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Statistical Methods and Results for WTP IHLW and ILAW Compliance

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Test Specification: 24590-WTP-TSP-RT-02-002, Rev. 0
Test Plan: TP-RPP-WTP-165, Rev. 1
Test Exceptions: 24590-WTP-TEF-RT-03-039
24590-WTP-TEF-RT-04-00017
24590-WTP-TEF-RT-04-00036
R&T Focus Area: Waste Form Qualification
Test Scoping Statements: B-60, B-62, B-69, and B-70

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Completeness of Testing

This report describes the results of work and testing specified by Test Specification 24590-WTP-TSP-RT-02-002; Test Exceptions 24590-WTP-TEF-RT-03-039, 24590-WTP-TEF-RT-04-00017, and 24590-WTP-TEF-RT-04-00036; and Test Plan TP-RPP-WTP-165, 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, Manager Date
WTP R&T Support Project

Testing Summary

The immobilized high-level waste (IHLW) and immobilized low-activity waste (ILAW) vitrification processes of the Waste Treatment Plant (WTP) will be subject to variation and several uncertainties. The compositions and compliance properties (e.g., Product Consistency Test (PCT) for IHLW and ILAW, Vapor Hydration Test (VHT) for ILAW, and waste loading for IHLW and ILAW) of the IHLW and ILAW melts and products will be subject to variation because the compositions of waste feeds will vary over time. In addition, the state of knowledge at any step of the IHLW or ILAW processes will be subject to mixing, sampling, chemical analysis, volume measurement, blending, weighing, transfer, and other uncertainties.

Several aspects of the WTP compliance strategies for IHLW and ILAW are statistically based. That is, those compliance strategies account for variations and uncertainties in meeting requirements of the specifications. This report documents the outcomes of the first of two phases of work at Battelle—Pacific Northwest Division (PNWD) to develop statistical methods and results associated with the WTP's statistically based compliance strategies for IHLW and ILAW. Each statistical method (developed so far) intended for use in demonstrating compliance during IHLW and ILAW production operations is illustrated with a realistic example.

The statistical methods and investigations in this report were originally scoped to address the compliance strategies as described in the WTP Rev. 0 Product Compliance Plans (PCPs) for IHLW (Nelson 2003) and ILAW (Nelson et al. 2003). During the course of the work, the IHLW portion of the work was rescoped to reflect (1) the WTP IHLW facility design change to eliminate the Concentrate Receipt Vessel (CRV), and (2) corresponding changes to the IHLW compliance strategy. Guidance for the rescoped work consisted of an overview of the revised compliance strategy prepared for a meeting,[(a)] verbal instructions from WTP Waste Form Qualification (WFQ) staff, and later an early revision of what would eventually become the Rev. 1 IHLW PCP. That revision still addressed the Waste Acceptance Product Specifications (WAPS) requirements (DOE-EM 1996), rather than the Waste Acceptance System Requirements Document (WASRD) requirements (DOE-RW 2002) that have since been mandated for use in place of the WAPS.[(b)] The Rev. 1 PCPs for IHLW (Nelson et al. 2004) and ILAW (Westsik et al. 2004) were issued after the work in this report was completed and the report was substantially written. Hence, this report addresses IHLW specifications in the WAPS (DOE-EM 1996) and the WTP contract (DOE-ORP 2003), and ILAW specifications in the WTP contract. The second phase of the PNWD work to develop statistical methods and results to implement the WTP IHLW and ILAW compliance strategies will address the Rev. 1 PCPs and the specifications they address (including the WASRD for IHLW), as well as any subsequent revisions in the IHLW and ILAW specifications and PCPs. These changes will be reflected in a final version of this report currently scheduled to be issued in 2007.

(a) "IHLW Product Qualification and Control Compliance Strategy," River Protection Project, Waste Treatment Plant, May 5, 2004.

(b) ORP memorandum from R.J. Schepens to J.P. Henschel, "Notification to Stop Using the Office of Environmental Management High Level Waste Product Acceptance Specifications (1996) to Control Waste Treatment and Immobilization Plant (WTP) Project Work Regarding the Immobilized High-Level Waste (IHLW) Product," 04-WED-019, dated May 18, 2004.

The balance of this Testing Summary section provides an overview of the work performed relative to objectives, success criteria, quality requirements, test conditions, and known discrepancies. Section 8 of the report provides a more detailed summary of the methods developed and the results of the investigations performed.

Objectives

The objectives from the Test Specification (Swanberg 2002) and the Test Plan (Piepel and Cooley 2003), as modified by the test exceptions described in Table S.2, are listed and discussed in Table S.1.

Test Exceptions

Three test exceptions are listed and described in Table S.2.

Results and Performance Against Success Criteria

The success criteria in the Test Plan (Piepel and Cooley 2003) and the performance against those criteria are listed and discussed in Table S.3.

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 (WTPSP) quality assurance project plan (QAPjP) (PNWD 2004a) 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 (ASME 1989), NQA-2a-1990, Part 2.7 (ASME 1990), and DOE/RW-0333P, Rev. 13, *Quality Assurance and Requirements Description* (QARD) (DOE-RW 2003) as appropriate per the Test Plan (Piepel and Cooley 2003). These quality requirements are implemented through PNWD's *Waste Treatment Plant Support Project (WTPSP) Quality Assurance Requirements and Description Manual* (PNWD 2004b).

For activities associated with HLW, the additional quality assurance requirements of the QARD (DOE-RW 2003) were satisfied. A listing of the procedures implementing the QARD quality assurance requirements is included in Attachment 1 of the Test Plan. A matrix that cross-references the NQA-1, NQA-2a, and QARD requirements with the PNWD's procedures for this work is given in Attachment 2 of the Test Plan (Piepel and Cooley 2003). The matrix includes justification for those requirements not implemented.

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 statistical method development, computer calculations, and statistical simulation

"experiments" were performed, in accordance with the WTPSP procedure QA-RPP-WTP-1101 (*Scientific Investigations*) and other applicable procedures. Computer calculations were performed in accordance with WTPSP procedure QA-RPP-WTP-SCP (*Software Control*). The statistical methods developed and 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 Test Specification 24590-WTP-TSP-RT-02-002, Rev. 0, *Statistics for IHLW and ILAW Waste Compliance* (Swanberg 2002), 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 (Piepel and Cooley 2003) objectives. The QA-RPP-WTP-604 review procedure is part of PNWD's *WTPSP Quality Assurance Requirements and Description Manual* (PNWD 2004b).

R&T Test Conditions

The test conditions applicable to this work from the Test Specification (Swanberg 2002), and clarified in the Test Plan (Piepel and Cooley 2003), are listed and discussed in Table S.4. The results corresponding to the test conditions are also summarized in Table S.4. More detailed summaries of the statistical compliance methods developed and investigation results obtained are presented in Section 8.1 for IHLW and Section 8.2 for ILAW.

Of particular interest are results on the numbers of samples required in the IHLW MFPV and the ILAW CRV to (1) meet possible goals for uncertainties in estimating IHLW and ILAW compositions for each MFPV batch, and (2) satisfy specifications that set limits on compliance quantities. The current WTP baseline is to take 8 samples per IHLW MFPV batch with 1 analysis per sample, and 3 samples per ILAW CRV batch with 1 analysis per sample. The results in this report provide for the following assessments of the baseline numbers of samples and analyses per sample.

Performance of WTP Baseline Numbers of Samples for Estimating Chemical and Radionuclide Compositions

Table S.5 summarizes the uncertainty (percent relative half-widths of 90% confidence intervals) in estimating the mass fraction of each reportable chemical composition and radionuclide composition component, based on the WTP baseline numbers of samples. Results are shown for the cases where all applicable uncertainties for each of IHLW and ILAW are at their low estimates, or all at their high

estimates. The total uncertainties in mass fractions of reportable chemical and radionuclide composition components are in the ranges of < 5%, 5 to 10%, 10 to 15%, 15 to 20%, and > 20% depending on the chemical or radionuclide composition component and whether uncertainties are at the low or high ends of estimated ranges.

Ability to Comply with Limiting Specifications Using WTP Baseline Numbes of Samples

For IHLW, 8 samples per MFPV batch with 1 analysis per sample provides for easily meeting the PCT B, Li, and Na release limits:

- for each MFPV batch. This was demonstrated with all uncertainties at their high estimated values.
- over a collection of batches corresponding to an HLW waste type. Conservative estimates of the uncertainties and variations for each of three HLW waste tanks (AY-102, AZ-102, and C-104) were considered in the calculations.

For ILAW, 3 samples per CRV batch with 1 analysis per sample and 1 determination of each vessel volume and using uncertainty estimates at their high estimated values provides the following results.

- Radionuclide concentration limits are easily met when considering each MFPV batch as well as over a collection of batches corresponding to each of three LAW waste types: AP-101 (Envelope A), AZ-101 (Envelope B), and AN-107 (Envelope C).
- VHT specification limits were also easily met for each MFPV batch and over each of the three LAW waste types.
- PCT B and Na specification limits were easily met when considering each MFPV batch for each of the three LAW tanks. Compliance over a waste type was also achieved for all LAW tanks considered except one. Using highly conservative estimates for the uncertainties and variation between batches and assuming a conservative 10 MFPV batches per LAW waste type of AP-101 resulted in the 95%/95% UTI for PCT normalized B release of 4.244 g/L being slightly higher than the limit of 4 g/L. Compliance can be obtained by having slightly lower uncertainties or variation, increasing the number of MFPV batches per LAW waste type from 10, or increasing the number of samples per ILAW CRV batch from 3.

The final report will use updated estimates of uncertainties and variations affecting the IHLW and ILAW processes to obtain the final recommendations of the numbers of samples, analyses, and volume determinations.

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

As discussed previously, the work in this report was planned and conducted to address

- IHLW specifications in the WAPS (DOE-EM 1996) and WTP contract (DOE-ORP 2003)
- WTP IHLW compliance strategies in the HLW PCP Rev. 0 (Nelson 2003) with modifications to address the removal of the HLW CRV
- ILAW specifications in the WTP contract
- ILAW PCP Rev. 0 (Nelson et al. 2003)

The impacts of revisions to the WTP compliance strategies in the IHLW Rev. 1 PCP (Nelson et al. 2004) to address the changes from IHLW WAPS to WASRD specifications, and the ILAW PCP Rev. 1 (Westsik et al. 2004) on the second phase of the PNWD compliance work will be determined in conjunction with the WTP WFQ staff. The second phase of work will be rescoped as necessary. The final version of this report, currently scheduled for release in 2007, will present the results from the second phase of work conducted according to the IHLW specifications and WTP compliance strategies applicable at the time of the work.

Table S.1. Summary of Objectives

Test Objective	Objective Met (Y/N)	Discussion of How Objective was Met
1. Statistical confidence interval methods are needed to demonstrate with high confidence that each batch of HLW or LAW melter feed will meet the requirements of applicable specifications after accounting for applicable uncertainties.	Yes	Statistical confidence interval methods based on Monte Carlo simulation for ILAW and variance propagation methods for IHLW have been developed to quantify the combined uncertainty in chemical composition, radionuclide composition, and product durability (*compliance quantities*, for short) of glass that would be produced from each MFPV batch in the IHLW and ILAW processes. A Monte Carlo simulation approach was required for ILAW because of the complicated mathematical forms of mass-balance-based equations for the compliance quantities. The statistical confidence interval methods are discussed in Sections 4 (IHLW) and 5 (ILAW). Results and illustrations based on the methods are presented in Sections 6 (IHLW) and 7 (ILAW). Tables 8.1 (IHLW) and 8.5 (ILAW) summarize the subsections where confidence interval methods for specific compliance quantities are discussed and illustrated.
2. Statistical analyses that account for applicable variations and uncertainties are needed to determine the number of process samples, analyses, and measurements required to: (i) control and report the IHLW and ILAW chemical compositions, radionuclide inventories, and their associated uncertainties, and (ii) demonstrate compliance with specifications having limits.	Partially	Calculations were performed varying the values of various parameters: (1) numbers of samples, analyses per sample, and other process measurements, and (2) applicable within-MFPV-batch uncertainties. For each combination of parameters: (i) a Monte Carlo simulation was performed for ILAW, and (ii) error propagation with standard statistical interval methods was performed for IHLW, to determine the half-widths of the statistical intervals for the compliance quantities. The results provide preliminary input on how the numbers of samples, analyses per sample, and measurements affect the total uncertainties in compliance quantities for glass that would result from a given MFPV batch. The investigations are described in Sections 4 (IHLW) and 5 (ILAW). The results are presented in Sections 6 (IHLW) and 7 (ILAW). Tables 8.2 (IHLW) and 8.6 (ILAW) summarize the subsections where the investigations for specific compliance quantities are discussed and results are reported. Work scheduled for the future will: (1) Address similar needs for specifications scheduled to be investigated in FY05, and (2) provide final recommendations on the numbers of samples, analyses per sample, and other process measurements that will be used during IHLW and ILAW production operations. The results will be included in the final version of this report currently scheduled for delivery to the WTP Project in 2007.

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

Test Objective	Objective Met (Y/N)	Discussion of How Objective was Met
3. Statistical tolerance interval methods are needed to control and report with high confidence (X%) that a high percentage (Y%) of the waste glass produced from a specified quantity of HLW or LAW feed, or for a specified production period, meet limits for leachability in the PCT (IHLW and ILAW) and VHT (ILAW) tests, as well as other applicable requirements in WAPS or Contract specifications. The number of process samples, analyses, and measurements required to meet or exceed the desired values for X% and Y% must be determined.	Partially	The report by Piepel and Cooley (2002) developed and illustrated X%/Y% upper tolerance interval (X%/Y% UTI) methods for the previous WTP IHLW and ILAW compliance strategies that involved sampling and analyzing at only a single point of the process (i.e., MFPV for IHLW, and glass shards for ILAW). That work also assessed the effects of: (1) various numbers of samples and analyses per sample, and (2) various magnitudes of batch-to-batch variation and within-batch (mixing/sampling and analytical) uncertainties. The current WTP IHLW compliance strategy (of sampling and analyzing IHLW MFPV samples) is the same as addressed by Piepel and Cooley (2002), so the work in that report has been used in Sections 4.3.5 and 6.3.3 of this report. This report also describes how the X%/Y% UTI method in Piepel and Cooley (2002) can be adapted to the current ILAW strategies for compliance with radionuclide Class C limits (Sections 5.3.3.1 and 7.3.3.1), PCT limits (Sections 5.4.5 and 7.4.3), and VHT limits (Sections 5.4.5 and 7.5.3). Future work is planned to: (1) verify the confidence (X%) and coverage (Y%) performance of the X%/Y% UTI method, and (2) perform final calculations on numbers of samples, analyses per sample, and other process measurements in order to meet the Class C radionuclide (ILAW), PCT (IHLW and ILAW), and VHT (ILAW) requirements.

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

Test Objective	Objective Met (Y/N)	Discussion of How Objective was Met
4. Methods are needed to properly calculate means and standard deviations (SDs) of IHLW and ILAW chemical compositions and radionuclide inventories over the course of a waste type in order to report these compositions and their uncertainties in the production records. The methods must account for the possibility of unbalanced data (e.g., different numbers of samples or analyses per sample) and multiple sources of variation or uncertainty. Standard, simple formulas for calculating means and SDs are not appropriate (i.e., can yield incorrect results) when data are unbalanced or have multiple sources of variation or uncertainty.	Partially	The equations for calculating means and SDs for most relevant IHLW and ILAW specifications are presented in Section 4 (IHLW) and Section 5 (ILAW). These methods are illustrated using realistic data in Sections 6 (IHLW) and 7 (ILAW). Tables 8.1 (IHLW) and 8.5 (ILAW) summarize the subsections where the equations for means and SDs for specific compliance quantities are discussed and illustrated. Still to be addressed in FY05 are the development of formulas for means and SDs to the extent required for WAPS 1.6 (IAEA Safeguards Reporting for IHLW) and 3.14 (Concentration of Plutonium in Each Canister). Such formulas are presented in this report for the situation where every radionuclide is analyzed in every IHLW MFPV batch, but the WTP compliance strategy has changed so that only a few radionuclides will be analyzed for every MFPV batch. Hence, formulas for calculating means and SDs consistent with the revised compliance strategy must be developed.

HLW = high-level waste; IAEA = International Atomic Energy Agency; IHLW = immobilized HLW; ILAW = immobilized LAW; LAW = low-activity waste; MFPV = Melter Feed Preparation Vessel; PCT = Product Consistency Test; UTI = Upper Tolerance Interval; VHT = Vapor Hydration Test; WAPS = Waste Acceptance Product Specifications; WTP = Waste Treatment and Immobilization Plant.

Table S.2. Summary of Test Exceptions

Test Exception	Description and Discussion
24590-WTP-TEF-RT-03-039	The Test Specification (Swanberg 2002) includes as test conditions requirements to develop statistical approaches to demonstrate compliance with (1) hazardous waste requirements for IHLW (WAPS 1.5 and Contract Specification 1.2.2.1.5) and for ILAW (Contract Specification 2.2.2.20) (2) heat generation for IHLW (WAPS 3.8.2) (3) compressive strength requirements The WTP Project determined that statistical compliance strategies were not required for these needs. The associated scope in the Statistical Analysis task of the WTPSP was deleted in BCR-BNI-62. The scope reduction is reflected in Rev. 1 of the Test Plan (Piepel and Cooley 2003).
24590-WTP-TEF-RT-04-00017	This Test Exception expands the scope of the work in two areas, only the second of which is relevant to this report. The first area is for TSS B-61 (IHLW) and B-65 (ILAW) to include quantifying variations and uncertainties in (1) IHLW viscosity, electrical conductivity, and percent crystallinity temperatures, and (2) ILAW viscosity and electrical conductivity. This expanded scope is not related to the focus of the current report. The second area is for TSS B-6069 (LAW) and B-6270 (IHLW) to include application of the tools developed to assess the impact of process biases, variations, and uncertainties on waste form product performance and processing properties. No specific scope activities reflecting these scope additions have yet been added to the baseline scope and schedule for the Statistical Analysis Task. Hence, there is no impact of this Test Exception for the present report.
24590-WTP-TEF-RT-04-00036	The Test Specification and Test Plan include as test conditions requirements to develop statistical methods to demonstrate compliance with IHLW and ILAW waste loading requirements. However, the WTP Project has revised its IHLW and ILAW compliance strategies to no longer require statistically based methods for waste loading compliance. Hence, the associated test conditions in the test specification and test plan are no longer needed. The associated scope in the Statistical Analysis task of the WTPSP was deleted in BCR-BNI-127. The scope reduction is reflected in ICN-TP-RPP-WTP-165R1.1 for Rev. 1 of the Test Plan (Piepel and Cooley 2003).
BCR = Baseline Change Request; BNI = Bechtel National Inc.; ICN = interim change notice; IHLW = immobilized high-level waste; ILAW = immobilized low-activity waste; WAPS = Waste Acceptance Product Specifications; WTP = Waste Treatment and Immobilization Plant; WTPSP = Waste Treatment Plant Support Project.	

Table S.3. Summary of Success Criteria and Performance

Success Criterion	Discussion of Performance on Success Criterion
1. Completing work in accordance with QA requirements as described in Section 5 of the Test Plan (Piepel and Cooley 2003)	All work was completed in accordance with QA requirements.
2. Issuing interim or technical reports as described in Section 7 of the Test Plan (Piepel and Cooley 2003)	This initial report is the first of two required technical reports. It is envisioned that the subsequent final report will be a revised and completed version of this initial report.
3. Determination by the WTP project (through review of technical reports/ deliverables) that the statistical techniques and tools described in Tables A and B of the Test Plan (Piepel and Cooley 2003) are satisfactory and appropriate for demonstrating compliance with WAPS and contract specifications.	This initial technical report has completed the internal PNWD review and revision cycle as well as the WTP Project review and revision cycle. This initial technical report has been cleared by the WTP Project for project use.

QA = Quality assurance; PNWD = Battelle – Pacific Northwest Division; WAPS = Waste Acceptance Product Specifications; WTP = Waste Treatment and Immobilization Plant.

Table S.4. Summary of R&T Test Conditions

R&T Test Condition	Discussion of Whether the Test Condition was Followed and Any Deviations if Necessary
1. Determine the numbers of samples, analyses per sample, and measurements required for controlling (each batch) and reporting (for a waste type or other production period) IHLW and ILAW chemical composition per the associated IHLW PCP and ILAW PCP compliance strategies.	The methods developed to determine the numbers of samples per IHLW MFPV batch and chemical analyses per MFPV sample required to estimate IHLW chemical composition for each MFPV batch are presented in Section 4.1.3. The results of applying the methods are presented in Section 6.1.1. The methods developed to determine the numbers of samples per LAW CRV batch, chemical analyses per CRV sample, and volume determinations per CRV and MFPV batch required to estimate ILAW chemical composition for each MFPV batch are presented in Section 5.1.3. The results of applying the methods are presented in Section 7.1.1. The only deviations from the test conditions were that it was not necessary to determine the number of IHLW MFPV and LAW CRV batches to be sampled and analyzed relative to reporting for a waste type because the WTP compliance strategies for IHLW and ILAW specify sampling and analyzing every batch for chemical composition. Also, note that the calculations for the numbers of samples, analyses, etc. are preliminary and will be updated in the final version of this report scheduled for 2007.
2. Develop methods for properly calculating the IHLW or ILAW chemical composition means and SDs over an HLW or LAW waste type (or other production period) to report in the IHLW or ILAW Production Records.	No deviations were necessary. The equations for calculating means, SDs, and percent relative standard deviations (%RSDs) for (1) IHLW are given in Section 4.1.4 and illustrated in Section 6.1.2, and (2) ILAW are given in Section 5.1.4 and illustrated in Section 7.1.2. These equations account for batch-to-batch variation as well as all within-batch sources of uncertainty.
3. Quantify HLW and LAW glass composition reporting uncertainties for inclusion in the IHLW Product Qualification Report (PQR) and ILAW PQR. Note: The Test Specification and Test Plan refer to the IHLW Waste Form Qualification Report (WQR) and ILAW Qualification Document (QD), but IHLW PQR and ILAW PQR are the current terms for these documents.	No deviations were necessary. Equations for calculating SDs and %RSDs were developed and illustrated as described in the previous item. The illustrations used simulated data based on outputs of the WTP Project's G2 dynamic simulation flowsheet for one HLW glass (AY-102/C-106) and one LAW glass (AP-101). Calculations for glass from two additional HLW tanks and LAW tanks will be included in a forthcoming report under scope B-61 and B-65 to specifically address variation in various compliance quantities (including glass composition) over an HLW or LAW waste type.
4. Develop statistical methods to demonstrate compliance with HLW and LAW waste loading requirements.	Work scope deleted per Test Exception 24590-WTP-TEF-RT-04-00036 and ICN-TP-RPP-WTP-165R1.1.

Table S.4. Summary of R&T Test Conditions (cont.)

R&T Test Condition	Discussion of Whether the Test Condition was Followed and Any Deviations if Necessary
5. Determine the numbers of samples, analyses per sample, and measurements required for controlling (each batch) and reporting (for a waste type or other production period) IHLW and ILAW radionuclide inventories per the associated IHLW PCP and ILAW PCP compliance strategies.	The methods developed to determine the numbers of samples per IHLW MFPV batch and radiochemical analyses per MFPV sample required to estimate IHLW radionuclide composition for each MFPV batch are presented in Section 4.2.3. The results of applying the methods are presented in Section 6.2.1. The methods developed to determine the numbers of samples per LAW CRV batch, radiochemical analyses per CRV sample, and volume determinations per CRV and MFPV batch required to estimate ILAW radionuclide composition for each MFPV batch are presented in Section 5.2.3. The results of applying the methods are presented in Section 7.2.1. As noted in Item 1, one deviation from the test conditions was that it was not necessary to determine the number of IHLW MFPV and LAW CRV batches to be sampled and analyzed relative to reporting for a waste type. This is because the WTP compliance strategies for IHLW and ILAW specify (1) sampling every IHLW MFPV batch, analyzing selected radionuclides in every batch, and the remaining reportable radionuclides only in the first MFPV batch of an HLW waste type, and (2) sampling every CRV batch and analyzing for every reportable radionuclide in every batch. Also, it was possible to address radionuclide composition rather than radionuclide inventory, because inventory calculations require the mass of glass per IHLW canister and ILAW container, which will be determined for every canister/container.
6. Develop methods for properly calculating means and SDs to represent the variations and uncertainties in IHLW or ILAW radionuclide inventories over an HLW or LAW waste type (or other production period) to report in the IHLW or ILAW Production Records.	No deviations were necessary for ILAW radionuclides, where the equations for calculating means, SDs, and %RSDs are given in Section 5.2.4 and illustrated in Section 7.2.2. For IHLW radionuclides analyzed in every MFPV batch, equations for calculating means, SDs, and %RSDs are given in Section 4.2.4 and illustrated in Section 6.2.2. For radionuclides that will only be analyzed in the first MFPV batch corresponding to an HLW waste type, methods will be developed in the future (and documented in the final version of this report) after the details of the WTP compliance strategy are determined. These equations developed account for batch-to-batch variation as well as all within-batch sources of uncertainty.

Table S.4. Summary of R&T Test Conditions (cont.)

R&T Test Condition	Discussion of Whether the Test Condition was Followed and Any Deviations if Necessary
7. Develop statistical interval methods to demonstrate compliance with radionuclide concentration limits for each batch (process control) and for a waste type or other specified period of production (reporting).	This test condition applies only to ILAW, and there were no deviations. CL% empirical upper confidence interval (CL% EUCI) methods for each MFPV batch are described in Section 5.3.3.2 and illustrated in Section 7.3.3.2. X%/Y% UTI methods for demonstrating compliance over an LAW waste type or other period of production are described in Section 5.3.3.1 and illustrated in Section 7.3.3.1.
8. Develop statistical interval methods for process control (each batch) and reporting (over a waste type or other production period) aspects of the PCT compliance strategies (for IHLW and ILAW) and of the VHT compliance strategy (for ILAW).	There were no deviations. CL% upper combined confidence interval (CL% UCCI) methods are described and illustrated respectively for (1) IHLW PCT in Sections 4.3.3.2 and 6.3.1, (2) ILAW PCT in Sections 5.4.3.2 and 7.4.1, and (3) ILAW VHT in Sections 5.4.3.2 and 7.5.1. X%/Y% UTI methods are described and illustrated respectively for (1) IHLW PCT in Sections 4.3.5 and 6.3.3, (2) ILAW PCT in Sections 5.4.5 and 7.4.3, and (3) ILAW VHT in Sections 5.4.5 and 7.5.3.
9. Determine the sample sizes (numbers of sampling events over a waste type, samples per sampling period, and analyses per sample) required to demonstrate PCT (IHLW and ILAW) or VHT (ILAW) compliance with requirements for: (i) Each IHLW or ILAW batch, using X% confidence interval (CI) methodology. An X% CI provides X% confidence that the mean of a distribution is less than the CI value. (ii) IHLW or ILAW produced from a waste type (or other production period) using the X%/Y% upper tolerance interval (UTI) methodology. An X%/Y% UTI provides X% confidence that at least Y% of a distribution is less than the UTI value.	The only deviation is that it was not necessary to determine the number of sampling events over a waste type (i.e., the number of IHLW MFPV batches or the number of LAW CRV batches) because the WTP compliance strategies call for sampling every batch. The investigations to determine the numbers of samples per IHLW MFPV batch and chemical analyses per MFPV sample required to demonstrate PCT compliance for (1) each MFPV batch are described in Section 4.3.4 and the results presented in Section 6.3.2, and (3) each HLW waste type are described in Section 4.3.6 and the results presented in Section 6.3.4. The investigations to determine the numbers of samples per LAW CRV batch, chemical analyses per CRV sample, and volume determinations per CRV and MFPV batch required to demonstrate PCT and VHT compliance for (1) each MFPV batch are described in Section 5.4.4 and the results presented for PCT in Section 7.4.2 and for VHT in Section 7.5.2, and (3) each LAW waste type are described in Section 5.4.6 and the results presented for PCT in Section 7.4.4 and for VHT in Section 7.5.4.

Table S.4. Summary of R&T Test Conditions (cont.)

R&T Test Condition	Discussion of Whether the Test Condition was Followed and Any Deviations if Necessary
10. Develop statistical methods to implement the WAPS 1.6 compliance strategy activities for U and Pu described in the IHLW PCP. This work will: (i) develop methods to account for variations in per-canister inventories and fill heights, and (ii) quantify variations and uncertainties in determining U and Pu inventories and concentrations per canister.	This work was not scheduled to be included in this initial compliance report, but some of the work was completed early and was included. The balance of the work will be completed in FY 2005 and documented in the final version of this report scheduled in 2007. The portion of the work that was completed is discussed in Sections 4.6.3, 4.6.4, and 4.6.5.
11. Develop statistical methods to demonstrate compliance with the WAPS 3.14 Pu concentration limit after accounting for variations and uncertainties, as described in the IHLW PCP.	This work was not scheduled to be included in this initial compliance report, but some of the work was completed early and was included. The balance of the work will be completed in FY 2005 and documented in the final version of this report scheduled in 2007. The portion of the work that was completed is discussed in Sections 4.8.3.

CL = confidence level; CI = confidence interval; CRV = Concentrate Receipt Vessel; EUCI = empirical upper confidence interval; HLW = high-level waste; ICN = interim change notice; IHLW = immobilized HLW; ILAW = immobilized LAW; LAW = low-activity waste; MFPV = Melter Feed Preparation Vessel; PCP = Product Compliance Plan; PCT = Product Consistency Test; %RSD = percent relative standard deviation; PQR = Product Qualifcation Report; QD = qualification document; UTI = Upper Tolerance Interval; VHT = Vapor Hydration Test; WAPS = Waste Acceptance Product Specifications; WQR = Waste Form Qualification Report; WTP = Waste Treatment and Immobilization Plant.

Table S.5. Uncertainty Ranges (%RHWs of 90% Confidence Intervals) for Each Reportable Chemical and Radionuclide Composition Component Given the WTP Baseline Number of Samples (Assuming One Analysis) and Uncertainty in All Other Factors (Low or High) Across Three Tanks Each of HLW and LAW

Chemical or Radionuclide Composition Component	"Low" Uncertainties		"High" Uncertainties	
	3 ILAW CRV Samples[a]	8 IHLW MFPV Samples[a]	3 ILAW CRV Samples[a]	8 IHLW MFPV Samples[a]
Al_2O_3	R[b] < 5%	R < 5%	R < 5%	10% < R < 15%
B_2O_3	R < 5%	R < 5%	R < 5%	10% < R < 15%
CaO	R < 5%	5% < R < 10%	R < 5%	R > 20%
CdO	-[c]	R > 20%	-	R > 20%
Cl	R < 5%	-	5% < R < 10%	-
Cr_2O_3	-	5% < R < 10%	-	15% < R < 20%
F	5% < R < 10%	-	15% < R < 20%	-
Fe_2O_3	R < 5%	R < 5%	R < 5%	10% < R < 15%
K_2O	5% < R < 10%	-	15% < R < 20%	-
Li_2O	5% < R < 10%	5% < R < 10%	15% < R < 20%	10% < R < 15%
MgO	R < 5%	R > 20%	R < 5%	R > 20%
MnO	-	R < 5%	-	10% < R < 15%
Na_2O	R < 5%	R < 5%	5% < R < 10%	5% < R < 10%
NiO	-	5% < R < 10%	-	15% < R < 20%
P_2O_5	R < 5%	5% < R < 10%	5% < R < 10%	15% < R < 20%
PdO	-	15% < R < 20%	-	R > 20%
Rh_2O_3	-	15% < R < 20%	-	R > 20%
RuO_2	-	R > 20%	-	R > 20%
SO_3	R < 5%	R > 20%	5% < R < 10%	R > 20%
Sb_2O_3	-	15% < R < 20%	-	R > 20%
SeO_2	-	R > 20%	-	R > 20%
SiO_2	R < 5%	R < 5%	R < 5%	10% < R < 15%
SrO	-	R < 5%	-	10% < R < 15%
ThO_2	-	R < 5%	-	10% < R < 15%
TiO_2	R < 5%	-	R < 5%	-
U_3O_8	-	10% < R < 15%	-	15% < R < 20%
ZnO	R < 5%	R < 5%	R < 5%	15% < R < 20%
ZrO_2	R < 5%	R < 5%	R < 5%	10% < R < 15%
$^{241}Am_2O_3$	5% < R < 10%	15% < R < 20%	15% < R < 20%	R > 20%
$^{242}Cm_2O_3$	-	R > 20%	-	R > 20%
$^{243+244}Cm_2O_3$	10% < R < 15%	R > 20%	R > 20%	R > 20%
^{60}CoO	5% < R < 10%	15% < R < 20%	15% < R < 20%	R > 20%
$^{134}Cs_2O$	-	R > 20%	-	R > 20%
$^{137}Cs_2O$	10% < R < 15%	R < 5%	15% < R < 20%	5% < R < 10%
$^{154}Eu_2O_3$	10% < R < 15%	10% < R < 15%	R > 20%	R > 20%
$^{155}Eu_2O_3$	5% < R < 10%	5% < R < 10%	15% < R < 20%	10% < R < 15%

Table S.5. Uncertainty Ranges (%RHWs of 90% Confidence Intervals) for Each Reportable Chemical and Radionuclide Composition Component Given the WTP Baseline Number of Samples (Assuming One Analysis) and Uncertainty in All Other Factors (Low or High) Across Three Tanks Each of HLW and LAW (cont.)

Chemical or Radionuclide Composition Component	"Low" Uncertainties		"High" Uncertainties	
	3 ILAW CRV Samples[(a)]	8 IHLW MFPV Samples[(a)]	3 ILAW CRV Samples[(a)]	8 IHLW MFPV Samples[(a)]
^{63}NiO	10% < R < 15%	-	R > 20%	-
$^{237}NpO_2$	5% < R < 10%	15% < R < 20%	10% < R < 15%	R > 20%
$^{238}PuO_2$	5% < R < 10%	15% < R < 20%	15% < R < 20%	R > 20%
$^{239}PuO_2$	10% < R < 15%	5% < R < 10%	R > 20%	10% < R < 15%
$^{241}PuO_2$	10% < R < 15%	15% < R < 20%	R > 20%	R > 20%
$^{125}Sb_2O_3$	5% < R < 10%	15% < R < 20%	10% < R < 15%	R > 20%
^{90}SrO	10% < R < 15%	10% < R < 15%	R > 20%	R > 20%
$^{99}Tc_2O_7$	5% < R < 10%	5% < R < 10%	10% < R < 15%	10% < R < 15%
$^{233}U_3O_8$	-	5% < R < 10%	-	10% < R < 15%
$^{234}U_3O_8$	-	R > 20%	-	R > 20%
$^{235}U_3O_8$	-	10% < R < 15%	-	R > 20%
$^{236}U_3O_8$	-	R > 20%	-	R > 20%
$^{238}U_3O_8$	-	10% < R < 15%	-	R > 20%

(a) The %RHW ranges listed correspond to the results for the largest necessary number of samples across the three HLW or LAW tanks being equal to the specific WTP baseline value for IHLW or ILAW.
(b) R represents the %RHW.
(c) A dash (-) indicates that the particular oxide or radionuclide was not reportable for IHLW or ILAW.

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Acronyms, Terms, and Abbreviations

ANOVA	analysis of variance
A_j	specific activity of the j^{th} analyte, which is a radionuclide (Ci/g)
A_q	specific activity of the q^{th} radionuclide (Ci/g)
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
a_{ik}^{GFC}	mass of the k^{th} GFC added to the i^{th} MFPV batch (g)
BCR	baseline change request
BNI	Bechtel National, Inc.
b_k^h	coefficient of a linear mixture model term for the k^{th} normalized component of (1) IHLW in the model for PCT normalized release of h = B, Li, or Na or (2) ILAW in the model for VHT alteration depth or PCT normalized release of h = B or Na
b_{kk}^h	coefficient of a squared mixture model term in a PQM model, corresponding to the k^{th} normalized component of ILAW in the model for VHT alteration depth or PCT normalized release of h = B or Na
b_{kl}^h	coefficient of a crossproduct mixture model term in a PQM model, corresponding to the k^{th} normalized component of ILAW in the model for VHT alteration depth or PCT normalized release of h = B or Na
$\boldsymbol{b}^h$	$p \times 1$ column vector of the coefficients for a property-composition model on the property denoted by h
CHEM	set of chemical composition components in IHLW
$CHW_{i,CL\%\ UCI}^h$	composition uncertainty half-width for a CL% upper confidence interval (CL% UCI) on property h of glass corresponding to the i^{th} MFPV batch [ln(g/L) for IHLW and ILAW PCT, and ln(μm) for ILAW VHT]
Chemical composition	The composition of IHLW or ILAW that can be determined by chemical analyses, not including radiochemical analyses. Chemical composition is

	expressed as weight percents or mass fractions of oxide or halogen components of the IHLW or ILAW.
Ci	Curies
CI	confidence interval (see CL% CI for definition)
CL%	confidence level (in percent)
CL% CI	CL% confidence interval—An interval that includes the true mean value of a quantity with CL% confidence.
CL% EUCI	CL% empirical upper confidence interval
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% Multiplier	statistical distribution percentile value appropriate to provide CL% confidence that the *CL% CI* contains the true mean compliance quantity
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.
$CL\%\ UCCI\left(y_i^h\right)$	CL% UCCI for the true, unknown mean value of $y_i^h = ln\left(r_i^{PCT\ h}\right)$ for the i^{th} MFPV batch [ln(g/L)]
c_{ij}^{MFPV}	analyzed concentration of analyte *j* in the i^{th} IHLW MFPV batch (μg/mL = mg/L)

$\bar{c}_{ij}^{MFPV}$	average concentration of the j^{th} analyte over n_A^{MFPV} analyses each of n_S^{MFPV} samples from the i^{th} IHLW MFPV batch (μg/mL = mg/L)
c_{ij}^{CRV}	concentration of the j^{th} element in the LAW CRV batch, a portion of which is transferred to the i^{th} MFPV batch (μg/mL = mg/L)
c_{iq}^{MFPV}	mass-per-volume concentration of the q^{th} radionuclide in the i^{th} IHLW MFPV batch (μg/mL = mg/L)
c_{iq}^{CRV}	mass-per-volume concentration of the q^{th} radionuclide in the LAW CRV batch contributing to the i^{th} MFPV batch (μg/mL = mg/L)
c_{ijlm}^{CRV}	analyzed concentration of the j^{th} analyte from the m^{th} analysis of the l^{th} sample from the CRV batch contributing to the i^{th} ILAW MFPV batch (μg/mL = mg/L)
c_{ijlm}^{MFPV}	analyzed concentration of the j^{th} analyte from the m^{th} analysis of the l^{th} sample from the i^{th} IHLW MFPV batch (μg/mL = mg/L)
$\bar{c}_{iq}^{MFPV}$	mean mass-per-volume concentration of the q^{th} radionuclide in the i^{th} IHLW MFPV batch (μg/mL = mg/L)
$\bar{c}_{iq}^{CRV}$	mass-per-volume concentration of the q^{th} radionuclide in the LAW CRV batch contributing to the i^{th} MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations (μg/mL = mg/L)
$\bar{c}_{1kq}^{MFPV}$	mass-per-volume concentration of the q^{th} isotope of k = U or Pu in the first IHLW MFPV batch of an HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (μg/mL = mg/L)
$\bar{c}_{d,Pu}^{Canister}$	mass-per-volume concentration of Pu isotopes in glass from the D IHLW canisters corresponding to the I IHLW MFPV batches for a given HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (g/m^3)
$c_{i,Pu}^{MFPV}$	mass-per-volume concentration of Pu isotopes in glass that would be made from the i^{th} IHLW MFPV batch from a given HLW waste type (g/m^3)

$\bar{c}_{i,Pu}^{MFPV}$	mean mass-per-volume concentration of Pu isotopes in glass that would be made from the i^{th} IHLW MFPV batch from a given HLW waste type, based on averages over multiple samples, analyses per sample, volume determinations, and density determinations per MFPV batch (g/m^3)
$\bar{\bar{c}}_{D,Pu}^{Canister}$	mean mass-per-volume concentration of Pu isotopes in glass from the *D* IHLW canisters corresponding to the *I* IHLW MFPV batches for a given HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (g/m^3)
CRV	Concentrate Receipt Vessel
CSV	Concentrate Storage Vessel
D	number of IHLW canisters or ILAW containers associated with the *I* MFPV batches corresponding to an HLW or LAW waste type
D^{VHT}	alteration depth on a test coupon from running the VHT (μm)
δ	non-centrality parameter for the non-central t-distribution used in calculating the *k* multiplier for an X%/Y% UTI
df	degrees of freedom
df_I	degrees of freedom for the *I* MFPV batches associated with an LAW waste type
df_m	degrees-of-freedom associated with a property-composition model. When *p* coefficients in the model are estimated from *n* data points, $df_m = n - p$.
$df_{\tilde{\sigma}}$	degrees-of-freedom associated with the estimate $\tilde{\sigma}$, which is used in calculating X%/Y% UTIs
DL	detection limit
DOE	U.S. Department of Energy
DOE-EM	U.S. DOE-Environmental Management
DOE-ORP	U.S. DOE-Office of River Protection
DOE-RW	U.S. DOE-Office of Civilian Radioactive Waste Management
DQO	data quality objectives

DWPF	Defense Waste Processing Facility
EA	environmental assessment
ECI	empirical confidence interval
f_j	factor for converting the concentration of analyte j to the concentration of oxide j ($g_{oxide}/g_{analyte}$)
$f(P)$	function (i.e., mathematical transformation) of a glass property P
$F_{1-\alpha}(p, n-p)$	100(1 – α) percentile of an F-distribution with p numerator degrees of freedom and $n - p$ denominator degrees of freedom, where n is the number of data points used to fit the model and p is the number of model parameters estimated from the data
GFC	glass former chemical
G2	WTP Dynamic Flowsheet Model based on G2™ software
g	grams
g/L	grams per liter
g/mL	grams per milliliter
g/m^2	grams per square meter
g/m^3	grams per cubic meter
g_{ij}^{MFPV}	mass fraction of the j^{th} glass oxide[(a)] component in the i^{th} IHLW or ILAW MFPV batch (g_{oxide}/g_{oxides})
g_{iq}^{MFPV}	mass fraction of the q^{th} radionuclide oxide in the i^{th} IHLW or ILAW MFPV batch (g_{oxide}/g_{lass})
g_{ijlm}^{MFPV}	mass fraction of the j^{th} glass-oxide component corresponding to the m^{th} analysis of the l^{th} sample from the i^{th} IHLW MFPV batch (g_{oxide}/g_{oxides})
$\bar{g}_{ij}^{MFPV}$	mean mass fraction of the j^{th} component (chemical composition or radionuclide composition) in IHLW or ILAW that would be made from the

(a) A few glass components (e.g., F and Cl) are not expressed as oxides. However, for simplicity in the presentation, the term oxides will be used to differentiate from situations where elements are the focus.

	i^{th} IHLW or ILAW MFPV batch. For IHLW, the mean mass fraction of the j^{th} component is an average of mass fractions from multiple samples per MFPV batch and at least one chemical analysis per MFPV sample. For ILAW, the "mean" mass fraction is based on separate averages of (1) multiple samples per CRV batch and one or more chemical analyses per CRV sample and (2) multiple volume determinations per CRV and MFPV volume if more than one determination per volume is made. (g_{oxide}/g_{oxides})
$\overline{g}_{iq}^{MFPV}$	mean mass fraction of the q^{th} radionuclide composition component in IHLW or ILAW that would be made from the i^{th} IHLW or ILAW MFPV batch. For IHLW, the mean mass fraction of the q^{th} radionuclide component is an average of mass fractions from multiple samples per MFPV batch and at least one radiochemical analysis per MFPV sample. For ILAW, the "mean" mass fraction is based on separate averages of (1) multiple samples per CRV batch and one or more radiochemical analyses per CRV sample and (2) multiple volume determinations per CRV and MFPV volume if more than one determination per volume is made. (g_{oxide}/g_{oxides})
$\widetilde{g}_{ij}^{MFPV}$	average mass fraction of the j^{th} glass oxide component resulting from n_A^{MFPV} analyses of each of n_S^{MFPV} samples from the i^{th} IHLW MFPV batch (g_{oxide}/g_{oxides})
$\overline{\overline{g}}_j^{MFPV}$	mean (mass-weighted-average) mass fraction of the j^{th} IHLW or ILAW chemical composition or radionuclide composition component over I MFPV batches. The mass fraction for each IHLW or ILAW MFPV batch is given by $\overline{g}_{ij}^{MFPV}$, and a weighted average of these values is calculated using the mass of IHLW or ILAW that would be produced from the MFPV batch. (g_{oxide}/g_{oxides})
$\overline{g}_q^{MFPV}$	mean (mass-weighted-average) mass fraction of the q^{th} radionuclide oxide over I IHLW or ILAW MFPV batches. This notation only applies when there is one sample, one analysis per sample, one determination of each volume, etc. (g_{oxide}/g_{oxides})
$\overline{\overline{g}}_q^{MFPV}$	mean (mass-weighted-average) mass fraction of the q^{th} IHLW or ILAW radionuclide component over I MFPV batches. The mass fraction for each IHLW or ILAW MFPV batch is given by $\overline{g}_{iq}^{MFPV}$, and a weighted average of these values is calculated using the mass of IHLW or ILAW that would be produced from the MFPV batch. (g_{oxide}/g_{oxides})

G_{ijk}^{GFC}	mass of the j^{th} glass oxide component per mass of the k^{th} GFC for the i^{th} IHLW MFPV batch ($g_{oxide\ j}/g_{GFC\ k}$)
HBV	HLW Feed Blend Vessel
HLW	high level waste
$H_{i,max}^{Canister}$	maximum heat per canister if 100% filled with glass that would be made from the i^{th} IHLW MFPV batch (W)
I	number of IHLW MFPV batches corresponding to an HLW waste type or ILAW MFPV batches corresponding to an LAW waste type or other period of production
IAEA	International Atomic Energy Agency
ICN	interim change notice
IHLW	immobilized high level waste
IHLW PCP	IHLW Product Compliance Plan
ILAW	immobilized low activity waste
ILAW PCP	ILAW Product Compliance Plan
$\overline{IR}_{kq}$	mean isotopic ratio by mass of the q^{th} isotope of k = U or Pu, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch ($g_{isotope}/g_{radionuclide}$)
ITR	independent technical review
J	number of IHLW or ILAW chemical and radionuclide composition components (oxides and halogens) estimated for the IHLW or ILAW composition corresponding to each MFPV batch
$k(X, Y)$	constant used in calculating an X%/Y% UTI that is implicitly a function of X, Y, degrees of freedom associated with $\tilde{\sigma}$, and other parameters
L	liters
L_k^s	limiting activity-per-mass concentration for the k^{th} group of radionuclides, as specified in 10 CFR 61.55 (nCi/g)

L_q^r	limiting activity-per-volume concentration for the q^{th} radionuclide as specified in 10 CFR 61.55 (Ci/m^3)
LAW	low activity waste
LCI	lower confidence interval (see CL% LCI for definition)
LDR	Land Disposal Restrictions
LTI	lower tolerance interval
m_{ij}^{GFCs}	mass of the j^{th} glass oxide component in GFCs for the i^{th} ILAW MFPV batch (g)
m_{ij}^{MFPV}	mass of the j^{th} glass oxide component in the i^{th} IHLW or ILAW MFPV batch (g)
$m_{ij}^{MFPV\ Heel}$	mass of the j^{th} glass oxide component in the MFPV Heel included in the i^{th} ILAW MFPV batch (g)
$m_{ij}^{CRV\ to\ MFPV}$	mass of the j^{th} glass oxide component in the portion of an LAW CRV batch transferred to the i^{th} ILAW MFPV batch (g)
m_{iq}^{MFPV}	mass of the q^{th} radionuclide oxide from the i^{th} IHLW or ILAW MFPV batch (g)
$\overline{m}_{ij}^{MFPV}$	mean mass of the j^{th} IHLW component for the i^{th} IHLW MFPV batch averaged over n_S^{MFPV} samples per MFPV batch, n_A^{MFPV} analyses per sample, and n_V^{MFPV} volume determinations per IHLW MFPV batch (g_{oxide})
$\overline{m}_{iq}^{MFPV}$	mean mass of the q^{th} oxide (non-radionuclides as well as radionuclides) from the i^{th} IHLW MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations for each IHLW MFPV batch (g_{oxide})
M_i^{GFCs}	total mass of all glass oxide components in GFCs for the i^{th} ILAW MFPV batch (g_{oxides})

M_i^{MFPV}	total mass of the i^{th} glass oxide component in the IHLW or ILAW MFPV (g_{oxide})
$M_i^{MFPV\ Heel}$	total mass of all glass oxide components in the ILAW MFPV Heel included in the i^{th} ILAW MFPV batch (g_{oxides})
$M_i^{CRV\ to\ MFPV}$	total mass of all glass oxide components in the portion of the LAW CRV batch transferred to the i^{th} ILAW MFPV batch (g_{oxides})
MS	mean squares estimate obtained from an analysis-of-variance table
MF	mass fraction (g_{oxide}/g_{oxides})
$m_d^{Canister}$	mass of glass in the d^{th} IHLW canister associated with an HLW waste type (g_{glass})
$m_d^{Container}$	mass of glass in the d^{th} ILAW container associated with an LAW waste type (g_{glass})
$\overline{m}_D^{Canister}$	mean mass of glass in the D IHLW canisters associated with an HLW waste type (g_{glass})
$\overline{m}_D^{Container}$	mean mass of glass in the D ILAW containers associated with an LAW waste type or other period of production (g_{glass})
$\overline{m}_{Dq}^{Canister}$	mean mass of the q^{th} radionuclide oxide over the D IHLW canisters associated with the I IHLW MFPV batches corresponding to an HLW waste type (g_{oxide})
$\overline{m}_{Dq}^{Container}$	mean mass of the q^{th} radionuclide oxide over the D ILAW containers associated with the I MFPV batches corresponding to an LAW waste type (g_{oxide})
$\overline{m}_{d,Nk}^{Canister}$	mass in the d^{th} IHLW canister of radionuclide k for the set N_k of isotopes of k = U or Pu, based on averages over multiple samples, analyses per sample, and volume determinations for each IHLW MFPV batch ($g_{radionuclide}$)
$\overline{\overline{m}}_{D,Nk}^{Canister}$	mean mass of radionuclide k for the set N_k of isotopes of k = U or Pu over the D IHLW canisters associated with the I IHLW MFPV batches comprising an

	HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each IHLW MFPV batch ($g_{radionuclide}$)
$m_{i,max}^{Canister}$	maximum mass of glass per canister if 100% filled with glass that would be made from the i^{th} IHLW MFPV batch (g_{glass})
$MHW_{i,CL\%\ SUCI}^{h}$	model uncertainty half-width for a CL% simultaneous upper confidence interval (CL% SUCI) on property *h* for glass corresponding to the i^{th} MFPV batch [ln(g/L) for IHLW and ILAW PCT, and ln(μm) for ILAW VHT]
Mixing/sampling uncertainty	Samples from the IHLW MFPV and ILAW CRV will be subject to uncertainties from random inhomogeneity related to the inability to perfectly mix the vessel contents as well as random uncertainties in the sampling system. Multiple samples taken from an IHLW MFPV or an ILAW CRV will be subject to both mixing and sampling uncertainties, and it is not possible to separately estimate these two sources of uncertainty from data on multiple samples. Hence, the combined uncertainties are referred to as mixing/sampling uncertainty.
MFPV	Melter Feed Preparation Vessel (in the WTP IHLW or ILAW facility)
MFV	Melter Feed Vessel (in the WTP IHLW or ILAW facility)
mg/L	milligrams per liter
MT	metric tonne
MW_j^{oxide}	molecular weight of oxide *j* (g/mole)
$MW_j^{analyte}$	molecular weights of analyte *j* (g/mole)
$\tilde{\mu}$	estimate of the population mean that is calculated by forming the average model-predicted ln(PCT release) or ln(VHT alteration depth) for each IHLW or ILAW MFPV batch and averaging them across all MFPV batches corresponding to an HLW (or LAW, as appropriate) waste type [ln(g/L) for PCT, ln(μm) for VHT]
N	the number of radionuclides contributing to heat generation
NQA	nuclear quality assurance
n_A^{CRV}	number of analyses per LAW CRV sample

n_S^{CRV}	number of samples per LAW CRV batch
n_V^{CRV}	number of volume determinations of the LAW CRV before and after transfers
n_A^{MFPV}	number of chemical analyses per IHLW MFPV sample
$n_A^{CRV_{il}}$	number of chemical analyses of the l^{th} sample from the LAW CRV batch, a portion of which is used in making the i^{th} ILAW MFPV batch
$n_A^{MFPV_{il}}$	number of chemical analyses made of the l^{th} sample from the i^{th} IHLW MFPV batch
n_S^{MFPV}	number of samples per IHLW MFPV batch
$n_S^{CRV_i}$	number of samples from the LAW CRV batch, a portion of which is used in making the i^{th} ILAW MFPV batch
$n_S^{MFPV_i}$	number of samples from the i^{th} IHLW MFPV batch
n_V^{MFPV}	number of volume determinations of the IHLW MFPV or ILAW MFPV before and after transfers
n_{mc}^{h}	number of normalized IHLW components in the model for PCT normalized release of h = B, Li, or Na; or the number of normalized ILAW components in the model for h = VHT alteration depth or PCT normalized release of h = B or Na
n_ρ	number of determinations of density of glass that would be made from the i^{th} IHLW MFPV batch from a given HLW waste type
Nk	either *Tk* (the set of all isotopes of k = U or Pu) or *Fk* (the set of fissile isotopes of k = U or Pu)
N_k	number of radionuclides in the k^{th} group of radionuclides (one, except for TRU)
ORP	Office of River Protection
PCP	Product Compliance Plan

