLW CRV mixing/sampling solids bias on compliance and processing properties will depend on the expressions used to calculate those properties. The discussion of this topic at the end of Section 6.0 applies here as well.

The resulting two-sided 90% CCIs and one-sided 90% LCCIs, UCCIs, and LCIs (calculated as previously discussed) are plotted in Figure 7.1 to Figure 7.5 for each of the compliance and processing conditions, except PCT. PCT results were not included due to the ease of meeting that criterion for all combinations of CRV mixing/sampling bias and random uncertainty. In each of Figure 7.1 to Figure 7.5, the 90% CCIs, LCCIs, UCCIs, and LCIs are plotted versus the HLW CRV mixing/sampling solids bias. Separate lines in each plot correspond to the HLW CRV mixing/sampling random uncertainty values of 5, 15, and 25 %RSD.

In general, the 90% CCIs, LCCIs, UCCIs, and LCIs[(a)] became wider as the HLW CRV mixing/sampling random uncertainty %RSD was increased, just as expected. Viscosity at 1100°C appears to be the least affected by an increase in HLW CRV mixing/sampling random uncertainty. The magnitudes of 90% UCCIs for T_L and $T_{0.01}$, and 90% LCIs for waste loading are significantly affected by the HLW CRV mixing/sampling bias. The magnitudes of 90% UCCIs for TCLP Cd release and two-sided 90% CCIs for viscosity at 1100°C are little affected by the HLW CRV mixing/sampling bias.

(a) LCCIs and UCCIs apply to compliance and processing properties for which composition uncertainty as well as property-composition model uncertainty are combined. LCIs apply only to waste loading, for which there is only composition uncertainty and no property-composition model uncertainty.

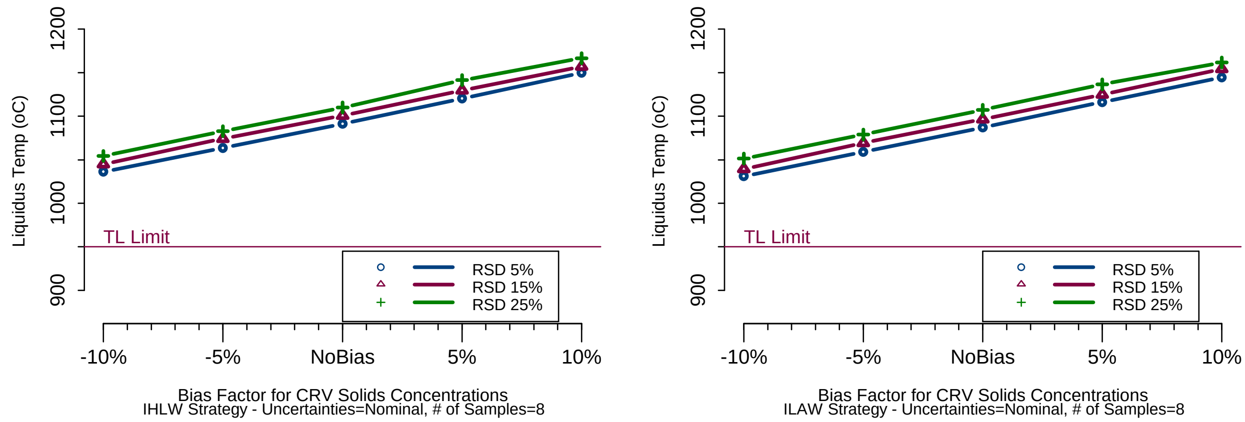

Figure 7.1. T_L 90% UCCI Results as Functions of HLW CRV Mixing/Sampling Bias and Random Uncertainty

When meeting the $T_{0.01}$ and WL conditions, the allowable range of HLW CRV mixing/sampling bias decreases significantly as the HLW CRV mixing/sampling random uncertainty %RSD increases. At 5 %RSD and with the IHLW strategy, the allowable range of HLW CRV mixing/sampling bias was -3% to 5%. At 25% RSD the allowable range of CRV mixing/sampling bias decreases, and was from -2% to +0.5%. The allowable ranges of HLW CRV mixing/sampling bias are wider with the ILAW strategy. At 5% RSD and with the ILAW strategy, -4% to +6.5% solids bias is allowable. However, at 25% RSD and with the ILAW strategy, -2.5% to 1% solids bias is allowable.