PCT	Product Consistency Test
PNWD	Battelle—Pacific Northwest Division
PQM	partial quadratic mixture
PQR	Product Qualification Report
p	number of fit parameters (coefficients) in a property-composition model
$p_{ij}^{CRV\ to\ MFPV}$	proportion that is from waste of the mass of the j^{th} glass oxide component in an LAW CRV transfer to the i^{th} ILAW MFPV batch
p_{ij}^{MFPV}	proportion that is from waste of the mass of the j^{th} glass oxide component in the i^{th} IHLW or ILAW MFPV batch
QA	quality assurance
QAPjP	quality assurance project plan
QARD	Quality Assurance and Requirements Description
RAD	set of radionuclide components in IHLW
Radionuclide composition	The composition of IHLW or ILAW that can be determined by radiochemical analyses. Radionuclide composition is expressed as weight percents or mass fractions of radionuclide oxide components of the IHLW or ILAW.
Radionuclide inventory	The Curies (Ci) of a radionuclide contained in a specified quantity of waste glass, such as an IHLW canister or ILAW container.
RCRA	Resource Conservation and Recovery Act
Reportable	A chemical or radionuclide composition component is "reportable" if it must be chemically analyzed or estimated to meet one or more applicable specifications. Included are components mentioned directly in a specification, or those needed to indirectly satisfy a specification through a property-composition model.
$R_{dq}^{Canister}$	inventory of radionuclide q for the d^{th} IHLW canister (Ci)
$R_{dq}^{Container}$	inventory of radionuclide q in the d^{th} ILAW container (Ci)

$\overline{R}_{dq}^{Canister}$	inventory of radionuclide q for the d^{th} IHLW canister based on averages over multiple samples, analyses per sample, and volume determinations of the corresponding i^{th} IHLW MFPV batch (Ci)
$\overline{R}_{dq}^{Container}$	inventory of radionuclide q for the d^{th} ILAW container, based on averages over multiple samples, analyses per sample, and volume determinations (Ci)
$R_{Dq}^{Canisters}$	total inventory of the q^{th} radionuclide in D IHLW canisters associated with an HLW waste type (Ci)
$\overline{R}_{Dq}^{Canister}$	mean inventory per canister of the q^{th} radionuclide over the D IHLW canisters associated with an HLW waste type (Ci/canister)
$\overline{R}_{Dq}^{Container}$	mean inventory per container of radionuclide q over the D ILAW containers associated with an LAW waste type (Ci/container)
$\overline{\overline{R}}_{Dq}^{Canister}$	mean inventory per canister of the q^{th} radionuclide over the D IHLW canisters associated with an HLW waste type (Ci/canister)
$\overline{\overline{R}}_{Dq}^{Container}$	mean inventory per container of the q^{th} radionuclide over the D ILAW containers associated with an LAW waste type, based on averages over multiple samples, analyses per sample, and volume determinations (Ci/container)
$\overline{\overline{R}}_{Dqk}^{Container}$	mean inventory per container of the q^{th} radionuclide in the k^{th} group of radionuclides in glass from D ILAW containers, based on averages over multiple samples, analyses per sample, and volume determinations (Ci/container)
R_j	ratio of moles of oxide per mole of analyte for oxide j ($moles_{oxide}/moles_{analyte}$)
$\overline{\overline{r}}_{Dq}^{Container}$	mean activity-per-volume concentration of the q^{th} radionuclide ($q = {}^{99}Tc$) in glass from D ILAW containers, based on averages over multiple samples, analyses per sample, and volume determinations (Ci/m^3)
$\overline{\overline{r}}_{Iq}^{MFPV}$	running average of activity-per-volume concentrations of the q^{th} radionuclide ($q = {}^{137}Cs$ and ${}^{90}Sr$) over the I ILAW MFPV batches produced through a given point in time, based on averages over multiple samples, analyses per sample, and volume determinations (Ci/m^3)

r_{iq}^{MFPV}	activity-per-volume concentration of the q^{th} radionuclide in the i^{th} IHLW MFPV batch (Ci/m^3)
$\bar{r}_{1kq}^{MFPV}$	activity-per-volume concentration of the q^{th} isotope of k = U or Pu in the first IHLW MFPV batch of an HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each IHLW MFPV batch (μCi/mL = mCi/L)
r_{iq}^{CRV}	activity-per-volume concentration of the q^{th} radionuclide in the LAW CRV batch contributing to the i^{th} ILAW MFPV batch (μCi/mL = mCi/L)
$\bar{r}_{iq}^{CRV}$	activity-per-volume concentration of the q^{th} radionuclide in the LAW CRV batch contributing to the i^{th} ILAW MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations (μCi/mL = mCi/L)
$\bar{r}_{iq}^{MFPV}$	mean activity-per-volume concentration of the q^{th} radionuclide in the i^{th} IHLW and ILAW MFPV batch (μCi/mL = mCi/L)
r_{ijlm}^{MFPV}	analyzed concentration of the j^{th} radionuclide from the m^{th} analysis of the l^{th} sample from the i^{th} IHLW MFPV batch (μCi/mL = mCi/L)
r_{iqlm}^{CRV}	activity-per-volume concentration of the q^{th} radionuclide in the i^{th} LAW CRV batch, based on the m^{th} radionuclide analysis of the l^{th} LAW CRV sample (μCi/mL = mCi/L)
r_{iqlm}^{MFPV}	activity-per-volume concentration of the q^{th} radionuclide in the i^{th} IHLW MFPV batch, based on the m^{th} radionuclide analysis of the l^{th} IHLW MFPV sample (μCi/mL = mCi/L)
R&T	Research and Technology
RHW	relative half-width
%RHW	percent relative half-width
RPP-WTP	River Protection Project-Waste Treatment and Immobilization Plant
RSD	relative standard deviation

%RSD	percent relative standard deviation (that is, the relative standard deviation multiplied by 100%)
$\%RSD_A$	%RSD arising from random analytical uncertainty
$\%RSD_S$	%RSD arising from random mixing/sampling uncertainty
$\%RSD_A(c_j^{MFPV})$	analytical %RSD in the concentration of the j^{th} element in an IHLW MFPV batch
$\%RSD_A(c_j^{CRV})$	analytical %RSD in the concentration of the j^{th} element in an LAW CRV batch
$\%RSD_S(c_j^{MFPV})$	mixing/sampling %RSD in the concentration of the j^{th} element in an IHLW MFPV batch
$\%RSD_S(c_j^{CRV})$	mixing/sampling %RSD in the concentration of the j^{th} element in an LAW CRV batch
$r_{ilm}^{PCT\ h}$	PCT normalized release of h = B, Li, or Na based on the m^{th} analysis of chemical composition of the l^{th} sample from the i^{th} IHLW MFPV batch (g/L = 2 g/m^2)
$r^{PCT\ B}$	PCT normalized boron release (g/L = 2 g/m^2)
$r^{PCT\ Li}$	PCT normalized lithium release (g/L = 2 g/m^2)
$r^{PCT\ Na}$	PCT normalized sodium release (g/L = 2 g/m^2)
ρ_i^{MFPV}	density of glass that would be made from the i^{th} IHLW MFPV batch (g_{glass}/m^3_{glass})
ρ_{ik}^{MFPV}	the k^{th} determination of density of glass that would be made from the i^{th} IHLW MFPV batch from a given HLW waste type (g_{glass}/m^3_{glass})
$\overline{\rho}_i^{MFPV}$	density of glass that would be made from the i^{th} IHLW MFPV batch from a given HLW waste type, based on an average of n_ρ determinations for glass that would be made from each IHLW MFPV batch (g_{glass}/m^3_{glass})

$\overline{\rho}_I^{MFPV}$	mean density of glass that would be made from I ILAW MFPV batches (g_{glass}/m^3_{glass})
$\overline{\rho}_D^{Canister}$	mean density of glass in the D IHLW canisters corresponding to the I IHLW MFPV batches for a given HLW waste type (g_{glass}/m^3_{glass})
$\overline{\rho}_D^{Container}$	mean density of glass in D ILAW containers (g_{glass}/m^3_{glass})
$\rho_d^{Container}$	density of glass for the d^{th} ILAW container (g_{glass}/m^3_{glass})
$\overline{\overline{s}}_{Dqk}^{Container}$	mean activity-per-mass concentration of the q^{th} radionuclide in the k^{th} group of radionuclides in glass from D ILAW containers, based on averages over multiple samples, analyses per sample, and volume determinations (nCi/g)
SD	standard deviation
SD_V^{CRV}	standard deviation of a volume determination on the LAW CRV (L)
SD_V^{MFPV}	standard deviation of a volume determination on the IHLW MFPV or ILAW MFPV (L)
$SD(Estimate)$	standard deviation of *Estimate*
$SD(G_{jk}^{GFC})$	GFC composition uncertainty, represented by the standard deviation in the mass fraction of the j^{th} component (oxide or halogen) in the k^{th} GFC ($g_{oxide\ j}/g_{GFC\ k}$)
$SD(a_k^{GFC})$	uncertainty in the mass of the k^{th} GFC added to an ILAW MFPV batch, expressed as a standard deviation (g)
$SD(\overline{\overline{SF}}_d^{Container})$	generic notation for the standard deviation of the sum-of-fractions for Class C radionuclides over the $d = 1, 2, \ldots, D$ ILAW containers. The notations $SD(\overline{SF1}_d^{Container})$ and $SD(\overline{SF2}_d^{Container})$ are specific to the sum-of-fractions of radionuclides in Tables 1 and of 10 CFR 61.55, respectively.
$SD(\overline{g}_{ij}^{MFPV})$	standard deviation of the average mass fraction of the j^{th} chemical composition component (oxide or halogen) in the i^{th} IHLW or ILAW MFPV batch. For IHLW, the average is based on multiple samples per MFPV batch and one or more chemical analyses per MFPV sample. For ILAW, the average is based on multiple samples per CRV batch, one or more chemical

	analyses per CRV sample, and one or more volume determinations per CRV and MFPV volume. (g_{oxide}/g_{oxides})
$SD(\overline{g}_{iq}^{MFPV})$	standard deviation of the average mass fraction of the q^{th} radionuclide composition component (oxide) in the i^{th} IHLW or ILAW MFPV batch. For IHLW, the average is based on multiple samples per MFPV batch and one or more radiochemical analyses per MFPV sample. For ILAW, the average is based on multiple samples per CRV batch, one or more radiochemical analyses per CRV sample, and one or more volume determinations per CRV and MFPV volume. (g_{oxide}/g_{oxides})
$SD(\overline{\overline{g}}_{q}^{MFPV})$	standard deviation of $\overline{\overline{g}}_{q}^{MFPV}$ (g_{oxide}/g_{oxides})
$SD(m_{d}^{Canister})$	standard deviation of the determined mass of glass in the d^{th} IHLW canister (g_{glass})
$SD(m_{d}^{Container})$	standard deviation of the determined mass of glass in the d^{th} ILAW container (g_{glass})
$SD(\overline{m}_{D}^{Canister})$	standard deviation of the mean mass of glass in the D IHLW canisters associated with an HLW waste type (g_{glass})
$SD(\overline{m}_{d,Nk}^{Canister})$	standard deviation of the mass of radionuclide k for the set N_k of isotopes of k = U or Pu in an individual IHLW canister across the D canisters associated with the I IHLW MFPV batches comprising an HLW waste type ($g_{radionuclide}$)
$SD(\overline{\overline{r}}_{Dq}^{Container})$	standard deviation of $\overline{\overline{r}}_{Dq}^{Container}$, which is sometimes referred to as a *standard error* because it is the standard deviation of an average (Ci/m^3)
$SD(R_{Dq}^{Canisters})$	standard deviation of the total inventory of the q^{th} radionuclide in D IHLW canisters associated with an HLW waste type (Ci)
$SD(\overline{R}_{dq}^{Canister})$	standard deviation of the average inventory of the q^{th} radionuclide in the d^{th} IHLW canister, where the average is based on multiple samples, analyses, and volume determinations for each IHLW MFPV batch (Ci)
$SD(\overline{R}_{dq}^{Container})$	standard deviation of the average inventory of the q^{th} radionuclide in the d^{th} ILAW container, where the average is based on multiple samples per LAW CRV batch, analyses per LAW CRV sample, and volume determinations for each CRV and MFPV batch (Ci)

$SD(\overline{\overline{R}}_{Dq}^{Canisters})$ standard deviation of the mean inventory per canister of the q^{th} radionuclide in D IHLW canisters associated with an HLW waste type (Ci/canister)

$SD(\rho_d^{Container})$ standard deviation of the density of glass in the d^{th} ILAW container (g_{glass}/m^3_{glass})

$SD_I(\hat{y}_{ilm}^h)$ standard deviation of $\hat{y}_{ilm}^h = \hat{l}n(r_{ilm}^{PCT\ h})$, i = 1, 2, … , I; l = 1, 2, … , n_S^{MFPV}; m = 1, 2, … , n_A^{MFPV} values corresponding to variation in IHLW composition over a waste type [ln(g/L)]

$SD_S^{MFPV}(\hat{y}_{ilm}^h)$ standard deviation of $\hat{y}_{ilm}^h$ values due to composition uncertainty resulting from mixing/sampling uncertainty for the i^{th} MFPV batch

$SD_A^{MFPV}(\hat{y}_{ilm}^h)$ standard deviation of $\hat{y}_{ilm}^h$ values due to composition uncertainty resulting from analytical uncertainty for the i^{th} MFPV batch

$SD_M[\hat{y}^h(\overline{\overline{\boldsymbol{x}}}_I^{MFPV})]$ standard deviation of the model prediction for the mass-weighted-average IHLW composition $\overline{\overline{\boldsymbol{x}}}_I^{MFPV}$

$SD_U\left(\hat{y}_i^h(\overline{\boldsymbol{x}}_i^{MFPV})\right)$ standard deviation in $\hat{\hat{y}}_i^h = ln(r_i^{PCT\ h})$ or $\hat{\hat{y}}_i^h = ln(D^{VHT})$ values representing all ILAW process uncertainties (e.g., CRV mixing/sampling, CRV analytical, CRV and MFPV volumes, GFC compositions and additions), where the process uncertainties in $\overline{\boldsymbol{x}}_i^{MFPV}$ are reduced by averaging over multiple determinations [ln(g/L) for PCT and ln(μm) for VHT]

$\overline{\overline{SF}}_d^{Container}$ generic notation for the sum-of-fractions for Class C radionuclides for the d^{th} ILAW container, based on averages over multiple samples, analyses per sample, and volume determinations. The notations $\overline{SF1}_d^{Container}$ and $\overline{SF2}_d^{Container}$ are specific to the sum-of-fractions of radionuclides in Tables 1 and of 10 CFR 61.55, respectively. (unitless)

$\overline{\overline{SF}}_i^{MFPV}$ generic notation for the sum-of-fractions for Class C radionuclides in ILAW that would be made from the i^{th} ILAW MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations. The notations $\overline{SF1}_i^{MFPV}$ and $\overline{SF2}_i^{MFPV}$ are specific to the sum-of-fractions of radionuclides in Tables 1 and of 10 CFR 61.55, respectively. (unitless)

$\overline{SF}_D^{Containers}$	generic notation for the mean sum-of-fractions for Class C radionuclides over *D* ILAW containers associated with *I* ILAW MFPV batches corresponding to an LAW waste type, based on averages over multiple samples, analyses per sample, and volume determinations. The notations $\overline{SF1}_D^{Containers}$ and $\overline{SF2}_D^{Containers}$ are specific to the sum-of-fractions of radionuclides in Tables 1 and of 10 CFR 61.55, respectively. (unitless)
σ	standard deviation of the distribution of possible $\bar{\hat{y}}_i^h$ values over the *I* IHLW MFPV batches corresponding to an HLW waste type
σ_g	standard deviation of the distribution of true ln(PCT normalized release) values for IHLW produced from a given HLW waste type
$\widetilde{\sigma}$	estimate of the population standard deviation that accounts for (1) variation in glass property values across MFPV batches corresponding to an HLW or LAW waste type, (2) mixing/sampling, analytical, and other uncertainties affecting the estimate of glass composition for each HLW or LAW MFPV batch, and (3) model uncertainty used to predict a glass property (or mathematical transformation thereof).
$\hat{\sigma}_U^2$	estimated mean square for error associated with the unweighted least squares fit of a property-composition model
$\hat{\sigma}_W^2$	estimated mean square for error associated with the weighted least squares fit of a property-composition model
$\boldsymbol{\Sigma_x}$	composition variance-covariance matrix for a vector $\boldsymbol{x}$ containing the composition for a particular glass
$\boldsymbol{\Sigma_b}$	variance-covariance matrix for the coefficients, $\boldsymbol{b}$, of a glass property-composition model
$\hat{\boldsymbol{\Sigma}}_b^h$	estimated $p \times p$ variance-covariance matrix of the model coefficient vector $\boldsymbol{b}^h$ for an IHLW property model (the PCT normalized release of h = B, Li, or Na) or for an ILAW property model (the PCT normalized release of h = B or Na or VHT alteration depth)
SME	Slurry Mix Evaporator
SUCI	simultaneous upper confidence interval (see CL% SUCI for definition)
TCLP	Toxicity Characteristic Leaching Procedure
$T_{1\%}$	temperature at which 1 volume percent of waste glass is crystalline (°C)

TI	tolerance interval
T_q	specific thermal output of the q^{th} radionuclide (W/Ci)
$t_{1-\alpha,df}$	100(1 – α) percentile of Student's t-distribution with *df* degrees of freedom
Δ_l	lower limit value specified for the triangular distribution
Δ_n	nominal value specified for the triangular distribution
Δ_u	upper limit value specified for the triangular distribution
u	units conversion factor for converting mg to g
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)
UTI	upper tolerance interval (see X%/Y% UTI for definition)
UTIHW	upper tolerance interval half-width
Variation	real changes in a variable over time or space (for example, *variation* in glass composition within a waste type)
VHT	Vapor Hydration Test
VSL	Vitreous State Laboratory (at The Catholic University of America)
$\overline{V}_D^{Container}$	mean volume of glass in *D* ILAW containers (m^3)
$V_i^{CRV\ before}$	volume of the LAW CRV before the transfer of material to the i^{th} ILAW MFPV batch (L)
$V_i^{CRV\ after}$	volume of the LAW CRV after the transfer of material to the i^{th} ILAW MFPV batch (L)
V_i^{MFPV}	volume of the i^{th} IHLW or ILAW MFPV batch (L)

$V_i^{MFPV\ Heel}$	volume of the MFPV Heel included in the i^{th} MFPV batch (L)
$V_i^{MFPV\ before}$	volume of the ILAW MFPV before receipt of LAW CRV material for the i^{th} ILAW MFPV batch (L)
$V_i^{MFPV\ after}$	volume of the ILAW MFPV after receipt of LAWCRV material for the i^{th} ILAW MFPV batch but before receipt of GFCs or any added water (L)
$\overline{V}_i^{MFPV}$	average volume over n_V^{MFPV} volume determinations of the i^{th} IHLW or ILAW MFPV batch (L)
V_{ih}^{MFPV}	h^{th} volume determination of the i^{th} MFPV batch (L)
$V_{max}^{Canister}$	the glass volume that would result from a 100% fill of an IHLW canister (m^3)
$V_i^{CRV\ to\ MFPV}$	volume transfer from the LAW CRV to the i^{th} ILAW MFPV batch (L)
$\boldsymbol{W}$	a diagonal matrix of weights associated with the data points used to fit a model to a glass property during the application of weighted least squares
WAPS	Waste Acceptance Product Specifications
WASRD	Waste Acceptance System Requirements Document
Waste type	a quantity of waste feed to a vitrification facility that is relatively constant in composition
WCP	Waste Form Compliance Plan
WFQ	waste form qualification
WL	waste loading (mass fraction or mass percent of glass that is from waste)
WL_{ij}^{MFPV}	waste loading of the j^{th} glass oxide component in the i^{th} IHLW or ILAW MFPV batch
WLS	weighted least squares
WQR	Waste Form Qualification Report

WSRC	Westinghouse Savannah River Company
WTP	Waste Treatment and Immobilization Plant
WTPSP	Waste Treatment Plant Support Project
wt%	weight percent
WVDP	West Valley Demonstration Project
$\bar{x}_{ik}^{MFPV}$	normalized mass fraction of the k^{th} component of ILAW corresponding to the i^{th} ILAW MFPV batch for use in the PQM model, such that $\sum_{k=1}^{p} x_{ik}^{MFPV} = 1$. The mass fractions are based on averages over multiple samples from a CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations (g_{oxide}/g_{oxides})
x_{iklm}^{MFPV}	normalized mass fraction of the k^{th} IHLW component from the m^{th} chemical analysis of the l^{th} sample from the i^{th} MFPV batch, where k is one of the IHLW components in a linear mixture model, such that $\sum_{k=1}^{n_{mc}^{h}} x_{iklm}^{MFPV} = 1$ (g_{oxide}/g_{oxides})
$\boldsymbol{x}_{ilm}^{MFPV}$	$p \times 1$ column vector of the IHLW normalized composition x_{iklm}^{MFPV}, $k = 1, 2, \ldots, p$ for which PCT model predictions are to be made (g_{oxide}/g_{oxides})
$\bar{\boldsymbol{x}}_{i}^{MFPV}$	$p \times 1$ column vector whose entries $\bar{x}_{ik}^{MFPV}, k = 1, 2, \cdots, p$ are means of the x_{ikl}^{MFPV} values for IHLW normalized composition, where $l = 1, 2, \ldots, n_S^{MFPV}$ (g_{oxide}/g_{oxides})
$\bar{\boldsymbol{x}}_{i}^{MFPV}$	$p \times 1$ column vector of the ILAW normalized composition $\bar{x}_{ik}^{MFPV}$, $k = 1, 2, \ldots, n_{mc}^{h}$ expanded to the form of the terms in the PQM model for PCT or VHT
$\bar{\bar{\boldsymbol{x}}}_{I}^{MFPV}$	$p \times 1$ column vector whose entries $\bar{\bar{x}}_{k}^{MFPV}, k = 1, 2, \cdots, p$ are model-component-normalized versions of the $\bar{\bar{g}}_{k}^{MFPV}, k = 1, 2, \cdots, p$, which are mass-weighted-average compositions over the $i = 1, 2, \ldots, I$ IHLW MFPV batches, with ordinary averaging over the $l = 1, 2, \ldots, n_S^{MFPV}$ samples per MPFV batch and $m = 1, 2, \ldots, n_A^{MFPV}$ analyses per sample (g_{oxide}/g_{oxides})

X%/Y% UTI	X%/Y% upper tolerance interval—At least Y% of a distribution is less than the UTI with X% confidence.
y_i^h	natural logarithm of the measured PCT normalized release of element *h* (for IHLW and ILAW) or the natural logarithm of the measured VHT alteration rate (LAW) for IHLW or ILAW corresponding to the i^{th} MFPV batch [ln(g/L) for PCT and ln(μm) for VHT]
$\hat{y}_i^h$	predicted natural logarithm of the PCT normalized release of *h* = B or Na [$\hat{l}n(r_i^{PCT\ h})$], or the predicted natural logarithm of the VHT alteration depth [$\hat{l}n(D_i^{VHT})$], for ILAW corresponding to the i^{th} MFPV batch, based on averages over multiple samples from a CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations. [ln(g/L) for PCT and ln(μm) for VHT]
$\hat{y}_{i,1-\alpha}^h$	100(1 – α) percentile of the empirical distribution of 1000 values of $\hat{y}_i^h$ resulting from 1000 Monte Carlo simulations of the i^{th} ILAW MFPV batch [ln(g/L) for PCT and ln(μm) for VHT]
$\hat{y}_{ilm}^h$	$\hat{l}n\left(r_{ilm}^{PCT\ h}\right)$ = predicted natural logarithm of the PCT normalized release of *h* = B, Li, or Na based on the m^{th} analysis of chemical composition of the l^{th} sample from the i^{th} IHLW MFPV batch [ln(g/L)]
$\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})$	model prediction of the PCT normalized release of *h* = B, Li, or Na for the mass-weighted-average IHLW composition $\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ [ln(g/L)]
$\bar{\hat{y}}_i^h$	mean of model-predicted $\hat{y}_{ilm}^h = \hat{l}n\left(r_{ilm}^{PCT\ h}\right)$ values over the n_S^{MFPV} samples and n_A^{MFPV} analyses per sample of the i^{th} IHLW MFPV batch [ln(g/L)]
$\bar{\bar{\hat{y}}}_I^h$	average of the $\bar{\hat{y}}_i^h$, *i* = 1, 2, … , *I* values for the *I* IHLW MFPV batches corresponding to an HLW waste type [ln(g/L)]
$z_{1-\beta}$	100(1 – β) percentile of the standard normal distribution

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Tables

1.0 Introduction

Various process samples, chemical analyses of composition, and measurements (e.g., volume and weight) will be required to control Waste Treatment and Immobilization Plant (WTP) vitrification facilities that will produce immobilized high-level waste (IHLW) and immobilized low-activity waste (ILAW). In addition, process and/or product samples, chemical and radiochemical analyses, and measurements will be required to satisfy applicable compliance requirements. For example, the Waste Acceptance System Requirements Document (WASRD, DOE-RW 2002) and the Waste Acceptance Product Specifications (WAPS, DOE-EM 1996) describe various compliance requirements for IHLW. Also, the contract between the U.S. Department of Energy (DOE) Office of River Protection (ORP) and Bechtel National, Inc. (BNI) specifies compliance requirements for ILAW as well as additional compliance requirements for IHLW (DOE-ORP 2003). This report focuses on the data and methods required to demonstrate compliance with the applicable requirements for IHLW and ILAW. However, the data and methods for demonstrating compliance will also play roles in controlling the IHLW and ILAW processes. Hence, although the focus of this report is on compliance, process-product control is also mentioned where relevant.

Although the process-product control and compliance strategies for the WTP IHLW and ILAW facilities are still under development and refinement, many aspects have been initially determined. The initial strategies are subject to potential change, however, as evidenced by DOE-ORP direction[(a)] to utilize the WASRD (DOE-RW 2002) rather than WAPS (DOE-EM 1996) as the primary compliance guidance document. The current compliance strategies for the WTP IHLW and ILAW facilities are described, respectively, in the IHLW Product Compliance Plan (IHLW PCP) by Nelson et al. (2004) and the ILAW Product Compliance Plan (ILAW PCP) by Westsik et al. (2004). However, these Rev. 1 PCPs were issued after the work in this report was completed and the report itself was substantially complete. The work in this report was performed to address the IHLW PCP Rev. 0 (Nelson 2003) with adjustments for the removal of the Concentrate Receipt Vessel (CRV) from the IHLW facility, and the ILAW PCP Rev. 0 (Nelson et al. 2003). Future work will address the IHLW and ILAW Rev. 1 PCPs and any subsequent revisions to applicable specifications and WTP compliance strategies.

Many of the compliance strategies outlined in the IHLW PCP and ILAW PCP are statistical in nature. That is, the strategies involve quantifying and accounting for variations and uncertainties in controlling the IHLW and ILAW vitrification processes and in satisfying compliance requirements. Statistically based strategies are being developed for pre-production activities (i.e., waste form qualification [WFQ] activities), production activities (i.e., batch-by-batch process-product control and compliance activities), and post-production activities (i.e., compliance and acceptance activities for product resulting from specified quantities of waste or periods of production). Strategies for environmental regulatory compliance (e.g., plant emissions or complying with Land Disposal Restriction [LDR] and delisting criteria) are described in the delisting/LDR data quality objectives document (Cook and Blumenkranz 2003). These strategies are also statistically based in that they account for applicable variations and uncertainties.

(a) ORP memorandum from R.J. Schepens to J.P. Henschel, "Notification to Stop Using the Office of Environmental Management High Level Waste Product Acceptance Specifications (1996) to Control Waste Treatment and Immobilization Plant (WTP) Project Work Regarding the Immobilized High-Level Waste (IHLW) Product," 04-WED-019, dated May 18, 2004.

Several aspects of the WTP IHLW and ILAW qualification, process-product control, and compliance strategies require estimates of variations and uncertainties of (1) incoming waste feed, (2) process materials and vessel contents at various steps of the IHLW and ILAW processes, and (3) the compositions and properties of IHLW and ILAW products. A report by Heredia-Langner et al. (2003) summarizes the initial work in quantifying variations and uncertainties that may affect the WTP IHLW and ILAW processes and the ability to demonstrate compliance with various specifications. That report is scheduled to be updated in the future as more WTP-specific data and results become available to provide better estimates of variations and uncertainties expected to be experienced by the WTP IHLW and ILAW processes.

Before continuing, it is important to clarify the use of the terms *variation* and *uncertainty* in this report. *Variation* refers to real changes in a variable over time or space (e.g., variation in glass composition because of variation in waste feed composition). *Uncertainty* refers to a lack of knowledge about a true, fixed state of affairs (e.g., analytical uncertainty in the chemical analysis of a glass sample). Hence, WTP IHLW and ILAW slurry and glass compositions will be subject to *variation* over time, whereas sampling, chemical and radiochemical analyses, volume determinations, weight measurements or determinations, density measurements, and other measurements or determinations at specific times will be subject to *uncertainty*.

There were four general objectives for the work summarized in this report per the Test Specification (Swanberg 2002) and Test Plan (Piepel and Cooley 2003).

- Statistical confidence interval (CI) methods are needed to demonstrate with high confidence that each batch of high-level waste (HLW) or low-activity waste (LAW) melter feed will meet the requirements of applicable specifications after accounting for applicable uncertainties.

- Statistical analyses that account for applicable variations and uncertainties are needed to determine the number of process samples, analyses, and measurements required to (1) control and report the IHLW and ILAW chemical compositions, radionuclide inventories, and their associated uncertainties, and (2) demonstrate compliance with IHLW and ILAW waste loading requirements. [Note that Item (2) was removed from the scope by Test Exception 24590-WTP-TEF-RT-04-00036.]

- Statistical tolerance interval (TI) methods are needed to control and report with high confidence (X%) that a high percentage (Y%) of the waste glass produced from a specified quantity of HLW or LAW feed (or for a specified production period) meets limits for leachability as well as other applicable requirements in WAPS or contract specifications. Measures of leachability include the Product Consistency Test (PCT), used for IHLW and ILAW, and the Vapor Hydration Test (VHT), used for ILAW. The number of process samples, analyses, and measurements required to meet or exceed the desired values for X% and Y% must be determined.

- Methods are needed to properly calculate means and standard deviations (SDs) of IHLW and ILAW chemical compositions and radionuclide inventories over the course of a waste type to report these compositions and their uncertainties in the production records. The methods must account for the possibility of unbalanced data (e.g., different numbers of samples or analyses per sample) and multiple sources of variation or uncertainty. Standard, simple formulas for calculating means and SDs are not appropriate (i.e., can yield incorrect results) when data are unbalanced or have multiple sources of variation or uncertainty.

The methods and results contained in this initial report at least partially address all four of the above objectives. Subsequent work will complete and finalize efforts for these objectives, which will be documented in a final report consisting of a revision of this initial report.

The remainder of this document is organized as follows. Section 2 provides an overview of the WTP IHLW and ILAW vitrification processes and compliance strategies. Section 3 describes the general statistical approaches used to implement the statistically based compliance strategies for IHLW and ILAW. Sections 4 and 5, respectively for IHLW and ILAW, present the statistical compliance methods for each WAPS (DOE-EM 1996) and WTP contract (DOE-ORP 2003) specification having a statistically based compliance strategy. Each subsection of Sections 4 and 5 corresponds to a specification, with sub-subsections (1) listing the specification verbatim, (2) describing the statistical aspects of the compliance strategy for that specification, and (3) presenting the statistical method(s) for implementing those aspects. Sections 6 and 7 contain results of applying the statistical methods to assess the effects of IHLW and ILAW process variations; uncertainties; and numbers of samples, analyses per sample, and other process measurements. Sections 6 and 7 also contain illustrations of compliance methods applied to realistic data such as might be collected during operation of the IHLW and ILAW vitrification facilities. Section 8 summarizes the work and results, and makes recommendations for data needed to support future efforts. Section 9 lists the references cited in the main body and appendices of the report. Appendices provide equations and other information too detailed to include in the main body of the report.

2.0 The WTP IHLW and ILAW Vitrification Processes and Compliance Strategies

Section 2.1 provides a general overview of the IHLW and ILAW vitrification processes and introduces the generic terms used to refer to IHLW and ILAW process vessels and other process steps. Sections 2.2 and 2.3 discuss the bases for the IHLW and ILAW compliance strategies, respectively. Section 2.4 discusses that the IHLW and ILAW compliance strategies for some specifications involve demonstrating compliance for (1) each Melter Feed Preparation Vessel (MFPV) batch and/or (2) a collection of MFPV batches corresponding to a specified quantity of HLW or LAW. Section 2.5 addresses the MFPV focus of the IHLW and ILAW compliance strategies.

2.1 IHLW and ILAW Vitrification Processes

Figure 2.1 and Figure 2.2, which were supplied by the WTP Project, display simplified overviews of the IHLW and ILAW vitrification processes. The figures illustrate the key process vessels, the glass former chemicals (GFCs) system, the melter, and possible sampling and measurement points. Symbols in the figures denote sampling points (S in a circle), non-routine sampling points (S_n in a circle), weight measurements (W in a diamond), and level measurements of vessels (L in a diamond).

In the IHLW vitrification facility (Figure 2.1), only the MFPV will be routinely sampled and analyzed. In the ILAW vitrification facility (Figure 2.2), only the Concentrate Receipt Vessel (CRV) will be routinely sampled and analyzed.

Weight measurements will be used to quantify the amounts of individual GFCs added to waste feed concentrates in the IHLW and ILAW MFPVs. Weights of individual GFCs will be determined as well as weights of combined GFCs in the GFC batch makeup hopper and the GFC feed hopper. Multiple weighing points provide for verifying transfers of individual and combined GFCs. Note that only GFC silos and not the hoppers are shown in Figure 2.1 and Figure 2.2, but it will be in the hoppers that GFC weight measurements are made.

Level measurements will be made in the CRV (ILAW only), MFPV (IHLW and ILAW), and Melter Feed Vessel (MFV) (IHLW and ILAW). A level-to-volume calibration equation for each vessel will then be used to calculate the vessel volume corresponding to a measured vessel level. Such measurements are important for estimating compositions and verifying transfers to and from the CRV (ILAW only), MFPV (IHLW and ILAW), and MFV (IHLW and ILAW). Fill levels of IHLW canisters and ILAW containers will also be measured, as shown in Figure 2.1 and Figure 2.2.

Although not indicted by symbols in Figure 2.1 and Figure 2.2, sampling and chemical analyses are planned in the pretreatment facility to verify that pretreated waste is acceptable for transfer to the IHLW or ILAW vitrification facility. Similarly, individual GFCs may be sampled and chemically analyzed to verify their compositions before being introduced to the GFC batch makeup facility. The density of material in the CRV (ILAW only) and MFPV (ILAW and IHLW) will be determined and used for process control purposes as well as compliance purposes in some cases.

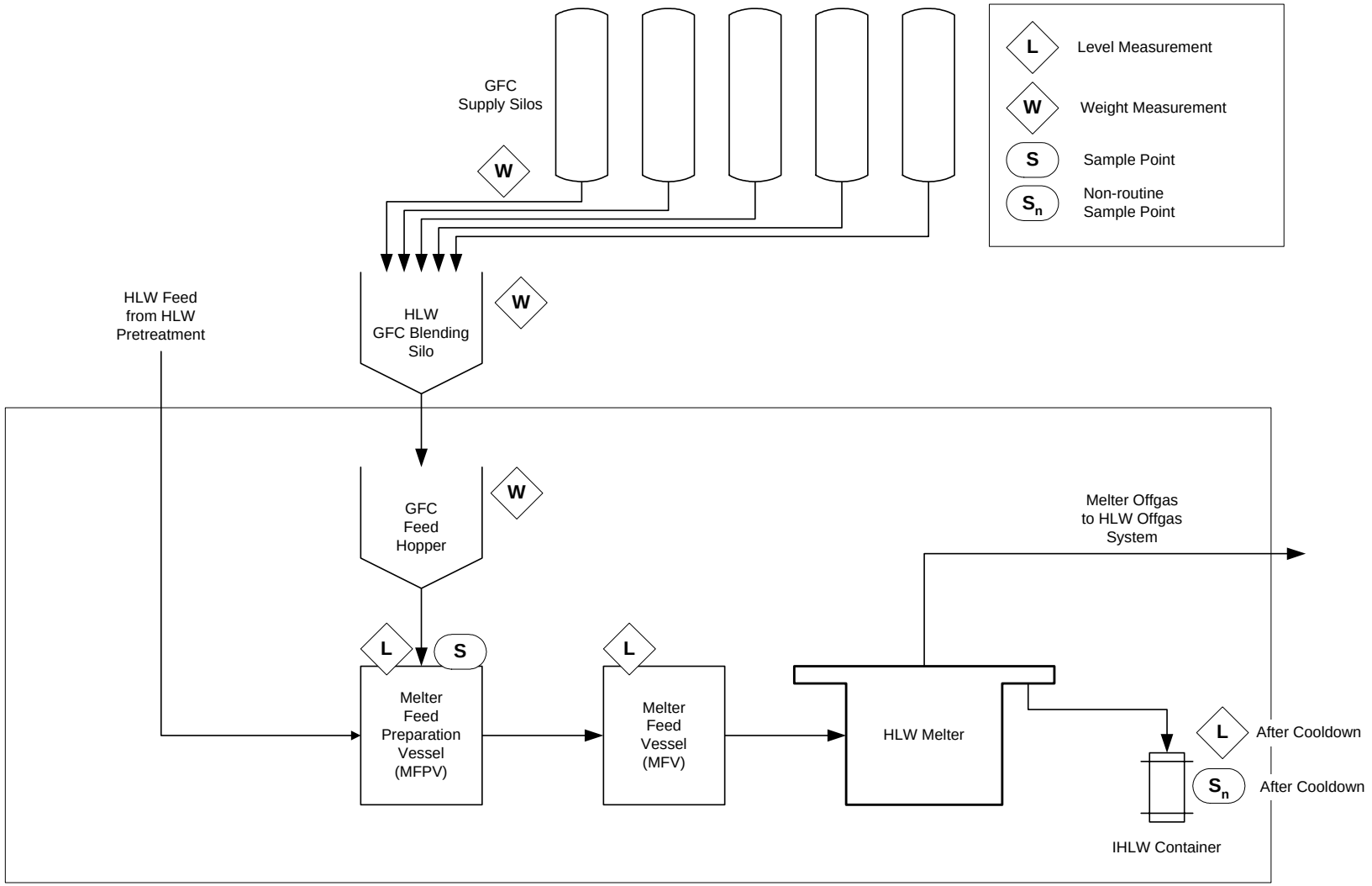

Figure 2.1. Overview of the HLW Vitrification Process

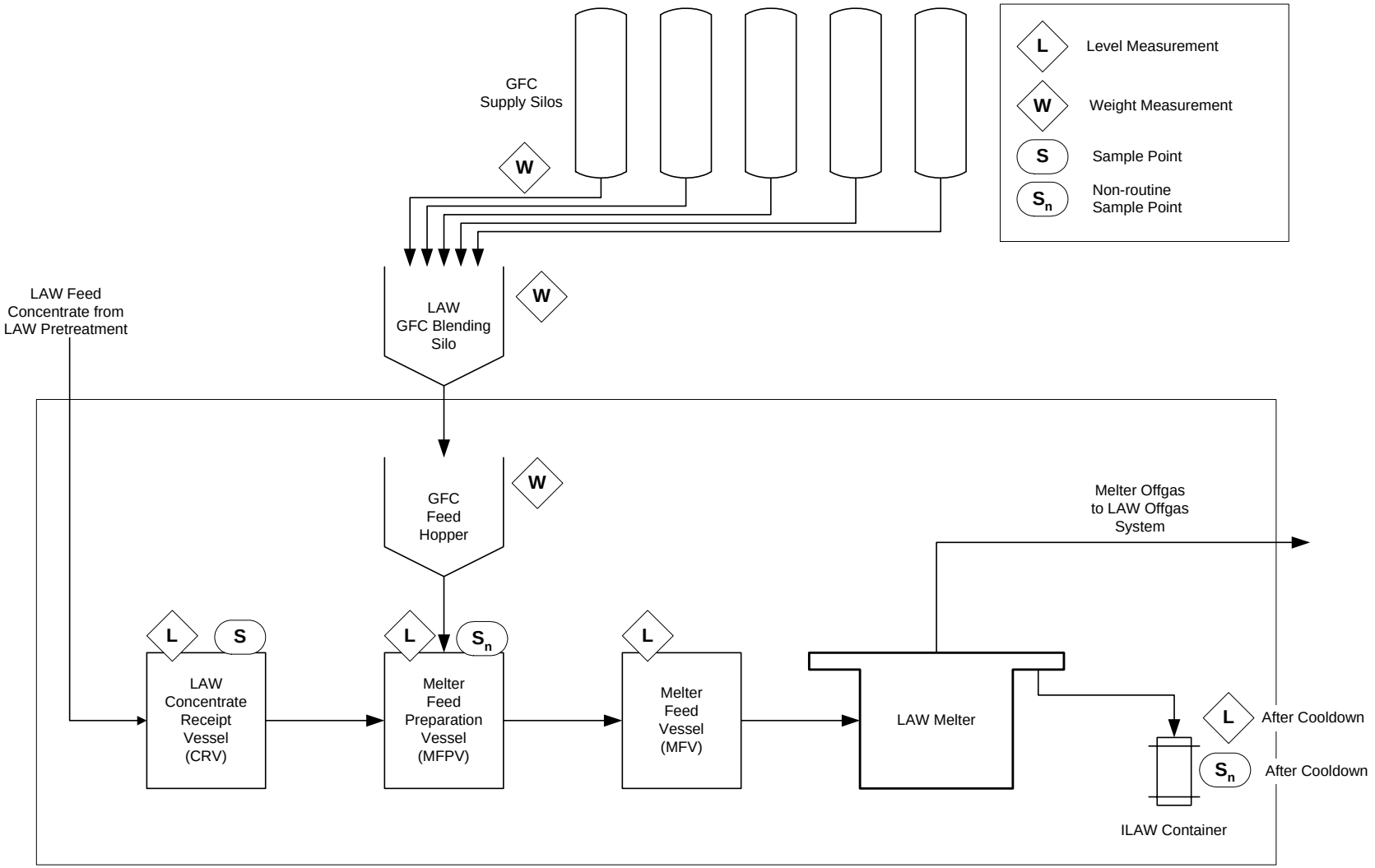

Figure 2.2. Overview of the LAW Vitrification Process

The possible sampling and measurement points in the IHLW and ILAW vitrification processes shown in Figure 2.1 and Figure 2.2, respectively, are not intended to present a comprehensive list of all possible sampling or measurement points that may be used for process-product control or specification compliance. As the WTP Project progresses in developing and finalizing IHLW and ILAW process-product control and compliance strategies, sampling and measurement points may be added or deleted.

2.2 Basis for the WTP IHLW Compliance Strategy

The current WTP IHLW compliance strategy is discussed in detail by Nelson et al. (2004), although the work in this report addresses interim revisions of the previous version of the compliance strategy (Nelson 2003).[(a)] The IHLW compliance strategy is based on direct characterization of each MFPV batch and verification of compliance before that batch is sent to the MFV. According to this strategy, the fundamental process samples, analyses, and measurements that will be used during production to control the process and demonstrate compliance with IHLW specifications are outlined in the following steps.

1. For each HLW MFPV batch, transfer a portion of the current HLW Feed Blend Vessel (HBV) to the HLW MFPV. Measure n_V^{MFPV} times the level of the HLW MFPV contents before and after the HBV-to-MFPV transfer. Apply level-to-volume calibration equations for the HLW MFPV to convert the measured vessel levels (before and after HBV transfers) to volumes. Use the before and after determinations of the HLW MFPV volumes to calculate the HBV-to-MFPV transfer volume (L).
2. After the transfer from the HBV to the HLW MFPV, sample and analyze the HLW MFPV
3. For each HLW MFPV batch,[(b)] obtain and/or calculate the oxide mass fraction compositions of each GFC from vendor certification sheets. The oxide mass fractions for a given GFC should be relative to the total GFC mass, including absorbed water or other volatiles that will not persist in the HLW melter.
4. Calculate the masses of GFCs to be added to each HLW MFPV batch so that when combined with the volume of waste transferred from the HBV and the HLW MFPV heel, the resulting HLW MFPV slurry will make HLW glass satisfying all processing constraints and compliance requirements. Add the calculated amounts of GFCs to the HLW MFPV.
5. For each HLW MFPV batch, measure the level of the HLW MFPV contents after adding the GFCs. Apply the level-to-volume calibration equation for the HLW MFPV to convert the measured MFPV level to a volume (L).
6. For each completed HLW MFPV batch, collect n_S^{MFPV} samples.
7. For each completed HLW MFPV batch, analyze n_A^{MFPV} times the chemical composition (element concentrations in μg/mL = mg/L) of each sample.

(a) See Section 1.0 for a discussion of why this report addresses IHLW PCP Rev. 0 (Nelson 2003) rather than IHLW PCP Rev. 1 (Nelson et al. 2004).

(b) Presumably, the nominal oxide mass fraction compositions of GFCs and uncertainties thereof will change infrequently, but the WTP Project must have the capability to change this information for any MFPV batch when appropriate.

8. For the first HLW MFPV batch from each HBV, analyze the concentrations of the radionuclides listed in the second column of Table 2.1. These radionuclides are more difficult to measure and thus will only be measured in the first MFPV batch of an HLW waste type. In subsequent MFPV batches of an HLW waste type, these radionuclide concentrations will be assigned values equal to those measured in the first MFPV batch.
9. For the remaining HLW MFPV batches from each HBV, analyze the radionuclides listed in the third column of Table 2.1. These radionuclides are more easily measured, and hence will be measured in each MFPV batch corresponding to an HLW waste type.
10. For each IHLW canister produced, determine the mass of glass in the canister.

In Steps 7 and 8, it is important that all detectable chemical composition and radionuclide components be quantified in chemical and radionuclide analyses. Only a subset of all detectable IHLW components are reportable[(a)] as shown in Table 2.1 and Table 2.2. However, failing to analyze for and quantify detectable components can lead to underestimating the mass of all IHLW components and thus result in biased estimates of IHLW composition (i.e., mass fractions of IHLW components).

Steps 1 to 5 are relevant to process control, whereas Steps 6 to 10 are relevant to demonstrating compliance with IHLW specifications during production. The main compliance quantities (e.g., chemical composition, radionuclide inventory, and PCT performance) addressed in this report can be calculated using the information in Steps 6 to 10. The equations for calculating compliance quantities associated with IHLW specifications are presented in Appendix A.

The statistical methods that will be used to demonstrate compliance during IHLW production are discussed in Section 4. The number of samples (n_S^{MFPV}) per IHLW MFPV batch and the number of analyses per sample (n_A^{MFPV}) necessary to provide high confidence in demonstrating compliance with applicable IHLW specifications are discussed in Section 6.

(a) A chemical composition or radionuclide component of IHLW is considered "reportable" if it must be used to satisfy one or more IHLW specifications, either directly or indirectly through a property-composition model.

Table 2.1. Reportable[(a)] Isotopes to be Analyzed in the WTP IHLW MFPV and ILAW CRV

Isotope	First HLW MFPV from Each HBV	Remaining HLW MFPVs from Each HBV	LAW from Each CRV
^{59}Ni	Y	-	-
^{60}Co	-[(b)]	-	Y
^{63}Ni	Y	-	Y
^{90}Sr	Y	Y	Y
^{93}Zr	Y	-	-
^{93}Nb	Y	-	-
^{99}Tc	Y	-	Y
^{125}Sb	-	-	Y
^{126}Sn	Y	-	-
^{135}Cs	Y	-	-
^{137}Cs	Y	Y	Y
^{151}Sm	Y	-	Y
^{152}Eu	Y	-	-
^{154}Eu	-	-	Y
^{155}Eu	-	-	Y
^{233}U	Y	-	Y
^{234}U	Y	-	-
^{235}U	Y	-	Y
^{236}U	Y	-	-
^{237}Np	Y	-	Y
^{238}U	Y	-	Y
^{238}Pu	Y	Y	Y
^{239}Pu	Y	^{239}Pu + ^{240}Pu	Y
^{240}Pu	Y	^{239}Pu + ^{240}Pu	Y
^{241}Pu	Y	-	Y
^{241}Am	Y	-	Y
^{242}Pu	Y	-	-
^{242}Cm	Y	-	-
^{243}Cm	-	-	Y[(b)]
^{244}Cm	Y[(c)]	-	Y[(b)]
^{243}Am	Y	-	-

(a) A chemical composition or radionuclide component of immobilized waste is considered "reportable" if it must be used to satisfy one or more applicable specifications, either directly or indirectly through a property-composition model. The lists of reportable radionuclides were provided by the WTP Project and are based in part on Kaiser et al. (2003, 2004).

(b) A dash (-) indicates that the isotope is not reportable for that particular location.

(c) The analytical methods typically used report only ^{243}Cm + ^{244}Cm.

Table 2.2. Reportable Chemical Composition Oxides for IHLW and ILAW

Oxide or Halogen	IHLW[(a)] Reportable?	ILAW[(b)] Reportable?
Al_2O_3	Y	Y
B_2O_3	Y	Y
CaO	Y	Y
CdO	Y	-
Cl	-[(c)]	Y
Cr_2O_3	Y	-
Fe_2O_3	Y	Y
K_2O	-	Y
Li_2O	Y	Y
MgO	Y	Y
MnO	Y	-
Na_2O	Y	Y
NiO	Y	-
P_2O_5	Y	Y
PdO	Y	-
Rh_2O_3	Y	-
RuO_2	Y	-
SO_3	Y	Y
Sb_2O_3	Y	-
SeO_2	Y	-
SiO_2	Y	Y
SrO	Y	-
ThO_2	Y	-
U_3O_8	Y	-
ZnO	Y	Y
ZrO_2	Y	Y
Others[(d)]	-	Y

(a) The list of reportable IHLW chemical composition components was provided by the WTP Project, and is based in part on Kaiser et al. (2003, 2004). It includes not only components that must be reportable according to one or more specifications, but also components expected to be present in one or more glass product or processing property-composition models.

(b) The list of reportable ILAW chemical composition components was provided by the WTP Project. It includes not only components that must be reportable according to one or more specifications, but also components expected to be present in one or more glass product or processing property-composition models. The list was developed by the WTP Project and is partially based on Table 3-4 of Nelson et al. (2002).

(c) A dash (-) indicates that the component is not reportable.

(d) Others is the sum of all other oxides or halogens not specifically listed.

2.3 Basis for the WTP ILAW Compliance Strategy

The WTP ILAW compliance strategy is discussed in detail by Westsik et al. (2004), although the work in this report addresses the previous version of the compliance strategy (Nelson 2003).[(a)] Similar to the IHLW, the ILAW compliance strategy is based on characterization of each MFPV batch before that batch is sent to the MFV. However, the IHLW compliance strategy uses direct characterization of each MFPV batch while the ILAW compliance strategy uses derived characterization of each MFPV batch. Therefore, according to the ILAW compliance strategy, the fundamental process samples, analyses, and measurements that will be used to comply with ILAW specifications are outlined in the following numbered list.

1. For each LAW CRV batch, collect n_S^{CRV} samples.
2. For each LAW CRV batch, analyze n_A^{CRV} times the chemical composition (element concentrations in μg/mL = mg/L) of each sample.
3. For each LAW CRV batch, analyze the concentrations of the radionuclides listed in the "LAW Each CRV" column of Table 2.1.
4. For each LAW MFPV batch, transfer a portion of the current LAW CRV batch to the LAW MFPV. Measure the levels of LAW CRV and LAW MFPV contents before and after the CRV-to-MFPV transfer. Apply level-to-volume calibration equations for the LAW CRV and MFPV to convert the measured vessel levels (before and after transfers) to volumes. Use the before and after determinations of the LAW CRV and MFPV volumes to calculate the CRV-to-MFPV transfer volume.
5. For each LAW MFPV batch,[(b)] obtain and/or calculate the oxide mass fraction compositions of each GFC from vendor certification sheets. The oxide mass fractions for a given GFC should be relative to the total GFC mass, including absorbed water or other volatiles that will not persist in the LAW melter.
6. Calculate the masses of GFCs to be added to each LAW MFPV batch so that when combined with the volume of waste transferred from the LAW CRV and the LAW MFPV heel, the resulting LAW MFPV slurry will make LAW glass satisfying all processing constraints and compliance requirements. Add the calculated amounts of GFCs to the LAW MFPV.
7. For each LAW MFPV batch, weigh the amounts of GFCs added to the LAW MFPV.
8. For each ILAW container produced, determine the mass of glass in the container.

In Steps 2 and 3, it is important that all detectable chemical composition and radionuclide components be quantified in chemical and radionuclide analyses. Only a subset of all detectable ILAW components are

(a) See Section 1.0 for a discussion of why this report addresses ILAW PCP Rev. 0 (Nelson et al. 2003) rather than ILAW PCP Rev. 1 (Westsik et al. 2004).

(b) Presumably, the nominal oxide mass fraction compositions of GFCs and uncertainties thereof will change infrequently, but the WTP Project must have the capability to change this information for any MFPV batch when appropriate.

reportable[a] as shown in Table 2.1 and Table 2.2. However, failing to analyze for detectable components can lead to underestimating the mass of all ILAW components and thus result in biased estimates of ILAW composition (i.e., mass fractions of ILAW components).

Steps 1 to 6 provide data for both process control and compliance aspects of the WTP strategy for ILAW. The main compliance quantities (i.e., chemical composition, radionuclide composition and inventory, PCT performance, and VHT performance) addressed in this report can be calculated using the information in Steps 1 to 6. The equations for calculating compliance quantities associated with ILAW specifications are presented in Appendix B.

The statistical approaches and methods that will be used to demonstrate compliance during ILAW production are discussed in Section 5. The number of LAW CRV samples (n_S^{CRV}), number of analyses per sample (n_A^{CRV}), and number of level/volume determinations (n_V^{CRV} and n_V^{MFPV}) necessary to provide high confidence in demonstrating compliance with applicable ILAW specifications are discussed in Section 7.

2.4 Compliance for Each MFPV Batch and over a Waste Type

The WTP IHLW and ILAW compliance strategies involve reporting or demonstrating compliance on different bases, depending on the specification. The strategies for several IHLW and ILAW specifications have two aspects (1) demonstrate compliance for each HLW or LAW MFPV batch before it is sent to the MFV and (2) report and demonstrate compliance for IHLW or ILAW that would be produced from MFPV batches corresponding to a specified quantity of HLW or LAW. Assessing compliance for each HLW or LAW MFPV batch before it is sent to the MFV is desirable because there is the option of adding additional GFCs to the MFPV if needed to adjust batches estimated to yield non-compliant glass. However, demonstrating compliance for each MFPV batch only accounts for within-batch uncertainties. On the other hand, reporting and demonstrating compliance over MFPV batches corresponding to specified quantities of HLW or LAW accounts for batch-to-batch variations as well as within-batch uncertainties.

In this report, the term *waste type* is used to refer to a specified quantity of HLW or LAW yielding a given number of MFPV batches (and the HLW or LAW glass that will be produced from those MFPV batches). The concept of a waste type is defined for HLW in the WAPS (DOE 1996) as follows: "Waste type—the waste material fed to each vitrification facility, whose composition and properties will remain relatively constant over an extended period of time during waste form production." Although this definition of waste type is contained in the WAPS for HLW, it is generic enough that it can be applied to LAW compliance also.

The WTP compliance strategy for IHLW addressed in this report (an interim modification of Nelson 2003)[b] specifies HLW waste types as corresponding to the contents of pretreatment HBVs. HBVs are

(a) A chemical composition or radionuclide component of ILAW is considered "reportable" if it must be used to satisfy one or more ILAW specifications, either directly or indirectly through a property-composition model.
(b) See Section 1.0 for a discussion of why this report addresses IHLW PCP Rev. 0 (Nelson 2003) rather than IHLW PCP Rev. 1 (Nelson et al. 2004).

the last vessels in the pretreatment facility that send HLW to the MFPV in the IHLW facility. An HBV will be filled and then emptied with successive transfers to the HLW MFPV before being refilled. In this sense, an HBV is "capped" and serves as an appropriate basis for defining an HLW waste type. An HBV will yield roughly 18 MFPV batches, with an MFPV batch roughly equivalent to 2 to 5 canisters of HLW glass depending on the HLW and waste loading. Hence, an HBV (and thus an HLW waste type) will yield 18 MFPV batches and roughly from 36 to 90 canisters of HLW glass.

The WTP ILAW compliance strategy (Nelson et al. 2003) addressed in this report[(a)] specifies the LAW from a given waste tank as an LAW waste type. The definition of a waste type is different for LAW than HLW for two main reasons. First, the composition of LAW is dominated by sodium with the next most important component being sulfate—hence, the composition of LAW from a waste tank will not vary as significantly as that of HLW. Second, the LAW Concentrate Storage Vessel (CSV) in the pretreatment facility that feeds the LAW CRV will not be "capped" as will the similar HBV for HLW. That is, more LAW will be added to the CSV after every transfer from the CSV to the LAW CRV. Because the composition of the LAW CSV will be continuously (albeit slowly) changing over a waste tank, an LAW tank was chosen by the WTP Project as defining an LAW waste type. Depending on the LAW waste tank, an LAW waste type is expected to yield varying numbers of MFPV batches and containers of LAW glass.

2.5 MFPV Focus of the IHLW and ILAW Compliance Strategies

As described in Sections 2.2 to 2.4, the focus of the WTP compliance strategies during IHLW and ILAW production is the MFPV batch. Compliance quantities (e.g., chemical composition, radionuclide composition, and product durability) and their uncertainties will be calculated for each MFPV batch. Then, for specifications with limits, compliance can be demonstrated for each MFPV batch before it is transferred to the MFV. Variations of the calculated compliance quantities and their uncertainties for MFPV batches corresponding to a waste type will be accounted for in demonstrating compliance over a waste type.

The "MFPV batch" approach to demonstrating compliance over a waste type has the disadvantage of not accounting for the reductions in variation resulting from (1) mixing each MFPV batch with the heel of the previous MFPV batch in the MFV and (2) mixing IHLW MFV batches in the IHLW melter and ILAW MFV batches in the ILAW melter. Hence, the canister-to-canister variation of compliance quantities for IHLW or ILAW corresponding to a specified quantity of HLW or LAW may be considerably less than the MFPV batch-to-batch variation. However, to take advantage of this reduction in variation, it would be necessary to model IHLW and ILAW composition that would result from mixing in the IHLW and ILAW MFVs and melters. The Defense Waste Processing Facility (DWPF), in developing their compliance strategy, investigated three approaches for modeling glass composition through the melter. However, none of the three approaches could accurately predict glass composition canister-by-canister (personal communication). Hence, DWPF adopted a Slurry Mix Evaporator (SME) based compliance strategy as described in the DWPF Waste Form Compliance Plan (Barnes 2003), which is analogous to the WTP's current MFPV-based compliance strategy for both IHLW and ILAW.

(a) See Section 1.0 for a discussion of why this report addresses ILAW PCP Rev. 0 (Nelson et al. 2003) rather than ILAW PCP Rev. 1 (Westsik et al. 2004).

The WTP Project has left open the possibility of switching to an alternative approach for compliance over a waste type if (1) the reduction in estimated variation in IHLW and ILAW compliance quantities would have significant benefits and (2) glass composition through the HLW and LAW melters could be accurately modeled. In the meantime, the MFPV-based compliance strategy over a waste type is conservative and avoids making the compliance equations (see Appendices A and B) even more complicated by including models for composition between the MFPV and the melter at any given point in time.

3.0 Approaches for Implementing Statistically Based IHLW and ILAW Compliance Strategies

The WTP IHLW and ILAW compliance strategies are statistically based for several IHLW and ILAW specifications. Statistically based strategies were chosen by the WTP Project in cases where:

- The specification requires quantifying and reporting (in qualification documentation and/or in production records) variations or uncertainties in compliance quantities (e.g., chemical composition, radionuclide composition, and waste loading).
- It was considered desirable to quantify and report (in qualification documentation and/or in production records) variations or uncertainties in compliance quantities (e.g., chemical composition, radionuclide composition, and waste loading).
- Compliance quantities may have the chance of approaching limiting values given in specifications. In such cases, a statistically based compliance strategy accounts for applicable variations and uncertainties in demonstrating that a compliance quantity is within its limit.

The general statistical approaches used to develop the statistically based compliance strategies presented later in the report are introduced in the following subsections. Section 3.1 introduces the confidence interval approach for demonstrating each MFPV batch is compliant. Section 3.2 introduces the tolerance interval approach for demonstrating glass made from an HLW or LAW waste type is compliant. Section 3.3 introduces the equations used to calculate basic compliance quantities. Section 3.4 introduces the approaches for assessing uncertainties and numbers of samples, analyses, and other process measurements for each MFPV batch. The approach for IHLW is discussed in Section 3.4.1, while the approach for ILAW is discussed in Section 3.4.2. Section 3.5 introduces the approach used to assess variation over multiple MFPV batches and numbers of samples, analyses, and other process measurements.

3.1 Confidence Interval Approach for Single-Batch Compliance

As discussed in Section 2.4, some compliance strategies involve demonstrating compliance for IHLW or ILAW corresponding to each HLW or LAW MFPV batch. A single HLW or LAW MFPV batch will have a corresponding "true" average glass composition as well as "true" average values of compliance quantities, such as chemical composition, radionuclide composition, and PCT releases. The true, average glass composition can only be estimated with uncertainty via process sampling, chemical analysis, and other process measurements (e.g., volume) according to the IHLW or ILAW compliance strategy summarized in Section 2.2 or 2.3, respectively. Similarly, property-composition models used to predict glass properties (e.g., PCT releases) as functions of glass composition are also subject to uncertainty.

Statistical CIs are the appropriate type of statistical statement to make when estimating the true average of a compliance quantity. A *CL% confidence interval* (CL% CI) provides CL% (confidence

level) confidence that the CI contains the true average compliance quantity.[(a)] A symmetric two-sided CL% CI has the generic form

$$CL\%\ CI = Estimate \pm CL\%\ Multiplier \times SD(Estimate) \tag{3.1}$$

where *Estimate* represents the estimate of the true mean compliance quantity for a single MFPV batch, *SD*(*Estimate*) represents the standard deviation of *Estimate*, and *CL% Multiplier* represents the statistical distribution percentile value appropriate to provide CL% confidence that *CL% CI* contains the true mean compliance quantity[(a)]. In cases where only a one-sided CL% lower confidence interval (CL% LCI) or a one-sided CL% upper confidence interval (CL% UCI) is required, only the minus or plus in Eq. (3.1) is used along with the appropriate change from a two-sided to one-sided value of the CL% Multiplier. Specific implementations of two-sided and one-sided CIs are presented in appropriate subsections of Sections 4 and 5.

The standard concept of a CL% CI is applicable for compliance quantities that do not involve property-composition models. For any compliance quantity calculated using a property-composition model, there are uncertainties associated with the model and with any estimated glass composition substituted into the model (see Section A.3 of Appendix A). Statistical theory for models fitted to data by least squares regression (Montgomery et al. 2001) provides a formula for CIs on model predictions. Standard CL% CI formulas provide for quantifying the uncertainty in predicted property values resulting from glass-composition uncertainty. In this report, CL% one-sided *upper combined confidence intervals* (CL% UCCIs) are used to account for both model uncertainty and glass-composition uncertainty in model-predicted glass properties. Upper intervals are used because all limiting specifications contain upper limits. The specifics of CL% UCCIs for compliance with different IHLW and ILAW specifications are presented in the relevant subsections of Sections 4 and 5, but they all have the generic form

$$\begin{aligned} CL\%\ UCCI\ &= Estimate\ via\ Property\text{-}Composition\ Model \\ &\quad + CL\%\ Composition\ Uncertainty\ Multiplier \times SD(Composition\ Uncertainty) \\ &\quad + CL\%\ Model\ Uncertainty\ Multiplier \times SD(Model\ Uncertainty), \end{aligned} \tag{3.2}$$

where the two SDs are both expressed in the same units as the property (or some mathematical transformation thereof, such as a logarithmic transformation) predicted by the property-composition model.

3.2 Tolerance Interval Approach for Multiple-Batch Compliance

As discussed in Section 2.4, some compliance strategies involve demonstrating compliance for IHLW or ILAW that would be made from a given number of HLW or LAW MFPV batches corresponding to a specified quantity of HLW or LAW (e.g., a waste type). For multiple MFPV batches, there is batch-to-batch variation (due to variation in the waste feed composition) as well as within-batch uncertainties due

(a) This statement is somewhat of a simplification. In practice, a CL% CI calculated from uncertain data will either contain the true average compliance quantity or not. For conceptual repeated collection of the uncertain data and calculation of a CL% CI, in the long run, the CL% of the calculated CIs would contain the true average compliance quantity. This is the proper interpretation of the CL% confidence for an CL% CI.

to sampling, chemical analyses, and other process measurements. Because there is actual variation in a compliance quantity over multiple MFPV batches (and the IHLW or ILAW that would be produced from them), an X%/Y% statistical tolerance interval (X%/Y% TI) is the appropriate type of statistical statement to make. An X%/Y% TI provides X% confidence that at least Y% of the IHLW or ILAW that would be produced from the multiple MFPV batches will have compliance quantity values inside the TI.[(a)] The general form of a symmetric two-sided X%/Y% TI is given by

$$\text{X\%/Y\% TI} = \tilde{\mu} \mp k(X,Y)\tilde{\sigma} \tag{3.3}$$

where $\tilde{\mu}$ is an estimate of the mean compliance quantity over the IHLW or ILAW corresponding to a waste type, *k(X, Y)* is a TI multiplier that provides the desired X% confidence and Y% coverage of the distribution of the compliance quantity over a waste type, and $\tilde{\sigma}$ is an estimate of the uncertainty in $\tilde{\mu}$. If a one-sided upper tolerance interval (UTI) is desired, only the "+" half of the formula in Eq. (3.3) is used. If a one-sided lower tolerance interval (LTI) is desired, only the "-" half of the formula in Eq. (3.3) is used.

Although the choice of values of X and Y in a X%/Y% TI are a matter of policy for the WTP Project to decide, it is recommended that X and Y have values between 90 and 100% (they can never equal 100% because of variation and uncertainty). With X and Y values in the 90 to 100% range, an X%/Y% TI will provide high (X%) confidence that a high (Y%) percentage of the IHLW or ILAW glass corresponding to the multiple MFPV batches have compliance quantities within the TI or satisfying a specification limit. The traditional approach of applying TIs involves selecting both X and Y (e.g., X = 95 and Y = 95) and calculating an X%/Y% TI to verify that its value satisfies the IHLW or ILAW limits of a given specification. However, it is more informative to determine the values of X and Y achieved corresponding to the specification limit. For example, perhaps it can be stated with 99% confidence that 99.9% of the IHLW produced from a given waste type satisfies the limits for a given IHLW specification. See Piepel and Cooley (2002) for further discussion and examples of TIs in general and the details (in their Section 3.8) on how to calculate achieved values of X and Y.

The question arises why it is necessary during IHLW and ILAW production to apply X%/Y% TIs to demonstrate compliance over multiple MFPV batches corresponding to a waste type when CL% CIs will have already been used to demonstrate the compliance of glass that will be made from each IHLW or ILAW MFPV batch. In calculating CL% CIs for compliance quantities and comparing them to specification limits, there is some statistical probability of incorrectly deciding that a given MFPV batch will make compliant glass when in fact the glass is not compliant. The probability of at least one such wrong decision increases with the number of decisions made (for MFPV batches corresponding to a waste type). The X%/Y% TI approach makes a single statistical statement about all MFPV batches corresponding to a waste type, ensuring that there is high confidence (low chance of wrong decision) that a high percentage of glass made from MFPV batches corresponding to a waste type will satisfy compliance quantity limits. Further, the X%/Y% TI accounts for variation in compliance quantities over

(a) This statement is somewhat of a simplification. In practice, an X%/Y% TI calculated from data subject to variation and uncertainty either will or will not contain at least Y% of the distribution of a compliance quantity over a waste type. Consider conceptual repeated collection of the data subject to variation and uncertainty. Then, for each conceptual repetition, consider calculating an X%/Y% TI. In the long run, X% of the calculated TIs would contain at least Y% of the distribution of the compliance quantity over a waste type. This is the proper interpretation of the X% confidence for an X%/Y% TI.

MFPV batches corresponding to a waste type, whereas the CL% CIs calculated for each MFPV batch do not. In summary, CL% CIs and X%/Y% TIs play complementary roles in demonstrating compliance during IHLW and ILAW production operations. The CL% CIs provide for demonstrating compliance for each MFPV batch while accounting for within-batch uncertainties. The X%/Y% TIs provide for demonstrating with high confidence that a high percentage of IHLW or ILAW produced from multiple MFPV batches is compliant with limiting specifications.

3.3 Equations for Calculating Compliance Quantities

Before the WTP compliance strategies (including, but not limited to, the statistically based strategies) can be implemented, equations are needed to calculate the basic compliance quantities associated with the IHLW and ILAW specifications. Equations to calculate several IHLW compliance quantities are presented in Appendix A, while equations to calculate several ILAW compliance quantities are presented in Appendix B. Appendices A and B include equations to calculate compliance quantities corresponding to all IHLW and ILAW specifications for which the WTP compliance strategy is statistically based. In a few cases, equations are also given for specifications where the WTP compliance strategy is not statistically based. For example, the equations to calculate ILAW waste loading had been developed before the WTP decision that a statistically based compliance strategy for waste loading compliance was no longer necessary. Because the ILAW waste loading equations were developed, they are presented in Section B.6 of Appendix B. Equations to calculate HLW loading had also been developed, but under the older compliance strategy in place when the IHLW vitrification facility still contained CRVs. Because those equations are no longer applicable, they are not presented in Appendix A.

The fundamental compliance quantity equations are for IHLW and ILAW glass compositions corresponding to completed MFPV batches (i.e., when they are ready for transfer to the MFV). These glass compositions are expressed as mass fractions of oxides or halogens for both non-radionuclides and radionuclides where the mass fractions of all oxides and halogens (non-radioactive as well as radioactive) must sum to unity. These equations are fundamental in that equations for other compliance quantities are based on the glass-composition equations. The ILAW compliance strategy (see Section 2.2) uses more process information to calculate glass composition than does the IHLW compliance strategy (see Section 2.3). The IHLW compliance strategy involves using only chemical analyses of MFPV samples (after GFCs have been added) to calculate HLW glass composition. On the other hand, the ILAW compliance strategy uses chemical analyses of CRV samples, level/volume measurements of the CRV and MFPV before and after transfers and GFC additions, and measured weights of GFCs added to the MFPV to calculate LAW glass composition. Hence, the equations for calculating HLW glass composition are relatively simple, whereas the equations for calculating LAW glass composition involve more complicated mass balances.

3.4 Approaches for Assessing Uncertainties and Numbers of Samples, Analyses, and Other Measurements for Single MFPV Batches

As discussed in Section 3.3, the equations for calculating ILAW compliance quantities are more complicated compared to the relatively simple nature of the equations for calculating IHLW compliance

quantities. The relatively simple nature of the IHLW equations means that closed-form (1) error (variance) propagation methods can be used to propagate single-MFPV-batch uncertainties through the equations, (2) statistical formulas for CL% CIs and CL% UCCIs can be used, and (3) calculations for numbers of samples, analyses per sample, and measurements can be performed. The more complicated nature of the equations for ILAW compliance quantities indicates that direct, closed-form methods cannot be used to quantify uncertainties and determine numbers of samples, analyses, and measurements. Rather, a Monte Carlo simulation approach must be used to propagate the various LAW vitrification process uncertainties and thus estimate the total uncertainties in compliance quantities for each MFPV batch. The Monte Carlo simulation approach also provides for obtaining CL% CIs and CL% UCCIs to demonstrate for each MFPV batch that ILAW compliance quantities satisfy their corresponding limits. Finally, the Monte Carlo simulation approach also provides the basis for determining the numbers of samples, analyses per sample, and other measurements required during ILAW production operations.

Estimates of process compositions and uncertainties affecting single MFPV batches were needed for both IHLW and ILAW to (1) assess total uncertainties in compliance quantities for single MFPV batches and (2) perform investigations and provide guidance to the WTP Project on the numbers of process samples, analyses, and other measurements required to meet process control and compliance requirements. The WTP Project provided estimates of process compositions and uncertainties for three waste tanks each of HLW (AY-102, AZ-102, and C-104) and LAW (AP-101, AZ-101, and AN-107). The three LAW waste tanks were selected to represent Envelopes A (AP-101), B (AZ-101), and C (AN-107).[(a)]

For each process variable, two bounding estimates of uncertainty referred to as "low" and "high" were provided by the WTP Project for this work. The goal of the low- and high-case uncertainty values for a given variable was to span the range within which the actual uncertainty (to be determined by subsequent WTP WFQ testing) is likely to fall. The estimates of process compositions and the ranges of uncertainties affecting single MFPV batches provided by the WTP Project are documented and discussed in Appendix C (IHLW) and Appendix D (ILAW).

Section 3.4.1 introduces the statistical error (variance) propagation methods used to (1) quantify uncertainties in IHLW compliance quantities and (2) assess the effects of different numbers of MFPV samples and analyses per MFPV sample on compliance with IHLW specifications. Section 3.4.2 introduces the Monte Carlo simulation approach used to (1) quantify uncertainties in ILAW compliance quantities and (2) assess the effects of different numbers of CRV samples, analyses per CRV sample, and other ILAW process measurements on compliance with ILAW specifications. The details of these methods and approaches for individual IHLW and ILAW specifications are presented in Chapters 4 and 5, respectively. The results of applying these methods are presented in Sections 6 (IHLW) and 7 (ILAW).

(a) Envelope A—LAW feed with lower concentrations of sulfate and varying potassium concentrations.
(b) Envelope B—LAW feed with higher ^{137}Cs and sulfate concentrations.
(c) Envelope C—LAW feed with organically complexed Sr and TRU requiring removal to meet specifications.

3.4.1 Approach for Assessing Uncertainty and Number of Samples and Analyses for Single IHLW MFPV Batches

During IHLW production operations, IHLW reporting and limiting specifications will be satisfied based only on analyzing samples from the IHLW MFPV. Hence, only mixing/sampling[(a)] and analytical uncertainties must be accounted for in statistically based compliance methods.

As discussed in Section 3.4, standard closed-form error (variance) propagation and statistical interval formulas will be used to assess uncertainties affecting the composition in a single HLW MFPV batch. The closed-form statistical interval formulas also provide the basis for assessing the effects of (1) different numbers of MFPV samples and analyses per sample and (2) different magnitudes of mixing/sampling and analytical uncertainties. Section 3.4.1.1 provides a brief overview of error (variance) propagation formulas. Section 3.4.1.2 discusses the approach used to assess the effects of number of MFPV samples, number of analyses per MFPV sample, and mixing/sampling and analytical uncertainties. Specific implementations of these methods for individual specifications are discussed in applicable subsections of Section 4. The results of investigations and example calculations using these methods are presented in applicable subsections of Section 6.

3.4.1.1 Overview of Error (Variance) Propagation

The quantities of interest for compliance are functions of several process variables, and each of these variables contributes to the overall uncertainty observed. To obtain an estimate of the uncertainty for the quantity of interest, it is necessary to apply error (variance) propagation techniques to the mathematical formula that relates the compliance quantity and the process variables. In general, if the relationship between a compliance quantity and the processing variables can be described as $Y = f(X_1, \ldots, X_q)$, where Y is the compliance quantity and $X_1, \ldots, X_q$ represent the process variables, then the variance of Y can be obtained by:

$$s_y^2 = \left(\frac{\partial Y}{\partial X_1}\right)^2 s_1^2 + \cdots + \left(\frac{\partial Y}{\partial X_q}\right)^2 s_q^2 + \left(\frac{\partial Y}{\partial X_1}\right)\left(\frac{\partial Y}{\partial X_2}\right) s_{12}^2 + \left(\frac{\partial Y}{\partial X_1}\right)\left(\frac{\partial Y}{\partial X_3}\right) s_{13}^2 + \cdots + \left(\frac{\partial Y}{\partial X_{q-1}}\right)\left(\frac{\partial Y}{\partial X_q}\right) s_{q-1,q}^2 \quad (3.4)$$

where s_i^2 represents the variance of the i^{th} variable and s_{ij}^2 is the covariance between the measurements of variables X_i and X_j. In many cases, it is possible to assume that the process variables are uncorrelated, making the s_{ij}^2 terms equal to zero, simplifying the expression for the variance of Y considerably (see for example Hines et al. [2002] or Hahn and Shapiro [1968, Section 7.2] for a more complete description). The specific formula for the variance of the product of two random variables has been presented by Goodman (1960) and is used in some instances in this report.

(a) See the entry for "mixing/sampling uncertainty" in the Acronyms, Terms, and Abbreviations section at the front of the report.

3.4.1.2 Assessment of Number of Samples, Number of Analyses, and Magnitudes of Uncertainties

To better understand (1) the total uncertainty associated with the IHLW compliance quantities, (2) how numbers of MFPV samples and analyses per sample affect total uncertainty, and (3) how magnitudes of mixing/sampling and analytical uncertainties affect total uncertainty in compliance quantities, an experimental design was implemented using variance propagation methods coupled with formulas for statistical CIs. The experimental design was intended to (1) determine the effects of the following six factors on the total uncertainty in compliance quantities at the IHLW MFPV and (2) provide a basis for the WTP Project to decide on the numbers of IHLW MFPV samples and analyses per sample needed during production:

- HLW tank
- statistical percent confidence level (CL%)
- mixing/sampling %RSD (percent relative standard deviation) in the concentration of the j^{th} element in a MFPV batch [$\%RSD_S(c_j^{MFPV})$]
- analytical %RSD in the concentration of the j^{th} element in a MFPV batch [$\%RSD_A(c_j^{MFPV})$]
- number of samples per MFPV batch (n_S^{MFPV})
- number of analyses per MFPV sample (n_A^{MFPV}).

The levels used for each of these factors are shown in Table 3.1.

Actual data were used from three HLW tanks (AY-102, AZ-102, and C-104) representing some of the initial tanks to be processed by the WTP. The MFPV nominal concentration data for each HLW tank are listed in Table C.1 (chemical composition analytes) and Table C.2 (radionuclides) of Appendix C. MFPV mixing/sampling uncertainties (%RSD values for low and high case) and MFPV analytical uncertainties (%RSD values for low and high case) are also listed in Table C.1 for chemical composition analytes and Tables C.2 and C.4 for radionuclides.

Table 3.1. Factors and Levels Used in IHLW Variance Propagation and Confidence Interval Investigations

HLW Tank	% Confidence	IHLW MFPV Mixing/Sampling %RSD[a]	IHLW MFPV Analytical %RSD[b]	Total Number of Analyses[c]
AY-102 AZ-102 C-104	90% 95%	Low High	Low High	1–30

(a) Low- and high-case values for HLW MFPV mixing/sampling uncertainty are listed in Table C.1 of Appendix C for chemical composition analyte concentrations and in Table C.2 for radionuclide concentrations.

(b) Low- and high-case values for HLW MFPV analytical uncertainty are given in Table C.1 of Appendix C for chemical composition analyte concentrations and in Table C.4 for radionuclide concentrations.

(c) Total number of analyses is equal to $n_S^{MFPV} \times n_A^{MFPV}$. All combinations were investigated up to a total of 30, using 1 to 3 analyses per sample.

An experimental test design (for a computer experiment) was used to run these factors at all combinations of levels, as shown in Table 3.2. This led to data analysis that determined which factors were contributing most to the uncertainty of chemical composition, radionuclide composition, and other compliance quantities. The results were used to assess how changing the numbers of samples and/or analyses per sample were contributing to the uncertainty of chemical composition, radionuclide composition, and other compliance quantities. The results were also used to assess (1) how changing the numbers of samples and/or analyses per sample would effectively decrease (through averaging) the uncertainty in compliance quantities and (2) how many samples and analyses would be needed in the compliance strategy during production.

Table 3.2. Experimental Design Used to Investigate Effects of Factors on Total Uncertainty and Compliance of IHLW Compliance Quantities

HLW Tank	% Confidence	IHLW MFPV Mixing/Sampling %RSD[a]	IHLW MFPV Analytical %RSD[b]	Total Number of Analyses[c]
AY-102	90	Low	Low	1–30
AY-102	90	Low	High	1–30
AY-102	95	Low	Low	1–30
AY-102	95	Low	High	1–30
AY-102	90	High	Low	1–30
AY-102	90	High	High	1–30
AY-102	95	High	Low	1–30
AY-102	95	High	High	1–30
AZ-102	90	Low	Low	1–30
AZ-102	90	Low	High	1–30
AZ-102	95	Low	Low	1–30
AZ-102	95	Low	High	1–30
AZ-102	90	High	Low	1–30
AZ-102	90	High	High	1–30
AZ-102	95	High	Low	1–30
AZ-102	95	High	High	1–30
C-104	90	Low	Low	1–30
C-104	90	Low	High	1–30
C-104	95	Low	Low	1–30
C-104	95	Low	High	1–30
C-104	90	High	Low	1–30
C-104	90	High	High	1–30
C-104	95	High	Low	1–30
C-104	95	High	High	1–30

(a) Low and high values for HLW MFPV mixing/sampling uncertainty are listed in Table C.1 of Appendix C for chemical composition analyte concentrations and in Table C.2 for radionuclide concentrations.

(b) Low and high values for HLW MFPV analytical uncertainty are given in Table C.1 of Appendix C for chemical composition analyte concentrations and in Table C.4 for radionuclide concentrations.

(c) Total number of analyses is equal to number of samples per MFPV batch × number of analyses per MFPV sample. All combinations were investigated up to a total of 30, using 1 to 3 analyses per sample.

3.4.2 Approach for Assessing Uncertainty and Numbers of Samples, Analyses, and Other Measurements for Single ILAW MFPV Batches

To better understand (1) the total uncertainty associated with the ILAW compliance quantities, (2) how numbers of samples, analyses, and other process measurements affect total uncertainty, and (3) how magnitudes of contributing process uncertainties affect total uncertainty in compliance quantities, an experimental design was implemented using Monte Carlo simulation. A brief overview of Monte Carlo simulation is provided in Section 3.4.2.1. The experimental design implemented via the Monte Carlo simulation approach is described in Section 3.4.2.2.

3.4.2.1 Overview of Monte Carlo Simulation

Monte Carlo simulation involves assuming statistical distributions for random (i.e., uncertain) variables, generating random realizations from these distributions, and performing calculations of interest using the random realizations of the random variables. In this report, the calculations of interest are various compliance quantities (e.g., ILAW chemical and radionuclide compositions, or concentrations of radionuclides in ILAW containers). Random variables of interest involve any process steps or measurements subject to uncertainty (e.g., mixing/sampling, or analytical).

3.4.2.2 Experimental Design to Investigate Effects of Various Factors on the Numbers of Samples, Analyses, and Other Measurements for Single ILAW MFPV Batches

The experimental design discussed in this section was intended to (1) determine the effects of the following nine factors on the total uncertainty in compliance quantities at the ILAW MFPV and (2) provide a basis for the WTP Project to decide on the numbers of ILAW process samples, analyses per sample, and other measurements needed during production:

- LAW tank and waste envelope
- mixing/sampling %RSD in the concentration of the j^{th} element in a CRV batch [$\%RSD_S(c_j^{MFPV})$]
- analytical %RSD in the concentration of the j^{th} element in a CRV batch [$\%RSD_A(c_j^{MFPV})$]
- GFC composition uncertainty, represented by the standard deviation in the mass fraction of the j^{th} component (oxide or halogen) in the k^{th} GFC [$SD(G_{jk}^{GFC})$]
- GFC mass uncertainty, represented by the standard deviation of the mass of the k^{th} GFC added to a MFPV batch. This uncertainty includes uncertainties due to batching, weighing, and transfers of GFCs [$SD(a_k^{GFC})$]
- volume uncertainties in the CRV and MFPV. The magnitudes of these uncertainties will depend on the level of contents in a vessel, but a generic notation is used for now (SD_V^{CRV} and SD_V^{MFPV})
- number of samples per CRV batch (n_S^{MFPV})

- number of analyses per CRV sample (n_A^{MFPV})
- number of volume determinations of the CRV and MFPV before and after transfers (n_V^{CRV} and n_V^{MFPV}).

The levels used for each of these factors are shown in Table 3.3. Note that the percent confidence level (CL%) does not appear in the above list or in Table 3.3 because it was not a factor varied in the Monte Carlo simulation study, but rather a factor considered in using the Monte Carlo simulation results.

Table 3.3. Factors and Levels Used in ILAW Monte Carlo Simulations

Waste Envelope	CRV Mixing/Sampling %RSD[a]	CRV Analytical %RSD[b]	GFC Composition Uncertainty[c]	GFC Batching Uncertainty[d]	Volume Uncertainty[e]	Number of Samples per CRV Batch	Number of Analyses per CRV Sample	Number of Volume Determinations
A (AP-101) B (AZ-101) C (AN-107)	Low High	Low High	Low High	Low High	Low High	1	1, 2, 3	1 3
						2	1, 2, 3	
						3	1, 2	
						4	1	
						5	1, 2	
						6	1	
						7	2	
						8	1	
						10	1	

(a) Low- and high-case values for LAW CRV mixing/sampling uncertainty are listed in Table D.1 for chemical composition analyte concentrations and in Table D.2 for radionuclide concentrations.
(b) Low- and high-case values for LAW CRV analytical uncertainty are given in Table D.1 for chemical composition analyte concentrations and in Table D.4 for radionuclide concentrations.
(c) Low- and high-case values for GFC composition uncertainties are given in Table D.7. Specifically, the nominal values and ranges in Table D.7 were used to define triangular distributions from which samples were taken in the Monte Carlo simulation.
(d) Low- and high-case values for GFC batching uncertainties are given in Table D.6.
(e) Low- and high-case values for volume uncertainties are given in Table D.9.

Actual data were used from three LAW tanks representing each of the three LAW waste envelopes: A (AP-101), B (AZ-101), and C (AN-107). The nominal CRV concentration data for each LAW tank are listed in Table D.1 (chemical composition analytes) and Table D.2 (radionuclides) of Appendix D. CRV mixing/sampling uncertainties (%RSD values for low and high case) are listed in Table D.1 (chemical composition analyte concentrations) and Table D.2 (radionuclide concentrations). CRV analytical uncertainties (%RSD values for low and high case) are listed in Table D.1 (chemical composition analyte

concentrations) and Table D.4 (radionuclide concentrations). Table D.5 contains the nominal masses of the GFCs added to the LAW MFPV for each LAW tank. Table D.6 contains the low- and high-case uncertainties associated with the masses of GFCs added to the ILAW MFPV shown in Table D.5. GFC composition data and corresponding low- and high-case uncertainties are found in Tables D.7 and D.8. Table D.9 contains the nominal LAW CRV and MFPV volumes as well as the low- and high-case uncertainties (SDs).

Numbers of LAW CRV samples and analyses were varied such that there were 15 different combinations tested. Table 3.3 shows that when 1 or 2 samples per CRV batch were taken, there were 1, 2, or 3 analyses per sample, which accounted for 6 of the 15 combinations. The other 9 combinations are listed in Table 3.3. The 1/1 case (1 sample with one analysis) was included as a baseline to measure the improvement when sampling more than once and/or analyzing each sample more than once.

A full-factorial design of the factors and levels in Table 3.3 would have resulted in 2880 runs ($3 \times 2^6 \times 15$). A full-factorial design is one in which all possible combinations of levels for each factor is run. For this analysis, there are six factors with two levels each, one factor with 15 levels and one factor with 3 levels, resulting in 2880 runs that would contain all possible combinations. To reduce the amount of time needed to perform a Monte Carlo simulation with this many runs, a half-replicate fractional-factorial experiment was designed such that only 1440 runs would be necessary ($3 \times 2^{6-1} \times 15$). This fractional factorial experiment results in using only half of all the possible combinations of factors and levels. Using a fractional factorial design results in each effect being confounded (masked) by another effect. In this case, the main effect of each of the six factors with only two levels is confounded with the five-factor interaction of the remaining factors. Also, each two-factor interaction is confounded with a four-factor interaction. Because four- and five-factor interactions are rarely significant or meaningful, this confounding structure should still be effective in determining significant main effects and two-factor interaction. For each of the 15 different combinations of numbers of samples and analyses-per-sample tested and each of the three tanks, the other six factors were varied such that there were 32 different runs performed in the simulation. Table 3.4 shows the factor levels tested for each of the 32 runs of the six two-level factors.

Table 3.4. Test Cases Used in the ILAW Fractional Factorial Design for the Six Two-Level Factors Studied in the ILAW Monte Carlo Investigation for each Combination of Waste Envelope, Number of Samples per CRV Batch, and Number of Analyses per CRV Sample, as defined in Table 3.3[a]

Run	CRV Sampling %RSD [b]	CRV Analytical %RSD [b]	GFC Composition Uncertainty [b]	GFC Batching Uncertainty [b]	Volume Uncertainty [b]	Number of Volume Determinations
1	Low	Low	Low	Low	Low	1
2	Low	Low	Low	Low	High	3
3	Low	Low	Low	High	Low	3
4	Low	Low	Low	High	High	1
5	Low	Low	High	Low	Low	3
6	Low	Low	High	Low	High	1
7	Low	Low	High	High	Low	1
8	Low	Low	High	High	High	3
9	Low	High	Low	Low	Low	3
10	Low	High	Low	Low	High	1
11	Low	High	Low	High	Low	1
12	Low	High	Low	High	High	3
13	Low	High	High	Low	Low	1
14	Low	High	High	Low	High	3
15	Low	High	High	High	Low	3
16	Low	High	High	High	High	1
17	High	Low	Low	Low	Low	3
18	High	Low	Low	Low	High	1
19	High	Low	Low	High	Low	1
20	High	Low	Low	High	High	3
21	High	Low	High	Low	Low	1
22	High	Low	High	Low	High	3
23	High	Low	High	High	Low	3
24	High	Low	High	High	High	1
25	High	High	Low	Low	Low	1
26	High	High	Low	Low	High	3
27	High	High	Low	High	Low	3
28	High	High	Low	High	High	1
29	High	High	High	Low	Low	3
30	High	High	High	Low	High	1
31	High	High	High	High	Low	1
32	High	High	High	High	High	3

(a) There were 15 different combinations of number of samples and number of analyses tested, along with 3 different waste envelopes, each containing 32 runs in the experiment. This resulted in 1440 runs (15 × 3 × 32).

(b) See the footnotes of Table 3.3 for the table references where the low- and high-case values for each factor may be found.

3.5 Approach to Assess Variation over Multiple MFPV Batches and Numbers of Samples, Analyses, and Other Measurements

As discussed in Section 3.2, X%/Y% TIs will be used to demonstrate compliance (for IHLW or ILAW corresponding to an HLW or LAW waste type) with certain IHLW and ILAW specifications that contain limits on compliance quantities. Work similar to that described in Section 3.4, except with the focus of using X%/Y TIs to demonstrate compliance over a waste type, has already been conducted and reported by Piepel and Cooley (2002).

At the time of the Piepel and Cooley (2002) work, both the IHLW and ILAW compliance strategies involved analyzing samples from a single location in the IHLW and ILAW processes. In the IHLW case, the strategy back then, as it is again now after recent changes, involved analyzing MFPV samples. Hence, the work by Piepel and Cooley (2002) is directly applicable to the current IHLW compliance strategy. In the ILAW case, the strategy back then was analyzing glass shard samples collected from the top of ILAW containers. While the current ILAW compliance strategy (see Section 2.3) is far removed from the previous one, the work of Piepel and Cooley (2002) can be adapted to the current strategy. The approach to implementing the current ILAW compliance strategy will result in an estimated glass composition (and corresponding SD for each glass component) for each ILAW MFPV batch. The X%/Y% TI method of Piepel and Cooley (2002) can be adapted to use these inputs for the ILAW situation. The specifics of this adaptation are discussed in Section 5.4.4.

Work to quantify variations in compliance IHLW and ILAW quantities over the course of HLW and LAW waste types is being conducted in FY 2005 (Piepel and Heredia-Langner 2003). The results of that work will be used in a future update of this report.

4.0 IHLW Compliance Strategies and Statistical Implementation Methods by Specification

This section describes the WTP IHLW compliance strategies and statistical implementation methods for each WAPS (DOE-EM 1996) or WTP contract (DOE-ORP 2003) specification having a statistical aspect to the compliance strategy. IHLW specifications not having statistical aspects to the corresponding WTP compliance strategies are not listed or discussed.

4.1 Compliance Approach and Methods for IHLW WAPS Specification 1.1.2: Chemical Composition During Production

Section 4.1.1 lists the applicable WAPS Specification 1.1.2. Section 4.1.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Sections 4.1.3 and 4.1.4 present the statistical methods that will be used to implement the statistical aspects of the compliance strategy.

4.1.1 WAPS Specification 1.1.2: Chemical Composition During Production

> *In the Production Records, the Producer shall report the oxide composition of the waste form. The reported composition shall include all elements, excluding oxygen, present in concentrations greater than 0.5 percent by weight of the glass, for each waste type. The Producer shall describe the method to be used for compliance in the WCP. An estimate of the error of the reported composition and the basis for the estimate shall be reported in the WQR.*

4.1.2 Statistical Aspects of the IHLW Compliance Strategy for WAPS 1.1.2

The following items describe the statistical and related aspects of the IHLW compliance strategy for WAPS Specification 1.1.2 (see the IHLW PCP, Nelson 2003) that are addressed in this report.[(a)]

Item 1: Determine the numbers of samples, chemical analyses per sample, and other process measurements necessary to adequately estimate IHLW chemical composition that would be produced from each MFPV batch.

Item 2: Develop equations for calculating the means and SDs of reportable glass components over the chemical-composition determinations of IHLW accumulated over the course of processing a waste type. The equations for SDs must account for applicable sources of variation and uncertainty.

The statistical methods to implement these aspects of the WTP IHLW compliance strategy for WAPS Specification 1.1.2 are discussed in Sections 4.1.3 and 4.1.4, respectively.

(a) See Section 1.0 for a discussion of why this report addresses WAPS specifications and IHLW PCP Rev. 0 (Nelson 2003) rather than IHLW PCP Rev. 1 (Nelson et al. 2004).

4.1.3 Statistical Method for Determining the Number of Samples and Analyses per Sample to Estimate IHLW Chemical Composition for an MFPV Batch

During IHLW production operations, the chemical composition will be calculated based on chemical analyses of samples from the MFPV. The applicable mass-balance equations for calculating IHLW chemical composition are given in Section A.1 of Appendix A. The balance of this subsection describes the statistical method to address Item 1 in Section 4.1.2.

Section 3.4.1 describes the general approach for assessing the impacts of the following factors:

- number of samples per MFPV batch (n_S^{MFPV})
- number of analyses per MFPV sample (n_A^{MFPV})
- mixing/sampling %RSD in the concentration of the j^{th} element in an MFPV batch [$\%RSD_S(c_j^{MFPV})$]
- analytical %RSD in the concentration of the j^{th} element in a MFPV batch [$\%RSD_A(c_j^{MFPV})$]
- statistical percent confidence level (CL%)
- IHLW produced from three HLW tanks (AY-102, AZ-102, and C-104)

on the total uncertainty in estimating IHLW chemical composition (mass fractions of oxides or halogens) for each MFPV batch. It is necessary at this time to consider a range of values for MFPV mixing/sampling and analytical uncertainties (as discussed in Section 3.4.1) because final estimates have not yet been produced by the WTP Project. A future update of this report will use final estimates of MFPV mixing/sampling and analytical uncertainties to provide a more definitive final recommended number of MFPV samples and number of chemical analyses per MFPV sample for estimating IHLW chemical composition.

To assess the total uncertainty in estimating IHLW chemical composition for a given MFPV batch, the percent relative half-width (%RHW) of a two-sided CL% CI (see Section 3.1) on the mass fraction of each IHLW component (oxide or halogen) is used. Piepel, Bates, and Gilbert (2001) discuss this uncertainty calculation in further detail. The formula for a %RHW, expressed as a percentage of the nominal value (mass fraction) of the j^{th} IHLW component (oxide or halogen) in an MFPV batch, is given by

$$\%RHW_{CL\%}(g_j^{MFPV}) = t_{1-\alpha/2,n_S^{MFPV}-1}\left[\frac{\left(\%RSD_S(g_j^{MFPV})\right)^2}{n_S^{MFPV}} + \frac{\left(\%RSD_A(g_j^{MFPV})\right)^2}{n_S^{MFPV}\,n_A^{MFPV}}\right]^{1/2} \qquad (4.1.1)$$

where

$\%RHW_{CL\%}(g_j^{MFPV})$ = percent relative half-width of a two-sided CL% CI on the mean mass fraction of the j^{th} component in IHLW corresponding to a MFPV batch (%)

$100(1-\alpha/2)$ = CL% = percent confidence for a two-sided CI (e.g., 90% when α = 0.10) (%)

$t_{1-\alpha/2, n_S^{MFPV}-1}$ = 100(1 – α/2) percentile of a Student's t-distribution with $n_S^{MFPV} - 1$ degrees of freedom

$\%RSD_S(g_j^{MFPV})$ = percent relative standard deviation for mixing/sampling uncertainty in the mass fraction of the j^{th} component of IHLW corresponding to a MFPV batch (%)

$\%RSD_A(g_j^{MFPV})$ = percent relative standard deviation for analytical uncertainty in the mass fraction of the *j*th component of IHLW corresponding to a MFPV batch (%)

n_S^{MFPV} = number of samples per MFPV batch

n_A^{MFPV} = number of analyses per MFPV sample.

In Eq. (4.1.1), note that $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ are used rather than $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ introduced earlier in the section. The difference is that $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ are uncertainties in mass fractions of the j^{th} IHLW component (oxide or halogen) in a MFPV batch, while $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ are uncertainties of analyzed concentrations of the j^{th} element in a MFPV batch. The quantities $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ can be obtained by propagating the uncertainties $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ through Eq. (A.1.3) in Section A.1 of Appendix A. Methodology to perform these propagations is scheduled for development in FY 2005 as part of other work in the Statistical Analysis task of the WTPSP (Piepel and Heredia-Langner 2003). The results of that work will be included and used in a future revision of this report. For the work in this report, a preliminary investigation indicated that propagated values of $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ tend to be close in magnitude to $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ values. Hence, calculations with Eq. (4.1.1) used values of the latter uncertainties as temporary substitutes for the former uncertainties in this version of the report. The next revision will use the appropriate uncertainties.

Equation (4.1.1) can be used to calculate %RHW values for various combinations of the factors described previously in this subsection. The results of such calculations can be used to determine the values of n_S^{MFPV} and n_A^{MFPV} that will provide estimates of glass components within a given percentage (i.e., the %RHW) of the true value with desired confidence (CL%). The results of such calculations are presented in Section 6.1.1.

4.1.4 Equations for Calculating Means and Standard Deviations of IHLW Chemical Composition over a Waste Type

The IHLW compliance strategy for WAPS 1.1.2 involves (1) calculating the IHLW chemical composition for each MFPV batch from analyses of MFPV samples and (2) calculating and reporting means and SDs of the calculated compositions over each HLW waste type. The chemical composition of IHLW corresponding to each MFPV is calculated in terms of mass fractions of J glass components (oxides and halogens). The mass fraction of the j^{th} IHLW component in the i^{th} MFPV batch is denoted by g_{ij}^{MFPV}, $j = 1, 2, \ldots, J$. By the nature of mass fractions, $\sum_{j=1}^{J} g_{ij}^{MFPV} = 1$.

This section presents the formulas for calculating means and SDs of IHLW chemical compositions (mass fractions of oxide and halogen glass components) over the I MFPV batches corresponding to an HLW waste type. Two situations are considered. Section 4.1.4.1 addresses the case of balanced data while Section 4.1.4.2 addresses the case of unbalanced data. The formulas in these subsections address Item 2 of Section 4.1.2.

4.1.4.1 Equations for Calculating Means and Standard Deviations of IHLW Chemical Composition over a Waste Type Using Balanced Data

In this section, we consider "balanced data" that occurs when (1) the same number of samples n_S^{MFPV} are collected from all MFPV batches $i = 1, 2, \ldots, I$ corresponding to an HLW waste type, (2) the same number of analyses n_A^{MFPV} are made for each MFPV sample of each MFPV batch corresponding to an HLW waste type, and (3) the same number of volume determinations n_V^{MFPV} are made for each MFPV batch. When $n_V^{MFPV} = 1$ for all MFPV batches and $n_A^{MFPV} = 1$ for all samples from all MFPV batches, balanced data occur when n_S^{MFPV} is the same for every MFPV batch and the single analysis of each MFPV sample is acceptable.

Section A.1 of Appendix A presents the mass-balance equations for calculating the IHLW chemical composition (in mass fractions) for a single MFPV batch. Specifically, Eq. (A.1.5) in Appendix A gives the formula for $\bar{g}_{ij}^{MFPV}$, the mass fraction of the j^{th} component in IHLW that would be made from the i^{th} MFPV batch averaged over the n_S^{MFPV} samples and n_A^{MFPV} analyses per sample for each MFPV batch. For each component j, formulas are required for the mean and SD of the $\bar{g}_{ij}^{MFPV}$, $i = 1, 2, \ldots, I$ values corresponding to an HLW waste type. Note that the volume of the i^{th} MFPV batch and the number of volume determinations n_V^{MFPV} do not appear in the equation for $\bar{g}_{ij}^{MFPV}$. This is because the MFPV volume is the same for all IHLW components corresponding to an MFPV batch, and hence cancels out of the equation.

In the case of balanced data, the formula for the mean (mass-weighted average) of mass fractions of the j^{th} IHLW component over the MFPV batches corresponding to an HLW waste type is given by:

$$\bar{\bar{g}}_j^{MFPV} = \frac{\sum_{i=1}^{I}\left(\frac{1}{n_S^{MFPV} n_A^{MFPV}}\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}} c_{ijlm}^{MFPV}\right)\left(\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV}\right) f_j}{\sum_{i=1}^{I}\sum_{j=1}^{J}\left(\frac{1}{n_S^{MFPV} n_A^{MFPV}}\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}} c_{ijlm}^{MFPV}\right)\left(\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV}\right) f_j} \qquad (4.1.2)$$

for $j = 1, 2, \ldots, J$, where:

$\bar{\bar{g}}_j^{MFPV}$ = mean (mass-weighted-average) mass fraction of the j^{th} IHLW component over I MFPV batches, based on averages over n_S^{MFPV} samples per MFPV batch, n_A^{MFPV} analyses per sample, and n_V^{MFPV} volume determinations per MFPV batch (g_{oxide}/g_{oxides})

I = number of MFPV batches corresponding to an HLW waste type

J = number of non-radionuclide oxides and radionuclide oxides estimated for the IHLW composition corresponding to each MFPV batch

f_j = $\frac{MW_j^{oxide}}{MW_j^{analyte}} R_j$ where MW_j^{oxide} and $MW_j^{analyte}$ are the molecular weights of oxide j and analyte j, respectively, and R_j is the ratio of moles of oxide per mole of analyte for oxide j. Hence, f_j is the factor for converting the concentration of analyte j (μg analyte j/mL = mg analyte j/L) to the concentration of oxide j (μg oxide j/mL = mg oxide/L). The quantity f_j is called the oxide factor for oxide j.

n_S^{MFPV} = number of samples per MFPV batch (≥ 1)

n_A^{MFPV} = number of chemical analyses per MFPV sample (≥ 1)

c_{ijlm}^{MFPV} = analyzed concentration of the j^{th} analyte from the m^{th} analysis of the l^{th} sample from the i^{th} MFPV batch (μg/mL = mg/L)

n_V^{MFPV} = number of volume determinations per MFPV batch (≥ 1)

V_{ih}^{MFPV} = the h^{th} volume determination of the i^{th} MFPV batch (L).

The derivation of Eq. (4.1.2) is presented in Section E.1 of Appendix E.

In the case of balanced data, the formula for the SD of mass fractions of the j^{th} IHLW component over the MFPV batches corresponding to an HLW waste type is given by:

$$SD\left(\overline{g}_{ij}^{MFPV}\right)=\left[\frac{\sum_{i=1}^{I}\left(\overline{g}_{ij}^{MFPV}-\overline{\overline{g}}_{j}^{MPFPV}\right)^2}{I-1}\right]^{0.5} \tag{4.1.3}$$

where

$SD\left(\overline{g}_{ij}^{MFPV}\right)$ = standard deviation of mass fractions for the j^{th} IHLW component over glass that would be made from the I MFPV batches corresponding to an HLW waste type (g_{oxide}/g_{oxides})

$\overline{g}_{ij}^{MFPV}$ = mass fraction of the j^{th} IHLW component in glass that would be made from the i^{th} MFPV batch (g_{oxide}/g_{oxides}).

The quantity $\overline{g}_{ij}^{MFPV}$ is calculated using Eq. (A.1.5) in Section A.1 of Appendix A, $\overline{\overline{g}}_{j}^{MFPV}$ is calculated using Eq. (4.1.2), and the remaining notation is as previously defined.