Bias significantly influenced $T_{0.01}$ and T_L, with an increase of approximately 6°C for each 1% increase in bias. WL was also significantly influenced with an increase of 0.15% $Al_2O_3 + Fe_2O_3 + ZrO_2$ for each 1% increase in bias. TCLP Cd Release and viscosity were not affected by the HLW CRV mixing/sampling solids bias. These conclusions were only based on solid bias in the -10% to 10% range.

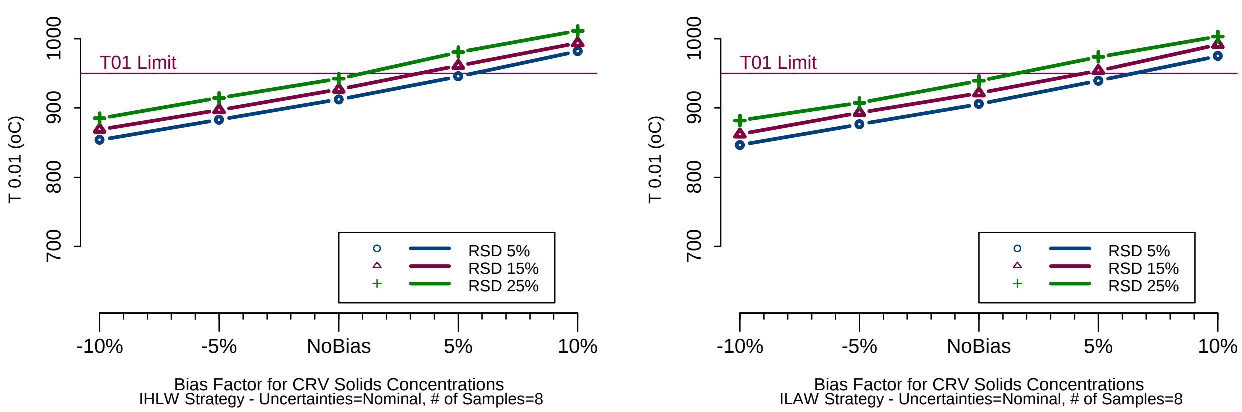

Figure 7.2. $T_{0.01}$ 90% UCCI Results as Functions of HLW CRV Mixing/Sampling Bias and Random Uncertainty

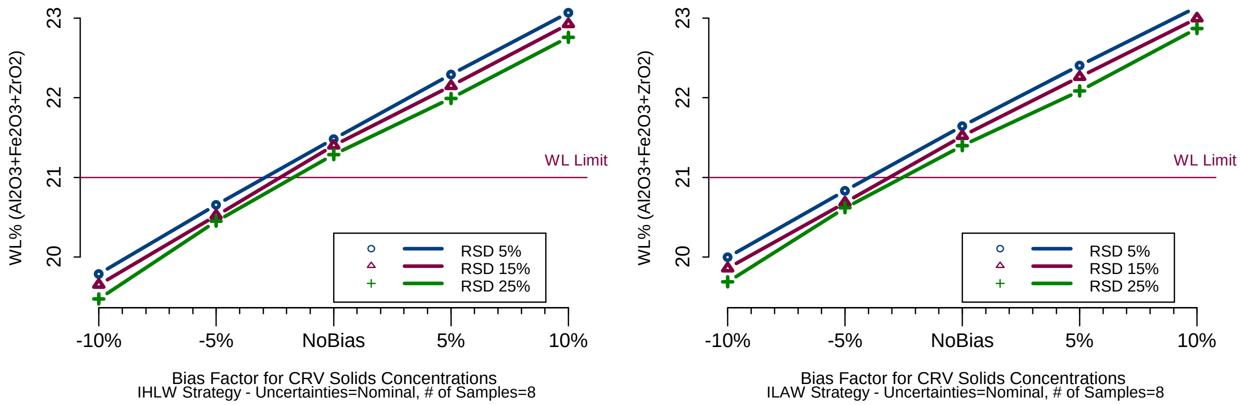

Figure 7.3. Waste Loading 90% LCI Results as Functions of HLW CRV Mixing/Sampling Bias and Random Uncertainty