A %RSD is simply the ratio of the standard deviation [$SD(\overline{g}_{ij}^{MFPV})$ in this case] to its corresponding mean, multiplied by 100. With the variables defined in this section, the %RSD for the j^{th} IHLW component in the i^{th} MFPV batch is given by

$$\%RSD(\overline{g}_{ij}^{MFPV})=100\left(\frac{SD(\overline{g}_{ij}^{MFPV})}{\overline{\overline{g}}_{j}^{MFPV}}\right). \tag{4.1.4}$$

In some cases, it may be preferred to report or consider the %RSD rather than the SD.

4.1.4.2 Equations for Calculating Means and Standard Deviations of IHLW Chemical Composition over a Waste Type Using Unbalanced Data

The case of unbalanced data is now addressed where (1) the number of samples per MFPV batch is not the same for the MFPV batches associated with an HLW waste type and/or (2) the number of analyses per MFPV sample is not the same for each sample from an MFPV batch or for different MFPV batches. Unbalanced data would occur during WTP IHLW production if (1) less than the desired number of samples were taken for every MFPV batch, (2) a sample from an MFPV batch were unusable for some reason, (3) the number of analyses were not the same for every MFPV sample, or (4) analytical results contain outliers that must be discarded.

Unbalanced data force changes in how the means and SDs for IHLW compositions are calculated. Several alternatives are available, but the simplest way to deal with unbalanced data is to calculate the means and SDs using the samples and analyses available. The process used is to take the mean of the analyses for each sample and then proceed to taking the mean of the sample means.

In the case of unbalanced data, the formula for the mean (mass-weighted average) of mass fractions of the j^{th} IHLW component over the MFPV batches corresponding to an HLW waste type is given by

$$\overline{\overline{g}}_j^{MFPV} = \frac{\sum_{i=1}^{I}\left[\frac{1}{n_S^{MFPV_i}}\sum_{l=1}^{n_S^{MFPV_i}}\left(\frac{1}{n_A^{MFPV_{il}}}\sum_{m=1}^{n_A^{MFPV_{il}}} c_{ijlm}^{MFPV}\right)\right]\left(\frac{1}{n_V^{MFPV_i}}\sum_{h=1}^{n_V^{MFPV_i}} V_{ih}^{MFPV}\right) f_j}{\sum_{i=1}^{I}\sum_{j=1}^{J}\left[\frac{1}{n_S^{MFPV_i}}\sum_{l=1}^{n_S^{MFPV_i}}\left(\frac{1}{n_A^{MFPV_{il}}}\sum_{m=1}^{n_A^{MFPV_{il}}} c_{ijlm}^{MFPV}\right)\left(\frac{1}{n_V^{MFPV_i}}\sum_{h=1}^{n_V^{MFPV_i}} V_{ih}^{MFPV}\right) f_j\right]} \tag{4.1.5}$$

for $j = 1, 2, \ldots, J$, where the notation is the same as defined after Eq. (4.1.2) except for the following differences

$n_S^{MFPV_i}$ = number of samples from the i^{th} MFPV batch

$n_A^{MFPV_{il}}$ = number of chemical analyses made of the l^{th} sample from the i^{th} MFPV batch

$n_V^{MFPV_i}$ = number of volume determinations for the i^{th} MFPV batch.

Hence, Eq. (4.1.5) for unbalanced data is similar to Eq. (4.1.2) for balanced data, but substitutes the preceding notation for unequal numbers of samples and analyses per MFPV sample.

In the case of unbalanced data, the SD of mass fractions for the j^{th} IHLW component over the I MFPV batches corresponding to an HLW waste type can again be calculated using Eq. (4.1.3). In that equation, $\overline{\overline{g}}_j^{MFPV}$ is given by Eq. (4.1.5) and $\overline{g}_{ij}^{MFPV}$ is given by the equation

$$\overline{g}_{ij}^{MFPV} = \frac{\overline{c}_{ij}^{MFPV} f_j}{\sum_{j=1}^{J}\overline{c}_{ij}^{MFPV} f_j} = \frac{\frac{1}{n_S^{MFPV_i}}\sum_{l=1}^{n_S^{MFPV_i}}\left(\frac{1}{n_A^{MFPV_{il}}}\sum_{m=1}^{n_A^{MFPV_{il}}} c_{ijlm}^{MFPV}\right) f_j}{\sum_{j=1}^{J}\left[\frac{1}{n_S^{MFPV_i}}\sum_{l=1}^{n_S^{MFPV_i}}\left(\frac{1}{n_A^{MFPV_{il}}}\sum_{m=1}^{n_A^{MFPV_{il}}} c_{ijlm}^{MFPV}\right) f_j\right]} \tag{4.1.6}$$

where the notation is as previously defined following Eq. (4.1.2) and Eq. (4.1.5). Equation (4.1.6) for unbalanced data is similar to Eq. (A.1.5) in Section A.1 of Appendix A for balanced data, but substitutes the notation for unequal numbers of samples and analyses. In Eqs. (4.1.6) and (A.1.5), note that the volume of the i^{th} MFPV batch does not appear because it cancels in the equation, as shown in Section A.1.

If the data are not greatly unbalanced, this simple way of calculating means and SDs for mass fractions of IHLW components over a waste type should produce reasonable results. However, other methods that are designed to work with unbalanced data could also be employed. Weighted least squares (WLS) can be used not only with unbalanced data but also if there is evidence that the variation across MFPV batches does not remain constant over the course of a waste type. WLS-based equations for means and SDs have not been developed at this time, but could be if deemed desirable by the WTP Project. Bootstrap methods, where available data are repeatedly re-sampled (i.e., with replacement) to obtain a balanced set, could also be used to solve the problem of unbalanced data. In general, bootstrapping methods take samples from available data, randomly and with replacement, until (in this case) a balanced set is obtained. The methods described to deal with balanced data can then be directly applied to this newly obtained set. This process is repeated numerous times (the precise number depends on the specific problem), obtaining every time estimates for all parameters of interest. Finally, the estimates obtained from every bootstrapped sample are combined to compute statistics (typically, average and variability estimates) for all parameters of interest.

4.2 Compliance Approach and Methods for IHLW WAPS Specification 1.2.2: Radionuclide Inventory During Production

Section 4.2.1 lists the applicable WAPS Specification 1.2.2 within the context of WAPS 1.2. Section 4.2.2 summarizes the statistical aspects of the WTP compliance strategy for WAPS 1.2.2. Sections 4.2.3 and 4.2.4 present the statistical methods that will be used to implement the statistical aspects of the compliance strategy.

4.2.1 WAPS Specification 1.2: Radionuclide Inventory Specification

The Producer shall report the inventory of radionuclides (in Curies) that have half-lives longer than 10 years and that are, or will be, present in concentrations greater than 0.05 percent of the total radioactive inventory for each waste type, indexed to the years 2015 and 3115.

1.2.2 Radionuclide Inventory During Production

The Producer shall provide in the Production Records estimates of the inventories of individual reportable radionuclides for each canister and for each waste type. The Producer shall also report the estimated error of these estimates in the WQR.

4.2.2 Statistical Aspects of the IHLW Compliance Strategy for WAPS 1.2.2

Items 1 and 2 following describe the statistical and related aspects of the IHLW compliance strategy for WAPS Specification 1.1.2, as described in Rev. 0 of the IHLW PCP (Nelson 2003). However, during the course of work documented in this report, the WTP Project substantially revised the IHLW compliance strategy and provided an informal description of the revisions to the compliance strategy. One of these revisions is to analyze all reportable radionuclides for samples from the first MFPV batch corresponding to an HLW waste type, and for the remaining MFPV batches to analyze only a small subset

of the radionuclides (see Table 2.1 in Section 2). Item 3 following was added based on the informal description of the revised IHLW compliance strategy.

Item 1: Determine the numbers of samples, analyses per sample, and other process measurements required to estimate radionuclide compositions, which are in turn used to estimate radionuclide inventories.

Item 2: Develop equations for calculating the means and SDs of the radionuclide inventory determinations for IHLW canisters produced from a given HLW waste type for each reportable radionuclide analyzed in every MFPV batch. Incorporate in the SD equation the variations and uncertainties affecting the radionuclide composition and the mass of glass in IHLW canisters.

Item 3: Develop statistical methods to quantify the variation and uncertainty present in determinations of radionuclide inventories over an HLW waste type for radionuclides analyzed in samples of the first MFPV batch only.

The statistical methods to implement these aspects of the WTP IHLW compliance strategy for WAPS Specification 1.2.2 are discussed in Sections 4.2.3 to 4.2.5.

4.2.3 Statistical Method for Determining the Numbers of Samples and Analyses Per Sample to Estimate the IHLW Radionuclide Composition for an MFPV Batch

During IHLW production operations, the radionuclide composition (mass fractions) will be calculated based on chemical analyses and radiochemical analyses of samples from the MFPV. Although mass fractions of IHLW radionuclide components (oxides) may be of limited interest directly, they play a key role in the equations developed to calculate IHLW radionuclide inventories (see Section A.2 of Appendix A). Hence, it is important to assess the numbers of IHLW MFPV samples and radiochemical analyses per sample required to adequately estimate IHLW radionuclide compositions (i.e., mass fractions).

The applicable mass-balance equations for calculating IHLW radionuclide composition (mass fractions) are given in Section A.2 of Appendix A. The balance of this subsection describes the statistical method to address Item 1 in Section 4.2.2.

Section 3.4.1 describes the general approach for assessing the impacts of the following factors:

- number of samples per MFPV batch (n_S^{MFPV})
- number of analyses per MFPV sample (n_A^{MFPV})
- mixing/sampling %RSD in the concentration of the q^{th} radionuclide in a MFPV batch [$\%RSD_S(c_q^{MFPV})$]
- analytical %RSD in the concentration of the q^{th} radionuclide in a MFPV batch [$\%RSD_A(c_q^{MFPV})$]
- statistical percent confidence level (CL%)

- IHLW produced from three HLW tanks (AY-102, AZ-102, and C-104)

on the total uncertainty in estimating IHLW radionuclide composition for each MFPV batch. It is necessary at this time to consider a range of values for process uncertainties (as discussed in Section 3.4.1) because final estimates have not yet been produced by the WTP Project. A future update of this report will use final estimates of MFPV mixing/sampling and analytical uncertainties to determine the final recommended number of MFPV samples and number of radiochemical analyses per MFPV sample for estimating IHLW radionuclide composition (and inventory).

To assess the total uncertainty in estimating IHLW radionuclide composition for a given MFPV batch, the %RHW of a two-sided CL% CI (see Section 3.1) on the mass fraction of each IHLW radionuclide component (oxide) is used. The %RHW for radionuclide composition can be calculated with the same formula as for chemical composition, which is given by Eq. (4.1.1) in Section 4.1.3. The only difference in Eq. (4.1.1) is substituting "*q,*" denoting a radionuclide component of IHLW in place of "*j,*" denoting a chemical composition component of IHLW. This formula can be used to calculate %RHW values for various combinations of the factors described previously in this subsection. The results of such calculations can be used to determine the values of n_S^{MFPV} and n_A^{MFPV} that will provide estimates of radionuclide glass components within a given percentage (i.e., the %RHW) of the true value with desired confidence (CL%). The results of such calculations are presented in Section 6.2.1.

4.2.4 Equations for Calculating Means and Standard Deviations of IHLW Radionuclide Inventories Using Information from All MFPV Batches Corresponding to an HLW Waste Type

During IHLW production operations, radionuclide inventories will be calculated based on (1) chemical and radiochemical analyses of MFPV samples, (2) determinations of content volumes in MFPV batches, and (3) determinations of the masses of glass in IHLW canisters. WAPS 1.2.2 calls for reporting inventories for each canister and for each waste type. However, it is not possible to easily relate the composition of MFPV batches to the composition of IHLW in canisters produced from those batches.

In the WTP IHLW compliance strategy, the radionuclides are divided in two groups. Radionuclides belonging to the first group will be analyzed only in samples from the first MFPV batch of each HLW waste type, while those in the second group will be analyzed in samples of every MFPV batch. See Table 2.1 for a listing of the reportable radionuclides in each of the two groups.

The compliance strategy for radionuclides in the second group is to report means and SDs of the radionuclide inventories over canisters (and associated MFPV batches) corresponding to an HLW waste type. This subsection presents the formulas for calculating means and SDs of the inventory of radionuclide *q* over the *D* IHLW canisters associated with the *I* MFPV batches corresponding to an HLW waste type. The formulas are based on average results over multiple samples, analyses, and volume determinations for each MFPV batch. Two situations are considered. Section 4.2.4.1 addresses the case of balanced data, while Section 4.2.4.2 addresses the case of unbalanced data. The formulas in these subsections address Item 2 of Section 4.2.2.

4.2.4.1 Equations for Calculating Means and Standard Deviations of IHLW Radionuclide Inventories over a Waste Type Using Balanced Data

Equations for calculating means and SDs of IHLW radionuclide inventories over a waste type using balanced data (as described at the start of Section 4.1.4.1) are presented in this subsection. These equations apply to those radionuclides that will be measured in every MFPV batch, as listed in Table 2.1 of Section 2.

Equation for the Mean Radionuclide Inventory over *D* IHLW Canisters Based on Averages of Balanced Multiple Samples, Analyses, and Volume Determinations for Each MFPV Batch

The expression for the mean inventory per canister of radionuclide q over the D IHLW canisters and I MFPV batches associated with an HLW waste type, based on averages over balanced multiple samples, analyses per sample, and volume determinations per MFPV batch, is given by

$$\overline{\overline{R}}_{Dq}^{Canister} = \frac{\overline{\overline{g}}_q^{MFPV}\,\overline{m}_D^{Canister}\,A_q}{f_q}$$

$$= \left(\frac{\left[\sum_{i=1}^{I} \left(\frac{\sum_{l=1}^{n_S^{MFPV}} \sum_{m=1}^{n_A^{MFPV}} r_{iqlm}^{MFPV}}{n_S^{MFPV}\, n_A^{MFPV}} \right) \left(\frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV}}{n_V^{MFPV}} \right) \right] \left[\frac{1}{D} \sum_{d=1}^{D} m_d^{Canister} \right]}{\sum_{i=1}^{I} \left(\sum_{j \in CHEM}^{J} \frac{\sum_{l=1}^{n_S^{MFPV}} \sum_{m=1}^{n_A^{MFPV}} c_{ijlm}^{MFPV} f_j}{n_S^{MFPV}\, n_A^{MFPV}} + \sum_{j \in RAD}^{J} \frac{\sum_{l=1}^{n_S^{MFPV}} \sum_{m=1}^{n_A^{MFPV}} r_{ijlm}^{MFPV} f_j / A_j}{n_S^{MFPV}\, n_A^{MFPV}} \right) \left(\frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV}}{n_V^{MFPV}} \right)} \right) \quad (4.2.1)$$

where

$\overline{\overline{R}}_{Dq}^{Canister}$ = mean inventory per canister of the q^{th} radionuclide over the D IHLW canisters associated with an HLW waste type, based on averages over multiple samples, analyses, and volume determinations for each MFPV batch (Ci)

$\overline{\overline{g}}_q^{MFPV}$ = mean (mass-weighted-average) mass fraction of the q^{th} IHLW radionuclide component over I MFPV batches, based on averages over n_S^{MFPV} samples per MFPV batch, n_A^{MFPV} analyses per sample, and n_V^{MFPV} volume determinations per MFPV batch (g_{oxide}/g_{oxides})

$\overline{m}_D^{Canister}$ = mean mass of glass in the D IHLW canisters associated with an HLW waste type (g_{glass})

A_q or A_j = specific activity of the q^{th} or j^{th} radionuclide ($Ci/g_{radionuclide}$)

I = number of MFPV batches corresponding to an HLW waste type

J = number of non-radionuclide oxides and radionuclide oxides estimated for the IHLW composition corresponding to each MFPV batch

$j \in CHEM$ = chemical composition components of IHLW

$j \in RAD$ = radionuclide composition components of IHLW

D = number of IHLW canisters associated with the I MFPV batches corresponding to an HLW waste type

f_j = $\frac{MW_j^{oxide}}{MW_j^{analyte}} R_j$ where MW_j^{oxide} and $MW_j^{analyte}$ are the molecular weights of oxide j and analyte j, respectively, and R_j is the ratio of moles of oxide per mole of analyte for oxide j. Hence, f_j is the factor for converting the concentration of analyte j (μg analyte j/mL = mg analyte j/L) to the concentration of oxide j (μg oxide j/mL = mg oxide/L). The quantity f_j is called the oxide factor for oxide j.

n_S^{MFPV} = number of samples per MFPV batch

n_A^{MFPV} = number of chemical and radiochemical analyses per MFPV sample

r_{ijlm}^{MFPV} = analyzed concentration of the j^{th} radionuclide from the m^{th} analysis of the l^{th} sample from the i^{th} MFPV batch (μCi/mL = mCi/L)

c_{ijlm}^{MFPV} = analyzed concentration of the j^{th} analyte from the m^{th} analysis of the l^{th} sample from the i^{th} MFPV batch (μg/mL = mg/L)

n_V^{MFPV} = number of volume determinations per MFPV batch

V_{ih}^{MFPV} = the h^{th} volume determination of the i^{th} MFPV batch (L)

$m_d^{Container}$ = mass of glass in the d^{th} IHLW container associated with an HLW waste type (g_{glass}).

The mean (mass-weighted average over IHLW MFPV batches) mass fraction of the q^{th} radionuclide ($\overline{\overline{g}}_q^{MFPV}$) plays an important role in calculating $\overline{\overline{R}}_{Dq}^{Canister}$, the mean inventory per canister of the q^{th} radionuclide over the D IHLW canisters associated with an HLW waste type. The quantity $\overline{\overline{g}}_q^{MFPV}$ is calculated for balanced data by Eq. (4.1.2) with q substituted for j in the numerator. Note that f_q does not appear in the final form of Eq. (4.2.1) because it cancels. This may be seen in the derivation of Eq. (4.2.1), which is presented in Section A.2.2.1 of Appendix A.

Despite the effective reductions of some within-batch uncertainties due to averaging, it should be recognized that values of $\overline{\overline{R}}_{Dq}^{Canister}$ calculated via Eq. (4.2.1) will still be subject to reduced within-MFPV-batch uncertainty as well as MFPV batch-to-batch variations.

Equation for the Standard Deviation of Radionuclide Inventory over *D* IHLW Canisters Based on Averages of Balanced Multiple Samples, Analyses, and Volume Determinations for Each MFPV Batch

The expression for the standard deviation of the inventory of radionuclide q over the D IHLW canisters and I MFPV batches associated with an HLW waste type, based on averages over balanced multiple samples, analyses per sample, and volume determinations per MFPV batch, is given by

$$SD(\overline{R}_{dq}^{Canister}) = \left(\frac{A_q}{f_q}\right)\left[\begin{array}{l}\left[\overline{\overline{g}}_q^{MFPV}\right]^2\left[SD(m_d^{Canister})\right]^2 + \left[\overline{m}_D^{Canister}\right]^2\left[SD(\overline{g}_{iq}^{MFPV})\right]^2 \\ -\left[SD(m_d^{Canister})\right]^2\left[SD(\overline{g}_{iq}^{MFPV})\right]^2\end{array}\right]^{1/2} \tag{4.2.2}$$

where

$SD(\overline{R}_{dq}^{Canister})$ = standard deviation of the average inventory of radionuclide q for the d^{th} IHLW canister where the average is based on multiple samples, analyses, and volume determinations for each MFPV batch (Ci)

$SD(m_d^{Canister})$ = standard deviation of the determined mass of glass in the d^{th} IHLW canister (g_{glass})

$SD(\overline{g}_{iq}^{MFPV})$ = standard deviation of the average mass fraction of the q^{th} radionuclide oxide in the i^{th} MFPV batch where the average is based on multiple samples, analyses, and volume determinations of the corresponding i^{th} MFPV batch (g_{oxide}/g_{oxides})

and the remaining notation is as previously defined following Eq. (4.2.1). The derivation of Eq. (4.2.2) is presented in Section A.2.2.2 of Appendix A.

As explained in Section A.2.2.2 in Appendix A, the term $SD(\overline{g}_{iq}^{MFPV})$ includes variation in mass fractions of the q^{th} radionuclide oxide across all I MFPV batches associated with an HLW waste type, as

well as mixing/sampling and analytical uncertainties associated with determining mass fractions of radionuclide oxides for each MFPV batch. A value of $SD(\bar{g}_{iq}^{MFPV})$ is calculated from the $\bar{g}_{iq}^{MFPV}$ (i = 1, 2, … , I) values using the usual standard deviation formula.

In a similar way, the term $SD(m_d^{Canister})$ includes uncertainties associated with determining the mass of glass in an IHLW canister as well as the variation in the masses of glass that occur across canisters associated with an HLW waste type. A value of $SD(m_d^{Canister})$ is calculated from the $m_d^{Canister}$ (d = 1, 2, … , D) values using the usual standard deviation formula.

4.2.4.2 Equations for Calculating Means and Standard Deviations of IHLW Radionuclide Inventories over a Waste Type Using Unbalanced Data

The case of unbalanced data (as described in Section 4.1.4.2) is now addressed, where $n_S^{MFPV_i} > 1$ denotes the number of samples taken from the i^{th} MFPV batch, $n_A^{MFPV_{il}} \geq 1$ denotes the number of chemical and radionuclide analyses made of the l^{th} sample from the i^{th} MFPV batch, and $n_V^{MFPV_i} \geq 1$ denotes the number of volume determinations for the i^{th} MFPV batch.

Equations for calculating means and SDs of IHLW radionuclide inventories over a waste type using unbalanced data are presented. These equations apply to those radionuclides that will be measured in every MFPV batch, as listed in Table 2.1 of Section 2. These equations also assume that the degree of unbalance is small. Otherwise, WLS methods or bootstrap methods (as described in the last paragraph of Section 4.1.4.2) should be applied.

Equation for the Mean Radionuclide Inventory over *D* IHLW Canisters Based on Averages of Unbalanced Multiple Samples, Analyses, and Volume Determinations for Each MFPV Batch

The expression for the mean inventory per canister of radionuclide q over the D IHLW canisters and I MFPV batches associated with an HLW waste type, based on averages over unbalanced multiple samples,

analyses per sample, and volume determinations per MFPV batch, is given by

$$\overline{\overline{R}}_{Dq}^{Canister} = \frac{\overline{\overline{g}}_q^{MFPV}\,\overline{m}_D^{Canister}\,A_q}{f_q}$$

$$= \frac{\left[\sum_{i=1}^{I}\left(\frac{1}{n_S^{MFPV_i}}\sum_{l=1}^{n_S^{MFPV_i}}\left[\frac{1}{n_A^{MFPV_{il}}}\sum_{m=1}^{n_A^{MFPV_{il}}} r_{iqlm}^{MFPV}\right]\right)\left(\frac{1}{n_V^{MFPV_i}}\sum_{h=1}^{n_V^{MFPV_i}} V_{ih}^{MFPV}\right)\right]\left[\frac{1}{D}\sum_{d=1}^{D} m_d^{Canister}\right]}{\sum_{i=1}^{I}\left[\sum_{j\in CHEM}^{J}\left(\frac{\sum_{l=1}^{n_S^{MFPV_i}}\frac{\sum_{m=1}^{n_A^{MFPV_i}} c_{ijlm}^{MFPV}}{n_A^{MFPV_i}}}{n_S^{MFPV_i}}\right) f_j + \sum_{j\in RAD}^{J}\left(\frac{\sum_{l=1}^{n_S^{MFPV_i}}\frac{\sum_{m=1}^{n_A^{MFPV_i}} r_{ijlm}^{MFPV}}{n_A^{MFPV_i}}}{n_S^{MFPV_i}}\right)\frac{f_j}{A_j}\right]\left[\frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV}}{n_V^{MFPV}}\right]} \quad (4.2.3)$$

where all notation is as previously defined following Eq. (4.2.1) and Eq. (4.1.5). Equation (4.2.3) is seen to be a modification of Eq. (4.2.1) with $n_S^{MFPV_i}$, $n_A^{MFPV_{il}}$, and $n_V^{MFPV_i}$ substituted for n_S^{MFPV}, n_A^{MFPV}, and n_V^{MFPV}, respectively. The mean (mass-weighted average over IHLW MFPV batches) mass fraction of the q^{th} radionuclide ($\overline{\overline{g}}_q^{MFPV}$) plays an important role in calculating $\overline{\overline{R}}_{Dq}^{Canister}$, the mean inventory per canister of the q^{th} radionuclide over the D IHLW canisters associated with an HLW waste type. The quantity $\overline{\overline{g}}_q^{MFPV}$ is calculated for unbalanced data by Eq. (4.1.5) with q substituted for j in the numerator. Note that f_q does not appear in the final form of Eq. (4.2.3) because it cancels in the derivation.

Equation for the Standard Deviation of Radionuclide Inventory over *D* IHLW Canisters Based on Averages of Unbalanced Multiple Samples, Analyses, and Volume Determinations for Each MFPV Batch

The expression for the SD of the inventory of radionuclide q over the D IHLW canisters and I MFPV batches associated with an HLW waste type, based on averages over unbalanced multiple samples, analyses per sample, and volume determinations per MFPV batch, is again given by Eq. (4.2.2). In Eq. (4.2.2), $\overline{g}_{iq}^{MFPV}$ is calculated using Eq. (4.1.6) and $\overline{\overline{g}}_q^{MFPV}$ is calculated by Eq. (4.1.5) where in both cases, q is one of the j in those equations.

4.2.5 Statistical Method for Calculating IHLW Radionuclide Inventories and Their Standard Deviations over an HLW Waste Type, Using Information from a Single MFPV Batch

This subsection is a placeholder for the description of the statistical method that will be used to address Item 3 of Section 4.2.2. The method will be described in this subsection in a future revision of the report.

4.3 Compliance Approach and Methods for IHLW WAPS Specification 1.3: Product Consistency

Section 4.3.1 lists the applicable WAPS Specification 1.3. Section 4.3.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Sections 4.3.3 to 4.3.6 present the statistical methods that will be used to implement the statistical aspects of the compliance strategy.

4.3.1 WAPS Specification 1.3: Product Consistency

The Producer shall demonstrate control of waste form production by comparing, either directly or indirectly, production samples to the Environmental Assessment (EA) benchmark glass. The Producer shall describe the method for demonstrating compliance in the WCP and shall provide verification in the Production Records. The Producer shall demonstrate the ability to comply with the specification in the WQR.

WAPS Specification 1.3.1: Acceptance Criterion

The consistency of the waste form shall be demonstrated using the Product Consistency Test (PCT). For acceptance, the mean concentrations of lithium, sodium and boron in the leachate, after normalizing for the concentrations in the glass, shall each be less than those of the benchmark glass described in the Environmental Assessment for selection of the DWPF waste form. The measured or projected mean PCT results for lithium, sodium, and boron shall be provided in the Production Records. The Producer shall define the statistical significance of the reported data in the WQR. One acceptable method of demonstrating that the acceptance criterion is met would be to ensure that the mean PCT results for each waste type are at least two standard deviations below the mean PCT results of the EA glass.

WAPS Specification 1.3.2: Method of Compliance

The capability of the waste form to meet this specification shall be derived from production glass samples and/or process control information. Production Records shall contain data derived from production samples, or process control information used for verification, separately or in combination. When using process control information to project PCT results, the Producer shall demonstrate in the WQR that the method used will provide information equivalent to the testing of samples of actual production glass.

4.3.2 Statistical Aspects of the IHLW Compliance Strategy for WAPS 1.3

The development of property-composition databases and models for PCT normalized releases of boron ($r^{PCT\ B}$), lithium ($r^{PCT\ Li}$), and sodium ($r^{PCT\ Na}$) are statistically based and play an important role in complying with this specification. This joint work involving Battelle—Pacific Northwest Division (PNWD) and the Vitreous State Laboratory (VSL) at The Catholic University of America is being documented in reports issued by VSL. Reports by Piepel et al. (2002) and Cooley et al. (2003) described the glass science and statistical approaches used to develop the property-composition database for the development of PCT and other IHLW property models. The Phase 1 (initial) IHLW PCT-composition models and uncertainty expressions for model predictions are documented in the report by Kot et al. (2005).

The following items describe the statistical and related aspects of the IHLW compliance strategy for WAPS Specification 1.3 (see the IHLW PCP, Nelson 2003) that are addressed in this report. [(a)]

Item 1: Develop a statistical interval method to demonstrate that the contents of each MFPV batch would produce IHLW compliant with WAPS 1.3. The method will account for uncertainties impacting the estimates of PCT boron, lithium, and sodium releases from IHLW that would be produced from each MFPV batch (e.g., sampling, analytical, other measurements, and property-composition model uncertainties).

Item 2: Determine the numbers of process samples, chemical analyses per sample, and other process measurements required to demonstrate that the PCT boron, lithium, and sodium releases from IHLW that would be produced from each MFPV batch will satisfy their respective limits. The calculations will require estimates of applicable process uncertainties (mixing/sampling, analytical, and other process measurements) as well as property-composition model uncertainties.

Item 3: Develop a statistical interval method to demonstrate that IHLW glass produced over a waste type complies with the PCT limits of WAPS 1.3. The method will account for the source of variation of interest (namely variation in PCT performance due to variation in IHLW composition over the course of a waste type). The method will also account for nuisance uncertainties (e.g., sampling, analytical, other measurements, and property-composition model uncertainties). Statistical X%/Y% upper tolerance intervals (X%Y% UTIs) may be used for this purpose.

Item 4: Determine the numbers of process samples, chemical analyses per sample, and other process measurements required to demonstrate that the PCT boron, lithium, and sodium releases from IHLW produced from a waste type will satisfy their respective limits. The calculations will require estimates of glass-composition variation over a waste type, applicable process uncertainties (mixing/sampling, analytical, and other process measurements), and property-composition model uncertainties.

(a) See Section 1.0 for a discussion of why this report addresses WAPS specifications and IHLW PCP Rev. 0 (Nelson 2003) rather than IHLW PCP Rev. 1 (Nelson et al. 2004).

Note that Items 1 and 2 do not appear specifically in Rev. 0 of the IHLW PCP (Nelson 2003). However, they are consistent with that version of the WTP Project's compliance strategy for WAPS Specification 1.3 to demonstrate compliance for each IHLW MFPV batch as well as over each HLW waste type. Items 1 and 2 are a part of the work scope in the Test Plan (Piepel and Heredia-Langner 2003) and hence the work and results are documented in this section.

The statistical methods to implement these aspects of the WTP IHLW compliance strategy for WAPS Specification 1.3 are discussed in Sections 4.3.3 to 4.3.6, respectively.

4.3.3 Statistical Interval Method to Demonstrate that IHLW from an MFPV Batch Will Satisfy PCT Limits

This subsection discusses and presents the formula for an appropriate statistical interval to satisfy Item 1 of Section 4.3.2. The statistical interval must (1) account for the uncertainty in the estimated IHLW composition corresponding to a given MFPV batch, (2) account for the uncertainties in property-composition models used to predict PCT normalized B, Li, and Na releases for the estimated IHLW composition corresponding to a given MFPV batch, and (3) provide high confidence that the true PCT normalized B, Li, and Na releases are less than the limits specified in WAPS 1.3. These normalized release limits, which are documented in Table 6 of a report by Jantzen et al. (1993)[(a)], are:

$$\begin{aligned} r^{PCT\ B} &\le 16.695 \text{ g/L } (= 8.35 \text{ g/m}^2) \\ r^{PCT\ Li} &\le 9.565 \text{ g/L } (= 4.78 \text{ g/m}^2) \\ r^{PCT\ Na} &\le 13.346 \text{ g/L } (= 6.67 \text{ g/m}^2) \end{aligned} \tag{4.3.1}$$

Section 4.3.3.1 presents the initial form of recommended property-composition models for PCT normalized releases of B, Li, and Na. Section 4.3.3.2 presents the equations for the appropriate type of statistical interval.

4.3.3.1 Property-Composition Model Form for PCT Normalized Releases of B, Li, and Na

The property-composition models developed by PNWD and VSL (Kot et al. 2005) for predicting PCT normalized releases of B, Li, and Na for IHLW compositions are of the general form

$$\hat{y}^h_{ilm} = \hat{ln}\left(r^h_{ilm}\right) = \sum_{k=1}^{n^h_{mc}} b^h_k \, x^{MFPV}_{iklm} \tag{4.3.2a}$$

$$= (\boldsymbol{b}^h)^T \, \boldsymbol{x}^{MFPV}_{ilm} \tag{4.3.2b}$$

where

(a) Jantzen et al. (1993) provide PCT normalized elemental releases from the DWPF EA glass in units of g/L. However, applying the standard assumption of a surface area-to-volume ratio of 2000 m^{-1}, the results were converted from g/L to g/m^2 and reported here in those units rounded to two decimal places.

$\hat{y}_{ilm}^{h}$ = $\hat{ln}\left(r_{ilm}^{PCT\,h}\right)$ = predicted natural logarithm of the PCT normalized release of h = B, Li, or Na based on the m^{th} analysis of chemical composition of the l^{th} sample from the i^{th} MFPV batch [ln(g/L)]

b_k^h = coefficient for the k^{th} normalized component of IHLW in the model for PCT normalized release of h = B, Li, or Na. The coefficients are obtained by fitting the linear mixture model form (see Cornell 2002) to a property-composition data set using least squares regression

x_{iklm}^{MFPV} = normalized mass fractions of the IHLW components in the linear mixture model, such that $\sum_{k=1}^{n_{mc}^h} x_{iklm}^{MFPV} = 1$

n_{mc}^h = number of normalized IHLW components in the model for PCT normalized release of h = B, Li, or Na. In the case of a linear mixture model as in Eq. (4.3.2a), it is also the number of model coefficients (parameters, denoted p) estimated from the property-composition data

$\boldsymbol{b}^h$ = $p \times 1$ column vector of the model coefficients b_k^h, $k = 1, 2, \ldots, p$. In this case with the model form given by Eq. (4.3.2.a), $p = n_{mc}^h$.

$\boldsymbol{x}_{ilm}^{MFPV}$ = $p \times 1$ column vector of the IHLW normalized composition x_{iklm}^{MFPV}, $k = 1, 2, \ldots, p$ for which PCT model predictions are to be made.

The normalized mass fraction compositions of IHLW in Eq. (4.3.2a) are obtained from the ordinary (unnormalized) mass fraction compositions by

$$x_{iklm}^{MFPV} = \frac{g_{ijlm}^{MFPV}}{\sum_{j}^{n_{mc}^h \text{ of } J} g_{ijlm}^{MFPV}} \quad k = 1,2,\cdots,n_{mc}^h \tag{4.3.3}$$

where g_{ijlm}^{MFPV} is calculated using Eq. (A.1.3) in Section A.1 of Appendix A. Note that the l and m subscripts are relevant but not shown in that equation, so it is appropriate for the current context.

Table 4.1 lists the model terms (k) and the coefficients (b_k^h) for each IHLW PCT release (h = B, Li, and Na) used for the work in this report. These results are from work performed at PNWD that is documented in the report by Kot et al. (2005).

Table 4.1. IHLW PCT Model Terms and Coefficients

Model Term[(a)]	ln(PCT B)[(b)] Coefficient	ln(PCT Li)[(b)] Coefficient	ln(PCT Na)[(b)] Coefficient
Al_2O_3	-16.0111	-11.5792	-13.7309
B_2O_3	6.0139	3.0320	1.7213
Li_2O	20.5142	15.7575	19.9566
MnO	3.7888	1.4622	3.6828
Na_2O	12.2908	7.4435	13.2619
SiO_2	-3.9574	-2.3693	-3.8031
ThO_2	6.1476	2.5351	3.1327
ZrO_2	-9.6868	-6.0292	-8.9994
Model and Data Info			
n[(c)]	97	97	97
p[(c)]	8	8	8
$df_m = n - p$[(d)]	89	89	89

(a) The model terms are expressed in normalized mass fractions of the eight oxide components shown, such that the normalized mass fractions sum to one.
(b) PCT releases are modeled in ln(g/L).
(c) The notation n denotes the number of data points used to estimate the coefficients in the model form given by Eq. (4.3.2.a). The notation p denotes the number of coefficients estimated.
(d) df_m denotes the model degrees of freedom, calculated as indicated.

4.3.3.2 Equation for CL% Upper Combined Confidence Interval for PCT Normalized Releases of B, Li, and Na for a Single IHLW MFPV Batch

An appropriate statistical interval for demonstrating that the PCT limits in Eq. (4.3.1) are satisfied for each MFPV batch is a CL% UCCI, the concept of which was introduced in Section 3.1. Section A.3 of Appendix A discusses the statistical method for combining model and composition uncertainties that is used in forming a CL% UCCI. The CL% UCCI formula is given in general by

$$CL\%\ UCCI\left(y_i^h\right) = \bar{\hat{y}}_i^h + CHW_{i,CL\%\ UCI}^h + MHW_{i,CL\%\ SUCI}^h \tag{4.3.4}$$

where

$CL\%\ UCCI\left(y_i^h\right)$ = CL% UCCI for the true, unknown mean value of $y_i^h = ln\left(r_i^{PCT\ h}\right)$, that is, the natural logarithm of the PCT normalized release of element h (= B, Li, or Na) from IHLW corresponding to the i^{th} MFPV batch [ln(g/L)]

$\bar{\hat{y}}_i^h$ = mean of model-predicted $\hat{y}_{ilm}^h = \hat{ln}\left(r_{ilm}^{PCT\ h}\right)$ values over the n_S^{MFPV} samples and n_A^{MFPV} analyses per sample of the i^{th} MFPV batch [ln(g/L)]

$CHW^{h}_{i,CL\%\ UCI}$ = composition uncertainty half-width for a CL% upper confidence interval (CL% UCI) for the PCT normalized release of element *h* for IHLW corresponding to the i^{th} MFPV batch

$MHW^{h}_{i,CL\%\ SUCI}$ = model uncertainty half-width for a CL% SUCI for the PCT normalized release of element *h* for IHLW corresponding to the i^{th} MFPV batch.

A CL% SUCI is one of several upper confidence intervals (UCIs) on the true mean values of predictions made by a glass property-composition model for a set of glass compositions. All of the UCIs 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. Thus, CL% SUCIs for many glass compositions provide high confidence of containing the true property mean values for those glass compositions. The CL% SUCI method has been used by the DWPF and the West Valley Demonstration Project (WVDP) in their strategies for complying with WAPS 1.3.

Figure 4.1 illustrates a 95% UCCI for the natural logarithm of a PCT normalized elemental release.

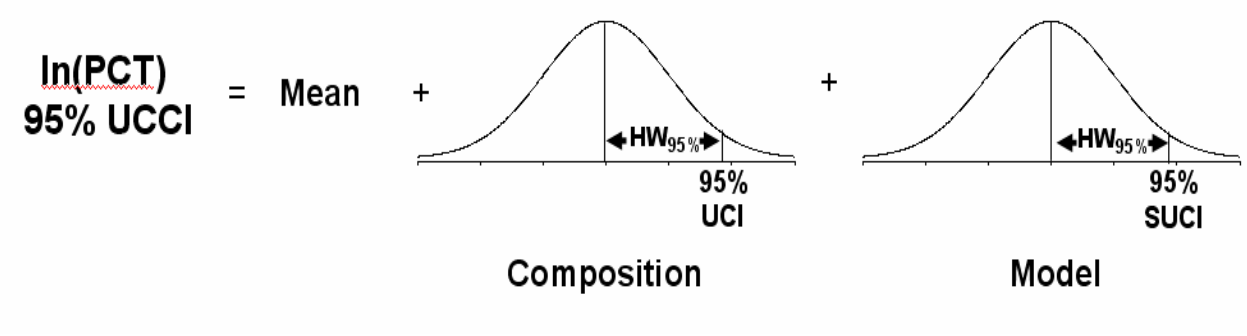

Figure 4.1. Graphical Illustration of a 95% Combined Confidence Interval for ln(PCT)

Equations for the terms on the right-hand side of Eq. (4.3.4) are given in Section E.2 of Appendix E for the case of $n_S^{MFPV} > 1$ samples and $n_A^{MFPV} \geq 1$ analyses per sample of the i^{th} MFPV batch. However, during operation of the WTP IHLW facility, it is expected that $n_A^{MFPV} = 1$ for reasons discussed in Section 6 of this report. Hence, the equations for the terms on the right hand side of Eq. (4.3.4) are now given for the case of $n_S^{MFPV} > 1$ samples and $n_A^{MFPV} = 1$ analyses per sample of the i^{th} MFPV batch.

The quantity $\bar{\hat{y}}_i^h$ in Eq. (4.3.4) is given by

$$\bar{\hat{y}}_i^h = \frac{\sum_{l=1}^{n_S^{MFPV}} \left(\sum_{k=1}^{n_{mc}^h} b_k^h \, x_{ikl}^{MFPV} \right)}{n_S^{MFPV}} \tag{4.3.5}$$

where all notation is as previously defined following Eq. (4.3.2a) and Eq. (4.2.1), except that the *m* subscript is missing because $n_A^{MFPV} = 1$.

The quantity $CHW_{i,CL\%\ UCI}^h$ in Eq. (4.3.4) is given by

$$CHW_{i,CL\%\ UCI}^h = t_{1-\alpha,df} \sqrt{\frac{\sum_{l=1}^{n_S^{MFPV}} \left(\hat{y}_{il}^h - \bar{\hat{y}}_i^h \right)^2 \Big/ \left(n_S^{MFPV} - 1 \right)}{n_S^{MFPV}}} \tag{4.3.6}$$

where

$t_{1-\alpha,df}$ = CL% = 100(1 – α) percentile of a Student's t-distribution with $df = n_S^{MFPV} - 1$ degrees of freedom, which provides CL% = 100(1–α) percent confidence for the one-sided UCI (e.g., 95% when α = 0.05)

$\hat{y}_{il}^h$ = model-predicted $\hat{y}_{il}^h = \hat{l}n\left(r_{il}^{PCT\ h}\right)$ values corresponding to the n_S^{MFPV} samples from the i^{th} MFPV batch [ln(g/L)]

$\bar{\hat{y}}_i^h$ = mean of model-predicted $\hat{y}_{il}^h$ values over the n_S^{MFPV} samples from the i^{th} MFPV batch [ln(g/L)]

and the remaining notation is as previously defined following Eq. (4.2.1), again with the subscript *m* missing because $n_A^{MFPV} = 1$.

The quantity $MHW_{i,CL\%\ SUCI}^h$ in Eq. (4.3.4) is given by

$$MHW_{i,CL\%\ SUCI}^h = \sqrt{p\, F_{1-\alpha}(p, n-p)} \left(\sqrt{(\bar{\mathbf{x}}_i^{MFPV})^T \, \hat{\boldsymbol{\Sigma}}_b^h \, \bar{\mathbf{x}}_i^{MFPV}} \right) \tag{4.3.7}$$

where

p = number of coefficients in the property-composition model for the PCT normalized release of element h = B, Li, or Na. For a model of the form in Eq. (4.3.2a), $p = n_{mc}^{h}$.

$F_{1-\alpha}(p, n-p)$ = CL% = 100(1 – α) percentile of an F-distribution with p numerator degrees of freedom and $n - p$ denominator degrees of freedom, where n is the number of data points used to fit the model for $ln\left(r^{PCT\ h}\right)$ and p is the number of model coefficients estimated from the data

$\bar{\boldsymbol{x}}_i^{MFPV}$ = $p \times 1$ column vector whose entries $\bar{x}_{ik}^{MFPV}, k = 1, 2, \cdots, p$ are means of the x_{ikl}^{MFPV} [as given by Eq. (4.3.3) with m = 1] values, where l = 1, 2, … , n_S^{MFPV}

$\hat{\boldsymbol{\Sigma}}_b^h$ = $p \times p$ variance-covariance matrix of the model coefficient vector $\boldsymbol{b}^h$ for the PCT normalized release of h = B, Li, or Na. The variances of the coefficients are located on the diagonal of the matrix, and the covariances between pairs of coefficients are located on the off-diagonal positions of the matrix

and the remaining notation is as previously defined following Eq. (4.3.2a). General equations for calculating model variance-covariance matrices such as $\hat{\boldsymbol{\Sigma}}_b^h$ are given in Section A.3 of Appendix A. The variance-covariance matrices for the IHLW PCT normalized B, Li, and Na models given in Table 4.1 are given in Appendix D of Kot et al. (2005).

An illustration of the CL% UCCI method is presented in Section 6.3.1.

4.3.4 Statistical Method for Determining the Numbers of Samples and Analyses per Sample to Demonstrate IHLW from an MFPV Batch Will Satisfy PCT Limits

This subsection discusses the methodology used to address Item 2 of Section 4.3.2. A modified version of the CL% UCCI formula given by Eqs. (4.3.4) to (4.3.7) in Section 4.3.3 can be used to calculate CL% UCCI values, given property-composition models for PCT normalized releases of B, Li, and Na, variance-covariance matrices for the model coefficients, and various combinations of values of the following factors

- number of samples per MFPV batch (n_S^{MFPV})
- number of analyses per MFPV sample (n_A^{MFPV})
- MFPV mixing/sampling composition uncertainty expressed in $ln(r_{ilm}^{PCT\ h})$ units [$SD_S(\hat{y}_{ilm}^h)$]

- MFPV analytical composition uncertainty expressed in $ln(r_{ilm}^{PCT\ h})$ units [$SD_A(\hat{y}_{ilm}^h)$]
- statistical percent confidence level (CL%)
- IHLW produced from three HLW tanks (AY-102, AZ-102, and C-104)

The modification to the CL% UCCI equations in Section 4.3.3 requires using

$$CHW_{i,CL\%\ UCI}^h = t_{1-\alpha,df}\sqrt{\frac{\left[SD_S(\hat{y}_{ilm}^h)\right]^2}{n_S^{MFPV}} + \frac{\left[SD_A(\hat{y}_{ilm}^h)\right]^2}{n_S^{MFPV} n_A^{MFPV}}} \tag{4.3.8}$$

in place of Eq. (4.3.6), where $SD_S(\hat{y}_{ilm}^h)$ and $SD_S(\hat{y}_{ilm}^h)$ are MFPV mixing/sampling and analytical uncertainties expressed in model [i.e., ln(PCT normalized release of h)] units. Note that process standard deviations $SD_S(\hat{y}_{ilm}^h)$ and $SD_A(\hat{y}_{ilm}^h)$ are used in Eq. (4.3.8), instead of RSDs. The natural logarithm of PCT values is used to model PCT and there is a strong approximate relationship of SD[ln(P)] ≈ RSD(P) for any property P. This relationship is explained in further detail in Section 3.2 of Piepel and Cooley (2002). This approximation allows RSD values [in original PCT release units] to be used as SD values [in ln(PCT) units] in this case.

The substitution of Eq. (4.3.8) for (4.3.6) in Eq. (4.3.4) is necessary for the investigation described in this section because the mixing/sampling and analytical uncertainties [expressed in ln(PCT) units] are chosen over a range of values rather than being estimated from production data as in Eq. (4.3.6). Also, notice that $n_A^{MFPV} = 1$ was assumed in Eq. (4.3.6), but the more general problem of $n_A^{MFPV} \geq 1$ is addressed by Eq. (4.3.8).

After calculating the CL% UCCI values for all of the combinations of input factors, the ones that satisfy the PCT limits are then inspected to find the least number of total analyses (number of samples × number of analyses) necessary to comply with the PCT limits. The results of these calculations are presented in Section 6.3.2.

4.3.5 Statistical Interval Method to Demonstrate that IHLW from an HLW Waste Type Will Satisfy PCT Limits

This subsection discusses and presents the formula for an appropriate statistical interval to satisfy Item 3 of Section 4.3.2. The statistical interval must account for (1) variation in PCT normalized releases of B, Li, and Na resulting from the variation in IHLW composition over the course of an HLW waste type, (2) uncertainty in the estimated IHLW composition corresponding to each MFPV batch resulting from mixing/sampling and analytical uncertainties, and (3) uncertainties in property-composition models used to predict PCT normalized B, Li, and Na releases for the estimated IHLW composition corresponding to a given MFPV batch. Finally, the statistical interval must provide high confidence that the true PCT normalized B, Li, and Na releases for the vast majority of IHLW produced from an HLW waste type are less than the limits specified in WAPS 1.3.

An appropriate statistical interval for demonstrating with high (X%) confidence that a high percentage (Y%) of IHLW produced from an HLW waste type satisfies the PCT limits in Eq. (4.3.1) is a X%/Y% UTI. The concept of a X%/Y% UTI was introduced in Section 3.2. Section A.3 of Appendix A discusses the statistical method for combining model and composition uncertainties that is used in forming a X%/Y% UTI. Piepel and Cooley (2002) derived the equations necessary to calculate an X%/Y% UTI. Sections 1.2 and 4.2 of Piepel and Cooley (2002) explain why the X%/Y% UTI approach is appropriate and preferred over the "two standard deviation" option mentioned in WAPS 1.3. A brief summary of the X%/Y% UTI equations developed by Piepel and Cooley (2002) will be presented here. Sections 3 and 4, and Appendix H in Piepel and Cooley (2002) provide more details and information.

Equation (3.3) in this report gives the general form of a two-sided X%Y% TI. To obtain a one-sided X%/Y% UTI, the equation changes to the following

$$\text{X\%/Y\% UTI} = \tilde{\mu} + k(X, Y)\,\tilde{\sigma} \tag{4.3.9}$$

where

X%/Y% UTI = a value that with X% confidence captures Y% of the distribution (population) of true mean ln(PCT releases) over the MFPV batches corresponding to an HLW waste type [ln(g/L)]

$\tilde{\mu}$ = estimate of the population mean that is calculated by forming the average model-predicted ln(PCT releases) for each MFPV batch and averaging them across all MFPV batches corresponding to an HLW waste type [ln(g/L)]

$k(X, Y)$ = UTI multiplier that is implicitly a function of X, Y, degrees of freedom associated with $\tilde{\sigma}$, and other parameters discussed subsequently in this section

$\tilde{\sigma}$ = estimate of the population standard deviation that properly accounts for (1) variation in ln(PCT releases) across MFPV batches corresponding to an HLW waste type, (2) mixing/sampling and analytical uncertainties for each MFPV batch, and (3) model uncertainty [ln(g/L)].

The quantities X and Y generally should have values between 95% (or 90%) and 100%, to provide high confidence that a high percentage of IHLW produced from an HLW waste type satisfies the WAPS 1.3 requirements. However, X and Y can never take values of 100%, because it is impossible to be 100% confident about 100% of the true distribution of ln(PCT releases) given estimated IHLW composition variation as well as IHLW composition and model uncertainties.

Equations for the terms on the right hand side of Eq. (4.3.9) are given in Section E.3 of Appendix E for the case of $n_S^{MFPV} > 1$ samples and $n_A^{MFPV} \geq 1$ analyses per sample of the i^{th} MFPV batch. However, during operation of the WTP IHLW facility, it is expected that $n_A^{MFPV} = 1$ for reasons discussed in Section 6. Hence, the equations for the terms on the right hand side of Eq. (4.3.9) are now given for the case of $n_S^{MFPV} > 1$ samples and $n_A^{MFPV} = 1$ analyses per sample of the i^{th} MFPV batch.

The equation for $\tilde{\mu}$ in Eq. (4.3.9) is given by

$$\tilde{\mu} = \bar{\bar{\hat{y}}}^{h} = \frac{\sum_{i=1}^{I} \bar{\hat{y}}_i^{h}}{I} = \frac{1}{I} \sum_{i=1}^{I} \left[\frac{\sum_{l=1}^{n_S^{MFPV}} \left(\sum_{k=1}^{p} b_k^h \, x_{ikl}^{MFPV} \right)}{n_S^{MFPV}} \right] \tag{4.3.10}$$

where the notation is as defined in previous subsections of Section 4.3. Note that Eq. (4.3.10) calculates the ordinary mean (average) of the model-predicted property values over the n_S^{MFPV} samples per MFPV batch and the *I* IHLW MFPV batches. An alternative approach would be to use $\hat{y}(\bar{\bar{\boldsymbol{x}}}^{MFPV})$, the model-predicted value for the normalized version of the mass-averaged composition over the *I* MFPV batches ($\bar{\bar{\boldsymbol{x}}}^{MFPV}$) that would result from supplying $\bar{\bar{\boldsymbol{g}}}^{MFPV}$ [calculated per Eq. (4.1.2) for balanced data and Eq. (4.1.5) for unbalanced data] to the normalizing transformation given in Eq. (4.3.3). Although this alternative approach would be consistent with some of the other compliance methods and calculations presented in this report, it is contrary to the typical method for developing TIs.

In general, *k* in Eq. (4.3.9) is calculated using the following equation

$$k(X,Y) = \frac{t(X,Y,df_{\tilde{\sigma}},\delta)}{\sqrt{I}} \tag{4.3.11}$$

where $t(X,Y,df_{\tilde{\sigma}},\delta)$ represents a non-centralized *t*-distribution with degrees of freedom $df_{\tilde{\sigma}}$ and non-centrality parameter δ, and *I* is the number of MFPV batches associated with an HLW waste type. This is Eq. (3.18d) in Piepel and Cooley (2002), adapted to the notation in this report. It is important to note that *k*(*X, Y*) is determined so as to compensate for the effects of MFPV mixing/sampling uncertainty and analytical uncertainty, which are "nuisance uncertainties" with respect to the population for which a X%/Y% UTI is desired.

The expression for $df_{\tilde{\sigma}}$ in Eq. (4.3.11) is given by

$$df_{\tilde{\sigma}} \approx \frac{\left[\left((\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^{\mathrm{T}} \, \hat{\boldsymbol{\Sigma}}_b^h \, \bar{\bar{\boldsymbol{x}}}_I^{MFPV} \right) + \sum_{i=1}^{I} (\bar{\hat{y}}_i^h - \bar{\bar{\hat{y}}}^h)^2 \Big/ (I-1) \right]^2}{\frac{\left((\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^{\mathrm{T}} \, \hat{\boldsymbol{\Sigma}}_b^h \, \bar{\bar{\boldsymbol{x}}}_I^{MFPV} \right)^2}{df_m} + \frac{\left[\sum_{i=1}^{I} (\bar{\hat{y}}_i^h - \bar{\bar{\hat{y}}}^h)^2 \Big/ (I-1) \right]^2}{I-1}} \tag{4.3.12}$$

where

$df_{\tilde{\sigma}}$ = approximate degrees of freedom associated with $\tilde{\sigma}$

$\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ = $p \times 1$ column vector whose entries $\bar{\bar{x}}_k^{MFPV}, k = 1, 2, \cdots, p$ are means of the x_{ikl}^{MFPV} [as given by Eq. (4.3.3) with m = 1] values, where i = 1, 2, … , I and l = 1, 2, … , n_S^{MFPV}. Note that $p = n_{mc}^h$ because of the model form in Eq. (4.3.2a).

$\hat{\boldsymbol{\Sigma}}_b^h$ = $p \times p$ variance-covariance matrix of the model coefficient vector $\boldsymbol{b}^h$ for the PCT normalized release of h = B, Li, or Na

df_m = degrees of freedom for the model relating PCT normalized releases of h = B, Li, or Na to IHLW composition. This quantity is given by $n - p$, where n is the number of data points used to fit the model and p is the number of model coefficients estimated using the data.

I = number of IHLW MFPV batches corresponding to an HLW waste type.

The expression in Eq. (4.3.12) is derived in Section E.3 of Appendix E for the case of $n_S^{MFPV} > 1$ samples and $n_A^{MFPV} \geq 1$ analyses per sample of the i^{th} MFPV batch. The expression in Eq. (4.3.12) is a special case of Eq. (E.3.4) when $n_A^{MFPV} = 1$.

The expression for δ in Eq. (4.3.11) is given by

$$\delta = z_{1-\beta}\sqrt{I}\,\frac{\sigma_g}{\sigma} \tag{4.3.13}$$

where

δ = non-centrality parameter for the non-central t-distribution used in calculating the $k(X, Y)$ multiplier for an X%/Y% UTI

$z_{1-\beta}$ = $100(1 - \beta)$ percentile of the standard normal distribution

I = number of IHLW MFPV batches corresponding to an HLW waste type

σ_g = standard deviation of the distribution of true ln(PCT normalized release) values for IHLW produced from a given HLW waste type [ln(g/L)]

σ = $\left[\sigma_{\text{g}}^2 + \bar{\sigma}_m^2 + \frac{(\sigma_S^{MFPV})^2 + (\sigma_A^{MFPV})^2}{n_S^{\text{MFPV}}}\right]^{0.5}$ = standard deviation of the distribution of possible $\bar{\hat{y}}_i^h$ values over the I IHLW MFPV batches corresponding to an HLW waste type [ln(g/L)].

Equations (4.3.12) and (4.3.13) for $df_{\tilde{\sigma}}$ and δ are based on Eqs. (3.18f) and (3.18e) in Section 3.7 and development work in Appendix H of Piepel and Cooley (2002). Note that σ_g includes only the true variation in ln(PCT normalized release) values, and not the true model, sampling, and chemical analysis "nuisance" uncertainties. On the other hand, σ (of which $\tilde{\sigma}$ is an estimate) includes true uncertainties for modeling, sampling, and chemical analyses. Hence, σ_g / σ is the fraction of the inflated (by model, sampling, and analytical nuisance uncertainties) standard deviation represented by the true standard deviation in ln(PCT normalized release) values over IHLW produced from an HLW waste type. Per Eq. (4.3.13) and the underlying theory (see Appendix H of Piepel and Cooley 2002), it is only necessary that the ratio σ_g / σ of these two true SDs be "known" (i.e., well-estimated). Scope discussed by Piepel and Heredia-Langner (2003) will produce estimates of the relevant variations and uncertainties based on information prior to commissioning testing. These estimates will provide for calculating preliminary estimates of the σ_g / σ ratio for different HLW waste types. It is also expected that cold commissioning testing of the WTP IHLW facility will provide updated estimates of variations and uncertainties that can be used to calculate updated estimates of the the σ_g / σ ratio for different HLW waste types. Section 6.3.3 and Section G.3 of Appendix G illustrate how to calculate the σ_g / σ ratio from simulated operating data (such as would be available during cold commissioning).

The estimate of the population standard deviation $\tilde{\sigma}$ in Eq. (4.3.9) is given by

$$\tilde{\sigma} = \left\{ \left[(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^T \boldsymbol{\Sigma}_{\boldsymbol{b}}^h \bar{\bar{\boldsymbol{x}}}_I^{MFPV} \right] + \sum_{i=1}^{I} \left(\bar{\hat{y}}_i^h - \bar{\bar{\hat{y}}}^h \right)^2 \Big/ (I-1) \right\}^{0.5} \tag{4.3.14}$$

where $\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ is a $p \times 1$ column vector, where because of the model form used, $p = n_{mc}^h$. The entries of $\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ are given by $\bar{\bar{x}}_k^{MFPV}$, $k = 1, 2, \cdots, n_{mc}^h$, which are calculated using

$$\bar{\bar{x}}_I^{MFPV} = \frac{1}{I} \sum_{i=1}^{I} \bar{x}_{ik}^{MFPV} = \frac{1}{I} \sum_{i=1}^{I} \left(\frac{\sum_{l=1}^{n_S^{MFPV}} x_{ikl}^{MFPV}}{n_S^{MFPV}} \right) . \tag{4.3.15}$$

In Eq. (4.3.15), x_{ikl}^{MFPV} is calculated using Eq. (4.3.3) with g_{ijl}^{MFPV} used as inputs calculated by Eq. (A.1.3), $\bar{\hat{y}}_i^h$ is given by Eq. (4.3.5), $\bar{\bar{\hat{y}}}^h$ is given by Eq. (4.3.10), and I is the number of MFPV batches associated with the HLW waste type for which an X%/Y% UTI is to be calculated. The remaining notation in Eqs. (4.3.14) and (4.3.15) is as defined in previous subsections of Section 4.3.

Equations (4.3.14) and (4.3.15) are special cases of more general equations applicable when $n_S^{MFPV} \geq 1$ and $n_A^{MFPV} = 1$. The more general equations for the case of $n_S^{MFPV} \geq 1$ and $n_A^{MFPV} \geq 1$ are presented in Section E.3 of Appendix E. From the derivations in Section E.3, it is seen that the first term in Eq. (4.3.14) represents model uncertainty while the second term represents composition uncertainty expressed in model units. The composition uncertainty includes (1) variation in IHLW composition over the *I* MFPV batches corresponding to an HLW waste type and (2) uncertainties associated with estimating IHLW composition for a single MFPV batch, reduced by averaging over multiple samples per MFPV batch and analyses per MFPV sample.

An illustration of the X%/Y% UTI method and equations is presented in Section 6.3.3.

4.3.6 Statistical Method for Determining the Numbers of Samples and Analyses per Sample to Demonstrate IHLW from a Waste Type Will Satisfy PCT Limits

This subsection discusses the methodology used to address Item 4 of Section 4.3.2. The X%/Y% UTI formula overviewed in Section 4.3.5 and discussed in detail by Piepel and Cooley (2002) can be used to calculate X/Y%% UTI values (or half-widths thereof), given various combinations of values of the following factors

- number of samples per MFPV batch (n_S^{MFPV})
- number of analyses per MFPV sample (n_A^{MFPV})
- MFPV mixing/sampling composition uncertainty expressed in $ln(r_{ilm}^{PCT\ h})$ units [$SD_S(\hat{y}_{ilm}^h)$]
- MFPV analytical composition uncertainty expressed in $ln(r_{ilm}^{PCT\ h})$ units [$SD_A(\hat{y}_{ilm}^h)$]
- statistical percent confidence (X%)
- percent coverage of the distribution of true PCT release values over a waste type (Y%)
- IHLW produced from three HLW tanks (AY-102, AZ-102, and C-104).

Piepel and Cooley (2002) calculated half-widths of X%/Y% UTIs (which they denoted UTIHW) for combinations of values of the preceding and other parameters (e.g., model uncertainty and model degrees of freedom). The results were summarized in their Tables 4.3 to 4.6, and are briefly summarized in Section 6.3.4.

In this report, additional calculations were performed varying selected factors listed in the bullets above. The X%/Y% UTI values that satisfy the PCT limits were then inspected to find the least number of total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) necessary to comply with the PCT limits. The results of these calculations are presented in Section 6.3.4.

4.4 Compliance Approach and Methods for IHLW WAPS Specification 1.5: Hazardous Waste

Section 4.4.1 lists the applicable WAPS Specification 1.5. Section 4.4.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Section 4.4.3 presents the statistical methods that will be used to implement the statistical aspects of the compliance strategy.

4.4.1 WAPS Specification 1.5: Hazardous Waste Specification

The Producer shall determine and report to DOE/RW the presence or absence of any hazardous waste listed in 40 CFR 261.31 through 40 CFR 261.33, in the waste or in any feed stream proposed for storage or disposal. Any RCRA-listed component in a waste shall require the Producer to petition EPA and receive exemption to delist the waste.

The Producer shall perform the appropriate tests and procedures, as described in 40 CFR 261.20 through 40 CFR 261.24 using samples from production runs or prototypical specimens to determine if the waste that will be received by DOE/RW for transportation and disposal has hazardous characteristics. Any waste that is shown to have hazardous characteristics shall be treated to remove such characteristics.

The Producer shall certify in the WQR that the waste is not hazardous, including the absence of any listed components. The characteristic testing methods to be used shall be described in the WCP and the results documented in the WQR. Any modification to these methods needs prior approval from DOE/RW.

4.4.2 Statistical Aspects of the IHLW Compliance Strategy for WAPS 1.5

Section 4.1.5 of the IHLW PCP (Nelson 2003) describes the compliance strategy for WAPS Specification 1.5. The strategy involves using a data quality objectives (DQO) process to establish criteria for developing adequate data with acceptable quality to support a delisting petition and a LDR treatability variance for IHLW. The DQO process involves several statistical aspects, including statistical experimental design and planning for statistical analysis of the resulting data. The results of the DQO process are documented in a report by Cook and Blumenkranz (2003). The results of the data development, quality assurance, and statistical data analyses in support of the IHLW LDR treatability variance petition are contained in a report by Kot et al. (2003). The results of the data development, quality assurance, and statistical data analyses in support of the IHLW delisting petition are contained in a report by Kot et al. (2004b).

4.4.3 Statistical Methods to Implement the IHLW Compliance Strategy for WAPS 1.5

Relevant statistical methods for the statistical aspects described in Section 4.4.2 are discussed in the reports by Cook and Blumenkranz (2003), Kot et al. (2003), and Kot et al. (2004b).

If the HLW LDR treatment variance and delisting processes lead to future revisions in the IHLW compliance strategy that include "during production" aspects of compliance, any associated statistical methods or equations will be included in a future revision of this subsection.

4.5 Compliance Approach and Methods for IHLW Contract Specification 1.2.2.1.5: Dangerous and Hazardous Waste Requirements

Section 4.5.1 lists the applicable Contract Specification 1.2.2.1.5. Section 4.5.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Section 4.5.3 presents the statistical methods that will be used to implement the statistical aspects of the compliance strategy.

4.5.1 Contract Specification 1.2.2.1.5: Dangerous and Hazardous Waste Requirements

The WTP shall be designed, constructed, and operated so that the IHLW product does not designate as characteristic or criteria for dangerous waste or extremely hazardous waste pursuant to WAC 173-303-070, and is not restricted from land disposal pursuant to WAC 173-303-140 and 40CFR268, Land Disposal Restrictions.

4.5.2 Statistical Aspects of the IHLW Compliance Strategy for Contract Specification 1.2.2.1.5

Section 4.1.5 of the IHLW PCP (Nelson 2003) describes the compliance strategy for WAPS Specification 1.5. The strategy involves using a DQO process to establish criteria for developing adequate data with acceptable quality to support a delisting petition and a LDR treatability variance for IHLW. The DQO process involves several statistical aspects, including statistical experimental design and planning for statistical analysis of the resulting data. The results of the DQO process are documented in a report by Cook and Blumenkranz (2003). The results of the data development, quality assurance, and statistical data analyses in support of the IHLW LDR treatability variance petition are contained in a report by Kot et al. (2003). The results of the data development, quality assurance, and statistical data analyses in support of the IHLW delisting petition are contained in a report by Kot et al. (2004b).

4.5.3 Statistical Methods to Implement IHLW Compliance Strategy for Contract Specification 1.2.2.1.5

Relevant statistical methods for the statistical aspects described in Section 4.5.2 are discussed in the reports by Cook and Blumenkranz (2003), Kot et al. (2003), and Kot et al. (2004b).

If the HLW LDR treatment variance and delisting processes lead to future revisions in the IHLW compliance strategy that include "during production" aspects of compliance, any associated statistical methods or equations will be included in a future revision of this subsection.

4.6 Compliance Approach and Methods for IHLW WAPS Specification 1.6: IAEA Safeguards Reporting for HLW

Section 4.6.1 lists the applicable WAPS Specification 1.6. Section 4.6.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Sections 4.6.3 to 4.6.6 present the statistical methods that will be used to implement the statistical aspects of the compliance strategy.

4.6.1 WAPS 1.6: IAEA Safeguards Reporting for HLW

The Producer shall report the following in the production records:

(1) The total and fissile uranium and plutonium content of each canister in grams.

(2) The concentration of plutonium in grams per cubic meter for each canister.

(3) The ratio by weight of the total element of the following isotopes: 233U, 234U, 235U, 236U, 238U, 238Pu, 239Pu, 240Pu, 241Pu, and 242Pu.

4.6.2 Statistical Aspects of the IHLW Compliance Strategy for WAPS 1.6

The following items describe the statistical and related aspects of the IHLW compliance strategy for WAPS Specification 1.6, as described in Rev. 0 of the IHLW PCP (Nelson 2003). Although Rev. 1 of the IHLW PCP has been recently released (Nelson et al. 2004), the work scope addressed in this report was based on the compliance strategy described in Rev. 0.

Item 1: Develop formulas for calculating the means and SDs of the total and fissile uranium and plutonium mass in IHLW canisters corresponding to an HLW waste type.

Item 2: Develop a statistical method for estimating the concentration of plutonium in IHLW canisters during production.

Item 3: Develop a statistical method for estimating the isotopic ratios of uranium and plutonium in IHLW canisters during production.

Item 4: Determine the numbers of samples, analyses per sample, and other process measurements required to adequately estimate the compliance quantities described in WAPS 1.6.

Items 1 through 2 are somewhat vague compared to the WAPS 1.6 compliance strategy in Rev. 0 of the IHLW PCP (Nelson 2003), which calls for developing methods to calculate means and SDs of the compliance quantities over each HLW waste type. The strategy also calls for the SDs to account for the variations and uncertainties affecting the radionuclide composition and the mass of glass in IHLW canisters. However, the current IHLW compliance strategy (Nelson et al. 2004) calls for analyzing the majority of the radionuclides in only one MFPV batch corresponding to an HLW waste type. In that case, during production there will not be multiple values over the MFPV batches and canisters corresponding to an HLW waste type to calculate means and SDs. An alternative may be to estimate variation over multiple MFPV batches and canisters before production and then use these prior estimates to quantify variation during production. In any case, it will be possible to quantify the uncertainty in the compliance quantities based on multiple samples and possibly multiple analyses per sample for the single MFPV batch for which all radionuclides are measured.

The statistical methods to implement the preceding aspects of the WTP IHLW compliance strategy for WAPS Specification 1.1.2 are discussed in Sections 4.6.3 to 4.6.6.

4.6.3 Statistical Method for Estimating the Total and Fissile Uranium and Plutonium Mass in IHLW Canisters During Production

This subsection addresses Item 1 in Section 4.6.2. Equations for calculating the means and SDs of the masses of total and fissile U and Pu are given in Section A.5.1 of Appendix A. However, these equations assume that estimates of each isotope of U and Pu will be available for every MFPV batch. That was the WTP compliance strategy according to Rev. 0 of the IHLW PCP (Nelson 2003).

Subsequent to the completion of the work presented in Section A.5.1 of Appendix A, Rev. 1 of the IHLW PCP (Nelson et al. 2004) was issued with revisions to the compliance strategy. A significant revision was that only selected radionuclides would be measured for every MFPV batch (see Table 2.1). The work to develop statistical methods to address Item 1 of Section 4.6.2 according to the revised IHLW compliance strategy in Rev. 1 of the IHLW PCP (Nelson et al. 2004) is scheduled for completion in FY 2005. The results will be documented in a future revision of this report.

4.6.4 Statistical Method for Estimating the Concentration of Plutonium in IHLW Canisters During Production

This subsection addresses Item 2 in Section 4.6.2. Equations for calculating the mean and SD of the concentration of Pu in IHLW canisters during production are given in Section A.5.2 of Appendix A. However, these equations assume that each isotope of U and Pu will be estimated in every MFPV batch. That was the WTP compliance strategy according to Rev. 0 of the IHLW PCP (Nelson 2003).

Subsequent to the completion of the work presented in Section A.5.2 of Appendix A, Rev. 1 of the IHLW PCP (Nelson et al. 2004) was issued with revisions to the compliance strategy. A significant revision was that only selected radionuclides would be measured for every MFPV batch (see Table 2.1). The work to develop statistical methods to address Item 2 of Section 4.6.2 according to the revised IHLW compliance strategy in Rev. 1 of the IHLW PCP (Nelson et al. 2004) is scheduled for completion in FY 2005. The results will be documented in a future revision of this report.

4.6.5 Statistical Method for Estimating the Isotopic Ratios of Uranium and Plutonium in IHLW Canisters During Production

Per the WTP Project's compliance strategy, the isotopic ratios of uranium and plutonium will be treated as constant over the MFPV batches corresponding to a waste type (an HBV). The reason for this is because all uranium isotopes behave the same chemically, as do all plutonium isotopes. Hence, the ratios by weight of the individual uranium isotopes to total uranium and the ratios by weight of the individual plutonium isotopes to total plutonium are expected to remain constant over a given HLW waste type (HBV). Neither pretreatment processing nor vitrification is expected to affect the isotopic ratios.

Even though the isotopic ratios are expected to remain constant over each HLW waste type, the estimates of the ratios for a given waste type will be uncertain because they will be calculated from

isotope measurements for a single MFPV batch. Hence, statistical methods must be developed to quantify the uncertainty in uranium and plutonium isotopic ratios. The first step in addressing this problem is to develop the equations to calculate isotopic ratios from a single IHLW MFPV batch. Section A.5.3 of Appendix A presents the development of these equations. Specifically, Equation (A.5.7) in Section A.5.3 of Appendix A provides for calculating mass isotopic ratios of U and Pu based on multiple samples and analyses per sample for a single MFPV batch corresponding to a given HLW waste type.

The work to develop the statistical method for quantifying uncertainties in reportable isotopic ratios [calculated according to Eq. (A.5.7)] is scheduled for FY 2005. This work will address Item 3 of Section 4.6.2. The results will be included in this section in a future revision of this report.

4.6.6 Statistical Method for Determining the Numbers of Samples, Analyses, and Measurements to Estimate the WAPS 1.6 Compliance Quantities During Production

Work is scheduled during FY 2005 to address Item 4 in Section 4.6.2. The method to determine the numbers of samples, analyses per sample, and other process measurements required to adequately estimate the compliance quantities described in WAPS 1.6 will be documented in this section in a future revision of this report.

4.7 Compliance Approach and Methods for WAPS Specification 3.8.2: Heat Generation at Year of Shipment

Section 4.7.1 lists the applicable WAPS Specification 3.8 and sub-specification 3.8.2. Section 4.7.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Section 4.7.3 presents the statistical methods that could be used to implement the statistical aspects of the compliance strategy.

4.7.1 WAPS Specification 3.8: Heat Generation Specification

The heat generation rate for each canistered waste form shall not exceed 1500 watts per canister at the year of shipment.

4.7.2 WAPS Specification 3.8.2: Heat Generation at Year of Shipment

The Producer shall report in the Storage and Shipping Records the estimated heat generation rate for each canistered waste form. The Producer shall describe the method for compliance in the WCP.

4.7.3 Statistical Aspects of the IHLW Compliance Strategy for WAPS 3.8.2

The "Compliance Strategy" portion of Section 4.3.8.2 of Rev. 0 of the IHLW PCP (Nelson 2003) describes the WTP Project's compliance strategy for WAPS 3.8.2 as follows:

> The WTP project's strategy for compliance with this specification is to calculate the heat generation rate over all canisters corresponding to a given waste type based on the estimated per-canister radionuclide inventories as described in response to WAPS Specification 1.2.2. The heat generation rate of the canistered waste forms at the time of delivery to the CSB will be calculated using a computer code (e.g., MicroShield [Grove 1996]). The mean and standard deviation of the heat generation rate of each canister over the course of a waste type will be reported in the Storage and Shipping Records.

The *Production Implementation* portion of Section 4.3.8.2 of Rev. 0 of the IHLW PCP (Nelson 2003) describes[(a)] relevant activities as including

- Determine per-canister radionuclide inventories over the course of a waste type as discussed in the response to WAPS Specification 1.2.2, Radionuclide Inventory During Production. These determinations of radionuclide inventories over the course of a waste type will account for variations over the course of a waste type in radionuclide concentrations and the amounts (i.e., fill heights) of IHLW glass in the canisters. The estimated inventories will be based on radiochemical analysis of the waste feed to HLW vitrification from pretreatment, or analysis of the IHLW product produced over the course of the waste type, or a combination of both.

- Calculate the heat generation rate over all canisters corresponding to a given waste type based on the estimated per-canister radionuclide inventories. The WTP project will use a computer code (e.g., MicroShield [Grove 1996]) to calculate the heat generation rate for the canistered waste forms at the time of delivery to the Canister Storage Building. Heat generation rates, as a function of time, will be calculated to account for radionuclide decay.

- Calculate the mean and SD for heat generation rates over the course of a given waste type. The SD of heat generation rates will be calculated based on the variations and uncertainties in the estimates of radionuclide inventories over the course of a waste type. Variations and uncertainties in radionuclide concentrations and the amount of glass in a canister (e.g., canister fill heights) over a waste type will be accounted for in the calculations of variation and uncertainty in per-canister radionuclide inventories, and hence in per-canister heat generation rates.

Currently, there is no work scope in the Statistical Analysis task of the PNWD WTPSP to address the statistical aspects of (1) the first bullet (accounting for variations in radionuclide concentrations and canister fill heights) and (2) the third bullet (calculating means and SDs, where the SDs must account for variations and uncertainties). At one point, there was scope to develop a statistical interval method to demonstrate with high confidence that a very high percentage of IHLW canisters corresponding to a waste type would have heat loadings meeting the 1500-watt limit. However, that scope was subsequently cut when the WTP Project decided that a statistical-interval-based compliance approach was not needed, which was based on the expectation that heat loadings of IHLW canisters would be well below the 1500-watt limit. However, no replacement scope corresponding to the "mean and SD" approach of the preceding

(a) The three bullets following were copied and pasted from Rev. 0 of the IHLW PCP (Nelson 2003), except for two minor changes. In the second bullet, Canister Storage Building was spelled out in place of an acronym. Also, the portion of the third bullet after the first sentence was copied and pasted from the middle of the second bullet for better clarity.

bullets was added. Regardless, some comments about statistical methods are made in the following section.

4.7.4 Statistical Methods to Implement the IHLW Compliance Strategy for WAPS 3.8.2

As noted in Section 4.7.2, the Statistical Analysis task of the WTPSP currently has no scope to develop statistical methods to address the statistical aspects of the WTP compliance strategy described in Section 4.7.2. If it were possible for the WTP Project to calculate a heat generation rate for each IHLW canister associated with an HLW waste type, then a mean and SD could be calculated over those canisters using standard formulas for those two statistics. However, as noted previously in Section 4.2.4, it will be very difficult to accurately associate IHLW compositions corresponding to MFPV batches with specific IHLW canisters to calculate per-canister inventories of radionuclides. Hence, it will be very difficult to accurately calculate the heat generation separately for each particular IHLW canister and in turn calculate the mean and SD over the canisters associated with an HLW waste type.

An alternative approach would be to use a Monte Carlo approach with a computer code such as MicroShield (Grove 1996). The means and SDs of radionuclide inventories per IHLW canister, calculated as discussed in Section 4.2.4 (and in Section A.2.2 of Appendix A) could serve as the basis for generating random sets of radionuclide inventories from which the mean and SD of heat generation rate per canister could be calculated.

Another approach is suggested by Eq. (A.6.1) presented in Section A.6 of Appendix A for calculating the maximum heat output of an IHLW canister with specified radionuclide composition/inventories. This approach would provide for calculating means and SDs reflecting the variation in IHLW radionuclide composition/inventory over MFPV batches corresponding to an HLW waste type. However, it would not reflect the variation in the mass of glass per canister over IHLW canisters corresponding to a waste type. A modification of Eq. (A.6.1) to include the determined mass of glass in an IHLW canister rather than the maximum would result in a conceptual equation that would allow for developing equations for the mean and SD of heat output, similar to what was done for radionuclide inventories in Section A.2.2 of Appendix A.

4.8 Compliance Approach and Methods for IHLW WAPS Specification 3.14: Concentration of Plutonium in Each Canister

Section 4.8.1 lists the applicable WAPS Specification 3.14. Section 4.8.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Section 4.8.3 presents the statistical methods that will be used to implement the statistical aspects of the compliance strategy.

4.8.1 WAPS Specification 3.14: Concentration of Plutonium in Each Canister

> *The concentration of plutonium in each HLW standard canister shall be less than 2500 grams/cubic meter.*

4.8.2 Statistical Aspects of the IHLW Compliance Strategy for WAPS 3.14

The majority of the WTP strategy for complying with WAPS 3.14, as described in Rev. 0 of the IHLW PCP (Nelson 2003), involves pre-production activities (i.e., WFQ activities). The following activity, copied from Rev. 0 of the IHLW PCP, is the only one that involves demonstrating compliance during IHLW production.

Item 1: Develop statistical methods to account for variations and uncertainties in per canister plutonium concentrations to demonstrate with high confidence that the limits of this specification will be satisfied for each canister produced from a given waste type.

Although Rev. 1 of the IHLW PCP has been recently released (Nelson et al. 2004), the work scope addressed in this report was based on the compliance strategy described in Rev. 0. However, the majority of the scope for the Statistical Analysis task of the WTPSP is scheduled for completion in FY 2005. Hence, this section of the report will be updated in a future revision to reflect the compliance strategy in Rev. 1 of the IHLW PCP (Nelson et al. 2004).

4.8.3 Statistical Method to Implement the IHLW Compliance Strategy for WAPS 3.14

Section A.7 discusses equations for calculating the mean and SD of Pu concentration per canister (g/m^3) over IHLW canisters associated with an HLW waste type. The work to address Item 1 of Section 4.8.2 is scheduled for completion in FY 2005. It is envisioned that a statistical X%/Y% UTI formula will be developed using the mean and SD equations from Section A.7. A X%/Y% UTI would provide high confidence (X%) that a high percentage (Y%) of IHLW corresponding to an HLW waste type will have Pu concentration per canister less than the prescribed limit. This, or another appropriate statistical method based on any revisions to the Rev. 1 IHLW PCP compliance strategy for this specification, will be addressed in a future revision of this report.

4.9 Compliance Approach and Methods for IHLW Contract Specification 1.2.2.1.6: Product Loading

Section 4.9.1 lists the applicable Contract Specification 1.2.2.1.6. Section 4.9.2 summarizes the WTP compliance strategy for this specification and explains why no statistical methods are required.

4.9.1 Contract Specification 1.2.2.1.6: Product Loading

> *Loading of non-volatile components in Envelope D, and, if directed by DOE, entrained solids after washing in accordance with Specification 12, Number of HLW Canisters Per Batch of Waste Envelope D, shall be achieved, such that, the concentration of at least one of the waste components or waste component combinations in Table TS-1.1, Minimum Component Limits in HLW Glass exceeds its minimum weight percent in HLW glass as identified in Table TS-1.1 (e.g., for a high-iron waste, the Contractor shall incorporate at least 12.5 weight percent iron oxide from the waste into the glass). The product loading shall not cause the limits in any other requirement of this specification to be violated.*

Product waste loading shall be calculated on an average basis for each batch transfer of Waste Envelope D. The waste loading may be adjusted downward if necessary to comply with Universal Treatment Standards (UTS) leaching requirements.

4.9.2 The IHLW Compliance Strategy for Contract Specification 1.2.2.1.6

The WTP Project's compliance strategy for this specification is described in Section 5.1.6 of the IHLW PCP (Nelson 2003).[(a)] During IHLW production, the compliance strategy will involve determining the IHLW chemical composition and verifying that at least one product loading limit from Table TS-1.1 is satisfied on an average basis for each batch transfer of an HLW waste type.

Before Baseline Change Request (BCR)-119, the Statistical Analysis task of the PNWD WTPSP included scope to develop a statistical approach for demonstrating that at least one product loading limit from Table TS-1.1 was satisfied. It was envisioned that the statistical approach would account for the (1) uncertainties affecting the IHLW chemical composition estimate for each MFPV batch, and (2) variations across MFPV batches in calculating average product loadings corresponding to a batch transfer of an HLW waste type. In fact, equations for calculating product (waste) loading were developed as part of the work scope before BCR-119. However, those equations were for the IHLW process before the CRVs were eliminated and were no longer applicable to the new IHLW process and approach for estimating IHLW chemical composition for each MFPV batch. Hence, those equations are not presented in Appendix A.

Ultimately, the WTP Project decided that it was sufficient to compare the average product loadings over a batch transfer of an HLW waste type without accounting for variations and uncertainties. Hence, the scope to develop a statistical approach for demonstrating compliance with Table TS-1.1 limits was removed in BCR-119.

(a) See Section 1.0 for a discussion of why this report addresses the IHLW PCP WAPS specifications and Rev. 0 (Nelson 2003) rather than Rev. 1 of the IHLW PCP Rev. 1 (Nelson et al. 2004).

5.0 ILAW Compliance and Statistical Implementation Methods by Specification

This section describes the WTP ILAW compliance strategies and statistical implementation methods for each WTP contract (DOE-ORP 2003) specification having one or more statistical aspects to the compliance strategy. ILAW specifications not having statistical aspects to the corresponding WTP compliance strategies are not listed or discussed.

5.1 Compliance Approach and Methods for ILAW Contract Specification 2.2.2.6.2: Chemical Composition During Production

Section 5.1.1 lists the applicable Contract Specification 2.2.2.6.2. Section 5.1.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Sections 5.1.3 and 5.1.4 present the statistical methods that will be used to implement the statistical aspects of the compliance strategy.

5.1.1 Contract Specification 2.2.2.6.2: Chemical Composition During Production

> *The production documentation (Table C.5-1.1, Deliverable 6.7) shall provide the chemical composition of each waste form, optional filler, and package. The reported composition shall include elements (excluding oxygen) present in concentrations greater than 0.5 percent by weight and elements and compounds required to meet regulatory or Contract requirements.*

5.1.2 Statistical Aspects of the ILAW Compliance Strategy for Contract Specification 2.2.2.6.2

The following items describe the statistical and related aspects of the ILAW compliance strategy for Contract Specification 2.2.2.6.2 (see the ILAW PCP, Nelson et al. 2003) that are addressed in this report.[(a)]

Item 1: Determine the numbers of samples, chemical analyses per sample, and other process measurements necessary to adequately estimate ILAW chemical composition that would be produced from each MFPV batch.

Item 2: Develop equations for calculating the means and SDs of reportable glass components over the chemical composition determinations of ILAW produced as a given LAW waste type (or production lot, to be defined by the WTP) is being processed. Equations for SDs will account for applicable sources of variation and uncertainty.

The statistical methods to implement these aspects of the WTP ILAW compliance strategy for Contract Specification 2.2.2.6.2 are discussed in Sections 5.1.3 and 5.1.4.

(a) See Section 1.0 for a discussion of why this report addresses ILAW PCP Rev. 0 (Nelson et al. 2003) rather than ILAW PCP Rev. 1 (Westsik et al. 2004).

5.1.3 Statistical Method for Determining the Numbers of Samples, Analyses per Sample, and Volume Determinations to Estimate the ILAW Chemical Composition for an MFPV Batch

During ILAW production operations, the chemical composition of the ILAW corresponding to an MFPV batch will be calculated by mass-balance equations using the following inputs:

- Chemical and radionuclide concentrations of pre-treated waste in an LAW CRV determined by chemical and radiochemical analyses of CRV samples
- GFC compositions and measured weights of GFCs added to the MFPV
- Calculated volumes of the CRV and MFPV before and after transfers (obtained by measuring the level of vessel contents and applying volume-level calibration equations)
- Chemical and radionuclide composition of the MFPV heel from the previous batch.

The applicable mass-balance equations for calculating ILAW chemical composition are given in Section B.1 of Appendix B. The balance of this subsection describes the statistical method to address Item 1 in Section 5.1.2.

Section 3.4.2 describes the Monte Carlo simulation approach for assessing the impacts of the following factors

- number of samples per CRV batch (n_S^{CRV})
- number of analyses per CRV sample (n_A^{CRV})
- number of volume determinations of the CRV and MFPV before and after transfers (n_V^{CRV} and n_V^{MFPV})
- mixing/sampling %RSD in the concentration of the j^{th} element in a CRV batch [$\%RSD_S(c_j^{CRV})$]
- analytical %RSD in the concentration of the j^{th} element in a CRV batch [$\%RSD_A(c_j^{CRV})$]
- GFC composition uncertainty, represented by the standard deviation in the mass fraction of the j^{th} component (oxide or halogen) in the k^{th} GFC [$SD(G_{jk}^{GFC})$]
- GFC mass uncertainty, represented by the standard deviation of the mass of the k^{th} GFC added to a MFPV batch. This uncertainty includes uncertainties due to batching, weighing, and transfers of GFCs.
  [$SD(a_k^{GFC})$]
- volume uncertainties in the CRV and MFPV. The magnitudes of these uncertainties will depend on the level of contents in a vessel, but a generic notation is used for now (SD_V^{CRV} and SD_V^{MFPV})
- statistical percent confidence level (CL%)

- ILAW produced from three LAW tanks representing one each of Envelopes A (AP-101), B (AZ-101), and C (AN-107)

on the total uncertainty in estimating ILAW chemical composition (mass fractions of oxides or halogens) for each MFPV batch. It is necessary at this time to consider a range of values for process uncertainties because final estimates have not yet been produced by the WTP Project. A future update of this report will use final estimates of process uncertainties to determine the final recommended numbers of CRV samples, chemical analyses per CRV sample, and volume determinations of the CRV and MFPV for estimating ILAW chemical composition.

To assess the total uncertainty in estimating ILAW chemical composition for a given MFPV batch, the %RHW of a two-sided CL% empirical confidence interval (ECI) on the mass fraction of each ILAW component (oxide or halogen) is used. A Monte Carlo simulation approach was used to obtain CL% ECIs and the corresponding %RHWs. The mass-balance equations in Section B.1 were used to develop the Monte Carlo simulation approach. The formula for a %RHW, expressed as a percentage of the nominal value (mass fraction) of a given glass component, is given by

$$\%RHW_{CL\%}(g_{sj}^{MFPV}) = \frac{100\left(MF_{sj}^{(1-\alpha/2)} - MF_{sj}^{(\alpha/2)}\right)/2}{MF_j^{Nominal}} \qquad (5.1.1)$$

where

$\%RHW_{CL\%}(g_{sj}^{MFPV})$ = percent relative half-width of the two-sided CL% ECI on the mean mass fraction of the j^{th} oxide in the MFPV for the s^{th} simulation test case (%)

$100(1-\alpha/2)$ = CL% = percent confidence for the two-sided ECI (e.g., 90% when α = 0.10)

$MF_{sj}^{(1-\alpha/2)}$ = $100(1-\alpha/2)^{th}$ percentile of the 1000 simulated mass fractions for the j^{th} oxide and the s^{th} simulation test case (g_{oxide}/g_{oxides})

$MF_{sj}^{(\alpha/2)}$ = $100(\alpha/2)^{th}$ percentile of the 1000 simulated mass fractions for the j^{th} oxide and the s^{th} simulation test case (g_{oxide}/g_{oxides})

$MF_j^{Nominal}$ = nominal mass fraction of the j^{th} oxide in the MFPV (g_{oxide}/g_{oxides}).

Note that $MF_j^{Nominal}$ does not depend on the simulation test case (subscript *i*) because the test cases represent different combinations of uncertainties and numbers of samples, analyses per sample, and volume determinations in factors affecting oxide mass fractions. Hence, the nominal oxide mass fraction for the j^{th} oxide is the same for all test cases.

Equation (5.1.1) can be used to calculate %RHW values for various combinations of the factors described previously in this subsection. The outcomes of such calculations based on the simulation results can then be used to determine the values of n_S^{CRV}, n_A^{CRV}, n_V^{CRV}, and n_V^{MFPV} that will provide estimates of glass components within a given percentage (i.e., the %RHW) of the true value with desired confidence (CL%). The results of such calculations are presented in Section 7.1.1.

5.1.4 Equations for Calculating Means and Standard Deviations of ILAW Chemical Composition over a Waste Type

The ILAW compliance strategy for Contract Specification 2.2.2.6.2 involves (1) calculating the ILAW chemical composition for each MFPV batch from analyses of CRV samples and other process information (see Section 2.3) and (2) calculating and reporting means and SDs of the calculated compositions over each LAW waste type. The chemical composition of ILAW corresponding to each MFPV is calculated in terms of mass fractions of *J* glass components (oxides and halogens). The mass fraction of the j^{th} ILAW component in the i^{th} MFPV batch is denoted by g_{ij}^{MFPV}, $j = 1, 2, \ldots, J$. By the nature of mass fractions, $\sum_{j=1}^{J} g_{ij}^{MFPV} = 1$.

This section presents the formulas for calculating means and SDs of ILAW chemical compositions (mass fractions of oxide and halogen glass components) over the *I* MFPV batches corresponding to an LAW waste type. Two situations are considered. Section 5.1.4.1 addresses the case of balanced data, while Section 5.1.4.2 addresses the case of unbalanced data. The formulas in these subsections address Item 2 of Section 5.1.2.

5.1.4.1 Equations for Calculating Means and Standard Deviations of ILAW Chemical Composition over a Waste Type Using Balanced Data

In this section, we consider "balanced data", which occurs when (1) the same number of samples n_S^{CRV} are collected from all CRV batches $i = 1, 2, \ldots, I$ corresponding to an LAW waste type, (2) the same number of analyses n_A^{CRV} are made for each CRV sample of each CRV batch corresponding to an LAW waste type, and (3) the same number of volume determinations n_V^{CRV} and n_V^{MFPV} are made for each CRV batch and MFPV batch corresponding to an LAW waste type. When $n_A^{CRV} = 1$ for all samples from all CRV batches, balanced data occur when n_S^{CRV} is the same for every CRV batch, and the single analysis of each CRV sample is acceptable.

Section B.1 of Appendix B presents the mass-balance equations for calculating the ILAW chemical composition (in mass fractions) for a single MFPV batch. Specifically, Eq. (B.1.11) in Appendix B gives the formula for $\bar{g}_{ij}^{MFPV}$, the mass fraction of the j^{th} component in ILAW that would be made from the i^{th} MFPV batch averaged over the n_S^{CRV} samples per CRV batch, n_A^{CRV} analyses per CRV sample, and

$n_V^{CRV} = n_V^{MFPV}$ volume determinations for each CRV batch. For each component j, formulas are required for the mean and SD of the $\overline{g}_{ij}^{MFPV}$, $i = 1, 2, \ldots, I$ values corresponding to an LAW waste type.

In the case of balanced data, the formula for the mean of mass fractions of the j^{th} ILAW component over the MFPV batches corresponding to an LAW waste type is given by

$$\overline{\overline{g}}_j^{MFPV} = \frac{\sum_{i=1}^{I}\left[\frac{1}{n_S^{CRV} n_A^{CRV}}\sum_{l=1}^{n_S^{CRV}}\sum_{m=1}^{n_A^{CRV}} c_{ijlm}^{CRV} f_j \overline{V}_i^{CRV\,to\,MFPV} u + \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \overline{m}_{i-1,j}^{MFPV}\left(\frac{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\,Heel}}{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV}}\right)\right]}{\sum_{i=1}^{I}\left[\sum_{j=1}^{J}\left(\frac{1}{n_S^{CRV} n_A^{CRV}}\sum_{l=1}^{n_S^{CRV}}\sum_{m=1}^{n_A^{CRV}} c_{ijlm}^{CRV} f_j \overline{V}_i^{CRV\,to\,MFPV} u\right) + \sum_{j=1}^{J}\sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \sum_{j=1}^{J}\overline{m}_{i-1,j}^{MFPV}\left(\frac{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\,Heel}}{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV}}\right)\right]} \tag{5.1.2}$$

with

$$\overline{m}_{i-1,j}^{MFPV} = \frac{1}{n_S^{CRV} n_A^{CRV}}\sum_{l=1}^{n_S^{CRV}}\sum_{m=1}^{n_A^{CRV}} c_{i-1,jlm}^{CRV} f_j \overline{V}_{i-1}^{CRV\,to\,MFPV} u + \sum_{k=1}^{K} a_{i-1,k}^{GFC} G_{i-1,jk}^{GFC} + \overline{m}_{i-2,j}^{MFPV}\left(\frac{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV\,Heel}}{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{i-2,h}^{MFPV}}\right) \tag{5.1.3}$$

and

$$\overline{V}_i^{CRV\,to\,MFPV} = \frac{\hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,before}}}{\hat{\sigma}^2_{\overline{V}_i^{CRV\,before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,before}}}\left(\frac{\sum_{h=1}^{n_V^{CRV}} V_{ih}^{CRV\,before}}{n_V^{CRV}} - \frac{\sum_{h=1}^{n_V^{CRV}} V_{ih}^{CRV\,after}}{n_V^{CRV}}\right)$$

$$+ \frac{\hat{\sigma}^2_{\overline{V}_i^{CRV\,before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\,after}}}{\hat{\sigma}^2_{\overline{V}_i^{CRV\,before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,before}}}\left(\frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV\,after}}{n_V^{MFPV}} - \frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV\,before}}{n_V^{MFPV}}\right) \tag{5.1.4}$$

where the bars in certain notations (e.g., $\overline{V}_{i-1}^{CRV\,to\,MFPV}$) denote averages. The $\hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}}$ notation in Eq. (5.1.4) represents the variance of $\overline{V}_i^{MFPV\,after} = \frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\,After}$. The other variance

notations in Eq. (5.1.4) have similar interpretations. Note that Eqs. (5.1.2) and (5.1.3) assume that the IHLW MFPV is uniformly mixed.

In Eqs. (5.1.2) to (5.1.4), the following notation is used

$\bar{\bar{g}}_j^{MFPV}$ = mean (mass-weighted-average) mass fraction of the j^{th} ILAW component over I MFPV batches, based on averages over n_S^{CRV} samples per CRV batch, n_A^{CRV} analyses per sample, and n_V^{CRV} and n_V^{MFPV} volume determinations per CRV and MFPV batches (g_{oxide}/g_{oxides})

I = number of MFPV batches per reporting or compliance period

n_S^{CRV} = number of samples per CRV batch

n_A^{CRV} = number of chemical analyses per CRV sample

c_{ijlm}^{CRV} = analyzed concentration of the j^{th} analyte from the m^{th} analysis of the l^{th} sample from the i^{th} CRV batch (μg/mL = mg/L)

J = number of glass oxide components

f_j = $\frac{MW_j^{oxide}}{MW_j^{analyte}} R_j$ where MW_j^{oxide} and $MW_j^{analyte}$ are the molecular weights of oxide j and analyte j, respectively, and R_j is the ratio of moles of oxide per mole of analyte for oxide j. Hence, f_j is the factor for converting the concentration of analyte j (μg analyte j/mL = mg analyte j/L) to the concentration of oxide j (μg oxide j/mL = mg oxide/L). The quantity f_i is called the oxide factor for oxide j.

u = $\frac{1\,(\text{g})}{1000\,(\text{mg})}$, a units conversion factor for converting mg to g

K = number of GFCs

a_{ik}^{GFC} = mass of the k^{th} GFC added to the i^{th} MFPV batch (g)

G_{ijk}^{GFC} = mass of the j^{th} glass oxide component per mass of the k^{th} GFC for the i^{th} MFPV batch ($g_{oxide\,j}/g_{GFC\,k}$). The mass fractions G_{ijk}^{GFC} $j = 1, 2, \ldots, J$ for the k^{th} GFC can sum to less than 1.0 to the extent the GFC contains interstitial water or other

components that will not survive in the glass. The nominal G_{ijk}^{GFC} mass fractions of glass oxide components in the GFCs should not change frequently over MFPV batches. However, the *i* subscript was retained in case these mass fractions change (1) from one vendor to another for the same GFC or (2) for different lots of a given GFC from the same vendor.

$\overline{m}_{i-1,j}^{MFPV}$ = mass of the j^{th} glass oxide component in the $(i-1)^{st}$ MFPV batch based on averages over multiple samples, analyses per sample, and volume determinations (g)

n_V^{MFPV} = number of volume determinations per MFPV batch

$V_i^{MFPV\ Heel}$ = volume of the MFPV Heel included in the i^{th} MFPV batch (L)

V_{i-1}^{MFPV} = volume of the $(i-1)^{st}$ MFPV batch (L). This is the total volume of the $(i\text{-}1)^{st}$ MFPV batch, including the MFPV Heel, waste transferred from the CRV, GFCs added, and any water that may be added. Water will typically be added to Envelope B LAW in the MFPV to lower the sodium molarity. It is not anticipated that LAW from Envelopes A and C will require adding water in the MFPV.

n_V^{CRV} = number of volume determinations per CRV batch

$V_i^{CRV\ before}$ = volume of the CRV before the transfer of material to the i^{th} MFPV batch (L)

$V_i^{CRV\ after}$ = volume of the CRV after the transfer of material to the i^{th} MFPV batch (L)

$V_i^{MFPV\ before}$ = volume of the MFPV before receipt of CRV material for the i^{th} MFPV batch

$V_i^{MFPV\ Heel}$ = volume of the MFPV Heel included in the i^{th} MFPV batch (L)

$V_i^{MFPV\ after}$ = volume of the MFPV after receipt of CRV material for the i^{th} MFPV batch but before receipt of GFCs or any added water (L).

The notations similar to V_{ih}^{MFPV}, but with different superscripts and subscripts, have similar meanings where the (1) superscripts indicate the different vessel conditions for which volume determinations are made, and (2) subscripts denote the MFPV batch (i.e., "*i*-1" or "*i*-2").

The derivation and explanation of Eq. (5.1.2) is presented in Section F.1 of Appendix F, while the derivations and explanations of Eqs. (5.1.3) and (5.1.4) are presented in Section B.1 of Appendix B.

In the case of balanced data, the formula for the standard deviation of mass fractions of the j^{th} ILAW component over the MFPV batches corresponding to an LAW waste type is given by:

$$SD(\bar{g}_{ij}^{MFPV}) = \left[\frac{\sum_{i=1}^{I} \left(\bar{g}_{ij}^{MFPV} - \bar{\bar{g}}_{j}^{MFPV} \right)^2}{I-1} \right]^{0.5} \qquad (5.1.5)$$

where

$SD(\bar{g}_{ij}^{MFPV})$ = standard deviation of mass fractions for the j^{th} ILAW component over glass that would be made from the I MFPV batches corresponding to an LAW waste type (g_{oxide}/g_{oxides})

$\bar{g}_{ij}^{MFPV}$ = mass fraction of the j^{th} ILAW component in glass that would be made from the i^{th} MFPV batch (g_{oxide}/g_{oxides})

$\bar{g}_{ij}^{MFPV}$ is calculated using Eq. (B.1.11) in Section B.1 of Appendix B, $\bar{\bar{g}}_{j}^{MFPV}$ is calculated using Eq. (5.1.2), and the remaining notation is as previously defined.

A %RSD is simply the ratio of the standard deviation [$SD(\bar{g}_{ij}^{MFPV})$ in this case] to its corresponding mean, multiplied by 100. With the variables defined in this section, the %RSD for the mass fraction of the j^{th} ILAW component in the i^{th} MFPV batch is given by

$$\%RSD(\bar{g}_{ij}^{MFPV}) = 100\left(\frac{SD(\bar{g}_{ij}^{MFPV})}{\bar{\bar{g}}_{j}^{MFPV}} \right) . \qquad (5.1.6)$$

In some cases, it is preferred to report or consider the %RSD rather than the SD.

5.1.4.2 Equations for Calculating Means and Standard Deviations of ILAW Chemical Composition over a Waste Type Using Unbalanced Data

The case of unbalanced data is now addressed, where (1) the number of samples per CRV batch is not the same for the CRV batches associated with an LAW waste type, (2) the number of analyses per CRV sample is not the same for each sample from a CRV batch or for different CRV batches, and/or (3) the number of volume determinations is not the same for each case where a vessel volume is required. Unbalanced data would occur during WTP ILAW production if (1) less than the desired number of samples were taken for every CRV batch, (2) a sample from a CRV batch were unusable for some reason, (3) the number of analyses were not the same for every CRV sample, or (4) analytical results contain outliers that must be discarded. Similar occurrences for volume determinations would also lead to unbalanced data.

Unbalanced data forces changes in how the means and SDs for ILAW compositions are calculated. Several alternatives are available, but the simplest way to deal with unbalanced data is to calculate the means and SDs using the samples, analyses, and volume determinations available.

In the case of unbalanced data, the formula for the mean of mass fractions of the j^{th} ILAW component over the MFPV batches corresponding to an LAW waste type is given by

$$\overline{\overline{g}}_j^{MFPV} = \frac{\sum_{i=1}^{I}\left[\frac{1}{n_S^{CRV_i}}\sum_{l=1}^{n_S^{CRV_i}}\left(\frac{1}{n_A^{CRV_{il}}}\sum_{m=1}^{n_A^{CRV_{il}}} c_{ijlm}^{CRV} f_i \overline{V}_i^{CRV\,to\,MFPV} u\right) + \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \overline{m}_{i-1,j}^{MFPV}\left(\frac{\frac{1}{n_V^{MFPV_i}}\sum_{h=1}^{n_V^{MFPV_i}} V_{i,h}^{MFPV\,Heel}}{\frac{1}{n_V^{MFPV_{i-1}}}\sum_{h=1}^{n_V^{MFPV_{i-1}}} V_{i-1,h}^{MFPV}}\right)\right]}{\sum_{i=1}^{I}\left[\sum_{j=1}^{J}\left(\frac{1}{n_S^{CRV_i}}\sum_{l=1}^{n_S^{CRV_i}}\left(\frac{1}{n_A^{CRV_{il}}}\sum_{m=1}^{n_A^{CRV_{il}}} c_{ijlm}^{CRV} f_i \overline{V}_i^{CRV\,to\,MFPV} u\right)\right) + \sum_{j=1}^{J}\sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \sum_{j=1}^{J}\overline{m}_{i-1,j}^{MFPV}\left(\frac{\frac{1}{n_V^{MFPV_i}}\sum_{h=1}^{n_V^{MFPV_i}} V_{i,h}^{MFPV\,Heel}}{\frac{1}{n_V^{MFPV_{i-1}}}\sum_{h=1}^{n_V^{MFPV_{i-1}}} V_{i-1,h}^{MFPV}}\right)\right]} \tag{5.1.7}$$

with

$$\overline{m}_{i-1,j}^{MFPV} = \frac{1}{n_S^{CRV_{i-1}}}\sum_{l=1}^{n_S^{CRV_{i-1}}}\left(\frac{\sum_{m=1}^{n_A^{CRV_{i-1,l}}} c_{i-1,jlm}^{CRV} f_j \overline{V}_{i-1}^{CRV\,to\,MFPV} u}{n_A^{CRV_{i-1,l}}}\right) + \sum_{k=1}^{K} a_{i-1,k}^{GFC} G_{i-1,jk}^{GFC} + \overline{m}_{i-2,j}^{MFPV}\left(\frac{\frac{1}{n_V^{MFPV_{i-1}}}\sum_{h=1}^{n_V^{MFPV_{i-1}}} V_{i-1,h}^{MFPV\,Heel}}{\frac{1}{n_V^{MFPV_{i-2}}}\sum_{h=1}^{n_V^{MFPV_{i-2}}} V_{i-2,h}^{MFPV}}\right) \tag{5.1.8}$$

and

$$\overline{V}_i^{CRV\,to\,MFPV} = \frac{\hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,before}}}{\hat{\sigma}^2_{\overline{V}_i^{CRV\,before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,before}}}\left(\frac{\sum_{h=1}^{n_V^{CRV_i}} V_{ih}^{CRV\,before}}{n_V^{CRV_i}} - \frac{\sum_{h=1}^{n_V^{CRV_i}} V_{ih}^{CRV\,after}}{n_V^{CRV_i}}\right)$$

$$+ \frac{\hat{\sigma}^2_{\overline{V}_i^{CRV\,before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\,after}}}{\hat{\sigma}^2_{\overline{V}_i^{CRV\,before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,before}}}\left(\frac{\sum_{h=1}^{n_V^{MFPV_i}} V_{ih}^{MFPV\,after}}{n_V^{MFPV_i}} - \frac{\sum_{h=1}^{n_V^{MFPV_i}} V_{ih}^{MFPV\,before}}{n_V^{MFPV_i}}\right) \tag{5.1.9}$$

In Eqs. (5.1.7) to (5.1.9), the notation is the same as in Eqs. (5.1.2) to (5.1.4), with the following differences

$n_S^{CRV_i}$ = number of samples from the CRV batch, a portion of which is used in making the i^{th} MFPV batch

$n_A^{CRV_{il}}$ = number of chemical analyses made of the l^{th} sample from the CRV batch, a portion of which is used in making the i^{th} MFPV batch

$n_V^{CRV_i}$ = number of volume determination for the CRV batch, a portion of which is used in making the i^{th} MFPV batch

$n_V^{MFPV_i}$ = number of volume determinations made for the i^{th} MFPV batch.