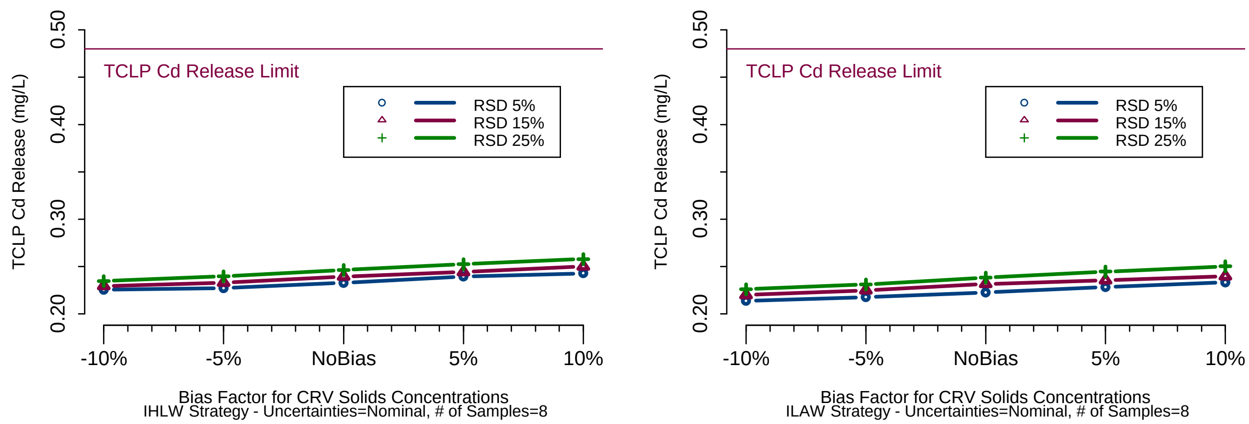

Figure 7.4. TCLP Cd Release 90% UCCI Results as Functions of HLW CRV Mixing/Sampling Bias and Random Uncertainty

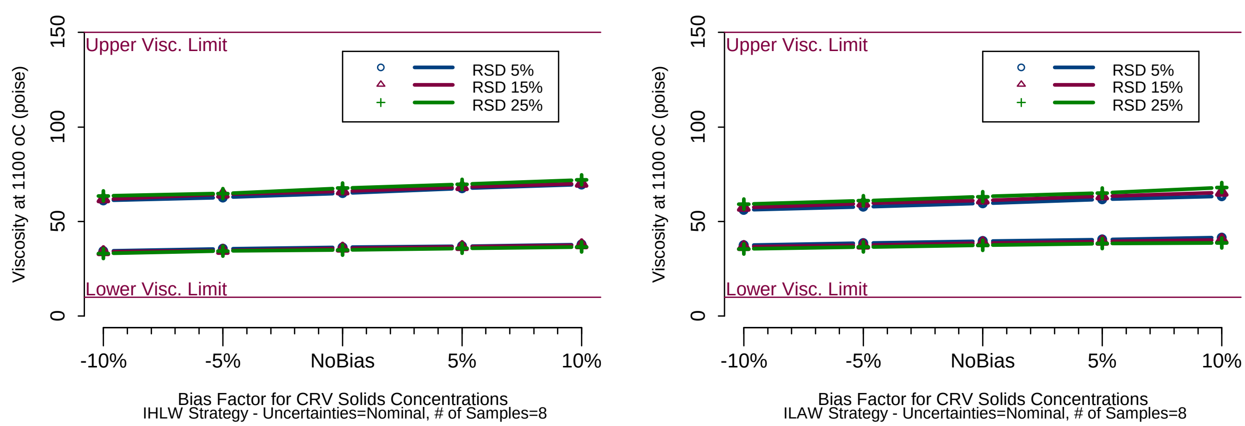

Figure 7.5. Viscosity at 1100°C Two-Sided 90% CCI Results as Functions of HLW CRV Mixing/Sampling Bias and Random Uncertainty

8.0 Summary and Discussion

The primary goal of the work summarized in this report was to assess how well a Waste Treatment and Immobilization Plant (WTP)[(a)] high-level waste (HLW) Concentrate Receipt Vessel (CRV) must be mixed and sampled to satisfy applicable compliance and processing conditions. Mixing and sampling effects were jointly assessed because during WTP production operations when the CRV is sampled, mixing and sampling effects (bias or random uncertainty) will be confounded. That is, any difference in the composition of a CRV sample and the true composition in the CRV could be due to mixing effects, sampling effects, or both. Taking multiple samples from a CRV and averaging the results can effectively reduce the mixing/sampling random uncertainty, but cannot reduce any mixing/sampling bias nor separate the mixing effects from the sampling effects.