Equations (5.1.7) to (5.1.9) for unbalanced data are similar to Eqs. (5.1.2) to (5.1.4) for balanced data, but substitute the preceding notation for unequal numbers of samples, analyses, and volume determinations. Eqs. (5.1.7) and (5.1.8) also assume uniform mixing in the IHLW MFPV.

In the case of unbalanced data, the standard deviation of mass fractions for the j^{th} ILAW component over the I MFPV batches corresponding to an LAW waste type can again be calculated using Eq. (5.1.5). In that equation, $\bar{g}_{ij}^{MFPV}$ is given by Eq. (5.1.7), and $\bar{g}_{ij}^{MFPV}$ is given by the equation

$$\bar{g}_{ij}^{MFPV} = \frac{\frac{1}{n_S^{CRV_i}} \sum_{l=1}^{n_S^{CRV_i}} \left(\frac{1}{n_A^{CRV_{il}}} \sum_{m=1}^{n_A^{CRV_{il}}} c_{ijlm}^{CRV} f_i \bar{V}_i^{CRV\,to\,MFPV} u \right) + \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \bar{m}_{i-1,j}^{MFPV} \left(\frac{\frac{1}{n_V^{MFPV_i}} \sum_{h=1}^{n_V^{MFPV_i}} V_{i,h}^{MFPV\,Heel}}{\frac{1}{n_V^{MFPV_{i-1}}} \sum_{h=1}^{n_V^{MFPV_{i-1}}} V_{i-1,h}^{MFPV}} \right)}{\sum_{j=1}^{J} \left(\frac{1}{n_S^{CRV_i}} \sum_{l=1}^{n_S^{CRV_i}} \left(\frac{1}{n_A^{CRV_{il}}} \sum_{m=1}^{n_A^{CRV_{il}}} c_{ijlm}^{CRV} f_i \bar{V}_i^{CRV\,to\,MFPV} u \right) \right) + \sum_{j=1}^{J} \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \sum_{j=1}^{J} \bar{m}_{i-1,j}^{MFPV} \left(\frac{\frac{1}{n_V^{MFPV_i}} \sum_{h=1}^{n_V^{MFPV_i}} V_{i,h}^{MFPV\,Heel}}{\frac{1}{n_V^{MFPV_{i-1}}} \sum_{h=1}^{n_V^{MFPV_{i-1}}} V_{i-1,h}^{MFPV}} \right)} \quad (5.1.10)$$

In Eq. (5.1.10), $\bar{m}_{i-1,j}^{MFPV}$ is given by Eq. (5.1.8), $\bar{V}_i^{CRV\,to\,MFPV}$ is given by Eq. (5.1.9), and all notation is as previously defined following Eqs. (5.1.2), (5.1.3), (5.1.4), (5.1.8), and (5.1.9). Note that Eq. (5.1.10) is similar to Eq. (B.1.11) in Section B.1 of Appendix B, except with modifications to reflect the unequal numbers of samples per CRV batch, unequal numbers of analyses per CRV sample, and/or unequal numbers of volume determinations.

After calculating $SD(\bar{g}_{ij}^{MFPV})$ values with unbalanced data using Eqs. (5.1.5) and (5.1.10), if $\%RSD(\bar{g}_{ij}^{MFPV})$ values are desired, they can be calculated using Eq. (5.1.6).

If the data are not greatly unbalanced, this simple way of calculating means and SDs for mass fractions of ILAW components over a waste type should produce reasonable results. However, other methods that are designed to work with unbalanced data could also be employed. WLS can be used not only with unbalanced data but also if there is evidence that the variation across CRV and MFPV batches does not remain constant over the course of a waste type. WLS-based equations for means and SDs have not been developed at this time, but could be if deemed desirable by the WTP Project. Bootstrap methods, where available data are repeatedly re-sampled (i.e., with replacement) to obtain a balanced set, could also be used to solve the problem of unbalanced data. A brief description of how bootstrap methods can be applied to unbalanced datasets can be found at the end of Section 4.1.4.2.

5.2 Compliance Approach and Methods for ILAW Contract Specification 2.2.2.7.2: Radionuclide Composition During Production

Section 5.2.1 lists the applicable Contract Specification 2.2.2.7.2. Section 5.2.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Sections 5.2.3 and 5.2.4 present the statistical methods that will be used to implement the statistical aspects of the compliance strategy.

5.2.1 Contract Specification 2.2.2.7.2: Radionuclide Composition During Production

The ILAW production documentation shall identify the radionuclide inventory in each ILAW package produced. The actual inventory indexed at the month of product transfer and the inventory indexed to December 31, 2002, shall be reported.

5.2.2 Statistical Aspects of the ILAW Compliance Strategy for Contract Specification 2.2.2.7.2

The following items describe the statistical and related aspects of the ILAW compliance strategy for Contract Specification 2.2.2.7.2 (see the ILAW PCP, Nelson et al. 2003) that are addressed in this report.[(a)]

Item 1: Determine the numbers of samples, analyses per sample, and other process measurements required to estimate radionuclide compositions for each ILAW MFPV batch, which are in turn used to estimate radionuclide inventories.

Item 2: Develop equations for calculating the means and SDs of the radionuclide inventory determinations for ILAW containers produced from a given ILAW production lot for each significant (i.e., reportable) radionuclide. Incorporate in the SDs the variations and uncertainties affecting the radionuclide composition and the mass of glass in ILAW containers.

The statistical methods to implement these aspects of the WTP ILAW compliance strategy for Contract Specification 2.2.2.7.2 are discussed in Sections 5.2.3 and 5.2.4.

(a) See Section 1.0 for a discussion of why this report addresses ILAW PCP Rev. 0 (Nelson et al. 2003) rather than ILAW PCP Rev. 1 (Westsik et al. 2004).

5.2.3 Statistical Method for Determining the Numbers of Samples, Analyses, and Volume Determinations to Estimate the ILAW Radionuclide Composition for an MFPV Batch

During ILAW production operations, the radionuclide composition (mass fractions) will be calculated based on chemical analyses and radiochemical analyses of samples from the CRV and other process measurements and determinations. Although mass fractions of ILAW radionuclide components (oxides) may be of limited interest directly, they play a key role in the equations developed to calculate ILAW radionuclide inventories and concentrations (see Section B.2 of Appendix B). Hence, it is important to assess the numbers of LAW CRV samples, radiochemical analyses per sample, and other process determinations required to adequately estimate ILAW radionuclide compositions.

The applicable mass-balance equations for calculating ILAW radionuclide composition (mass fractions) are given in Section B.2 of Appendix B. The balance of this subsection describes the statistical method to address Item 1 in Section 5.2.2.

Section 3.4.2 describes the Monte Carlo simulation approach for assessing the impacts of the following factors

- number of samples per CRV batch (n_S^{CRV})
- number of radiochemical analyses per CRV sample (n_A^{CRV})
- number of volume determinations of the CRV and MFPV before and after transfers (n_V^{CRV} and n_V^{MFPV})
- mixing/sampling %RSD in the concentration of the j^{th} element in a CRV batch [$\%RSD_S(c_j^{CRV})$]
- analytical %RSD in the concentration of the j^{th} element in a CRV batch [$\%RSD_A(c_j^{CRV})$]
- GFC composition uncertainty, represented by the standard deviation in the mass fraction of the j^{th} component (oxide or halogen) in the k^{th} GFC [$SD(G_{jk}^{GFC})$]
- GFC mass uncertainty, represented by the standard deviation of the mass of the k^{th} GFC added to a MFPV batch. This uncertainty includes uncertainties due to batching, weighing, and transfers of GFCs.
  [$SD(a_k^{GFC})$]
- volume uncertainties in the CRV and MFPV. The magnitudes of these uncertainties will depend on the level of contents in a vessel, but a generic notation is used for now (SD_V^{CRV} and SD_V^{MFPV})
- statistical percent confidence level (CL%)
- ILAW produced from three tanks representing one each of Envelopes A (AP-101), B (AZ-101), and C (AN-107)

on the total uncertainty in estimating ILAW radionuclide composition (mass fractions of oxides) for each MFPV batch. It is necessary at this time to consider a range of values for process uncertainties (as discussed in Section 3.4.2) because final estimates have not yet been produced by the WTP Project. A future update of this report will use final estimates of process uncertainties to determine the final recommended numbers of CRV samples, radiochemical analyses per CRV sample, and volume determinations of the CRV and MFPV for estimating ILAW radionuclide composition (and inventory).

To assess the total uncertainty in estimating ILAW radionuclide composition for a given MFPV batch, the percent relative half-width (%RHW) of a two-sided CL% ECI on the mass fraction of each ILAW component (radionuclide oxide) is used. A Monte Carlo simulation approach was used to obtain CL% ECIs and the corresponding %RHWs. The mass-balance equations in Section B.2 were used to develop the Monte Carlo simulation approach. The formula for a %RHW, expressed as a percentage of the nominal value (mass fraction) of a given glass component, is given by Eq. (5.1.1) presented previously, where now "*j*" in that equation represents a radionuclide oxide.

Equation (5.1.1) can be used to calculate %RHW values for various combinations of the factors described previously in this subsection. The outcomes of such calculations based on the simulation results can then be used to determine the values of n_S^{CRV}, n_A^{CRV}, n_V^{CRV}, and n_V^{MFPV} that will provide estimates of glass components within a given percentage (i.e., the %RHW) of the true value with desired confidence (CL%). The results of such calculations are presented in Section 7.2.1.

5.2.4 Equations for Calculating Means and Standard Deviations of ILAW Radionuclide Inventories over MFPV Batches Corresponding to an LAW Waste Type

During ILAW production operations, radionuclide inventories will be calculated based on (1) chemical and radiochemical analyses of CRV samples, (2) volume determinations of CRV and MFPV batches, and (3) determined masses of glass in ILAW containers. Contract Specification 2.2.2.7.2 calls for reporting inventories for each canister and for each waste type. However, it is not possible to easily relate the composition of MFPV batches to the composition of ILAW in canisters produced from those batches.

In the WTP ILAW compliance strategy, every reportable radionuclide (see Table 2.1) will be analyzed in every sample of every CRV batch. Also, the mass of glass in every ILAW container will be determined. Then, using this information, the means and SDs of the radionuclide inventories over containers (and associated MFPV batches) corresponding to an LAW waste type will be calculated and reported for every container associated with the LAW waste type.

This subsection presents the formulas for calculating means and SDs of the inventory of radionuclide *q* over the *D* ILAW containers associated with the *I* MFPV batches corresponding to an LAW waste type. The formulas are based on average results over multiple samples, analyses, and measurements at different stages of the ILAW process. Two situations are considered. Section 5.2.4.1 addresses the case of balanced data, while Section 5.2.4.2 addresses the case of unbalanced data. The formulas in these subsections address Item 2 of Section 5.2.2.

5.2.4.1 Equations for Calculating Means and Standard Deviations of ILAW Radionuclide Inventories over a Waste Type Using Balanced Data

Equations for calculating means and SDs of ILAW radionuclide inventories over a waste type using balanced data (as described at the start of Section 5.1.4.1) are presented in this subsection. These equations apply to all reportable radionuclides, as listed in Table 2.1 of Section 2.

Equation for the Mean Radionuclide Inventory over *D* ILAW Containers Based on Averages of Balanced Multiple Samples, Analyses, and Volume Determinations for Each Batch

The expression for the mean inventory per container of radionuclide q over the D ILAW canisters and I MFPV batches associated with an LAW waste type, based on averages over balanced multiple samples per CRV batch, analyses per CRV sample, and volume determinations per CRV and MFPV batches is given by

$$\overline{\overline{R}}_{Dq}^{Container} = \frac{\overline{\overline{g}}_q^{MFPV}\,\overline{m}_D^{Container}\,A_q}{f_q}$$

$$= \sum_{i=1}^{I}\left[\begin{array}{l}\left(\dfrac{\sum_{l=1}^{n_S^{CRV}}\sum_{m=1}^{n_A^{CRV}} r_{iqlm}^{CRV}\,/\,A_q}{n_S^{CRV}\,n_A^{CRV}}\right)\overline{V}_i^{CRV\ to\ MFPV} f_q u + \\ \sum_{k=1}^{K} a_{ik}^{GFC} G_{iqk}^{GFC} + \overline{m}_{i-1,q}^{MFPV}\left(\dfrac{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\ Heel}}{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV}}\right)\end{array}\right]\left[\left(\frac{1}{D}\sum_{d=1}^{D} m_d^{Container}\right)\frac{A_q}{f_q}\right]$$

$$\left[\sum_{i=1}^{I}\left[\left(\sum_{j\in CHEM}^{J}\frac{\sum_{l=1}^{n_S^{CRV}}\sum_{m=1}^{n_A^{CRV}} c_{ijlm}^{CRV} f_j u}{n_S^{CRV}\,n_A^{CRV}} + \sum_{j\in RAD}^{J}\frac{\sum_{l=1}^{n_S^{CRV}}\sum_{m=1}^{n_A^{CRV}} r_{ijlm}^{CRV} f_j u\,/\,A_j}{n_S^{CRV}\,n_A^{CRV}}\right)\overline{V}_i^{CRV\ to\ MFPV}\right]\right.$$

$$\left. + \sum_{i=1}^{I}\sum_{j=1}^{J}\left(\sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \overline{m}_{i-1,j}^{MFPV}\left(\frac{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\ Heel}}{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV}}\right)\right)\right] \qquad (5.2.1)$$

where

$\overline{\overline{R}}_{Dq}^{Container}$ = mean inventory per container of the q^{th} radionuclide over the D ILAW containers associated with an LAW waste type, based on averages over multiple samples, analyses, and volume determinations (Ci)

$\overline{\overline{g}}_{q}^{MFPV}$ = mean (mass-weighted-average) mass fraction of the q^{th} ILAW radionuclide component over I MFPV batches, based on averages over n_S^{CRV} samples per CRV batch, n_A^{CRV} analyses per sample, and n_V^{CRVV} and n_V^{MFPV} volume determinations per CRV and MFPV batches (g_{oxide}/g_{oxides})

$\overline{m}_{D}^{Container}$ = mean mass of glass in the D ILAW containers associated with an LAW waste type (g_{glass})

A_q or A_j = specific activity of the q^{th} or j^{th} radionuclide ($Ci/g_{radionuclide}$)

I = number of MFPV batches corresponding to an LAW waste type

J = number of non-radionuclide oxides and radionuclide oxides estimated for the ILAW composition corresponding to each MFPV batch

$j \in CHEM$ = chemical composition components of ILAW

$j \in RAD$ = radionuclide composition components of ILAW

D = number of ILAW containers associated with the I MFPV batches corresponding to an LAW waste type

f_j = $\frac{MW_j^{oxide}}{MW_j^{analyte}} R_j$ where MW_j^{oxide} and $MW_j^{analyte}$ are the molecular weights of oxide j and analyte j, respectively, and R_j is the ratio of moles of oxide per mole of analyte for oxide j. Hence, f_j is the factor for converting the concentration of analyte j (µg analyte j/mL = mg analyte j/L) to the concentration of oxide j (µg oxide j/mL = mg oxide/L). The quantity f_i is called the oxide factor for oxide j.

n_S^{CRV} = number of samples per CRV batch

n_A^{CRV} = number of chemical and radiochemical analyses per CRV sample

r_{ijlm}^{CRV} = analyzed concentration of the j^{th} radionuclide from the m^{th} analysis of the l^{th} sample from the i^{th} CRV batch (μCi/mL = mCi/L)

c_{ijlm}^{CRV} = analyzed concentration of the j^{th} analyte from the m^{th} analysis of the l^{th} sample from the i^{th} CRV batch (μg/mL = mg/L)

n_V^{CRV} = number of volume determinations per CRV batch

$\overline{V}_i^{CRV\ to\ MFPV}$ = weighted average estimate of the volume of material transferred from the CRV to the i^{th} MFPV batch, as calculated by Eq. (5.1.4)

$m_d^{Container}$ = mass of glass in the d^{th} ILAW container associated with an LAW waste type (g_{glass}).

and the remaining notation is as previously defined. The mean (mass-weighted average over ILAW MFPV batches) mass fraction of the q^{th} radionuclide ($\overline{\overline{g}}_q^{MFPV}$) plays an important role in calculating $\overline{\overline{R}}_{Dq}^{Container}$, the mean inventory per container of the q^{th} radionuclide over the D ILAW containers associated with an LAW waste type. The quantity $\overline{\overline{g}}_q^{MFPV}$ is calculated for balanced data by Eq. (5.1.2) with q substituted for j in the numerator. The derivation of Eq. (5.2.1), which assumes uniform mixing in the MFPV, is presented in Section B.2.2.1 of Appendix B.

Despite the effective reductions of some within-batch uncertainties due to averaging, it should be recognized that values of $\overline{\overline{R}}_{Dq}^{Container}$ calculated via Eq. (5.2.1) will still be subject to reduced ILAW process uncertainties as well as MFPV batch-to-batch variations.

Equation for the Standard Deviation of Radionuclide Inventory over *D* ILAW Containers Based on Averages of Balanced Multiple Samples, Analyses, and Volume Determinations for Each Batch

The expression for the standard deviation of the inventory of radionuclide q over the D ILAW containers and I MFPV batches associated with an LAW waste type, based on averages over balanced multiple samples per CRV batch, analyses per CRV sample, and volume determinations per CRV and MFPV batches is given by

$$SD(\overline{R}_{dq}^{Container}) = \left(\frac{A_q}{f_q}\right)\left[\begin{array}{l}\left[\overline{\overline{g}}_q^{MFPV}\right]^2\left[SD(m_d^{Container})\right]^2 + \left[\overline{m}_D^{Container}\right]^2\left[SD(\overline{g}_{iq}^{MFPV})\right]^2 \\ -\left[SD(m_d^{Container})\right]^2\left[SD(\overline{g}_{iq}^{MFPV})\right]^2\end{array}\right]^{1/2} \quad (5.2.2)$$

where

$SD(\overline{R}_{dq}^{Container})$ = standard deviation of the average inventory of radionuclide q for the d^{th} ILAW container, where the average is based on multiple samples, analyses, and volume determinations (Ci)

$SD(m_d^{Container})$ = standard deviation of the determined mass of glass in the d^{th} ILAW container (g_{glass})

$SD(\overline{g}_{iq}^{MFPV})$ = standard deviation of the average mass fraction of the q^{th} radionuclide oxide in the i^{th} MFPV batch, where the average is based on multiple samples, analyses and volume determinations (g_{oxide}/g_{oxides})

and the remaining notation is as previously defined following Eq (5.2.1). The derivation of Eq. (5.2.2) is presented in Section B.2.2.2 of Appendix B.

As explained in Section B.2.2.2 in Appendix B, the term $SD(\overline{g}_{iq}^{MFPV})$ includes variation in mass fractions of the q^{th} radionuclide oxide across all I MFPV batches associated with an LAW waste type as well as uncertainties in determining mass fractions of radionuclide oxides for each MFPV batch. These uncertainties include random inhomogeneities in mixing the CRV contents, random uncertainties associated with the CRV sampling system, random irreproducibility of the chemical-analysis techniques employed, random uncertainties in volume determinations, and random uncertainties in the masses of GFCs added to the MFPV. The first four of these can be effectively reduced by averaging when multiple samples, analyses per sample, and volume determinations per CRV and MFPV batch are made. A value of $SD(\overline{g}_{iq}^{MFPV})$ is calculated from the $\overline{g}_{iq}^{MFPV}$ ($i = 1, 2, \ldots, I$) values using the usual standard deviation formula.

In a similar way, the term $SD(m_d^{Container})$ includes uncertainties associated with determining the mass of glass in an ILAW container as well as the variation in the masses of glass that occur across containers associated with an LAW waste type. A value of $SD(m_d^{Container})$ is calculated from the $m_d^{Container}$ ($d = 1, 2, \ldots, D$) values using the usual standard deviation formula.

5.2.4.2 Equations for Calculating Means and Standard Deviations of ILAW Radionuclide Inventories over a Waste Type Using Unbalanced Data

The case of unbalanced data (as described in Section 5.1.4.2) is now addressed, where $n_S^{CRV_i} \geq 3$ denotes the number of samples taken from the CRV batch corresponding to the i^{th} MFPV batch, $n_A^{CRV_{il}} \geq 1$ denotes the number of chemical and radionuclide analyses made of the l^{th} sample from the i^{th} CRV batch, $n_V^{CRV_i} \geq 1$ denotes the number of volume determinations for the CRV batch corresponding to the i^{th} MFPV batch, and $n_V^{MFPV_i} \geq 1$ denotes the number of volume determinations for the i^{th} MFPV batch.

Equations for calculating means and SDs of ILAW radionuclide inventories over a waste type using unbalanced data are presented. These equations apply to all reportable radionuclides (which will be measured in every CRV batch) as listed in Table 2.1 of Section 2. These equations also assume that the degree of unbalance is small. Otherwise, WLS methods or bootstrap methods (as described in the last paragraph of Section 4.1.4.2) should be applied.

Equation for the Mean Radionuclide Inventory over *D* ILAW Canisters Based on Averages of Unbalanced Multiple Samples, Analyses, and Volume Determinations for Each Batch

The expression for the mean inventory per container of radionuclide q over the D ILAW canisters and I MFPV batches associated with an LAW waste type, based on averages over unbalanced multiple samples per CRV batch, analyses per CRV sample, and volume determinations per CRV and MFPV batches (assuming uniform mixing) is given by

$$\overline{\overline{R}}_{Dq}^{Container} = \frac{\overline{\overline{g}}_q^{MFPV}\,\overline{m}_D^{Container}\,A_q}{f_q}$$

$$= \sum_{i=1}^{I}\left[\begin{array}{l}\left(\dfrac{\sum_{l=1}^{n_S^{CRV_i}}\sum_{m=1}^{n_A^{CRV_i}} r_{iqlm}^{CRV} / A_q}{n_S^{CRV_i}\,n_A^{CRV_i}}\right)\overline{V}_i^{CRV\ to\ MFPV} f_q u + \\ \sum_{k=1}^{K} a_{ik}^{GFC} G_{iqk}^{GFC} + \overline{m}_{i-1,q}^{MFPV}\left(\dfrac{\frac{1}{n_V^{MFPV_i}}\sum_{h=1}^{n_V^{MFPV_i}} V_{i,h}^{MFPV\ Heel}}{\frac{1}{n_V^{MFPV_i}}\sum_{h=1}^{n_V^{MFPV_i}} V_{i-1,h}^{MFPV}}\right)\end{array}\right]\left[\left(\frac{1}{D}\sum_{d=1}^{D} m_d^{Container}\right)\frac{A_q}{f_q}\right]$$

$$\sum_{i=1}^{I}\left[\left(\sum_{j\in CHEM}^{J}\frac{\sum_{l=1}^{n_S^{CRV_i}}\sum_{m=1}^{n_A^{CRV_i}} c_{ijlm}^{CRV} f_j u}{n_S^{CRV_i}\,n_A^{CRV_i}} + \sum_{j\in RAD}^{J}\frac{\sum_{l=1}^{n_S^{CRV_i}}\sum_{m=1}^{n_A^{CRV_i}} r_{ijlm}^{CRV} f_j u / A_j}{n_S^{CRV_i}\,n_A^{CRV_i}}\right)\overline{V}_i^{CRV\ to\ MFPV}\right] \qquad (5.2.3)$$

$$+ \sum_{i=1}^{I}\sum_{j=1}^{J}\left[\sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \overline{m}_{i-1,j}^{MFPV}\left(\frac{\frac{1}{n_V^{MFPV_i}}\sum_{h=1}^{n_V^{MFPV_i}} V_{i,h}^{MFPV\ Heel}}{\frac{1}{n_V^{MFPV_i}}\sum_{h=1}^{n_V^{MFPV_i}} V_{i-1,h}^{MFPV}}\right)\right]$$

where

$\overline{\overline{R}}_{Dq}^{Canister}$ = mean inventory per container of the q^{th} radionuclide over the D ILAW containers associated with an LAW waste type, based on averages over multiple samples per CRV batch, analyses per CRV sample, and volume determinations for CRV and MFPV batches (Ci)

$\overline{\overline{g}}_q^{MFPV}$ = mass weighted average of the mass fractions of the q^{th} radionuclide oxide over the I ILAW containers associated with an LAW waste type, based on averages over multiple samples per CRV batch, analyses per CRV sample, and volume determinations ($g_{oxide\ q}/g_{oxides}$)

A_q = specific activity of the q^{th} radionuclide ($Ci/g_{radionuclide}$)

I = number of MFPV batches corresponding to an LAW waste type

J = number of non-radionuclide oxides and radionuclide oxides estimated for the ILAW composition corresponding to each MFPV batch

$j \in CHEM$ = chemical composition components of ILAW

$j \in RAD$ = radionuclide composition components of ILAW

D = number of ILAW containers associated with the I MFPV batches corresponding to an LAW waste type

f_q = $\frac{MW_j^{oxide}}{MW_j^{analyte}} R_j$ where MW_j^{oxide} and $MW_j^{analyte}$ are the molecular weights of oxide j and analyte j, respectively, and R_j is the ratio of moles of oxide per mole of analyte for oxide j. Hence, f_j is the factor for converting the concentration of analyte j (μg analyte j/mL = mg analyte j/L) to the concentration of oxide j (μg oxide j/mL = mg oxide/L). The quantity f_i is called the oxide factor for oxide j.

and the remaining notation is as previously defined for the equations in Section 5.1 and following Eq. (5.2.1). The mean (mass-weighted average over ILAW MFPV batches) mass fraction of the q^{th} radionuclide ($\overline{\overline{g}}_q^{MFPV}$) plays an important role in calculating $\overline{\overline{R}}_{Dq}^{Container}$, the mean inventory per container of the q^{th} radionuclide over the D ILAW containers associated with an LAW waste type. The quantity $\overline{\overline{g}}_q^{MFPV}$ is calculated for unbalanced data by Eq. (5.1.7) with q substituted for j in the numerator.

Despite the effective reductions of some within-batch uncertainties due to averaging, it should be recognized that values of $\overline{\overline{R}}_{Dq}^{Canister}$ calculated via Eq. (5.2.3) will still be subject to reduced within-MFPV-batch uncertainty as well as MFPV batch-to-batch variations.

Equation for the Standard Deviation of Radionuclide Inventory over *D* ILAW Canisters Based on Averages of Unbalanced Multiple Samples, Analyses, and Volume Determinations for Each CRV Batch

The expression for the standard deviation of the inventory of radionuclide *q* over the *D* ILAW containers and *I* MFPV batches associated with an LAW waste type, based on averages over unbalanced multiple samples per CRV batch, analyses per CRV sample, and volume determinations of CRV and MFPV batches is again given by Eq. (5.2.2). In Eq. (5.2.2), $\overline{\overline{g}}_{q}^{MFPV}$ is calculated by Eq. (5.1.7), and $\overline{g}_{iq}^{MFPV}$ is calculated using Eq. (5.1.10) where in both cases, *q* is one of the *j* in those equations.

5.3 Compliance Approach and Methods for ILAW Contract Specification 2.2.2.8: Radionuclide Concentration Limits

Section 5.3.1 lists the applicable Contract Specification 2.2.2.8. Section 5.3.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Sections 5.3.3 to 5.3.6 present the statistical methods that will be used to implement the statistical aspects of the compliance strategy.

5.3.1 Contract Specification 2.2.2.8: Radionuclide Concentration Limits

> *The radionuclide concentration of the ILAW form shall be less than Class C limits as defined in 10 CFR 61.55. In addition, the average concentrations of ^{137}Cesium (^{137}Cs) and ^{90}Strontium (^{90}Sr) shall be limited as follows: $^{137}Cs < 3$ Ci/m^3 and $^{90}Sr < 20$ Ci/m^3. The method used to perform concentration averaging should be identified in the ILAW Product Compliance Plan.*

5.3.2 Statistical Aspects of the ILAW Compliance Strategy for Contract Specification 2.2.2.8

The following items describe the statistical and related aspects of the ILAW compliance strategy for Contract Specification 2.2.2.8 (see the ILAW PCP, Nelson et al. 2003) that are addressed in this report.[(a)]

Item 1: Develop a statistical method to demonstrate that ILAW radionuclide concentrations over a waste type are below Class C limits.

Item 2: Determine the numbers of samples, analyses per sample, and other process measurements required to demonstrate that radionuclide concentrations over a waste type are below Class C limits.

(a) See Section 1.0 for a discussion of why this report addresses ILAW PCP Rev. 0 (Nelson et al. 2003) rather than ILAW PCP Rev. 1 (Westsik et al. 2004).

Item 3: Develop a statistical method to demonstrate that running averages of ^{137}Cs and ^{90}Sr concentrations (over all ILAW containers presented to date for acceptance on a waste-type basis) are below the specified limits.

Item 4: Determine the numbers of samples, analyses per sample, and other process measurements required to demonstrate that running averages of ^{137}Cs and ^{90}Sr concentrations are below their specified limits.

The statistical methods to implement these aspects of the WTP ILAW compliance strategy for Contract Specification 2.2.2.8 are discussed in Sections 5.3.3 to 5.3.6. The equations to calculate the "compliance quantities" involved in Specification 2.2.2.8 are presented in Section B.3 of Appendix B.

5.3.3 Statistical Methods to Demonstrate that ILAW Radionuclide Concentrations Meet Class C Limits

This subsection describes the statistical methods to address Item 1 in Section 5.3.2. The statistical methods are applied within the framework of the compliance requirements discussed in 10 CFR 61.55(a)(5) and 10 CFR 61.55(a)(7). Clause (5) is applicable because WTP LAW is expected to contain both long-lived radionuclides (identified in Table 1 of 10 CFR 61.55) and short-lived radionuclides (identified in Table 2 of 10 CFR 61.55). Clause (7) is applicable because WTP LAW is expected to contain a mixture (i.e., more than one) of the radionuclides listed in each of Table 1 and Table 2.

Parts of 10 CFR 61.55(a)(5) and 10 CFR 61.55(a)(7) provide for identifying whether waste is Class A, B, or C and verifying radionuclides meet their respecitive limits. However, Contract Specification 2.2.2.8 only requires demonstrating that Class C limits are met. The Class C limits on concentrations of radionuclides listed in Table 1 and Table 2 of 10 CFR 61.55 are summarized in Table B.1 of Appendix B.

According to 10 CFR 61.55(a)(7), the *sum-of-fractions rule* must be used to determine whether the Class C limits on radionuclide concentrations in Tables 1 and 2 of 10 CFR 61.55 are met.[(a)] The sum-of-fractions of radionuclide concentrations in Table 1 or 2 is determined by dividing the concentration of each radionuclide in Table 1 or Table 2 by the corresponding Class C limit and adding the resulting values. The sum-of-fractions for Table 1 radionuclides (SF1) and for Table 2 radionuclides (SF2) must then be less than 1.0 for the Class C limits of Table 1 and Table 2 to be satisfied.[(b)]

After eliminating radionuclides determined by the WTP Project as not present in LAW, the SF1 and SF2 calculations include the following 10 CFR 61.55 Table 1 and Table 2 radionuclides with their Class C concentration limits (from Table B.1 in Appendix B) listed in parentheses:

- SF1: ^{99}Tc (3 Ci/m^3), alpha emitting TRU (100 nCi/g), ^{241}Pu (nCi/g), and ^{242}Cm (20,000 nCi/g)

(a) The sum-of-fractions of radionuclide concentrations can be calculated for Class A, B, or C limits in Table 2 of 10 CFR 61.55. However, only Class C limits are of concern per Contract Specification 2.2.2.8.

(b) It can be inferred from 10 CFR 61.55(a)(5)(i) that it is not necessary to calculate SF1 if each of the radionuclides in Table 1 has concentrations less than 0.1 times their corresponding limits. In that case, SF1 would necessarily be less than 1.0. If one or more radionuclides in Table 1 are greater than 0.1 times their limits, SF1 must be calculated because it may then exceed 1.0. However, it is sufficient to always calculate SF1 and compare it to 1.0 to verify that the Class C limits in Table 1 of 10 CFR 61.55 are satisfied.

- SF2: ^{63}Ni (700 Ci/m^3), ^{90}Sr (7000 Ci/m^3), and ^{137}Cs (4600 Ci/m^3)

Two statistical methods have been developed for demonstrating compliance with Class C limits using the sum-of-fractions rule. The first method addresses Item 1 of Section 5.3.2, namely demonstrating compliance over the *D* ILAW containers associated with an LAW waste type. The second method provides for assessing compliance of the ILAW that would result from each MFPV batch. These methods are described in Sections 5.3.3.1 and 5.3.3.2, respectively.

5.3.3.1 Statistical Method to Demonstrate that ILAW Radionuclide Concentrations over ILAW Containers Associated with an LAW Waste Type Meet Class C Limits

To demonstrate that ILAW radionuclide concentrations meet Class C limits over ILAW containers associated with an LAW waste type, an X%/Y% UTI method is appropriate. The X%/Y% UTI method is applied to sum-of-fractions of ILAW Class C radionuclides in Table 1 (SF1) and Table 2 (SF2) of 10 CFR 61.55 as discussed in Section 5.3.3. The concept of a TI was introduced in Section 3.2, with Eq. (3.3) providing the general formula for X%/Y% TIs. In this situation, the formulas for X%/Y% UTIs are given by

$$X\%/Y\%\ UTI(SF1_D^{Containers}) = \overline{SF1}_D^{Containers} + k(X,Y)\ SD(\overline{SF1}_d^{Container}) \tag{5.3.1a}$$

$$X\%/Y\%\ UTI(SF2_D^{Containers}) = \overline{SF2}_D^{Containers} + k(X,Y)\ SD(\overline{SF2}_d^{Container}) \tag{5.3.1b}$$

where

$X\%/Y\%\ UTI(SF1_D^{Containers})$ = X%/Y% UTI on $SF1_D^{Containers}$, the sum-of-fractions of ILAW radionuclides in Table 1 of 10 CFR 61.55 over the *D* ILAW containers associated with an LAW waste type

$X\%/Y\%\ UTI(SF2_D^{Containers})$ = X%/Y% UTI on $SF2_D^{Containers}$, the sum-of-fractions of ILAW radionuclides in Table 2 of 10 CFR 61.55 over the *D* ILAW containers associated with an LAW waste type

$\overline{SF1}_D^{Containers}$ and $\overline{SF2}_D^{Containers}$ are calculated using Eq. (B.3.4) and Eq. (B.3.5), respectively; $SD(\overline{SF1}_d^{Container})$ and $SD(\overline{SF1}_d^{Container})$ are calculated using Eq. (B.3.7) and Eq. (B.3.9), respectively; and $k(X, Y)$ is calculated as described in Section F.2 of Appendix F. Equations (B.3.4), (B.3.5), (B.3.7) and (B.3.9) are derived and discussed in Section B.3.1.1 of Appendix B.

Compliance with Class C limits for ILAW corresponding to an LAW waste type is demonstrated by calculating the X%/Y% UTIs on SF1 and SF2 using Eqs. (5.3.1a) and (5.3.1b), respectively, and verifying that the results are less than 1. An illustration of the application of the X%/Y% UTI formulas in Eqs. (5.3.1a) and (5.3.1.b) to realistic ILAW data is presented in Section 7.3.1.1.

5.3.3.2 Statistical Method for Assessing Whether ILAW Radionuclide Concentrations for ILAW from Each MFPV Batch Meet Class C Limits

Although not required by the WTP ILAW compliance strategy, presumably it is of interest to assess whether the ILAW that would be made from each MFPV batch satisfies the Class C limits. Again, the sum-of-fractions rule is used to make this assessment. Equations (B.3.10) and (B.3.11) in Section B.3.1.2 of Appendix B provide for calculating $\overline{SF1}_i^{MFPV}$ and $\overline{SF2}_i^{MFPV}$, the sum-of-fractions of radionuclides for Class C limits (in Tables 1 and 2 of 10 CFR 61.55) for ILAW that would be made from the i^{th} MFPV batch.

The Monte Carlo simulation approach described in Section 3.4.2 provides for quantifying the total uncertainties in $\overline{SF1}_i^{MFPV}$ and $\overline{SF2}_i^{MFPV}$ values resulting from the various ILAW process uncertainties affecting a given MFPV batch. During ILAW production, a Monte Carlo simulation could be run for each MFPV batch "*i,*" resulting in 1000 (say) values each of $\overline{SF1}_i^{MFPV}$ and $\overline{SF2}_i^{MFPV}$ calculated using Eqs. (B.3.10) and (B.3.11), respectively.[(a)] From these 1000 values, CL% empirical upper confidence intervals (CL% EUCIs) on $\overline{SF1}_i^{MFPV}$ and $\overline{SF2}_i^{MFPV}$ can be obtained. Equations for these CL% EUCIs are given by

$$\text{CL\% EUCI}(\overline{SF1}_i^{MFPV}) = \overline{SF1}_i^{(1-\alpha)} \tag{5.3.2a}$$

$$\text{CL\% EUCI}(\overline{SF2}_i^{MFPV}) = \overline{SF2}_i^{(1-\alpha)} \tag{5.3.2b}$$

where

$\text{CL\% EUCI}(\overline{SF1}_i^{MFPV})$ = CL% EUCI on $\overline{SF1}_i^{MFPV}$, the sum-of-fractions of ILAW radionuclides in Table 1 of 10 CFR 61.55 for ILAW corresponding to the i^{th} ILAW MFPV batch

$\overline{SF1}_i^{(1-\alpha)}$ = CL% [= $100(1-\alpha)^{th}$] percentile of the 1000 simulated values of $\overline{SF1}_i^{MFPV}$

and $\text{CL\% EUCI}(\overline{SF2}_i^{MFPV})$ and $\overline{SF2}_i^{(1-\alpha)}$ are similarly defined except for radionuclides in Table 2 of 10 CFR 61.55.

(a) Although the Monte Carlo simulations for a large number of test cases (such as described in Section 3.4.2) can be time consuming, during ILAW production, the estimates of uncertainties and number of samples, analyses, and other process measurements would all be set. Hence, this would be like running the Monte Carlo simulation for one test case, which requires only a few seconds computing time. Alternately, tentative discussions with the WTP Project have considered running Monte Carlo simulations for a matrix of combinations before production. Then a table lookup or interpolation process would be used to obtain the desired total uncertainties rather than actually performing Monte Carlo simulations for each MFPV batch during ILAW production.

If the values of CL% EUCI ($\overline{SF1}_i^{MFPV}$) and CL% EUCI ($\overline{SF2}_i^{MFPV}$) are less than 1, then that ILAW MFPV batch would be statistically demonstrated as satisfying Class C limits with CL% confidence. An illustration of the method is presented in Section 7.3.1.2.

5.3.4 Statistical Method for Determining the Numbers of Samples, Analyses, and Volume Determinations to Demonstrate that ILAW Radionuclide Concentrations for Each MFPV Batch Meet Class C Limits

This subsection describes the statistical method to address Item 2 in Section 5.3.2. Specifically, a method is described for determining the numbers of samples per CRV batch, numbers of radiochemical analyses per CRV sample, and numbers of volume determinations of CRV and MFPV batches necessary to demonstrate that ILAW radionuclide concentrations for each MFPV batch meet Class C limits in Tables 1 and 2 of 10 CFR 61.55 (these limits are summarized in Table B.1 of Section B.3 in Appendix B). The method uses the sum-of-fractions rule, as described in Section 5.3.3.

Section 3.4.2 describes the Monte Carlo simulation approach that was used to assess the impacts of several factors on the total uncertainty in estimating the sum-of-fractions, where the magnitude of the total uncertainty affects the ability to demonstrate that ILAW from each MFPV batch complies with Class C limits. These factors are listed in Section 5.2.3, and include (1) the numbers of samples per CRV batch, analyses per CRV sample, and volume determinations on CRV and MFPV batches, and (2) several uncertainties in the ILAW process. It is necessary at this time to consider a range of values for process uncertainties (as discussed in Section 3.4.2) because final estimates have not yet been produced by the WTP Project. A future update of this report will use final estimates of process uncertainties to determine the final recommended numbers of CRV samples, radiochemical analyses per CRV sample, and volume determinations of the CRV and MFPV for demonstrating compliance with Class C limits.

The methodology described in Section 5.3.3.2 was implemented as part of the Monte Carlo simulation described in Section 3.4.2. Compliance for each test case (combination of factor levels) in the ILAW simulation was determined by comparing the values of CL% EUCI ($\overline{SF1}_i^{MFPV}$) and CL% EUCI ($\overline{SF2}_i^{MFPV}$) to the limiting value of 1. Test cases with values of n_S^{CRV}, n_A^{CRV}, n_V^{CRV}, and n_V^{MFPV} that yield CL% EUCI ($\overline{SF1}_i^{MFPV}$) and CL% EUCI ($\overline{SF2}_i^{MFPV}$) values less than 1 provide for meeting Class C limits. For given values of n_V^{CRV} and n_V^{MFPV}, the test case with the minimal number of total analyses ($n_S^{CRV} \times n_A^{CRV}$) that demonstrates compliance is the number of CRV samples and analyses necessary for meeting Class C limits. The results of such calculations are presented in Section 7.3.2.

5.3.5 Statistical Method to Demonstrate that Running-Average Concentrations of ^{137}Cs and ^{90}Sr Meet Specified Limits

This subsection describes the statistical method to address Item 3 in Section 5.3.2. The goal of the method is to demonstrate that running-average concentrations of ^{137}Cs and ^{90}Sr over some specified period of ILAW production (e.g., an ILAW production lot, ILAW production corresponding to an LAW

waste type, or all ILAW production up to some point in time) meet the limits given in Contract Specification 2.2.2.8.

The appropriate statistical method is to calculate CL% UCIs for the true, unknown running-average concentrations of ^{137}Cs and ^{90}Sr and then verify that the CL% UCI values are less than the limits in Specification 2.2.2.8. The formula is given by

$$CL\%\ UCI = \bar{\bar{r}}_{Dq}^{Container} + t_{1-\alpha,df}\ SD(\bar{\bar{r}}_{Dq}^{Container}) \tag{5.3.3}$$

where

$\bar{\bar{r}}_{Dq}^{Container}$ = running average of activity-per-volume concentrations of the q^{th} radionuclide (q = ^{137}Cs and ^{90}Sr) over the D ILAW containers produced through a given point in time, based on averages over multiple samples, analyses per sample, and volume determinations (Ci/m^3)

$t_{1-\alpha,df}$ = 100(1−α) percentile of a Student's t-distribution with df degrees of freedom, which provides CL% = 100(1−α) percent confidence for the one-sided UCI (e.g., 95% when $\alpha = 0.05$)

$SD(\bar{\bar{r}}_{Dq}^{Container})$ = standard deviation of $\bar{\bar{r}}_{Dq}^{Container}$, which is sometimes referred to as a *standard error* because it is the standard deviation of an average (Ci/m^3).

The running average $\bar{\bar{r}}_{Dq}^{Container}$ can be calculated using Eq. (B.3.13) in Section B.3.2.1 of Appendix B. The quantity $SD(\bar{\bar{r}}_{Dq}^{Container})$ can be calculated using Eq. (F.3.3) in Section F.3 of Appendix F. A formula for df is given as Eq. (F.3.4) in Section F.3 of Appendix F.

An illustration of the method is presented in Section 7.3.3.

5.3.6 Statistical Method for Determining the Numbers of Samples, Analyses, and Volume Determinations to Demonstrate that Running-Average Concentrations of ^{137}Cs and ^{90}Sr Meet Specified Limits

This subsection describes the statistical method to address Item 4 in Section 5.3.2. Specifically, a method is described for determining the numbers of samples per CRV batch, numbers of radiochemical analyses of ^{137}Cs and ^{90}Sr per CRV sample, and numbers of volume determinations of CRV and MFPV batches necessary to demonstrate that ILAW ^{137}Cs and ^{90}Sr concentrations meet the Contract Specification 2.2.2.8 limits of ^{137}Cs ≤ 3 Ci/m^3 and ^{90}Sr ≤ 20 Ci/m^3.

The statistical method involves calculating CL% UCIs via Eq. (5.3.3) for combinations of levels of

- the factors described in Section 3.4.2, including the various uncertainties affecting the ILAW process
- a factor corresponding to variations in ^{137}Cs or ^{90}Sr concentrations over the *I* MFPV batches and *D* ILAW containers corresponding to an LAW waste type.

Then, the resulting CL% UCIs would be compared to the ^{137}Cs and ^{90}Sr concentration limits given in Contract Specification 2.2.2.8. Test cases (combinations of factor levels) with values of n_S^{CRV}, n_A^{CRV}, n_V^{CRV}, and n_V^{MFPV} that yield CL% UCI values less than the limiting concentrations for ^{137}Cs and ^{90}Sr provide for meeting the specification. For given values of n_V^{CRV} and n_V^{MFPV}, the test case with the minimal number of total analyses ($n_S^{CRV} \times n_A^{CRV}$) that demonstrates compliance is the number of CRV samples and analyses necessary for meeting the ^{137}Cs and ^{90}Sr concentration limits.

The details of the statistical method for combining variations over ILAW MFPV batches corresponding to an LAW waste type and uncertainties within MFPV batches have not yet been developed. Implementing such a method is complicated because (1) ILAW uncertainties are propagated in a Monte Carlo simulation, and (2) variations over ILAW MFPV batches corresponding to an LAW waste type are not amenable to treatment via Monte Carlo simulation. Item (2) is the case because variation over MFPV batches is not expected to follow a nice statistical distribution (e.g., a Gaussian distribution). Thus, what is ideally required is a way to combine the Monte Carlo simulation software with software such as, or which could emulate, the WTP Project's G2 dynamic simulation flowsheet (Deng 2004; Vora 2004). However, such a development effort is beyond the current scope.

An alternative method was used to provide a basis for assessing the numbers of samples per ILAW CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations. Specifically, only uncertainties affecting single MFPV batches were considered, as discussed in Section 3.4.2. This approach is the same as used to address other specifications in this report. The results of calculations using this method to provide input on values of n_S^{CRV}, n_A^{CRV}, n_V^{CRV}, and n_V^{MFPV} required to comply with ^{137}Cs and ^{90}Sr limits for each MFPV batch are presented in Section 7.3.4.

5.4 Compliance Approach and Methods for ILAW Contract Specification 2.2.2.17: Waste Form Testing

Section 5.4.1 lists the applicable Contract Specification 2.2.2.17 and its sub-specifications 2.2.2.17.2 (PCT) and 2.2.2.17.3 (VHT). Section 5.4.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Sections 5.4.3 to 5.4.6 present the statistical methods that will be used to implement the statistical aspects of the compliance strategy.

5.4.1 Contract Specification 2.2.2.17: Waste Form Testing

Contract Specification 2.2.2.17.2: Product Consistency Test (PCT)

The normalized mass loss of sodium, silicon, and boron shall be measured using a seven day product consistency test run at 90°C as defined in ASTM C1285-98. The test shall be conducted with a glass to water ratio of 1 gram of glass (-100 +200 mesh) per 10 milliliters of water. The normalized mass loss shall be less than 2.0 grams/m^2. Qualification testing shall include glass samples subjected to representative waste form cooling curves. The product consistency test shall be conducted on waste form samples that are statistically representative of the production glass.

Contract Specification 2.2.2.17.3: Vapor Hydration Test (VHT)

The glass corrosion rate shall be measured using at least a seven day vapor hydration test run at 200°C as defined in the DOE concurred upon ILAW Product Compliance Plan. The measured glass alteration rate shall be less than 50 grams/(m^2 day). Qualification testing shall include glass samples subjected to representative waste form cooling curves. The vapor hydration test shall be conducted on waste form samples that are representative of the production glass.

5.4.2 Statistical Aspects of the ILAW Compliance Strategy for Contract Specifications 2.2.2.17.2 and 2.2.2.17.3

The following items describe the statistical and related aspects of the ILAW compliance strategy for Contract Specifications 2.2.2.17.2 and 2.2.2.17.3 (see the ILAW PCP, Nelson et al. 2003) that are addressed in this report.[(a)]

Item 1: Develop a statistical interval method to demonstrate that the contents of each MFPV batch would produce ILAW compliant with the PCT and VHT specifications. The method will account for uncertainties impacting the estimate of PCT and VHT responses for ILAW that would be produced from each MFPV batch (e.g., sampling, analytical, other measurements, and property-composition model uncertainties).

Item 2: Determine the numbers of process samples, chemical analyses per sample, and other process measurements required to demonstrate that the PCT and VHT responses for ILAW that would be produced from each MFPV batch will satisfy their respective limits. The calculations will require estimates of applicable process uncertainties (mixing/sampling, analytical, and other process measurements) as well as property-composition model uncertainties.

Item 3: Develop a statistical interval method to demonstrate that ILAW glass produced over a waste type complies with the PCT and VHT specifications. The method will account for the source of variation of interest (namely variation in PCT or VHT performance due to variation in ILAW composition over the course of a waste type). The method will also account for nuisance

(a) See Section 1.0 for a discussion of why this report addresses ILAW PCP Rev. 0 (Nelson et al. 2003) rather than ILAW PCP Rev. 1 (Westsik et al. 2004).

uncertainties (e.g., sampling, analytical, other measurements, and property-composition model uncertainties). Statistical X%/Y% UTIs may be used for this purpose.

Item 4: Determine the numbers of process samples, chemical analyses per sample, and other process measurements required to demonstrate that the PCT and VHT responses for ILAW produced from a waste type will satisfy their respective limits. The calculations will require estimates of glass-composition variation over a waste type, applicable process uncertainties (mixing/sampling, analytical, and other process measurements), and property-composition model uncertainties.

Note that Items 1 and 2 do not appear specifically in the ILAW PCP (Nelson et al. 2003) addressed in this report. However, they are consistent with that version of the WTP Project's compliance strategy for Contract Specifications 2.2.2.17.2 and 2.2.2.17.3 to demonstrate compliance for each ILAW MFPV batch as well as over each LAW waste type. Items 1 and 2 are a part of the work scope covered in this report (Piepel and Heredia-Langner 2003) and hence were included in this section.

The statistical methods to implement these aspects of the WTP ILAW compliance strategy for Contract Specifications 2.2.2.17.2 and 2.2.2.17.3 are discussed in Sections 5.4.3 to 5.4.6.

5.4.3 Statistical Interval Method to Demonstrate that ILAW Corresponding to an MFPV Batch Will Satisfy PCT and VHT Limits

This subsection discusses and presents the formula for an appropriate statistical interval to satisfy Item 1 of Section 5.4.3. The statistical interval must (1) account for the uncertainty in the estimated ILAW composition corresponding to a given MFPV batch, (2) account for the uncertainties in property-composition models used to predict natural logarithms of PCT normalized B, Na, and Si releases ($r^{PCT\,B}$, $r^{PCT\,Na}$, and $r^{PCT\,Si}$ in units of g/L) and predict the natural logarithm of VHT alteration depth (D^{VHT} in units of μm) at 24 ± 2 days for the estimated ILAW composition corresponding to a given MFPV batch, and (3) provide high confidence that the true PCT and VHT values are less than the limits specified in Contract Specifications 2.2.2.17.2 and 2.2.2.17.3. These limits are:

$$\begin{aligned} r^{PCT\,B} &\le 2\ \text{g/m}^2 = 4\ \text{g/L} \\ r^{PCT\,Na} &\le 2\ \text{g/m}^2 = 4\ \text{g/L} \\ r^{PCT\,Si} &\le 2\ \text{g/m}^2 = 4\ \text{g/L} \\ R^{VHT} &\le 50\ \text{g/m}^2\text{day or } D^{VHT} \le 453\ \mu\text{m} \end{aligned} \tag{5.4.1}$$

It is important to note that VHT is modeled in natural logarithm of alteration depth (in μm) at 24 ± 2 days, but the specification limit is in alteration rate (g/m^{2}day). An alteration depth from the model can be converted to alteration rate (in g/m^{2}day) using the following equation:

$$R^{VHT} = e^{\ln(D^{VHT})} \times \frac{2.65}{24} \tag{5.4.2}$$

where $\ln(D^{VHT})$ is the natural logarithm of the alteration depth as calculated from the VHT model, 2.65 represents the assumed glass density (g/cm^3), and 24 represents the number of test days. A slight modification of Eq. (5.4.2) converts the VHT alteration rate limit of 50 g/m^{2}day to the VHT alteration depth limit of 453 μm listed in Eq. (5.4.1).