The work documented in this report was conducted in a short time frame to address a WTP need. Hence, it was necessary to use and adapt the software already developed (for related but separate work) to simulate the WTP immobilized high-level waste (IHLW) and immobilized low-activity waste (ILAW) compliance strategies involving the CRV, glass forming chemicals (GFCs), and the Melter Feed Preparation Vessel (MFPV). That simulation software was designed to account for several uncertainties affecting a single MFPV batch. However, it did not have the capability to separately simulate CRV or MFPV mixing and sampling uncertainties. Further, there was not time to modify the software to incorporate that capability prior to beginning the work. Also, although batch-to-batch variation is important in assessing whether compliance and processing property conditions are satisfied, the simulation software did not account for this type of variation. Statistical methods other than simulation are being developed as part of other activities in the Test Plan (TP-RPP-WTP-193, Rev. 1, *Test Plan: Statistical Methods for Estimating Variations in HLW and LAW Waste Types*) to account for batch-to-batch variation in assessing whether compliance and processing property conditions are satisfied.

8.1 Summary of Simulation Studies

Three simulation studies were performed to assess the effects of HLW CRV mixing/sampling bias and random uncertainty, as well as other factors, on the ability to satisfy processing and compliance conditions. The other factors include glass formulation, other random uncertainties, and number of CRV and MFPV samples (with one chemical analysis per sample assumed). All three simulation studies used two calculation approaches, corresponding to the IHLW and ILAW compliance strategies. The "other random uncertainties", which depend on the compliance strategy, are listed in Section 3.2. The current IHLW compliance strategy involves sampling, analyzing, and making volume determinations for both the CRV and MFPV. Although masses of GFCs added to each MFPV batch will be determined during the IHLW process, they are not used as part of the IHLW compliance strategy. Under the IHLW compliance strategy, the GFC masses will be estimated using the analyses of MFPV samples and other process information. This is expected to add additional uncertainty to the calculated glass composition that would be produced from an MFPV batch. However, it will reduce the risk of possible biases due to GFC mis-batching. Hence, the work scope included investigating the ILAW compliance strategy applied to the IHLW process. The ILAW compliance strategy uses analyses of CRV samples and masses of GFCs added to the MFPV to calculate the composition of glass that would be produced from an MFPV batch.

(a) All acronyms are re-introduced for the benefit of those only reading this Summary and Discussion section.

The ILAW compliance strategy was expected to yield calculated glass compositions, as well as calculated glass compliance and processing properties, with less uncertainty than the IHLW compliance strategy.

Five glass formulations (denoted A, B, C, D, and E) for AZ-102 HLW were investigated in the first simulation study. These five AZ-102 glass formulations were found to be bounding for glass formulations corresponding to other initial HLWs to be processed by the WTP. Further, glasses A to E offered a progression of trade-offs between waste loading compliance and satisfying the $T_{0.01}$[a] constraint, the two most limiting compliance and processability constraints (see Figure 2.1).

In the first simulation study, the effects of HLW CRV mixing/sampling random uncertainty and other factors were studied for each of Glasses A to E using both the IHLW and ILAW compliance strategies. The other factors included HLW CRV mixing/sampling random uncertainty (%RSD[b] = 1, 5, 10, 15), number of CRV (IHLW and ILAW strategies) and MFPV (IHLW strategy) samples (4 or 8), and other random uncertainties depending on the compliance strategy as discussed in Section 3.2 and Sections 4.1 to 4.3.[c] Glass formulations A and B had difficulty complying with the waste loading (WL) requirement when accounting for composition uncertainty. This was especially evident in cases with high uncertainties and 4 samples (one analysis each) from each of the CRV and MFPV. However, Glass A was designed to exactly satisfy the WL requirement for a nominal composition without uncertainties, and Glass B to satisfy it with only a small margin. Hence, these results were expected. Glass formulations C, D, and E had difficulty satisfying the $T_{0.01}$ processability condition in the high uncertainties case. With nominal uncertainties, only E had difficulty satisfying the $T_{0.01}$ condition. Because of these findings, it was decided to use glass formulation C in the second and third simulation studies to assess the effects of CRV mixing/sampling bias and other factors.