Section 5.4.3.1 presents the initial forms of recommended property-composition models for PCT normalized releases of B and Na, and VHT alteration depth. PCT normalized releases of Si from simulated LAW glasses are dominated by B and Na releases, and so the WTP Project made the decision that PCT Si releases need not be modeled (see Muller et al. 2005). Section 5.4.3.2 presents the equations for the appropriate type of statistical interval.

5.4.3.1 Property-Composition Model Forms for PCT Normalized Releases of B and Na and VHT Alteration Depth

Reduced partial quadratic mixture (PQM) models were developed by PNWD and VSL (Muller et al. 2005) for predicting PCT normalized releases of B and Na, as well as VHT alteration depth, for ILAW compositions. These models are of the general form

$$\hat{\bar{y}}_i^h = \sum_{k=1}^{n_{mc}^h} b_k^h \, \bar{x}_{ik}^{MFPV} + Selected\left\{ \sum_{k=1}^{n_{mc}^h} b_{kk}^h \left(\bar{x}_{ik}^{MFPV}\right)^2 + \sum_{k=1}^{n_{mc}^h - 1} \sum_{l>k}^{n_{mc}^h} b_{kl}^h \bar{x}_{ik}^{MFPV} \bar{x}_{il}^{MFPV} \right\} \qquad (5.4.3a)$$

$$= (\boldsymbol{b}^h)^T \, \bar{\boldsymbol{x}}_i^{MFPV} \qquad (5.4.3b)$$

where

$\hat{\bar{y}}_i^h$ = predicted natural logarithm of the PCT normalized release of h = B or Na [$\hat{ln}(r_i^{PCT\ h})$], or the predicted natural logarithm of the VHT alteration depth [$\hat{ln}(D_i^{VHT})$], for ILAW corresponding to the i^{th} MFPV batch, based on averages over multiple samples from a CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations. For PCT, the units are ln(g/L), and for VHT, the units are ln(μm).

n_{mc}^h = number of normalized ILAW components used in the model for property h = PCT normalized release of B or Na, or VHT alteration depth

b_k^h, b_{kk}^h, b_{kl}^h = coefficients for the PQM model form involving normalized components (k and l) of ILAW in the model for h = PCT normalized release of B or Na, or VHT alteration depth. The coefficients are obtained by fitting the PQM model form to a property-composition data set using least squares regression.

$\bar{x}_{ik}^{MFPV}$ = normalized mass fractions of the ILAW components in the PQM model, such that $\sum_{k=1}^{p} x_{ik}^{MFPV} = 1$. The mass fractions are based on averages over multiple samples from a CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations.

p = number of coefficients (including linear, squared, and crossproduct terms) in a PQM model

$\boldsymbol{b}^h$ = $p \times 1$ column vector of the model coefficients b_k^h, b_{kk}^h, and b_{kl}^h

$\bar{\boldsymbol{x}}_i^{MFPV}$ = $p \times 1$ column vector of the ILAW normalized composition $\bar{x}_{ik}^{MFPV}$, $k = 1, 2, \ldots,$ n_{mc}^h expanded to the form of the terms in the PQM model for PCT or VHT.

In Eq. (5.4.3a), "Selected" means that only a subset of the squared and crossproduct terms in the curly brackets are included in the model. The subset is selected using standard stepwise regression or similar methods. See Piepel et al. (2002) for further discussion and illustrations of PQM models.

The normalized mass-fraction compositions of ILAW in Eq. (5.4.3a) are obtained from the ordinary (unnormalized) mass-fraction compositions by

$$\bar{x}_{ik}^{MFPV} = \frac{\bar{g}_{ij}^{MFPV}}{\sum_{j}^{n_{mc}^h \text{ of } J} \bar{g}_{ij}^{MFPV}} \quad k = 1,2,\cdots,n_{mc}^h \tag{5.4.4}$$

where $\bar{g}_{ij}^{MFPV}$ is calculated using Eq. (B.1.11) in Section B.1 of Appendix B.

Finally, it is important to understand the difference in notation of $\hat{\bar{y}}_i^h$ introduced in this section for ILAW compliance and the notation of $\bar{\hat{y}}_i^h$ introduced in Section 4.3.3.2 for IHLW compliance. In the ILAW notation of $\hat{\bar{y}}_i^h$, the "bar" appears first and denotes the averaging over multiple samples, analyses per sample, and volume determinations that takes place to yield an ILAW composition estimate for the i^{th} MFPV batch. Then, a PCT or VHT model is applied to this averaged ILAW composition estimate, so the "hat" (denoting a model prediction) appears above the "bar." In the IHLW notation of $\bar{\hat{y}}_i^h$, the "hat" appears first because model predictions are made for each of the $n_S^{MFPV} \times n_A^{MFPV}$ separate estimates of IHLW composition for the i^{th} MFPV batch ($g_{iklm}^{MFPV} \rightarrow x_{iklm}^{MFPV}$, $l = 1, 2, \ldots, n_S^{MFPV}$ and $m = 1, 2, \ldots, n_A^{MFPV}$). Then, these $n_S^{MFPV} \times n_A^{MFPV}$ model predictions are averaged, so that the "bar" appears above the "hat." The more complicated nature of the WTP's ILAW compliance strategy (see Section 2.3) precludes obtaining multiple separate estimates of ILAW for each MFPV batch.

Table 5.1 lists the PQM model terms and the coefficients for PCT B, PCT Na, and VHT used for the work in this report. These models and coefficients are documented in the report by Muller et al. (2005).

Table 5.1. ILAW PCT and VHT Model Terms and Coefficients

PQM Model Term	ln(PCT B)[(a)] Coefficient	ln(PCT Na)[(a)] Coefficient	ln(VHT)[(b)] Coefficient
Al_2O_3	-19.9158	-17.2629	49.8620
B_2O_3	1.6716	2.2622	8.5808
CaO	-1.5471	3.9240	-21.4725
Fe_2O_3	-0.8289	2.1598	18.3252
K_2O	4.9225	41.2770	137.6727
Li_2O	-6.9721	-5.4762	113.4367
MgO	-25.7905	-9.9926	-31.3959
Na_2O	15.2327	12.9487	35.2036
SO_3	(c)	(c)	-707.4950
SiO_2	-3.1991	-3.4173	-15.5899
TiO_2	-11.0586	-8.1687	-20.1469
ZnO	(c)	(c)	1.8503
ZrO_2	-18.0010	-19.8097	-73.6987
Others	(c)	(c)	-83.5317
Al_2O_3 * K_2O	(c)	(c)	-1206.9348
B_2O_3 * CaO	(c)	(c)	-731.6002
B_2O_3 * K_2O	(c)	-199.2665	(c)
B_2O_3 * MgO	493.3071	267.6811	(c)
B_2O_3 * SO_3	(c)	(c)	6505.9075
CaO * Fe_2O_3	(c)	(c)	-486.3382
CaO * SiO_2	(c)	(c)	304.4759
Fe_2O_3 * K_2O	(c)	-266.2859	(c)
Fe_2O_3 * Li_2O	349.7992	201.4967	(c)
K_2O * ZnO	(c)	(c)	-1288.2916
Li_2O * ZrO_2	541.9078	526.3173	(c)
MgO * Others	(c)	(c)	1733.1272
MgO * TiO_2	(c)	(c)	1430.2732
Model and Data Information			
n[(d)]	69	69	70
p[(d)]	14	16	22
$df_m = n - p$[(e)]	55	53	48

(a) PCT normalized elemental releases are modeled in ln(g/L).
(b) VHT alteration depth is modeled in ln(μm).
(c) A missing value indicates that the model term was not included for that particular property.
(d) The notation n denotes the number of data points used to estimate the coefficients in the model form given by Eq. (5.4.3.a). The notation p denotes the number of coefficients estimated.
(e) df_m denotes the model degrees of freedom, calculated as indicated.

5.4.3.2 Equation for CL% Upper Combined Confidence Interval for PCT Normalized Releases of B and Na, and VHT Alteration Depth for a Single ILAW MFPV Batch

An appropriate statistical interval for demonstrating that the PCT and VHT limits in Eq. (5.4.1) are satisfied for each MFPV batch is a CL% UCCI, the concept of which was introduced in Section 3.1. Section B.4 of Appendix B discusses the statistical method for combining model and composition uncertainties that is used in forming a CL% UCCI. The CL% UCCI formula is given in general by

$$CL\%\ UCCI(y_i^h) = \hat{\bar{y}}_i^h + CHW_{i,CL\%\ UCI}^h + MHW_{i,CL\%\ SUCI}^h \qquad (5.4.5)$$

where

$CL\%\,UCCI(y_i^h)$ = CL% UCCI for the true, unknown mean value of the property y_i^h [that is, the natural logarithm of the PCT normalized release of element h (= B or Na) or natural logarithm of the VHT alteration depth] from ILAW corresponding to the i^{th} MFPV batch. This is in units of ln(g/L) for PCT and ln(μm) for VHT.

$\hat{\bar{y}}_i^h$ = predicted natural logarithm of the PCT normalized release of h = B or Na [$\hat{ln}(r_{ilm}^{PCT\ h})$], or the predicted natural logarithm of the VHT alteration depth [$\ln(D^{VHT})$] for ILAW corresponding to the i^{th} MFPV batch, based on averages over multiple samples from a CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations. For PCT, the units are ln(g/L), and for VHT, the units are ln(μm).

$CHW_{i,CL\%\ UCI}^h$ = composition uncertainty half-width for a CL% upper confidence interval (CL% UCI) for PCT or VHT for ILAW corresponding to the i^{th} MFPV batch

$MHW_{i,CL\%\ SUCI}^h$ = model uncertainty half-width for a CL% simultaneous upper confidence interval (CL% SUCI) for PCT or VHT for ILAW corresponding to the i^{th} MFPV batch.

A CL% SUCI is one of several UCIs on the true mean values of predictions made by a glass property-composition model for a set of glass compositions. All of the UCIs 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. Thus, CL% SUCIs for many glass compositions provide high confidence of containing the true property mean values for those glass compositions. The CL% SUCI method has been used by DWPF and WVDP in their strategies for complying with WAPS 1.3 for IHLW and is also proposed for that use by the WTP Project (see Section 4.3.3.2). Figure 4.1 in Section 4.3.3.2 illustrates the general concept of a CL% UCCI.

During operation of the WTP ILAW facility, it is expected that $n_A^{CRV} = 1$ for reasons discussed elsewhere in this report. However, equations for the terms on the right hand side of Eq. (5.4.5) are the same given the notation used for the cases of (1) $n_S^{CRV} > 1$ samples and $n_A^{CRV} > 1$ analyses per sample of the i^{th} MFPV batch and (2) $n_S^{CRV} > 1$ samples and $n_A^{CRV} = 1$ analyses per sample of the i^{th} MFPV batch. The difference in these two cases occurs in the calculation of $\overline{\boldsymbol{g}}_i^{MFPV}$ as shown in Section B.1.2 of Appendix B. Otherwise, the equations for the terms on the right hand side of Eq. (5.4.5) are the same.

The quantity $\hat{\bar{y}}_i^h$ in Eq. (5.4.5) is calculated using Eq. (5.4.3a) in Section 5.4.3.1. The quantity $CHW_{CL\%\ UCI}^{ih}$ in Eq. (5.4.5) is obtained using the Monte Carlo simulation approach. Specifically, each of 1000 simulations of the i^{th} ILAW MFPV batch yields an ILAW composition estimate $\overline{\boldsymbol{g}}_i^{MFPV}$ (mass fractions of oxides or halogens), which is converted to a reduced normalized composition $\overline{\boldsymbol{x}}_i^{MFPV}$ using Eq. (5.4.4), and then the property-composition model in Eq. (5.4.3a) is applied. The result is 1000 simulated values of $\hat{\bar{y}}_i^h$ for the i^{th} ILAW MFPV batch. Then, $CHW_{i,CL\%\ UCI}^h$ is determined from the CL% EUCI (CL% empirical upper confidence interval) obtained from the 1000 simulated values of $\hat{\bar{y}}_i^h$ according to

$$CHW_{i,CL\%\ UCI}^h = \hat{\bar{y}}_{i,1-\alpha}^h - \hat{\bar{y}}_i^h \tag{5.4.6}$$

where

$\hat{\bar{y}}_{i,1-\alpha}^h$ = CL% = 100(1 – α) percentile of the empirical distribution of 1000 values of $\hat{\bar{y}}_i^h$ resulting from 1000 Monte Carlo simulations of the i^{th} ILAW MFPV batch

and the remaining notation is as previously defined. Recall that the "bar" notation appearing in $\hat{\bar{y}}_{i,1-\alpha}^h$ and $\hat{\bar{y}}_i^h$ denotes model predictions for an estimate of ILAW composition of the i^{th} MFPV batch obtained by averaging over multiple samples per MFPV batch, analyses per MFPV sample, and volume determinations per MFPV batch. If $n_A^{CRV} = 1$, then the averaging would only occur with respect to the multiple samples per MFPV batch and multiple volume determinations if volumes are determined more than once for each MFPV batch.

The quantity $MHW_{i,CL\%\ SUCI}^h$ in Eq. (5.4.5) is given by

$$MHW_{i,CL\%\ SUCI}^h = \sqrt{p\ F_{1-\alpha}(p, n-p)}\left(\sqrt{(\overline{\mathbf{x}}_i^{MFPV})^{\mathrm{T}}\ \hat{\boldsymbol{\Sigma}}_b^h\ \overline{\mathbf{x}}_i^{MFPV}}\right) \tag{5.4.7}$$

where

p = number of coefficients in the appropriate PCT or VHT model. Note that this is not the same as the number of model components because of using a PQM model.

$F_{1-\alpha}(p, n-p)$ = CL% = 100(1 – α) percentile of an F-distribution with p numerator degrees of freedom and $n - p$ denominator degrees of freedom, where n is the number of data points used to fit the model, and p is the number of model coefficients estimated from the data

$\bar{\boldsymbol{x}}_i$ = $p \times 1$ column vector whose first n_{mc}^h entries $\bar{x}_{ik}^{MFPV}, k = 1, 2, \cdots, n_{mc}^h$ are given by Eq. (5.4.4). The remaining entries $\bar{x}_k^{MFPV}, k = n_{mc}^h + 1, \cdots, p$ are squares and/or crossproducts of the initial entries according to the form of the PQM model.

$\hat{\boldsymbol{\Sigma}}_b^h$ = $p \times p$ variance-covariance matrix of the model coefficient vector $\boldsymbol{b}^h$ for the PCT normalized release of h = B, Li, or Na. The variances of the coefficients are located on the diagonal of the matrix, and the covariances between pairs of coefficients are located on the off-diagonal positions of the matrix

and the remaining notation is as previously defined. General equations for calculating model variance-covariance matrices such as $\hat{\boldsymbol{\Sigma}}_b^h$ are given in Section B.4 of Appendix A. The variance-covariance matrices for the ILAW PCT normalized B and Na models given in Table 5.1 are included in Appendix D of Muller et al. (2005).

An illustration of the methods applied to PCT normalized releases is presented in Section 7.4.1. An illustration of the methods applied to VHT alteration depth is presented in Section 7.5.1.

5.4.4 Statistical Method for Determining the Numbers of Samples, Analyses per Sample, and Volume Determinations to Demonstrate ILAW from an MFPV Batch Will Satisfy PCT and VHT Limits

This subsection discusses the methodology used to address Item 2 of Section 5.4.2. The CL% UCCI formula given by Eqs. (5.4.5) to (5.4.7) in Section 5.4.3 can be used to calculate CL% UCCI values given property-composition models for PCT and VHT responses, variance-covariance matrices for the model coefficients, and various combinations of values of the following factors:

- number of LAW CRV samples (n_S^{CRV})
- number of analyses per CRV sample (n_A^{CRV})
- numbers of volume determinations of the CRV and MFPV before and after transfers (n_V^{CRV} and n_V^{MFPV})

- mixing/sampling %RSD in the concentration of the j^{th} element in a CRV batch [$\%RSD_S(c_j^{CRV})$]
- analytical %RSD in the concentration of the j^{th} element in a CRV batch [$\%RSD_A(c_j^{CRV})$]
- GFC composition uncertainty, represented by the standard deviation in the mass fraction of the j^{th} component (oxide or halogen) in the k^{th} GFC [$SD(G_{jk}^{GFC})$]
- GFC mass uncertainty, represented by the standard deviation of the mass of the k^{th} GFC added to a MFPV batch. This uncertainty includes uncertainties due to batching, weighing, and transfers of GFCs.
  [$SD(a_k^{GFC})$]
- volume uncertainties in the CRV and MFPV. The magnitudes of these uncertainties will depend on the level of contents in a vessel, but a generic notation is used for now (SD_V^{CRV} and SD_V^{MFPV}).
- statistical percent confidence level (CL%)
- ILAW produced from three tanks representing one each of Envelopes A (AP-101), B (AZ-101), and C (AN-107).

After calculating the CL% UCCI values for all of the combinations of input factors, the ones that satisfy the PCT limits or VHT limits are then inspected to find the least number of total analyses (number of samples × number of analyses) necessary to comply with the appropriate limits. The results of these calculations as applied to PCT are presented in Section 7.4.2. The results of these calculations as applied to VHT are presented in Section 7.5.2.

5.4.5 Statistical Interval Method to Demonstrate that ILAW from an LAW Waste Type Will Satisfy PCT and VHT Limits

This subsection discusses and presents the formula for an appropriate statistical interval to satisfy Item 3 of Section 5.4.2. The statistical interval must account for (1) variation in property values (i.e., PCT normalized releases of B and Na, and VHT alteration rate) resulting from the variation in ILAW composition over the course of an LAW waste type, (2) uncertainty in the estimated ILAW composition corresponding to each MFPV batch resulting from applicable ILAW process uncertainties, and (3) uncertainties in property-composition models used to predict (a) the natural logarithm of PCT normalized B and Na releases and (b) the natural logarithm of VHT alteration depth for the estimated ILAW composition corresponding to a given MFPV batch. Finally, the statistical interval must provide high confidence that the true PCT and VHT values for the vast majority of ILAW produced from an LAW waste type are less than the limits given in Contract Specifications 2.2.2.17.2 and 2.2.2.17.3.

An appropriate statistical interval for demonstrating with high (X%) confidence that a high percentage (Y%) of ILAW produced from an LAW waste type satisfies the property limits in Eq. (5.4.1) is a X%/Y% UTI. The concept of a X%/Y% UTI was introduced in Section 3.2. Section B.4 of Appendix B discusses the statistical method for combining model and composition uncertainties that is used in forming a X%/Y% UTI. Piepel and Cooley (2002) derived the equations necessary to calculate an

X%/Y% UTI. They also explained (Sections 1.2 and 4.2) why the X%/Y% UTI approach is appropriate and preferred over the "two standard deviation" approach as mentioned in WAPS 1.3 for IHLW.

The X%/Y% UTI equations developed by Piepel and Cooley (2002) are applicable for production compliance strategies that involve estimating glass composition from analyses of samples from a single process location. At the time the Piepel and Cooley (2002) work was performed, the WTP ILAW compliance strategy was to estimate glass composition for reporting and compliance purposes based on analyses of shard samples taken from the tops of ILAW containers before closure. However, the current ILAW compliance strategy is more complicated, as discussed in Section 2.3. The strategy is more complicated because it involves using analyses of CRV samples, weights of GFCs, volume determinations, and other process information all subject to uncertainty. However, the X%/Y% UTI equations developed by Piepel and Cooley (2002) can be adapted for use to account for the current ILAW compliance strategy.

Equation (3.3) in this report gives the general form of a two-sided X%Y% TI. To obtain a one-sided X%/Y% UTI, the equation changes to the following

$$\text{X\%/Y\% UTI} = \tilde{\mu} + k(X, Y)\,\tilde{\sigma} \tag{5.4.8}$$

where

X%/Y% UTI = a value that with X% confidence captures Y% of the distribution (population) of true mean ln(PCT releases) or ln(VHT alteration depth) over the MFPV batches corresponding to an LAW waste type

$\tilde{\mu}$ = estimate of the population mean that is calculated by forming the model-predicted ln(PCT release) or ln(VHT alteration depth) for each MFPV batch and averaging them across all MFPV batches corresponding to an LAW waste type

$k(X, Y)$ = UTI multiplier that is implicitly a function of X, Y, degrees of freedom associated with $\tilde{\sigma}$ and other parameters

$\tilde{\sigma}$ = estimate of the population standard deviation that properly accounts for (1) variation in ln(PCT releases) or ln(VHT alteration depth) across MFPV batches corresponding to an LAW waste type, (2) all ILAW process uncertainties affecting each MFPV batch, and (3) model uncertainty [ln(g/L) for PCT and ln(μm) for VHT].

The quantities X and Y generally should have values between 90% (or 95%) and 100%, to provide high confidence that a high percentage of ILAW produced from an LAW waste type satisfies the requirements of Contract Specifications 2.2.2.17.2 and 2.2.2.17.3. However, X and Y can never take values of 100% because it is impossible to be 100% confident about 100% of the true distribution of ln(PCT releases) or ln(VHT alteration depth) given estimated ILAW composition variation as well as ILAW composition and model uncertainties.

During operation of the WTP ILAW facility, it is expected that $n_A^{CRV} = 1$ for reasons discussed elsewhere in this report. However, equations for the terms on the right hand side of Eq. (5.4.8) are the same given the notation used for the cases of (1) $n_S^{CRV} > 1$ samples and $n_A^{CRV} > 1$ analyses per sample of the i^{th} MFPV batch and (2) $n_S^{CRV} > 1$ samples and $n_A^{CRV} = 1$ analyses per sample of the i^{th} MFPV batch. The difference in these two cases occurs in the calculation of $\bar{\boldsymbol{g}}_i^{MFPV}$ as shown in Section B.1.2 of Appendix B. Otherwise, the equations for the terms on the right hand side of Eq. (5.4.8) are the same. Section F.4 of Appendix F presents additional detail regarding the following equations for the terms in Eq. (5.4.8).

The equation for $\tilde{\mu}$ in Eq. (5.4.8) is given by

$$\begin{aligned} \tilde{\mu} = \bar{\hat{y}}^h &= \frac{\sum_{i=1}^{I} \hat{\bar{y}}_i^h}{I} \\ &= \frac{1}{I}\sum_{i=1}^{I}\left[\left(\sum_{k=1}^{n_{mc}^h} b_k^h \, \bar{x}_{ik}^{MFPV} + Selected\left\{\sum_{k=1}^{n_{mc}^h} b_{kk}^h \left(\bar{x}_{ik}^{MFPV}\right)^2 + \sum_{k=1}^{n_{mc}^h - 1}\sum_{l>k}^{n_{mc}^h} b_{kl}^h \bar{x}_{ik}^{MFPV}\bar{x}_{il}^{MFPV}\right\}\right)\right] \end{aligned} \tag{5.4.9}$$

where the notation is as defined in previous subsections of Section 5.4. Note that Eq. (5.4.9) calculates the ordinary mean (average) of the model-predicted property values over the *I* ILAW MFPV batches. An alternative approach would be to use $\hat{y}(\bar{\bar{\boldsymbol{x}}}^{MFPV})$, the model-predicted value for the normalized version of the mass-averaged composition over the *I* MFPV batches ($\bar{\bar{\boldsymbol{x}}}^{MFPV}$) that would result from supplying $\bar{\bar{\boldsymbol{g}}}^{MFPV}$ [calculated per Eq. (5.1.2) for balanced data and Eq. (5.1.7) for unbalanced data] to the normalizing transformation given in Eq. (5.4.5). Although this alternative approach would be consistent with some of the other compliance methods and calculations adopted in this report, it is contrary to the typical method for developing TIs.

In general, *k* in Eq. (5.4.8) is calculated using the following equation

$$k(X,Y) = \frac{t(X,Y,df_{\tilde{\sigma}},\delta)}{\sqrt{I}} \tag{5.4.10}$$

where $t(X,Y,df_{\tilde{\sigma}},\delta)$ represents a non-centralized *t*-distribution with degrees of freedom $df_{\tilde{\sigma}}$ and non-centrality parameter δ, and *I* is the number of MFPV batches associated with an LAW waste type. This is Eq. (3.18d) in Piepel and Cooley (2002), adapted to the notation in this report. It is important to note that $k(X, Y)$ is determined so as to compensate for the effects of ILAW process uncertainties affecting estimation of ILAW composition in the MFPV, which are "nuisance uncertainties" with respect to the population for which a X%/Y% UTI is desired.

The expression for $df_{\tilde{\sigma}}$ in Eq. (5.4.10) is given by

$$df_{\tilde{\sigma}} \approx \frac{\left[\left((\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^{\mathrm{T}}\,\boldsymbol{\Sigma}_b^h\,\bar{\bar{\boldsymbol{x}}}_I^{MFPV}\right)+\sum_{i=1}^{I}(\hat{\bar{y}}_i^h-\bar{\hat{\bar{y}}}^h)^2/(I-1)\right]^2}{\frac{\left((\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^{\mathrm{T}}\,\boldsymbol{\Sigma}_b^h\,\bar{\bar{\boldsymbol{x}}}_I^{MFPV}\right)^2}{df_m}+\frac{\left[\sum_{i=1}^{I}(\hat{\bar{y}}_i^h-\bar{\hat{\bar{y}}}^h)^2/(I-1)\right]^2}{I-1}} \tag{5.4.11}$$

where

$df_{\tilde{\sigma}}$ = approximate degrees of freedom associated with $\tilde{\sigma}$

$\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ = $p \times 1$ column vector whose first n_{mc}^h entries $\bar{\bar{x}}_k^{MFPV}$, $k = 1, 2, \cdots, n_{mc}^h$ are mass-weighted-averages of the $\bar{x}_{ik}^{MFPV}$, i = 1, 2, …, I values, which in turn are ordinary averages over the n_S^{CRV} samples per CRV batch, n_A^{CRV} analyses per sample, n_V^{CRV} determinations per CRV volume, and n_V^{MFPV} determinations per MFPV volume. The remaining entries $\bar{\bar{x}}_k^{MFPV}$, $k = n_{mc}^h + 1, \cdots, p$ are squares and/or crossproducts of the first n_{mc}^h entries according to the form of the PCT or VHT PQM model.

$\hat{\boldsymbol{\Sigma}}_b^h$ = $p \times p$ variance-covariance matrix of the model coefficient vector $\boldsymbol{b}^h$ for h = PCT B, PCT Na, or VHT alteration depth.

df_m = degrees of freedom for the model relating ln(PCT normalized release) of h = B or Na to ILAW composition or the model relating ln(VHT alteration depth) to ILAW composition. This quantity is given by $n - p$, where n is the number of data points used to fit the model, and p is the number of model coefficients estimated using the data.

I = number of ILAW MFPV batches corresponding to an LAW waste type

and the remaining notation is as previously defined. The expression in Eq. (5.4.11) is derived in Section F.4 of Appendix F.

The expression for δ in Eq. (5.4.10) is given by

$$\delta = z_{1-\beta}\sqrt{I}\,\frac{\sigma_g}{\sigma} \tag{5.4.12}$$

where

δ = non-centrality parameter for the non-central t-distribution used in calculating the

$k(X, Y)$ multiplier for an X%/Y% UTI

$z_{1-\beta}$ = 100(1 – β) percentile of the standard normal distribution

I = number of ILAW MFPV batches corresponding to an LAW waste type

σ_g = standard deviation of the distribution of true ln(PCT normalized release) values [ln(g/L)] or true ln(VHT alteration depth) values [ln(μm)] for ILAW produced from a given LAW waste type

σ = $\left[\sigma_{\mathrm{g}}^2 + \bar{\sigma}_m^2 + (\bar{\sigma}_{\mathrm{S}}^{\mathrm{MFPV}})^2 + (\bar{\sigma}_A^{MFPV})^2\right]^{0.5}$ = standard deviation of the distribution of possible $\hat{\bar{y}}_i^h$ values over the I ILAW MFPV batches corresponding to an LAW waste type for h = PCT B or Na [ln(g/L)] or VHT alteration depth [ln(μm)].

Equations (5.4.11) and (5.4.12) for f and δ are based on equations in Section 3.7 and Appendix F of Piepel and Cooley (2002) with appropriate modifications corresponding to the ILAW compliance strategy. Note that σ_g includes only the true variation in ln(PCT normalized release) values or ln(VHT alteration depth) values and not the true model, sampling, and chemical analysis "nuisance" uncertainties. On the other hand, σ (of which $\tilde{\sigma}$ is an estimate) includes true uncertainties for modeling, sampling, and chemical analyses. Hence, σ_g/σ is the fraction of the inflated (by model, sampling, and analytical nuisance uncertainties) standard deviation represented by the true standard deviation in ln(PCT normalized release) values or ln(VHT alteration depth) values over ILAW produced from an LAW waste type. Per Eq. (5.4.12) and the underlying theory (see Appendix H of Piepel and Cooley 2002), it is only necessary that the ratio σ_g/σ of these two true SDs be "known" (i.e., well-estimated). Scope discussed by Piepel and Heredia-Langer (2003) will produce estimates of the relevant variations and uncertainties based on information prior to commissioning testing. These estimates will provide for calculating preliminary estimates of the σ_g/σ ratio for different HLW waste types. It is also expected that cold commissioning testing of the WTP ILAW facility will provide updated estimates of variations and uncertainties that can be used to calculate updated estimates of the σ_g/σ ratio for different HLW waste types.

The estimate of the population standard deviation $\tilde{\sigma}$ in Eq. (5.4.8) is given by

$$\tilde{\sigma} = \left\{ \left((\bar{\bar{\boldsymbol{x}}}_I^{MFPV}) \boldsymbol{\Sigma}_{\boldsymbol{b}}^h \bar{\bar{\boldsymbol{x}}}_I^{MFPV} \right) + \sum_{i=1}^{I} \left(\hat{\bar{y}}_i^h - \bar{\bar{\tilde{y}}}^h \right)^2 \Big/ (I-1) \right\}^{0.5} \tag{5.4.13}$$

where $\bar{\bar{\boldsymbol{x}}}_I$ is a $p \times 1$ column vector whose first n_{mc}^h entries $\bar{\bar{x}}_k^{MFPV}, k = 1, 2, \cdots, n_{mc}^h$ are calculated by

$$\bar{\bar{x}}_I^{MFPV} = \frac{1}{I} \sum_{i=1}^{I} \bar{x}_{ik}^{MFPV} \tag{5.4.14}$$

and the remaining entries $\bar{\bar{x}}_k^{MFPV}$, $k = n_{mc}^h + 1, \cdots, p$ are squares and/or crossproducts of the initial entries according to the form of the PQM model. In Eq. (5.4.13), the $\bar{x}_{ik}^{MFPV}$, $k = 1, 2, \cdots, n_{mc}^h$ are calculated using Eq. (5.4.4) with $\bar{g}_{ij}^{MFPV}$ used as inputs calculated by Eq. (B.1.11), $\hat{\bar{y}}_i^h$ is given by Eq. (5.4.3a), $\bar{\hat{\bar{y}}}^h$ is given by Eq. (5.4.9), and I is the number of MFPV batches associated with the LAW waste type for which an X%/Y% UTI is to be calculated. The remaining notation in Eqs. (5.4.13) and (5.4.14) is as defined in previous subsections of Section 5.3.

From the derivations in Section F.4, it is seen that the first term in Eq. (5.4.13) represents model uncertainty, while the second term represents composition uncertainty expressed in model units. The composition uncertainty includes (1) variation in ILAW composition over the I MFPV batches corresponding to an LAW waste type and (2) uncertainties associated with estimating ILAW composition for a single MFPV batch, reduced by averaging over multiple samples per CRV batch, analyses per CRV sample, and volume determinations of the CRV and MFPV.

An illustration of the X%/Y% UTI method and equations for PCT is presented in Section 7.4.3. An illustration for VHT is presented in Section 7.5.3.

5.4.6 Statistical Method for Determining the Numbers of Samples, Analyses, and Volume Determinations to Demonstrate ILAW from a Waste Type Will Satisfy PCT and VHT Limits

This subsection discusses the methodology used to address Item 4 of Section 5.4.2. The X%/Y% UTI formula presented in Section 5.4.5 and the ILAW Monte Carlo simulation results (see Section 3.4.2 for more details) can be used to calculate X/Y%% UTI values (or half-widths thereof) given various combinations of values of the following factors:

- number of MFPV batches per LAW waste type (I)
- number of samples per CRV batch (n_S^{CRV})
- number of analyses per CRV sample (n_A^{CRV})
- number of volume determinations of the CRV and MFPV before and after transfers (n_V^{CRV} and n_V^{MFPV})
- mixing/sampling %RSD in the concentration of the j^{th} element in a CRV batch [$\%RSD_S(c_j^{CRV})$]
- analytical %RSD in the concentration of the j^{th} element in a CRV batch [$\%RSD_A(c_j^{CRV})$]
- GFC composition uncertainty, represented by the standard deviation in the mass fraction of the j^{th} component (oxide or halogen) in the k^{th} GFC [$SD(G_{jk}^{GFC})$]

- GFC mass uncertainty, represented by the standard deviation of the mass of the k^{th} GFC added to a MFPV batch. This uncertainty includes uncertainties due to batching, weighing, and transfers of GFCs. [$SD(a_k^{GFC})$]
- volume uncertainties in the CRV and MFPV. The magnitudes of these uncertainties will depend on the level of contents in a vessel, but a generic notation is used for now (SD_V^{CRV} and SD_V^{MFPV})
- statistical percent confidence level (CL%)
- ILAW produced from three tanks representing one each of Envelopes A (AP-101), B (AZ-101), and C (AN-107).

Piepel and Cooley (2002) calculated half-widths of X%/Y% UTIs for a compliance strategy that involves estimating glass composition based on analyses of samples from a single location, such as a completed MFPV batch or glass shards from the top of a canister/container. The WTP IHLW compliance strategy is of this type, but the WTP ILAW compliance strategy (see Section 2.3) is not. However, it was possible to adapt the results in Tables 4.3 to 4.6 of Piepel and Cooley (2002) for the WTP ILAW compliance strategy. The results of this adaptation are summarized in Section 7.4.4 for PCT and in Section 7.5.4 for VHT.

In this report, additional calculations were performed varying selected factors listed in the bullets above. The X%/Y% UTI values that satisfy the PCT or VHT limits were then inspected to find the least number of total analyses (number of samples × number of analyses) necessary to comply with the PCT or VHT limits. The results of these calculations as applied to PCT are presented in Section 7.4.4. The results of these calculations as applied to VHT are presented in Section 7.5.4.

5.5 Compliance Approach and Methods for ILAW Contract Specification 2.2.2.20: Dangerous Waste Limitations

Section 5.5.1 lists the applicable Contract Specification 2.2.2.20. Section 5.5.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Section 5.5.3 discusses the statistical methods that will be used to implement the statistical aspects of the compliance strategy.

5.5.1 Contract Specification 2.2.2.20: Dangerous Waste Limitations

> *The ILAW product shall be acceptable for land disposal under the State of Washington Dangerous Waste Regulations, WAC 173-303, and RCRA LDR in 40 CFR 268.*

5.5.2 Statistical Aspects of the ILAW Compliance Strategy for Contract Specification 2.2.2.20

Section 4.1.2 of the ILAW PCP (Nelson et al. 2003) addressed in this report[(a)] describes the compliance strategy for Contract Specification 2.2.2.20. The strategy involves using a DQO process to

(a) See Section 1.0 for a discussion of why this report addresses ILAW PCP Rev. 0 (Nelson et al. 2003) rather than ILAW PCP Rev. 1 (Westsik et al. 2004).

establish criteria for developing adequate data with acceptable quality to support the petition for an LDR treatability variance for ILAW. The DQO process involves several statistical aspects, including statistical experimental design and planning for statistical analysis of the resulting data. The results of the DQO process are documented in a report by Cook and Blumenkranz (2003). The results of the data development, quality assurance, and statistical data analyses are included in a report by Kot et al. (2003).

5.5.3 Statistical Methods to Implement the ILAW Compliance Strategy for Contract Specification 2.2.2.20

Relevant statistical methods for the statistical aspects described in Section 5.5.2 are discussed in the reports by Cook and Blumenkranz (2003) and Kot et al. (2003).

5.6 Compliance Approach and Methods for ILAW Contract Specification 2.2.2.2: Waste Loading

Section 5.6.1 lists the applicable Contract Specification 2.2.2.2. Section 5.6.2 summarizes the statistical aspects of the WTP compliance strategy for this specification. Section 5.6.3 discusses mass-balance equations and statistical methods that could be used to implement the specific aspects of the compliance strategy.

5.6.1 Contract Specification 2.2.2.2: Waste Loading

> *The loading of waste sodium from Envelope A in the ILAW glass shall be greater than 14 weight percent based on Na_2O. The loading of waste sodium from Envelope B in the ILAW glass shall be greater than 3.0 weight percent based on Na_2O. The loading of waste sodium from Envelope C in the ILAW glass shall be greater than 10 weight percent based on Na_2O.*

5.6.2 Statistical Aspects of the ILAW Compliance Strategy for Contract Specification 2.2.2.2

The following items describe the statistical and related aspects of the ILAW compliance strategy for Contract Specification 2.2.2.2 (see the ILAW PCP, Nelson et al. 2003) that are addressed in this report.[(a)]

Item 1: Develop a method for determining waste Na_2O loading through sampling and analyses of pretreated LAW feed, measurements of GFCs added during processing, including effects of heel mixing, and accounting for volatilization during the vitrification process. Mass-balance methods will be used to calculate the mass fractions of non-volatile oxides and waste Na_2O expected to be produced by vitrifying pretreated LAW feed and added GFCs.

Item 2: Determine the number of process samples, analyses, and measurements required to certify compliance using statistical sample size methods, considering control and compliance goals.

(a) See Section 1.0 for a discussion of why this report addresses ILAW PCP Rev. 0 (Nelson et al. 2003) rather than ILAW PCP Rev. 1 (Westsik et al. 2004).

Item 3: Develop a statistical interval method to summarize waste Na_2O loading determinations over a waste type. The statistical interval method will establish with high confidence that the ILAW produced from a waste type meets the applicable envelope-specific minimums. The method will be demonstrated before and during cold commissioning.

The statistical methods that could be used to implement these aspects of the WTP ILAW compliance strategy for Contract Specification 2.2.2.2 are discussed in the following section.

5.6.3 Statistical Methods to Implement the ILAW Compliance Strategy for Contract Specification 2.2.2.2

Scope to address the statistical aspects of the ILAW waste loading compliance strategy described in Section 5.6.2 was originally included in the work covered by this report per the applicable test plan (Piepel and Cooley 2003a). However, this scope was removed by the WTP Project in the early stages of the preparation of the report and documented in Test Exception 24590-WTP-TEF-RT-04-00036. The scope reduction was based on a decision that waste loading requirements would be easily met during ILAW production and hence that a statistical approach for demonstrating compliance was not needed. We briefly describe work completed before the scope reduction and options for addressing the items in Section 5.6.2 should they remain as part of the WTP ILAW compliance strategy or be re-included at a future time.

In relation to Item 1 in Section 5.6.2, mass-balance equations were developed for calculating waste Na_2O loading in ILAW. These equations are presented in Section B.6 of Appendix B at the stage of development when work was halted. At the direction of the WTP Project, initial work did not account for volatilization during the vitrification process. However, it was envisioned that volatilization would be addressed in subsequent work.

In relation to Item 2 in Section 5.6.2, equations for waste Na_2O loading in ILAW from Section B.6 of Appendix B were implemented in the ILAW single-MFPV-batch Monte Carlo simulation work described in Section 3.4.2. The data from those simulation runs were saved and could be accessed in the future to provide guidance to the WTP Project on numbers of CRV samples, analyses per sample, and volume determinations required to demonstrate, with high confidence, compliance with the waste Na_2O limits for each MFPV batch.

In relation to Item 3 in Section 5.6.2, two types of statistical intervals are applicable.

- As described in Section 3.1, a CL% ECI based on Monte Carlo simulation would be appropriate to account for process uncertainties and demonstrate compliance with waste Na_2O limits for each MFPV batch. In fact, the CL% ECI method was already developed and incorporated in the Monte Carlo simulation software developed to propagate ILAW process uncertainties through the complicated mass-balance-based equation for ILAW chemical composition. However, that method is not described or illustrated in the report because of the WTP change to a non-statistical compliance strategy for the waste loading specification.

- As described in Section 3.2, a statistical TI would be appropriate to account for process uncertainties (affecting each MFPV batch) and variations (over MFPV batches associated with an LAW waste type) in demonstrating compliance with waste Na_2O limits for LAW waste types. Specifically, an X%/Y% LTI would be appropriate. An X%/Y% LTI equation for waste loading could be developed by adapting the work of Piepel and Cooley (2002) as discussed in previous sections of the report.

These approaches are not discussed further because of the change to a non-statistical compliance strategy for Contract Specification 2.2.2.2.

6.0 Results and Illustrations of Statistical Methods for IHLW Compliance

This section presents the results of statistical WFQ activities performed per the IHLW compliance strategies for applicable specifications, as discussed in Section 4.0. This section also presents for each specification an example illustrating the application of the statistically based compliance method(s) for that specification as described in the corresponding subsection of Section 4.0. The examples are intended to illustrate (using realistic, simulated data) the statistical methods that will be used to demonstrate compliance with specifications during IHLW production.

6.1 Compliance Results for IHLW WAPS Specification 1.1.2: Chemical Composition During Production

Section 6.1.1 presents the results of the investigations described in Section 4.1.3 to assess the effects of several factors (the number of samples per MFPV batch, the number of analyses per MFPV sample, MFPV mixing/sampling uncertainty, and MFPV analytical uncertainty) on the IHLW chemical composition from a single MFPV batch. These results provide a basis for (1) assessing the sensitivity of IHLW chemical composition estimates to the ranges of possible uncertainties, and (2) the WTP Project to decide on the numbers of samples per MFPV batch, chemical analyses per MFPV sample, and volume determinations per MFPV batch.

Section 6.1.2 illustrates, using realistic example data, the methodology presented in Section 4.1.4 for calculating means and SDs of IHLW chemical composition over MFPV batches corresponding to a given HLW waste type.

6.1.1 Results of Investigations to Assess the Effects of Process Uncertainties, Number of Samples per MFPV Batch, and Number of Analyses per MFPV Sample on Uncertainties in Chemical Composition of IHLW from a MFPV Batch

This section uses the methodology described in Section 4.1.3 to assess the number of samples per MFPV batch and analyses per MFPV sample necessary to estimate the IHLW composition corresponding to an IHLW MFPV batch with a given precision (i.e., within a specified percentage of the true value) and confidence.

Given values of n_S^{MFPV}, n_A^{MFPV}, $\%RSD_S(g_j^{MFPV})$, $\%RSD_A(g_j^{MFPV})$, and the selected statistical confidence level (CL%), Eq. (4.1.1) can be used to calculate $\%RHW_{CL\%}(g_j^{MFPV})$ values (i.e., the precision of the estimated mass fraction of the j^{th} component in IHLW corresponding to an MFPV batch). As discussed in Section 4.1.3, the methodology to calculate $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ uncertainties from $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ uncertainties is scheduled for development in FY 2005. Based on preliminary calculations showing that $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$

values are relatively close to $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ values, the latter were used in place of the former in Eq. (4.1.1) for the investigations and results discussed in this section.

Values of $\%RHW_{CL\%}(g_j^{MFPV})$ were calculated for each IHLW component j for each of the combinations of variables listed in Table 3.2. The low (L) and high (H) values of $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ shown in Table 3.2 are listed in Table C.1 of Appendix C for three HLW tanks (AY-102, AZ-102, and C-104). The results of these calculations are summarized in Table 6.1. Because $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ were treated as values of $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ for the calculations, the latter notation is used in column headings of Table 6.1 (as well as Table 6.2, Table 6.3, and G.1 to G.14 subsequently discussed).

Table 6.1 shows the numbers of samples and analyses per sample from an MFPV batch that resulted in the minimal number of total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) yielding %RHW = $\%RHW_{CL\%}(g_j^{MFPV})$ values in specified ranges for each of the combinations of variables considered. The results in Table 6.1 apply to any IHLW component (oxide or halogen) having values of $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ shown. To illustrate using Table 6.1, suppose the j^{th} IHLW component has $\%RSD_S(g_j^{MFPV}) = 5$, $\%RSD_A(g_j^{MFPV}) = 5$, and is to be estimated with %RHW ≤ 10 and CL% = 90% confidence. Then, Table 6.1 shows that 4 samples would need to be taken from each MFPV batch with 1 analysis each. It is interesting to note that in no case was more than 1 analysis per sample recommended. When trying to minimize the total number of analyses needed, it can be seen from Eq. (4.1.1) that greater reduction in the chemical composition uncertainty (%RHW) can be achieved by increasing the number of samples than by increasing the number of analyses per sample. However, even though only one analysis per sample is needed, the number of samples needed still depends on the analytical uncertainty.

Tables similar to Table 6.1 were produced for each reportable IHLW component (oxide or halogen) using its specific sampling and analytical uncertainties as provided in Table C.1. These results can be found in Tables G.1 to G.14 in Appendix G. Only 14 tables in Appendix G were needed to summarize the results for the 23 reportable IHLW components because components with the same uncertainties required only one table. For example, Table G.1 is for components (oxides) Al_2O_3, B_2O_3, Fe_2O_3, MnO, SiO_2, SrO, and ZrO_2 because they each are expected to have the same sampling and analytical uncertainties.

Table 6.2 and Table 6.3 display a summary of the results from Tables G.1 to G.14. Each table displays the number of samples per MFPV batch necessary to achieve a %RHW = $\%RHW_{CL\%}(g_j^{MFPV})$ below a specified amount (e.g., 10%), given combinations of low or high estimates of the MFPV sampling and analytical uncertainties [$\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$] for each IHLW component j. Table 6.2 presents results for a confidence level of 90%, while Table 6.3 presents results for a confidence level of 95%.

Table 6.1. Numbers of IHLW MFPV Samples and Analyses per Sample[a] to Satisfy Certain %RHWs on IHLW Component Mass Fractions Given Mixing/Sampling and Analytical Uncertainties Representative of Those Expected in IHLW MFPV Data

$\%RSD_S(g_j^{MFPV})$[b]	$\%RSD_A(g_j^{MFPV})$[c]	% Confidence	Percent Relative Half-width (%RHW) on the Mass Fraction of an IHLW Chemical Composition Component							
			< 5%		< 10%		< 15%		< 20%`	
			n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
1	5	90	5	1	3	1	3	1	3	1
		95	7	1	4	1	3	1	3	1
	10	90	13	1	5	1	4	1	3	1
		95	18	1	7	1	5	1	4	1
	20	90	-[d]	-	13	1	7	1	5	1
		95	-	-	18	1	10	1	7	1
	25	90	-	-	19	1	10	1	7	1
		95	-	-	27	1	14	1	9	1
	40	90	-	-	-	-	22	1	13	1
		95	-	-	-	-	30	1	18	1
	50	90	-	-	-	-	-	-	19	1
		95	-	-	-	-	-	-	27	1
5	5	90	8	1	4	1	3	1	3	1
		95	11	1	5	1	4	1	3	1
	10	90	16	1	6	1	4	1	3	1
		95	22	1	8	1	5	1	4	1
	20	90	-	-	14	1	8	1	5	1
		95	-	-	19	1	10	1	7	1
	25	90	-	-	20	1	10	1	7	1
		95	-	-	28	1	14	1	9	1
	40	90	-	-	-	-	22	1	13	1
		95	-	-	-	-	-	-	19	1
	50	90	-	-	-	-	-	-	19	1
		95	-	-	-	-	-	-	27	1
15	5	90	29	1	9	1	6	1	4	1
		95	-	-	13	1	7	1	5	1
	10	90	-	-	11	1	6	1	5	1
		95	-	-	15	1	9	1	6	1
	20	90	-	-	19	1	10	1	7	1
		95	-	-	27	1	14	1	9	1
	25	90	-	-	25	1	13	1	8	1
		95	-	-	-	-	17	1	11	1
	40	90	-	-	-	-	24	1	15	1
		95	-	-	-	-	-	-	20	1
	50	90	-	-	-	-	-	-	21	1
		95	-	-	-	-	-	-	29	1

(a) This table lists the minimum total number of analyses ($n_S^{MFPV} \times n_A^{MFPV}$) necessary to satisfy the %RHW category.

(b) Components with low category mixing/sampling uncertainties had low and high values of 1 and 5 %RSD. Components with high category mixing/sampling uncertainties had low and high values of 5 and 15 %RSD.

(c) Depending on the component, low analytical uncertainties were 5, 10, 15, 20, 25, and 50 and high uncertainties were twice these values. Not shown in the table are results for 15, 30, and 100 analytical %RSD.

(d) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy the %RHW category.

Table 6.2. Numbers of IHLW MFPV Samples (with One Analysis per Sample) to Satisfy Certain %RHWs with 90% Confidence for Reportable IHLW Oxides Given Low and High Estimates of Mixing/Sampling and Analytical Uncertainties for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$	$\%RSD_A(g_j^{MFPV})$	%RHW [a]	Al_2O_3, B_2O_3, Fe_2O_3, MnO, SiO_2, SrO, ZrO_2	CaO, Cr_2O_3, P_2O_5	CdO	LiO_2	MgO	Na_2O	NiO	PdO, Rh_2O_3	RuO_2, SeO_2	SO_3	Sb_2O_3	ThO_2	U_3O_8	ZnO	Max (MF > 0.005)' [b]	Max (MF > 0.02) [b]
AY-102	L	L	10	4	6	- [c]	5	-	3	6	(d)		9	20		14	4	14	5
			15	3	4	-	4	-	3	4			5	10		8	3	8	4
			20	3	3	19	3	19	3	3			4	7		5	3	5	3
		H	10	6	14	-	13	-	5	14			27	-		-	6	-	13
			15	4	8	-	7	-	4	8			13	-		22	4	22	7
			20	3	5	-	5	-	3	5			9	19		13	3	13	5
	H	L	10	9	11	-	6	-	4	11			9	25		19	9	19	6
			15	6	6	-	4	-	3	6			6	13		10	6	10	4
			20	4	5	21	3	21	3	5			4	8		7	4	7	3
		H	10	11	19	-	14	-	6	19			27	-		-	11	-	14
			15	6	10	-	8	-	4	10			14	-		24	6	24	8
			20	5	7	-	5	-	3	7			9	21		15	5	15	5
AZ-102	L	L	10	4	6	4	5	-	3	4			-			6	6	6	4
			15	3	4	3	4	-	3	3			-			4	4	4	3
			20	3	3	3	3	19	3	3			19			3	3	3	3
		H	10	6	14	6	13	-	5	6			-			14	14	14	6
			15	4	8	4	7	-	4	4			-			8	8	8	4
			20	3	5	3	5	19	3	3			-			5	5	5	3
	H	L	10	9	11	9	6	-	4	9			-			11	11	11	9
			15	6	6	6	4	-	3	6			-			6	6	6	6
			20	4	5	4	3	21	3	4			21			5	5	5	4
		H	10	11	19	11	14	-	6	11			-			19	19	19	11
			15	6	10	6	8	-	4	6			-			10	10	10	6
			20	5	7	5	5	21	3	5			-			7	7	7	5
C-104	L	L	10	4	6	-	3	-	3	6	20	-	-		4	4	4	4	4
			15	3	4	-	3	-	3	4	10	-	-		3	3	3	3	3
			20	3	3	19	3	19	3	3	7	19	19		3	3	3	3	3
		H	10	6	14	-	5	-	5	14	-	-	-		6	6	6	6	6
			15	4	8	-	4	-	4	8	-	-	-		4	4	4	4	4
			20	3	5	19	3	19	3	5	19	-	-		3	3	3	3	3
	H	L	10	9	11	-	4	-	4	11	25	-	-		9	9	9	9	9
			15	6	6	-	3	-	3	6	13	-	-		6	6	6	6	6
			20	4	5	21	3	21	3	5	8	21	21		4	4	4	4	4
		H	10	11	19	-	6	-	6	19	-	-	-		11	11	11	11	11
			15	6	10	-	4	-	4	10	-	-	-		6	6	6	6	6
			20	5	7	21	3	21	3	7	21	-	-		5	5	5	5	5

(a) Only %RHW ≤ 10, 15, and 20 results are shown because of few acceptable results (i.e., $n_S^{MFPV} \leq 10$) for %RHW ≤ 5.