The second and third simulation studies assessed the effects of varying amounts of HLW CRV mixing/sampling bias, as well as other factors, using both the IHLW and ILAW compliance strategies. In the second simulation study, the other factors included HLW CRV mixing/sampling random uncertainty (%RSD = 5, 10), and a combined factor with either 8 CRV/MFPV samples and nominal values of all other random uncertainties or 4 CRV/MFPV samples and high values of all other random uncertainties. In the third simulation study, the only other factor studied was the HLW CRV mixing/sampling random uncertainty. The number of CRV/MFPV samples was held constant at 8, and the other uncertainties were held constant at their nominal values. The other random uncertainties depend on the compliance strategy as discussed in Section 3.2, and the values used are discussed in Sections 4.1 to 4.3. In both the second and third simulation studies, varying percentages of HLW CRV mixing/sampling bias were applied to the concentrations of the insoluble elements ("solids") in the CRV samples, with corresponding biases applied to the soluble elements. In these simulation studies, the nominal amounts of GFCs added to an MFPV batch were the same for the biased cases as for the unbiased cases, which is what would be expected during actual WTP IHLW production if CRV information was biased but that fact was undetected.

(a) $T_{0.01}$ = the temperature (°C) at which the volume fraction of crystals in glass is 0.01.
(b) %RSD = percent relative standard deviation.
(c) The other random uncertainties included CRV and MFPV analytical, MFPV mixing/sampling, CRV volume before and after transfers to the MFPV, MFPV volume before and after transfers from the CRV and addition of GFCs, GFC oxide compositions, and masses of GFCs added to the MFPV.

8.2 Summary of Simulation Study Results

For all combinations of bias and other investigation factors: PCT normalized boron, lithium, and sodium releases; viscosity at 1100°C; and Toxicity Characteristic Leaching Procedure (TCLP) Cd release all satisfied their respective compliance or processability constraints based on 90% combined confidence intervals (90% CCIs, see the "Acronyms, Terms, and Abbreviations" section) that accounted for composition and property-composition model uncertainties. The 90% CCIs for liquidus temperature (T_L) did not satisfy a 950°C processability constraint under any of the testing or bias conditions used. However, this result was expected because that constraint was not imposed in developing the glass formulations used in the simulations. Rather, a 950°C processability constraint on $T_{0.01}$ was imposed.

WL and $T_{0.01}$ were the compliance and processability criteria most affected by the factors varied in the simulation studies, as anticipated based on the glass formulation optimization work. As random composition uncertainties were reduced and numbers of HLW CRV and MFPV samples increased, the probability of satisfying the WL and $T_{0.01}$ conditions increased. This probability also increased when using the ILAW strategy instead of the IHLW strategy.

Figure 8.1 shows for each of four situations, the HLW CRV mixing/sampling solids bias range predicted to satisfy the limiting WL and $T_{0.01}$ conditions (as well as all other compliance and processing conditions). The allowable range of HLW CRV mixing/sampling solids bias is dependent on the HLW CRV mixing/sampling random uncertainty as shown for each of the four situations in Figure 8.1. The two plots on the left display the results for the IHLW compliance strategy, while the two plots on the right display the results for the ILAW compliance strategy. The top two plots display results for "nominal" levels of random uncertainties and 8 samples per MFPV and/or CRV, while the bottom two plots display results for "high" levels of random uncertainties and 4 samples per MFPV and/or CRV. The worst situation occurs in the lower left plot of Figure 8.1, corresponding to the IHLW compliance strategy, high random uncertainties, and 4 samples per MFPV and/or CRV. In that situation, there is no range of HLW CRV mixing/sampling solids bias allowable, even with the HLW CRV mixing/sampling random uncertainty as low as 5 %RSD. The best situation occurs in the upper right plot of Figure 8.1, corresponding to the ILAW compliance strategy, low random uncertainties, and 8 samples per MFPV and/or CRV. In that situation, the allowable range of HLW CRV mixing/sampling bias is –3% to +2% (relative) when HLW CRV mixing/sampling random uncertainty = 25 %RSD. For HLW CRV mixing/sampling random uncertainty = 5%RSD, the allowable bias range is –4% to +6.5% (relative). Figure 8.1 shows that as the CRV mixing/sampling random uncertainty %RSD increases, the allowable HLW CRV mixing/sampling bias range decreases.

The plots in Figure 8.1 illustrate that it will be difficult to satisfy the WL and $T_{0.01}$ conditions unless the uncertainty values for all the factors are kept at the nominal levels, there are 8 samples taken in the CRV (for the IHLW and ILAW strategies) and MFPV (for the IHLW strategy), and that the CRV mixing/sampling random uncertainty %RSD is less than 15%. Figure 8.1 shows that as the CRV mixing/sampling random uncertainty %RSD increases, the allowable CRV mixing/sampling bias range decreases. These plots illustrate that it will be difficult to satisfy the WL and $T_{0.01}$ conditions unless the uncertainty values for all the factors are kept at the nominal levels, there are 8 samples taken in the CRV and MFPV, and that the CRV mixing/sampling random uncertainty %RSD is less than 15%.

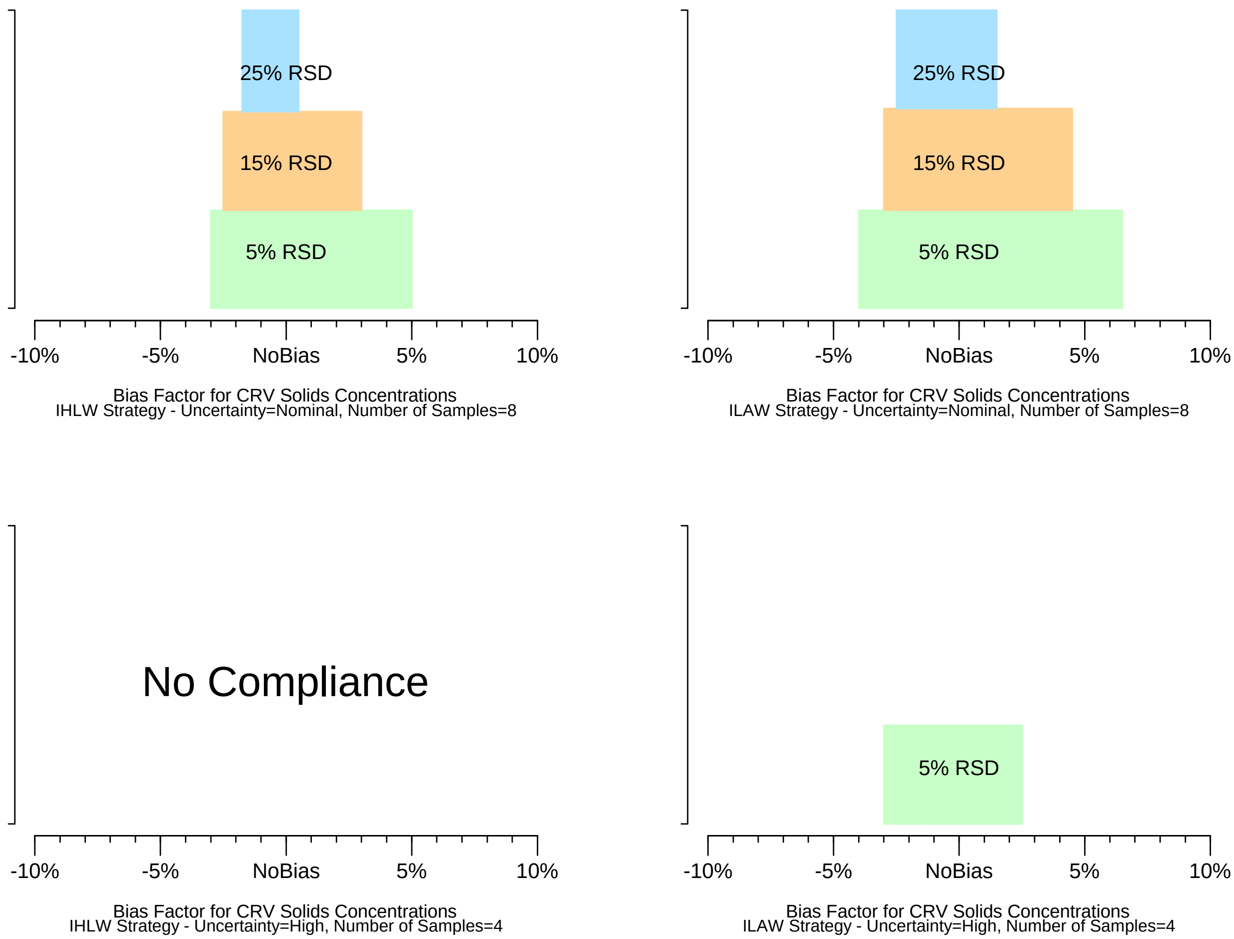

Figure 8.1. Ranges of HLW CRV Mixing/Sampling Bias that Allow Compliance and Processing Properties to be Satisfied with 90% Confidence. The dependence of the ranges on HLW CRV mixing/sampling random uncertainty %RSD is shown.

An example is now presented to clarify the meaning of the results in Figure 8.1 relative to operating the WTP HLW vitrification facility. Consider an HLW CRV containing two batches for transfer to the MFPV, as illustrated in Figure 8.2. Suppose that the HLW CRV samples taken from the sampling location have an average of 20 weight percent (wt%) solids. Further, suppose that the situation is represented by the upper left panel of Figure 8.1 (i.e., the IHLW compliance strategy, 8 CRV and MFPV samples, and nominal values random uncertainties), with 5 %RSD mixing/sampling random uncertainty. In this case, the allowable HLW CRV mixing/sampling solids bias is -3% to +5%, relative to the average of 20 wt% solids at the sampling location. This means that the average solids loading for Batch 1 (and Batch 2 as well) must be between 19.4 and 21.0 wt% solids[(a)] to produce acceptable glass.

(a) The lower limit is calculated as 20 – 0.03(20) = 19.4, while the upper limit is calculated as 20 + 0.05(20) = 21.0.

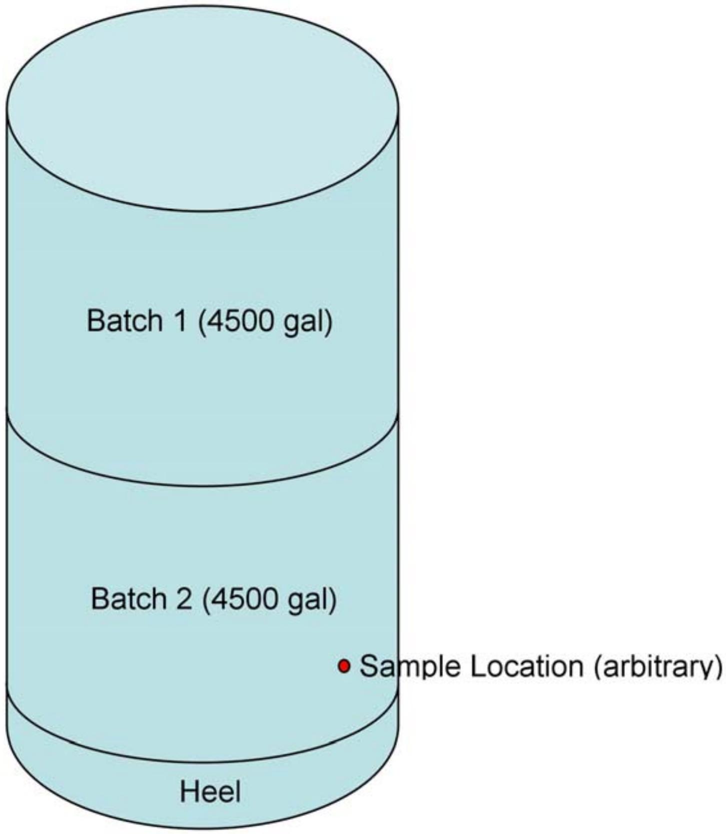

Figure 8.2. Illustration of HLW CRV and Two Batches for Transfer to the MFPV

8.3 Discussion of Results

The allowable HLW CRV mixing/sampling bias ranges in Figure 8.1 are based on the use of 90% confidence intervals (CIs) to account for uncertainties in assessing whether WL and $T_{0.01}$ conditions are satisfied. As discussed in Section 3.3, a 90% lower confidence interval (90% LCI)[a] was used to account for composition uncertainty in WL, while a 90% upper combined confidence interval (90% UCCI)[a] was used to account for composition and property-composition model uncertainties in $T_{0.01}$. Using CIs with confidence levels higher than 90% would further narrow the allowable ranges for HLW CRV mixing/sampling solids bias. However, it should be noted that the WTP is considering modifying the WL compliance strategy to not account for composition uncertainties in WL. That change would widen allowable ranges of HLW CRV mixing/sampling bias, and/or allow the selection of glass formulations closer to the WL compliance limits and farther from the $T_{0.01}$ processing limit.

Another consideration is which compliance calculation strategy to use. The ILAW strategy would allow for more bias to be present and still satisfy all compliance and processing conditions. Under the nominal uncertainty circumstances with eight samples, the allowable HLW CRV mixing/sampling solids bias corresponding to CRV mixing/sampling random uncertainties of 5, 15, and 25 %RSD are shown in the upper right panel of Figure 8.1. However, because the ILAW strategy does not involve sampling and

(a) See "Acronyms, Terms, and Abbreviations" for the definition of this term.

analyzing the MFPV, another way would be needed to confirm that any bias in solids remains within the allowable range.

The results in this report are dependent on the preliminary property-composition models used, and the uncertainties in property predictions made with those models. Uncertainties in preliminary property-composition models currently account for a substantial portion of the total uncertainties in demonstrating that compliance and processing conditions are satisfied. Work to develop property-composition models with smaller uncertainties is ongoing, as discussed in TP-RPP-WTP-179, Rev. 1, *Test Plan: Statistics for IHLW and ILAW Property-Composition Modeling*. Smaller model uncertainties, specifically for the $T_{0.01}$ model, would widen the allowable ranges of CRV mixing/sampling bias and random uncertainty.

The question arises as to what would happen during operation of the WTP HLW vitrification facility if the allowable range for HLW CRV mixing/sampling solids bias (depending on the level of random uncertainty, as summarized in Figure 8.1) was not satisfied. Under the IHLW compliance strategy, the "unallowable" HLW CRV bias may be detected because of the analysis of MFPV samples. Calculations performed for the affected MFPV batch(es) may fail to satisfy the compliance and/or processing conditions. In such a case, the WTP could modify the MFPV composition by adding more GFCs or waste, as needed. However, under the ILAW compliance strategy, "unallowable" bias would not be detected because that strategy relies on analyses of CRV samples and measurement of GFC additions. Hence, calculations performed for affected MFPV batches would mistakenly indicate that compliance and processing properties are satisfied. The ILAW strategy applied to the IHLW process would thus require confirmation from other data that HLW CRV mixing/sampling bias is within the allowable range for the level of HLW CRV mixing/sampling random uncertainty present.

Finally, it is interesting to compare the allowable HLW CRV mixing/sampling bias results in Figure 8.1 to the analytical accuracy requirements in Table D.3 of Kaiser et al. (2003). Whereas this report indicates that HLW CRV mixing/sampling bias can be at most -4% to +6.5% relative, Table D.3 of Kaiser et al. (2003) suggests that analytical bias from to -25% to +25% is acceptable. The magnitudes of allowable analytical biases in the HLW MFPV and/or CRV were not assessed as part of the work in this report. However, it seems unlikely that a -25% to +25% bias range would be found acceptable if such an assessment were to be performed. Thus, future work is recommended to determine the actual ranges of HLW CRV and MFPV analytical biases that can be tolerated and still allow all compliance and processing conditions to be met.

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