(b) Maximum values of n_S^{MFPV} are given for reportable components with mass fractions (MFs) > 0.005 and 0.02.

(c) A dash (–) indicates that over 30 samples per MFPV batch would be necessary to satisfy the %RHW category.

(d) Empty cells indicate that no data were recorded for that particular analyte and HLW tank.

Table 6.3. Numbers of IHLW MFPV Samples (with One Analysis per Sample) to Satisfy Certain %RHWs with 95% Confidence for Reportable IHLW Oxides Given Low and High Estimates of Mixing/Sampling and Analytical Uncertainties for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$	$\%RSD_A(g_j^{MFPV})$	%RHW [a]	Al_2O_3, B_2O_3, Fe_2O_3, MnO, SiO_2, SrO, ZrO_2	CaO, Cr_2O_3, P_2O_5	CdO	LiO_2	MgO	Na_2O	NiO	PdO, Rh_2O_3	RuO_2, SeO_2	SO_3	Sb_2O_3	ThO_2	U_3O_8	ZnO	Max (MF > 0.005) [b]	Max (MF > 0.02) [b]
AY-102	L	L	10	5	8	- [c]	7	-	4	8	(d)		12	28		19	5	19	7
			15	4	5	-	5	-	3	5			7	14		10	4	10	5
			20	3	4	27	4	27	3	4			5	9		7	3	7	4
		H	10	8	19	-	18	-	7	19			-	-		-	8	-	18
			15	5	10	-	10	-	5	10			18	-		-	5	-	10
			20	4	7	-	7	-	4	7			12	27		19	4	19	7
	H	L	10	13	15	-	8	-	5	15			13	-		27	13	27	8
			15	7	9	-	5	-	4	9			7	17		14	7	14	5
			20	5	6	29	4	29	3	6			5	11		9	5	9	4
		H	10	15	27	-	19	-	8	27			-	-		-	15	-	19
			15	9	14	-	10	-	5	14			19	-		-	9	-	10
			20	6	9	-	7	-	4	9			12	29		20	6	20	7
AZ-102	L	L	10	5	8	5	7	-	4	5			-			8	8	8	5
			15	4	5	4	5	-	3	4			-			5	5	5	4
			20	3	4	3	4	27	3	3			27			4	4	4	3
		H	10	8	19	8	18	-	7	8			-			19	19	19	8
			15	5	10	5	10	-	5	5			-			10	10	10	5
			20	4	7	4	7	-	4	4			-			7	7	7	4
	H	L	10	13	15	13	8	-	5	13			-			15	15	15	13
			15	7	9	7	5	-	4	7			-			9	9	9	7
			20	5	6	5	4	29	3	5			29			6	6	6	5
		H	10	15	27	15	19	-	8	15			-			27	27	27	15
			15	9	14	9	10	-	5	9			-			14	14	14	9
			20	6	9	6	7	-	4	6			-			9	9	9	6
C-104	L	L	10	5	8	-	4	-	4	8	28	-	-		5	5	5	5	5
			15	4	5	-	3	-	3	5	14	-	-		4	4	4	4	4
			20	3	4	27	3	27	3	4	9	27	27		3	3	3	3	3
		H	10	8	19	-	7	-	7	19	-	-	-		8	8	8	8	8
			15	5	10	-	5	-	5	10	-	-	-		5	5	5	5	5
			20	4	7	-	4	-	4	7	27	-	-		4	4	4	4	4
	H	L	10	13	15	-	5	-	5	15	-	-	-		13	13	13	13	13
			15	7	9	-	4	-	4	9	17	-	-		7	7	7	7	7
			20	5	6	29	3	29	3	6	11	29	29		5	5	5	5	5
		H	10	15	27	-	8	-	8	27	-	-	-		15	15	15	15	15
			15	9	14	-	5	-	5	14	-	-	-		9	9	9	9	9
			20	6	9	-	4	-	4	9	29	-	-		6	6	6	6	6

(a) Only %RHW ≤ 10, 15, and 20 results are shown because of few acceptable results (i.e., $n_S^{MFPV} \leq 10$) for %RHW ≤ 5.

(b) Maximum values of n_S^{MFPV} are given for reportable components with mass fractions (MFs) > 0.005 and 0.02.

(c) A dash (–) indicates that over 30 samples per MFPV batch would be necessary to satisfy the %RHW category.

(d) Empty cells indicate that no data were recorded for that particular analyte and HLW tank.

As an illustration of the use of Table 6.2 and Table 6.3, suppose it is desired to estimate the mass fraction of Al_2O_3 within 15% relative of the true value (i.e., %RHW ≤ 15%) having 90% confidence. Then, Table 6.2 shows that for high sampling and analytical uncertainties, 6 samples per MFPV batch would need to be taken (with 1 analysis per sample). This outcome is consistent across all three of the HLW tanks considered in the calculations (AY-102, AZ-102, and C-104).

The second-to-last column in each of Table 6.2 and Table 6.3 lists the maximum values of n_S^{MFPV} across the reportable chemical composition components with nominal mass fractions greater than 0.005 (0.5 wt%)[(a)]. This list of reportable components includes those with mass fraction > 0.02 (mentioned previously) along with the following added components: P_2O_5 (only AY-102), CdO (only AZ-102), NiO (only AZ-102), U_3O_8 (AY-102 and AZ-102), and ZnO (AY-102 and C-104). With 95% confidence (Table 6.3), 20% RHWs or less can be obtained with at most 7 samples when assuming "low" uncertainty values. The numbers of samples necessary for Tank AY-102 are larger because of the presence of U_3O_8 and its large analytical uncertainty. Without U_3O_8, the necessary numbers of samples decrease to at most 8 samples necessary to obtain 10% RHWs or less when assuming "low" uncertainty values, and at most 7 samples necessary to obtain 20% RHWs or less when assuming "high" uncertainty values.

The last column in each of Table 6.2 and Table 6.3 lists the maximum values of n_S^{MFPV} across the reportable chemical composition components with nominal mass fractions greater than 0.02 (2 wt%).[(a)] With 95% confidence (Table 6.3), 20% RHWs or less can be obtained with at most 7 samples when using "high" mixing/sampling and analytical uncertainty values. At most, 10 samples are necessary to obtain RHWs of 15% or less. Using "high" uncertainty values, 19 samples would be necessary to obtain 10% RHWs or less, while "low" uncertainty values only require 7 samples to obtain 10% RHWs or less.

6.1.2 Illustration of Calculating Means and Standard Deviations of IHLW Chemical Composition over an HLW Waste Type

This section uses realistic data to illustrate the equations presented in Section 4.1.4 for calculating means and SDs of IHLW chemical composition (mass fractions) over an HLW waste type. Equations are presented in Section 4.1.4.1 for the case of balanced data (equal numbers of samples per MFPV batch and equal numbers of analyses for each MFPV batch), and in Section 4.1.4.2 for the case of unbalanced data (unequal numbers of samples per MFPV batch and/or unequal numbers of analyses for each MFPV batch). The equations for the balanced data set are illustrated in this section.

A realistic balanced dataset to illustrate the use of Eqs. (4.1.2), (4.1.3), and (4.14) for calculating means, SDs, and %RSDs was obtained as follows. First, simulated IHLW chemical and radionuclide composition data (expressed in mass fractions) consisting of one estimate per MFPV batch were available for a blend of HLW from Tanks AY-102/C-106. This set of simulated data was obtained (Vienna 2004a) from the WTP Project's Run 3.1vv of the G2 dynamic simulation flowsheet (Deng 2004; Vora 2004). A subset of these data, corresponding to 18 MFPV batches associated with an HLW waste type (i.e., a HBV), were selected for this example.

[(a)] A mass fraction of 0.005 (0.5 wt%) corresponds to the level for reporting IHLW chemical composition specified in WAPS 1.1.2. A mass fraction of 0.02 (2 wt%) as selected as a cutoff that provided smaller numbers of samples and analyses per sample than the 0.005 case.

Note that G2 does not simulate multiple MFPV samples and/or analyses per sample as in the WTP IHLW compliance strategy and thus does not simulate MFPV mixing/sampling and analytical uncertainties. To address this issue, normally distributed random disturbances for mixing/sampling and analytical uncertainties (using the values given in Table C.1) were added to the elemental (and radionuclide) concentration data for the 18 MFPV batches from G2. This process created eight observations (elemental or radionuclide concentrations) per MFPV batch that simulated mixing/sampling and analytical uncertainties in the AY-102/C-106 G2 run. For the j^{th} element or radionuclide, the 8 concentrations per MFPV batch were averaged, yielding the results in Table I.1 in Section I.1 of Appendix I. Table I.2 contains the 18 MFPV batch volumes from the G2 run used. These were treated as single determinations of volume for use in Eq. (4.1.2) as discussed subsequently. Then, Eq. (A.1.5) in Section A.1 of Appendix A was applied to calculate the average mass fraction of the j^{th} IHLW component in the i^{th} MFPV batch (denoted $\bar{g}_{ij}^{MFPV}$). Table I.3 in Section I.1 of Appendix I lists these simulated average IHLW chemical compositions (mass fractions) corresponding to 18 MFPV batches selected from the G2 output.

Table 6.4 contains, for the reportable IHLW chemical composition components (listed in Table 2.2), the means, SDs, and %RSDs of mass fractions over the 18 MFPV batches corresponding to an HLW waste type from AY-102/C-106. Equations (4.1.2) to (4.1.4) were employed to calculate the results in Table 6.4. As an example, consider the case of Fe_2O_3. Substituting the concentrations used to produce the average concentrations from Table I.1 into Eq. (4.1.2), the mean mass fraction of Fe_2O_3 over the 18 MFPV batches[(a)] corresponding to an HLW waste type is obtained by

$$\bar{\bar{g}}_{Fe_2O_3}^{MFPV} = \frac{\left[\frac{1}{8}(213.8\ \text{g/L} + 215.4 + \cdots)\cdot(1\cdot 25718.3\ \text{L})\cdot 1.4286 + \frac{1}{8}(217.5\ \text{g/L} + 204.7 + \cdots)\cdot(1\cdot 24888.5\ \text{L})\cdot 1.4286 + \cdots\right]}{\left[\frac{1}{8}(121.56\ \text{g/L} + 111.99 + \cdots)\cdot(1\cdot 25718.3\ \text{L})\cdot 1.8889 + \cdots \frac{1}{8}(653.3\ \text{g/L} + 626.8 + \cdots)\cdot(1\cdot 24846.5\ \text{L})\cdot 2.1429 + \cdots\right]}$$

$$= 0.1096\ \ g_{Fe_2O_3}/g_{glass}.$$

Similarly, substituting the appropriate quantities from Table I.3 into Eq. (4.1.3), the standard deviation of Fe_2O_3 mass fractions over the 18 MFPV batches corresponding to an HLW waste type is given by

$$SD(\bar{g}_{Fe_2O_3}^{MFPV}) = \sqrt{\frac{[(0.1095) - (0.1096)]^2 + \cdots + [(0.1109) - (0.1096)]^2}{17}} = 0.0037\ \ g_{Fe_2O_3}/g_{glass}.$$

Finally, the variation plus uncertainty in mass fractions of Fe_2O_3 over the 18 MFPV batches corresponding to an HLW waste type can be expressed as a %RSD using Eq. (4.1.4)

$$\%RSD(\bar{g}_{Fe_2O_3}^{MFPV}) = 100\left(\frac{SD(\bar{g}_{Fe_2O_3}^{MFPV})}{\bar{\bar{g}}_{Fe_2O_3}^{MFPV}}\right) = 100\left(\frac{0.0037}{0.1096}\right) = 3.34\ .$$

(a) The mean mass fractions calculated by Eq. (4.1.2) are mass-weighted average mass fractions over the 18 MFPV batches.

The rest of the chemical composition (mass fractions) means, SDs, and %RSDs in Table 6.4 were calculated in a similar manner.

For this AY-102/C-106 IHLW example, the variations of the mass fractions (over the 18 IHLW MFPV batches corresponding to an HLW waste type) summarized in Table 6.4 range from approximately 2.5 to 4.0 %RSD for the majority of the reportable IHLW chemical composition components. Larger %RSD values were 8.66 for SiO_2, 18.76 for Li_2O, 21.55 for Na_2O, 52.40 for B_2O_3, and 109.22 for Al_2O_3. These larger values appear to be the results of large variations for those components in the original G2 dataset. If actual WTP IHLW data behave in similar manner to the G2 data, then such large variations may be representative of what could occur over a waste type during production operations.

Table 6.4. Example Results from Applying Equations for Calculating Means, SDs, and %RSDs of Mass Fractions for Reportable IHLW Chemical Composition Components. Results were obtained using data from 18 simulated IHLW MFPV batches corresponding to a blend of wastes from HLW Tanks AY-102/C-106.

Chemical Composition Component[(a)]	Mass Fraction ($g_{component}/g_{oxides}$)		
	Mean	SD	%RSD
Al_2O_3	0.0091	0.0099	109.22
B_2O_3	0.1129	0.0591	52.40
CaO	0.0060	0.0002	2.92
CdO	7.59E-05	2.27E-06	2.99
Cr_2O_3	0.0013	4.03E-05	3.08
Fe_2O_3	0.1096	0.0037	3.34
Li_2O	0.0419	0.0078	18.76
MgO	0.0028	8.85E-05	3.19
MnO	0.0111	0.0003	2.81
Na_2O	0.0675	0.0146	21.55
NiO	0.0026	6.36E-05	2.49
P_2O_5	0.0030	9.51E-05	3.15
PdO	1.53E-08	6.08E-10	3.96
Rh_2O_3	1.71E-05	5.71E-07	3.35
RuO_2	0.0004	1.30E-05	3.14
SO_3	0.0006	1.58E-05	2.76
Sb_2O_5	2.89E-06	7.53E-08	2.60
SeO_2	2.93E-06	7.17E-08	2.45
SiO_2	0.4636	0.0410	8.66
SrO	0.0002	7.74E-06	3.42
ThO_2	0.0004	1.23E-05	3.04
U_3O_8	0.0021	6.60E-05	3.16
ZnO	0.0001	4.17E-06	3.07
ZrO_2	2.84E-05	7.98E-07	2.93
Total	0.8353	N/A	N/A

(a) Only the components marked as reportable for IHLW in Table 2.2 are included in this table.
(b) The total is significantly below 1, indicating many components not listed in Table 2.2 have mass fractions significant above the reporting cut-off of 0.005 (0.5 wt%).

6.2 Compliance Results for IHLW WAPS Specification 1.2.2: Radionuclide Inventory During Production

Section 6.2.1 presents the results of investigations described in Section 4.2.3 to assess the effects of several factors (e.g., magnitudes of mixing/sampling and analytical uncertainties as well as the numbers of samples, analyses per sample, and volume determinations per MFPV batch) on the radionuclide composition of IHLW from a single MFPV batch. These results provide a basis for (1) assessing the sensitivity of single-MFPV-batch radionuclide composition estimates to the range of possible uncertainties, and (2) the WTP Project to decide on the numbers of samples, chemical analyses per sample, and volume determinations per MFPV batch.

Section 6.2.2 illustrates, using realistic example data, the methodology presented in Section 4.2.4 for calculating means and SDs of IHLW radionuclide inventories over MFPV batches corresponding to a given waste type.

Section 6.2.3 illustrates, using realistic data, the methodology presented in Section 4.2.5 for quantifying the variation and uncertainty present in determinations of radionuclide inventories over an HLW waste type for radionuclides analyzed in samples of the first MFPV batch only.

6.2.1 Results of Investigations to Assess the Effects of Process Uncertainties, Number of Samples, and Number of Analyses per Sample on Uncertainties in IHLW Radionuclide Composition from an MFPV Batch

This section uses the methodology described in Section 4.2.3 to assess the number of samples and analyses per sample of an MFPV batch necessary to estimate the IHLW radionuclide composition with a given precision (i.e., within a specified percentage of the true value) and confidence. As noted at the start of Section 4.2.3, mass fractions of IHLW radionuclide components (oxides) may be of limited interest directly, but they play a key role in the equations developed to calculate IHLW radionuclide inventories (see Section A.2 of Appendix A). Hence, it is important to assess the numbers of IHLW MFPV samples and radiochemical analyses per sample required to adequately estimate IHLW radionuclide compositions.

The methodology is the same as was used for IHLW chemical composition, as described in Section 4.1.3 and illustrated in Section 6.1.1. That is, Eq. (4.1.1) was used to calculate values of $\%RHW_{CL\%}(g_j^{MFPV})$ for various combinations of n_S^{MFPV}, n_A^{MFPV}, $\%RSD_S(g_j^{MFPV})$, $\%RSD_A(g_j^{MFPV})$, and the selected statistical confidence level (CL%) for each reportable radionuclide component j. As discussed in Section 6.1.1, values of $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ were used as representative replacements for values of $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$.

Values of $\%RHW_{CL\%}(g_j^{MFPV})$ were calculated for each reportable IHLW radionuclide component j for each of the combinations of variables listed in Table 3.2. The low (L) and high (H) values of $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ shown in Table 3.2 are listed in Tables C.2 and C.4 of Appendix C for three HLW tanks (AY-102, AZ-102, and C-104). The results of these calculations are

summarized in Table 6.5. Because $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ were treated as values of $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ for the calculations, the latter notation is used in column headings of Table 6.5 (as well as Table 6.6 and 6.7, and G.16 to G.29 subsequently discussed).

Table 6.5 shows the numbers of samples and analyses per sample from an MFPV batch that resulted in the minimal number of total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) yielding %RHW = $\%RHW_{CL\%}(g_j^{MFPV})$ values in specified ranges for each of the combinations of variables considered. The results in Table 6.5 apply to any IHLW radionuclide component having values of $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ shown. To illustrate using Table 6.5, suppose the j^{th} IHLW radionuclide component has $\%RSD_S(g_j^{MFPV})$ = 5, $\%RSD_A(g_j^{MFPV})$ = 15, and is to be estimated with %RHW ≤ 10 and CL% = 90% confidence. Then, Table 6.5 shows that 9 samples would need to be taken from each MFPV batch with 1 analysis each. However, if only %RHW ≤ 15 is desired with CL% = 90% for $\%RSD_S(g_j^{MFPV})$ = 5 and $\%RSD_A(g_j^{MFPV})$ = 15, then 6 samples per MFPV batch with 1 analysis per sample is sufficient.

To illustrate the use of Table 6.5 for radionuclides with larger analytical uncertainties, consider $\%RSD_S(g_j^{MFPV})$ = 5 and $\%RSD_A(g_j^{MFPV})$ = 50. Estimating radionuclides having these uncertainties with %RHW ≤ 20 and 90% confidence would require 19 samples per MFPV batch. However, estimating radionuclides having these uncertainties with %RHW ≤ 50 would only require 5 samples per MFPV batch. As in Section 6.1.1 for chemical composition components, in no case for radionuclide components was more than 1 analysis per sample recommended. The reason for this is the same as discussed in Section 6.1.1.

Tables similar to Table 6.5 were produced for each reportable IHLW radionuclide using its specific sampling and analytical uncertainties provided in Tables C.2 and C.4. These results can be found in Tables G.15 to G.28 in Appendix G. Only 14 tables in Appendix G were needed to summarize the results for the 20 reportable IHLW radionuclide components because components with the same uncertainties required only one table. For example, Table G.19 is for radionuclide components ^{60}CoO and $^{238}PuO_2$ because they each are expected to have the same uncertainties.

Table 6.6 and 6.7 display a summary of the results from Tables G.15 to G.28. Each table displays the number of samples per MFPV batch necessary to achieve a %RHW = $\%RHW_{CL\%}(g_j^{MFPV})$ below a specified amount (e.g., 10%), given combinations of low or high estimates of the MFPV sampling and analytical uncertainties [$\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$] for IHLW radionuclide j. Table 6.6 presents results for a confidence level of 90% while Table 6.7 presents results for a confidence level of 95%.

As an illustration of the use of Table 6.6 and Table 6.7, suppose it is desired to estimate the mass fraction of $^{137}Cs_2O$ within 15% relative (i.e., %RHW ≤ 15%) having 90% confidence. Then, Table 6.6 shows that for high sampling and analytical uncertainties (5 and 10 %RSD, respectively, according to Tables C.2 and C.4), 4 samples per MFPV batch would need to be taken (with 1 analysis per sample).

Table 6.5. Numbers of IHLW MFPV Samples and Analyses Per Sample[a] to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions Given Mixing/Sampling and Analytical Uncertainties Representative of Those Expected in IHLW MFPV Data

$\%RSD_S(g_j^{MFPV})$	$\%RSD_A(g_j^{MFPV})$[b]	% Confidence	Percent Relative Half-width (%RHW) on the Mass Fraction of an IHLW Radionuclide Component							
			< 10%		< 15%		< 20%		< 50%	
			n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
1	5	90	3	1	3	1	3	1	1	1
		95	4	1	3	1	3	1	2	1
	10	90	5	1	4	1	3	1	2	1
		95	7	1	5	1	4	1	3	1
	15	90	9	1	5	1	4	1	3	1
		95	12	1	7	1	5	1	3	1
	20	90	13	1	7	1	5	1	3	1
		95	18	1	10	1	7	1	3	1
	25	90	19	1	10	1	7	1	3	1
		95	27	1	14	1	9	1	4	1
	30	90	27	1	13	1	9	1	4	1
		95	-[c]	-	18	1	12	1	4	1
	40	90	-	-	22	1	13	1	4	1
		95	-	-	30	1	18	1	5	1
	50	90	-	-	-	-	19	1	5	1
		95	-	-	-	-	27	1	7	1
	60	90	-	-	-	-	27	1	6	1
		95	-	-	-	-	-	-	9	1
5	5	90	4	1	3	1	3	1	1	1
		95	5	1	4	1	3	1	3	1
	10	90	6	1	4	1	3	1	2	1
		95	8	1	5	1	4	1	3	1
	15	90	9	1	6	1	4	1	3	1
		95	13	1	7	1	5	1	3	1
	20	90	14	1	8	1	5	1	3	1
		95	19	1	10	1	7	1	4	1
	25	90	20	1	10	1	7	1	3	1
		95	28	1	14	1	9	1	4	1
	30	90	27	1	14	1	9	1	4	1
		95	-	-	19	1	12	1	4	1
	40	90	-	-	22	1	13	1	4	1
		95	-	-	-	-	19	1	6	1
	50	90	-	-	-	-	19	1	5	1
		95	-	-	-	-	27	1	7	1
	60	90	-	-	-	-	27	1	6	1
		95	-	-	-	-	-	-	9	1

(a) This table lists the minimum total number of analyses ($n_S^{MFPV} \times n_A^{MFPV}$) necessary to satisfy the %RHW category.

(b) Depending on the radionuclide component, low analytical uncertainties were 5, 10, 15, 20, 25, 30, and 50 and high uncertainties were twice these values. Not shown in the table are results for analytical %RSD = 100.

(c) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy the %RHW category.

Table 6.6. Numbers of IHLW MFPV Samples (with One Analysis per Sample) to Satisfy Certain %RHWs with 90% Confidence for Reportable IHLW Radionuclides Given Low and High Estimates of Mixing/Sampling and Analytical Uncertainties for Each of Three HLW Tanks

HLW Tank	$\%RSD_S$ (g_j^{MFPV})	$\%RSD_A$ (g_j^{MFPV})	%RHW [a]	Am^{241}	Cm^{242}	$Cm^{243} + Cm^{244}$, Cs^{134}	Co^{60}, Pu^{238}	Cs^{137}	Eu^{154}	Eu^{155}, Pu^{239}, Tc^{99}	Np^{237}	Pu^{241}, Sb^{125}	Sr^{90}	U^{233}	U^{234}, U^{236}	U^{235}	U^{238}	Max (wt% > 0.001) [b]	Max (wt% > 0.1) [b]
AY-102	L	L	10	19	(d)		19	3	9	5			5				9	5	(e)
			15	10			10	3	5	4			4				5	4	
			20	7			7	3	4	3			3				4	3	
			50	3			3	1	3	2			2				3	2	
		H	10	-[c]			-	5	27	13			13				27	13	
			15	-			-	4	13	7			7				13	7	
			20	19			19	3	9	5			5				9	5	
			50	5			5	2	4	3			3				4	3	
	H	L	10	20			20	4	9	6			6				9	6	
			15	10			10	3	6	4			4				6	4	
			20	7			7	3	4	3			3				4	3	
			50	3			3	1	3	2			2				3	2	
		H	10	-			-	6	27	14			14				27	14	
			15	-			-	4	14	8			8				14	8	
			20	19			19	3	9	5			5				9	5	
			50	5			5	2	4	3			3				4	3	
AZ-102	L	L	10	3		27	19	3	9	5	5	19	5	5	-	13	3	13	3
			15	3		13	10	3	5	4	4	10	4	4	-	7	3	7	3
			20	3		9	7	3	4	3	3	7	3	3	19	5	3	5	3
			50	1		4	3	1	3	2	2	3	2	2	5	3	1	3	1
		H	10	5		-	-	5	27	13	13	-	13	13	-	-	5	-	5
			15	4		-	-	4	13	7	7	-	7	7	-	22	4	22	4
			20	3		27	19	3	9	5	5	19	5	5	-	13	3	13	3
			50	2		6	5	2	4	3	3	5	3	3	13	4	2	4	2
	H	L	10	4		27	20	4	9	6	6	20	6	6	-	14	4	14	4
			15	3		14	10	3	6	4	4	10	4	4	-	8	3	8	3
			20	3		9	7	3	4	3	3	7	3	3	19	5	3	5	3
			50	1		4	3	1	3	2	2	3	2	2	5	3	1	3	1
		H	10	6		-	-	6	27	14	14	-	14	14	-	-	6	-	6
			15	4		-	-	4	14	8	8	-	8	8	-	22	4	22	4
			20	3		27	19	3	9	5	5	19	5	5	-	13	3	13	3
			50	2		6	5	2	4	3	3	5	3	3	13	4	2	4	2

(a) Only %RHW ≤ 10, 15, 20, and 50 results are shown because of few acceptable results (i.e., $n_S^{MFPV} \leq 10$) for %RHW ≤ 5.

(b) Maximum values of n_S^{MFPV} are given for reportable components with wt% > 0.001 and 0.1.

(c) A dash (–) indicates that over 30 samples per MFPV batch would be necessary to satisfy the %RHW category.

(d) Empty cells indicate that no data were recorded for that particular analyte and HLW tank.

(e) No radionuclide nominal wt% was greater than 0.1 for AY-102.

Table 6.6. Numbers of IHLW MFPV Samples (with One Analysis per Sample) to Satisfy Certain %RHWs with 90% Confidence for Reportable IHLW Radionuclides Given Low and High Estimates of Mixing/Sampling and Analytical Uncertainties for Each of Three HLW Tanks (cont.)

HLW Tank	$\%RSD_S(g_j^{MFPV})$	$\%RSD_A(g_j^{MFPV})$	%RHW [(a)]	Am^{241}	Cm^{242}	$Cm^{243}+Cm^{244}, Cs^{134}$	Co^{60}, Pu^{238}	Cs^{137}	Eu^{154}	$Eu^{155}, Pu^{239}, Tc^{99}$	Np^{237}	Pu^{241}, Sb^{125}	Sr^{90}	U^{233}	U^{234}, U^{236}	U^{235}	U^{238}	Max (wt% > 0.001) [(b)]	Max (wt% > 0.1) [(b)]
C-104	L	L	**10**	19	-	27	19	3	9	5	19	19	13	5	-	13	3	13	3
			15	10	-	13	10	3	5	4	10	10	7	4	-	7	3	7	3
			20	7	27	9	7	3	4	3	7	7	5	3	19	5	3	5	3
			50	3	6	4	3	1	3	2	3	3	3	2	5	3	1	3	1
		H	**10**	-	-	-	-	5	27	13	-	-	-	13	-	-	5	-	5
			15	-	-	-	-	4	13	7	-	-	22	7	-	22	4	22	4
			20	19	-	27	19	3	9	5	19	19	13	5	-	13	3	13	3
			50	5	25	6	5	2	4	3	5	5	4	3	13	4	2	4	2
	H	L	**10**	20	-	27	20	4	9	6	20	20	14	6	-	14	4	14	4
			15	10	-	14	10	3	6	4	10	10	8	4	-	8	3	8	3
			20	7	27	9	7	3	4	3	7	7	5	3	19	5	3	5	3
			50	3	6	4	3	1	3	2	3	3	3	2	5	3	1	3	1
		H	**10**	-	-	-	-	6	27	14	-	-	-	14	-	-	6	-	6
			15	-	-	-	-	4	14	8	-	-	22	8	-	22	4	22	4
			20	19	-	27	19	3	9	5	19	19	13	5	-	13	3	13	3
			50	5	25	6	5	2	4	3	5	5	4	3	13	4	2	4	2

(a) Only %RHW ≤ 10, 15, 20, and 50 results are shown because of few acceptable results (i.e., $n_S^{MFPV} \leq 10$) for %RHW ≤ 5.

(b) Maximum values of n_S^{MFPV} are given for reportable components with wt% > 0.001 and 0.1.

(c) A dash (–) indicates that over 30 samples per MFPV batch would be necessary to satisfy the %RHW category.

(d) Empty cells indicate that no data were recorded for that particular analyte and HLW tank.

Table 6.7. Numbers of IHLW MFPV Samples (with One Analysis per Sample) to Satisfy Certain %RHWs with 95% Confidence for Reportable IHLW Radionuclides Given Low and High Estimates of Mixing/Sampling and Analytical Uncertainties for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$	$\%RSD_A(g_j^{MFPV})$	%RHW [a]	Am^{241}	Cm^{242}	$Cm^{243}+Cm^{244}, Cs^{134}$	Co^{60}, Pu^{238}	Cs^{137}	Eu^{154}	$Eu^{155}, Pu^{239}, Tc^{99}$	Np^{237}	Pu^{241}, Sb^{125}	Sr^{90}	U^{233}	U^{234}, U^{236}	U^{235}	U^{238}	Max (wt% > 0.001) [b]	Max (wt% > 0.1) [b]
AY-102	L	L	10	27	(d)		27	4	12	7			7				12	7	(e)
			15	14			14	3	7	5			5				7	5	
			20	9			9	3	5	4			4				5	4	
			50	4			4	2	3	3			3				3	3	
		H	10	-[c]			-	7	-	18			18				-	18	
			15	-			-	5	18	10			10				18	10	
			20	27			27	4	12	7			7				12	7	
			50	7			7	3	4	3			3				4	3	
	H	L	10	28			28	5	13	8			8				13	8	
			15	14			14	4	7	5			5				7	5	
			20	9			9	3	5	4			4				5	4	
			50	4			4	3	3	3			3				3	3	
		H	10	-			-	8	-	19			19				-	19	
			15	-			-	5	19	10			10				19	10	
			20	27			27	4	12	7			7				12	7	
			50	7			7	3	4	4			4				4	4	
AZ-102	L	L	10	4		-	27	4	12	7	7	27	7	7	-	18	4	18	4
			15	3		18	14	3	7	5	5	14	5	5	-	10	3	10	3
			20	3		12	9	3	5	4	4	9	4	4	27	7	3	7	3
			50	2		4	4	2	3	3	3	4	3	3	7	3	2	3	2
		H	10	7		-	-	7	-	18	18	-	18	18	-	-	7	-	7
			15	5		-	-	5	18	10	10	-	10	10	-	30	5	30	5
			20	4		-	27	4	12	7	7	27	7	7	-	18	4	18	4
			50	3		9	7	3	4	3	3	7	3	3	18	5	3	5	3
	H	L	10	5		-	28	5	13	8	8	28	8	8	-	19	5	19	5
			15	4		19	14	4	7	5	5	14	5	5	-	10	4	10	4
			20	3		12	9	3	5	4	4	9	4	4	27	7	3	7	3
			50	3		4	4	3	3	3	3	4	3	3	7	4	3	4	3
		H	10	8		-	-	8	-	19	19	-	19	19	-	-	8	-	8
			15	5		-	-	5	19	10	10	-	10	10	-	-	5	-	5
			20	4		-	27	4	12	7	7	27	7	7	-	19	4	19	4
			50	3		9	7	3	4	4	4	7	4	4	18	6	3	6	3

(a) Only %RHW ≤ 10, 15, 20, and 50 results are shown because of few acceptable results (i.e., $n_S^{MFPV} \leq 10$) for %RHW ≤ 5.

(b) Maximum values of n_S^{MFPV} are given for reportable components with wt% > 0.1 and 0.001.

(c) A dash (–) indicates that over 30 samples per MFPV batch would be necessary to satisfy the %RHW category.

(d) Empty cells indicate that no data were recorded for that particular analyte and HLW tank.

(e) No radionuclide nominal wt% values were greater than 0.1 for AY-102.

Table 6.7. Numbers of IHLW MFPV Samples (with One Analysis per Sample) to Satisfy Certain %RHWs with 95% Confidence for Reportable IHLW Radionuclides Given Low and High Estimates of Mixing/Sampling and Analytical Uncertainties for Each of Three HLW Tanks (cont.)

HLW Tank	$\%RSD_S$ (g_j^{MFPV})	$\%RSD_A$ (g_j^{MFPV})	%RHW [a]	Am^{241}	Cm^{242}	Cm^{243} + Cm^{244}, Cs^{134}	Co^{60}, Pu^{238}	Cs^{137}	Eu^{154}	Eu^{155}, Pu^{239}, Tc^{99}	Np^{237}	Pu^{241}, Sb^{125}	Sr^{90}	U^{233}	U^{234}, U^{236}	U^{235}	U^{238}	Max (wt% > 0.001%) [b]	Max (wt% > 0.1%) [b]
C-104	L	L	**10**	27	-	-	27	4	12	7	27	27	18	7	-	18	4	18	4
			15	14	-	18	14	3	7	5	14	14	10	5	-	10	3	10	3
			20	9	-	12	9	3	5	4	9	9	7	4	27	7	3	7	3
			50	4	9	4	4	2	3	3	4	4	3	3	7	3	2	3	2
		H	**10**	-[c]	-	-	-	7	-	18	-	-	-	18	-	-	7	-	7
			15	-	-	-	-	5	18	10	-	-	30	10	-	30	5	30	5
			20	27	-	-	27	4	12	7	27	27	18	7	-	18	4	18	4
			50	7	25	9	7	3	4	3	7	7	5	3	18	5	3	5	3
	H	L	**10**	28	-	-	28	5	13	8	28	28	19	8	-	19	5	19	5
			15	14	-	19	14	4	7	5	14	14	10	5	-	10	4	10	4
			20	9	-	12	9	3	5	4	9	9	7	4	27	7	3	7	3
			50	4	9	4	4	3	3	3	4	4	4	3	7	4	3	4	3
		H	**10**	-	-	-	-	8	-	19	-	-	-	19	-	-	8	-	8
			15	-	-	-	-	5	19	10	-	-	-	10	-	-	5	-	5
			20	27	-	-	27	4	12	7	27	27	19	7	-	19	4	19	4
			50	7	25	9	7	3	4	4	7	7	6	4	18	6	3	6	3

(a) Only %RHW ≤ 10, 15, 20, and 50 results are shown because of few acceptable results (i.e., $n_S^{MFPV} \leq 10$) for %RHW ≤ 5.

(b) Maximum values of n_S^{MFPV} are given for reportable components with wt% > 0.1 and 0.001.

(c) A dash (–) indicates that over 30 samples per MFPV batch would be necessary to satisfy the %RHW category.

(d) Empty cells indicate that no data were recorded for that particular analyte and HLW tank.

For 95% confidence, 4 samples are also sufficient per Table 6.7. These outcomes are consistent for $^{137}Cs_2O$ across all three of the HLW tanks considered in the calculations (AY-102, AZ-102, and C-104). However they will not be consistent across all three tanks for radionuclide components with tank-dependent analytical uncertainties.

The second-to-last column in each of Table 6.6 and Table 6.7 lists the maximum values of n_S^{MFPV} across the reportable radionuclides with nominal mass fractions greater than 0.00001 (0.001 wt%). In addition to $^{238}U_3O_8$ for AZ-102 and C-104, this list of reportable radionuclides with mass fraction > 0.00001 includes $^{241}Am_2O_3$ (AZ-102), $^{237}NpO_2$ (AZ-102), $^{239}PuO_2$, ^{90}SrO (AY-102 and AZ-102), $^{233}U_3O_8$ (C-104), and $^{235}U_3O_8$ (AZ-102 and C-104). With 95% confidence (Table 6.7), at most 7 samples are necessary to obtain RHWs of 20% or less when assuming "low" mixing/sampling and analytical

uncertainties. When "high" mixing/sampling and analytical uncertainties are assumed, then at most 6 samples would be necessary to obtain RHWs of 50% or less.

The last column in each of Table 6.6 and Table 6.7 lists the maximum values of n_S^{MFPV} across the reportable radionuclides with nominal mass fractions greater than 0.001 (0.1 wt%). The only reportable radionuclide with mass fraction > 0.001 was $^{238}U_3O_8$ for AZ-102 and C-104. Results from AY-102 were not reported in this column because no radionuclides contained compositions larger than 0.1 wt%. With 95% confidence (Table 6.7), for AZ-102 and C-104 at the most 8 samples are necessary to obtain RHWs of 10% or less when "high" mixing/sampling and analytical uncertainties are assumed.

6.2.2 Illustration of Calculating Means and Standard Deviations of IHLW Radionuclide Compositions and Inventories over an HLW Waste Type for Radionuclides Analyzed in Every MFPV Batch

This section uses realistic data to illustrate the equations presented in Section 4.2.4 for calculating means and SDs of IHLW radionuclide inventories per IHLW canister (Ci/canister) over an HLW waste type. Equations were presented in Section 4.2.4.1 for the case of balanced data (equal numbers of samples per MFPV batch and equal numbers of analyses for each MFPV batch), and in Section 4.2.4.2 for the case of unbalanced data (unequal numbers of samples per MFPV batch and/or unequal numbers of analyses for each MFPV batch). These equations are applicable for the radionuclides listed in Table 2.1 that will be analyzed in every IHLW MFPV batch.

The equations for calculating the means and SDs of radionuclide inventories per IHLW canister have embedded in them equations for calculating the means and SDs of IHLW radionuclide compositions (mass fractions of radionuclide oxide components) per IHLW canister. These equations are the same as presented in Section 4.1.4 and illustrated in Section 6.1.2.

A realistic balanced dataset to illustrate the use of Eqs. (4.1.2), (4.1.3), and (4.14) for the means, SDs, and %RSDs of IHLW radionuclide compositions (mass fractions) and Eqs. (4.2.1) and (4.2.2) for the means and SDs of radionuclide inventories per IHLW canister was obtained as previously described in Section 6.1.2. Specifically, results from G2 simulation Run 3.1vv (Deng 2004; Vora 2004) performed by the WTP Project for HLW Tank AY-102/C-106 were obtained (Vienna 2004a) and augmented with randomly generated MFPV mixing/sampling and analytical uncertainties. For each of the 18 MFPV batches selected, radionuclide concentrations for 8 samples with one analysis per sample were generated for each of the 18 MFPV batches. The average radionuclide concentrations (across the 8 samples) for each of the 18 MFPV batches are listed in Table I.4 in Section I.2 of Appendix I. Table I.5 in Section I.2 of Appendix I lists the mean IHLW radionuclide compositions (oxide mass fractions) for each of the 18 MFPV batches. The radionuclide concentrations and mass-fraction compositions in Tables I.4 and I.5 correspond to the same 18 batches for which chemical composition concentrations and mass fractions are listed in Tables I.1 and I.3. Simulated masses of glass in the 75 IHLW canisters calculated to be produced from the 18 MFPV batches[(a)] are shown in Table I.6 in Section I.2 of Appendix I. The values in Table I.6 were produced by adding randomly generated disturbances (based on available data for six IHLW canisters, Andre 2004) to the average mass of glass (assumed to be 3.089×10^6 g) in an IHLW canister.

(a) The average number of canisters produced per MFPV batch was calculated by the WTP Project and provided in an Excel spreadsheet "HLW can count for waste type.xls" (January 19, 2005).

Table 6.8 contains the illustrative results of applying the previously mentioned equations for calculating the means, SDs, and %RSDs of IHLW radionuclide compositions and inventories per IHLW canister over the 18 MFPV batches corresponding to one AY-102/C-106 waste type. Only those radionuclides analyzed in every MFPV batch of an HLW waste type are listed in Table 6.8. Note that the

Table 6.8. Example Results from Applying Equations for Calculating Means, SDs, and %RSDs of IHLW Radionuclide Oxide Compositions and Radionuclide Inventories per IHLW Canister. Results were obtained using data from 18 simulated IHLW MFPV batches corresponding to a blend of wastes from Tanks AY-102/C-106.

Radionuclide Oxide Component	Radionuclide Oxide Compositions			Radionuclide	Radionuclide Inventories per IHLW Canister[b]		
	Mean (MF)[a]	SD (MF)	%RSD		Mean (Ci)	SD (Ci)	%RSD
^{59}NiO	1.2791E-06	4.7123E-08	3.68	^{59}Ni	0.2487	1.0488E-02	4.22
^{60}CoO	3.2993E-13	9.7566E-15	2.96	^{60}Co	8.8505E-04	3.1869E-05	3.60
^{63}NiO	1.5313E-07	5.2961E-09	3.46	^{63}Ni	21.4876	0.8648	4.02
^{90}SrO	2.3698E-05	8.7519E-07	3.69	^{90}Sr	8701.6447	367.7163	4.23
$^{93}ZrO_2$	1.1380E-06	2.6055E-08	2.29	^{93}Zr	6.5382E-03	2.0115E-04	3.08
$^{93}Nb_2O_5$	1.2045E-11	3.3003E-13	2.74	^{93}Nb	6.2438E-03	2.1384E-04	3.42
$^{99}TcO_2$	4.5367E-07	1.3394E-08	2.95	^{99}Tc	1.8004E-02	6.4758E-04	3.60
$^{125}Sb_2O_5$	1.0795E-12	3.9881E-14	3.69	^{125}Sb	2.5262E-03	1.0678E-04	4.23
$^{126}SnO_2$	2.9415E-08	9.9942E-10	3.40	^{126}Sn	2.0289E-03	8.0555E-05	3.97
$^{135}Cs_2O$	N/A[c]	N/A	N/A	^{135}Cs	N/A	N/A	N/A
$^{137}Cs_2O$	5.8217E-06	2.6806E-06	46.04	^{137}Cs	1.4782E03	6.8117E02	46.10
$^{151}Sm_2O_3$	6.2723E-08	1.8118E-09	2.89	^{151}Sm	4.3467	0.1541	3.54
$^{152}Eu_2O_3$	1.8977E-10	5.7908E-12	3.05	^{152}Eu	9.1129E-02	3.3523E-03	3.68
$^{154}Eu_2O_3$	1.0448E-08	3.0469E-10	2.92	^{154}Eu	7.2600	0.2590	3.57
$^{155}Eu_2O_3$	3.0154E-09	7.5907E-11	2.52	^{155}Eu	3.9522	0.1284	3.25
$^{233}U_3O_8$	3.9687E-10	1.4691E-11	3.70	^{233}U	1.0051E-05	4.2550E-07	4.23
$^{234}U_3O_8$	1.4851E-07	4.6573E-09	3.14	^{234}U	2.4056E-03	9.0187E-05	3.75
$^{235}U_3O_8$	9.0407E-06	2.9071E-07	3.22	^{235}U	5.1998E-05	1.9841E-06	3.82
$^{236}U_3O_8$	9.0174E-07	2.5375E-08	2.81	^{236}U	1.5333E-04	5.3426E-06	3.48
$^{237}Np_2O_5$	4.3517E-06	1.4446E-07	3.32	^{237}Np	8.1660E-03	3.1879E-04	3.90
$^{238}U_3O_8$	2.0873E-03	6.5970E-05	3.16	^{238}U	1.8589E-03	7.0074E-05	3.77
$^{238}PuO_2$	2.1864E-08	7.1857E-10	3.29	^{238}Pu	1.0121	3.9226E-02	3.88
$^{239}PuO_2$	1.6635E-05	5.1898E-07	3.12	^{239}Pu	2.8097	0.1050	3.74
$^{240}PuO_2$	8.3064E-08	2.7043E-08	3.26	^{240}Pu	0.5207	2.0046E-02	3.85
$^{241}PuO_2$	2.4705E-08	7.8621E-10	3.18	^{241}Pu	6.7368	2.5519E-01	3.79
$^{241}Am_2O_3$	1.5889E-06	5.5226E-08	3.47	^{241}Am	15.1760	0.6127	4.04
$^{242}PuO_2$	8.2473E-09	2.5698E-10	3.12	^{242}Pu	8.7752E-05	3.2751E-06	3.73
$^{242}Cm_2O_3$	2.8795E-12	8.2671E-14	2.87	^{242}Cm	0.0267	9.4278E-04	3.53
$^{243}Am_2O_3$	1.9685E-09	6.0356E-11	3.07	^{243}Am	1.1068E-03	4.0851E-05	3.69
$^{244}Cm_2O_3$	2.0747E-10	6.7853E-12	3.27	^{244}Cm	4.7263E-02	1.8254E-03	3.86

(a) MF = mass fraction

(b) The radionuclide inventories per IHLW canister are calculated for the present time based on the G2 output. It was beyond the scope of the Statistical Analysis task to index the inventories to 2015 or 3115 as required by WAPS 1.2.

(c) N/A = not available

%RSD values for radionuclide inventories per IHLW canister are somewhat larger than the corresponding %RSD values for radionuclide component mass fractions, because the former is affected by variation in mass of glass in IHLW canisters as well as by the variation in radionuclide composition.

Equations (4.1.2) to (4.1.4) were employed to calculate the radionuclide composition (mass fractions) results in Table 6.8. As an example, consider the case of $^{137}Cs_2O$. Substituting the appropriate quantities that were used to obtain the averages shown in Table I.4 into Eq. (4.1.2), the mean (mass-weighted average) mass fraction of $^{137}Cs_2O$ over the 18 MFPV batches corresponding to an HLW waste type is obtained by

$$\bar{\bar{g}}^{\text{MFPV}}_{^{137}Cs_2O} = \frac{\left[\frac{1}{8}(0.0224\ \text{g/L} + 0.0236 + \cdots)\cdot(1\cdot 25718.3\ \text{L})\cdot 1.0584 + \frac{1}{8}(0.0218\ \text{g/L} + 0.0215 + \cdots)\cdot(1\cdot 24888.5\ \text{L})\cdot 1.0584 + \cdots\right]}{\left[\frac{1}{8}(121.56\ \text{g/L} + 111.99 + \cdots)\cdot(1\cdot 25718.3\ \text{L})\cdot 1.8889 + \cdots \frac{1}{8}(653.3\ \text{g/L} + 626.8 + \cdots)\cdot(1\cdot 24846.5\ \text{L})\cdot 2.1429 + \cdots\right]}$$

$$= 5.8217\times 10^{-6}\ \ g_{Cs_2O}/g_{glass}$$

Similarly, substituting the appropriate quantities from Table I.5 into Eq. (4.1.3), the standard deviation of $^{137}Cs_2O$ mass fractions over the 18 MFPV batches corresponding to an HLW waste type is given by

$$SD(\bar{g}^{\text{MFPV}}_{^{137}Cs_2O}) = \sqrt{\frac{[(8.7017E-06)-(5.8217E-06)]^2 + \cdots + [(2.4040E-06)-(5.8217E-06)]^2}{17}}$$

$$= 2.6806\times 10^{-6}\ \ g_{Cs_2O}/g_{glass}$$

Finally, the variation plus uncertainty in mass fractions of $^{137}Cs_2O$ over the 18 MFPV batches corresponding to an HLW waste type can be expressed as a %RSD using Eq. (4.1.4)

$$\%RSD(\bar{g}^{MFPV}_{^{137}Cs_2O}) = 100\left(\frac{SD(\bar{g}^{MFPV}_{^{137}Cs_2O})}{\bar{\bar{g}}^{MFPV}_{^{137}Cs_2O}}\right) = 100\left(\frac{2.6806\times 10^{-6}}{5.8217\times 10^{-6}}\right) = 46.04\ .$$

The rest of the radionuclide composition (mass fractions) means, SDs, and %RSDs in Table 6.8 were calculated in a similar manner.

As an example of the application of Eq. (4.2.1), the available data in Tables I.5 and I.6 produce the following result for the mean inventory per IHLW canister of ^{137}Cs across 75 IHLW canisters from 18 IHLW MFPV batches corresponding to an AY-102/C-106 waste type:

$$\overline{\overline{R}}^{Canister}_{D,^{137}Cs} = \frac{\overline{\overline{g}}^{MFPV}_{^{137}Cs_2O}\,\overline{m}^{Canister}_{D}\,A_{^{137}Cs}}{f_{^{137}Cs_2O}}$$

$$= \frac{\left(5.8217\text{E}-06\,\frac{\text{g}_{^{137}Cs_2O}}{\text{g}_{\text{glass}}}\right)\left(3.07\text{E}06\ \text{g}_{\text{glass}}\right)\left(87\,\frac{\text{Ci}}{\text{g}_{^{137}Cs}}\right)}{1.0584\,\frac{\text{g}_{^{137}Cs_2O}}{\text{g}_{^{137}Cs}}} = 1468.89\ \text{Ci}\ ^{137}\text{Cs/canister}$$

As an example of the application of Eq. (4.2.2), the available data in Tables I.5 and I.6 produce the following result for the SD of inventory per IHLW canister of ^{137}Cs across 75 IHLW canisters from 18 IHLW MFPV batches corresponding to an AY-102/C-106 waste type:

$$SD(\overline{R}^{Canister}_{d,^{137}Cs}) = \left(\frac{A_{^{137}Cs}}{f_{^{137}Cs_2O}}\right)\left\{\begin{array}{l}\left[\overline{\overline{g}}^{MFPV}_{^{137}Cs_2O}\right]^2\left[SD(m_d^{Canister})\right]^2 + \left[\overline{m}_D^{Canister}\right]^2\left[SD(\overline{g}^{MFPV}_{i,^{137}Cs_2O})\right]^2 \\ -\left[SD(m_d^{Canister})\right]^2\left[SD(\overline{g}^{MFPV}_{i,^{137}Cs_2O})\right]^2\end{array}\right\}^{1/2}$$

$$= \left(\frac{87\,\frac{\text{Ci}}{\text{g}_{^{137}Cs}}}{1.0584\,\frac{\text{g}_{^{137}Cs_2O}}{\text{g}_{^{137}Cs}}}\right)\left\{\begin{array}{l}\left[\left(5.8217\text{E}-06\,\frac{\text{g}_{^{137}Cs_2O}}{\text{g}_{\text{glass}}}\right)\right]^2\left[70936.57\ \text{g}_{\text{glass}}\right]^2 + \left[3.07E06\ \text{g}_{\text{glass}}\right]^2\left[2.6806E-06\frac{\text{g}_{^{137}Cs_2O}}{\text{g}_{\text{glass}}}\right]^2 \\ -\left[70936.57\ \text{g}_{\text{glass}}\right]^2\left[2.6806E-06\frac{\text{g}_{^{137}Cs_2O}}{\text{g}_{\text{glass}}}\right]^2\end{array}\right\}^{1/2}$$

$$= 677.02\ \text{Ci}\ ^{137}\text{Cs/canister}$$

Finally, the variation plus uncertainty in ^{137}Cs inventory per IHLW canister across 75 IHLW canisters from 18 MFPV batches corresponding to an AY-102/C-106 waste type can be expressed as a %RSD using Eq. (4.1.4)

$$\%RSD(\overline{R}^{Canister}_{^{137}Cs}) = 100\left(\frac{SD(\overline{R}^{Canister}_{d,^{137}Cs})}{\overline{\overline{R}}^{Canister}_{D,^{137}Cs}}\right) = 100\left(\frac{677.02}{1468.89}\right) = 46.09\,.$$

The rest of the radionuclide inventory per IHLW canister means, SDs, and %RSDs in Table 6.8 were obtained in a similar manner.

6.2.3 Illustration of the Statistical Method for Calculating IHLW Radionuclide Inventories and Their Standard Deviations over an HLW Waste Type, Using Information from a Single MFPV Batch

This subsection is a placeholder for an illustration, using realistic data, of the statistical method described in Section 4.2.5. That methodology, which has not yet been developed, will address reporting IHLW radionuclide inventories and their SDs over an HLW waste type for those radionuclides that are analyzed in only the first MFPV batch of an HLW waste type.

6.3 Compliance Results for IHLW WAPS Specification 1.3: Product Consistency

Section 6.3.1 illustrates, using a realistic example, the statistical methods presented in Section 4.3.3 for demonstrating that IHLW from a single MFPV batch satisfies PCT limits.

Section 6.3.2 presents the results from the investigation described in Section 4.3.4 for assessing the effects of (1) MFPV mixing/sampling and analytical uncertainties and (2) the numbers of samples per MFPV batch and analyses per MFPV sample on the ability to demonstrate PCT compliance for IHLW from a single MFPV batch. These results provide a basis for (1) assessing the sensitivity of single-MFPV-batch PCT estimates to the ranges of possible process uncertainties, and (2) the WTP Project to decide on the number of samples per MFPV batch and the number of chemical analyses per MFPV sample necessary to demonstrate PCT compliance for IHLW from a single MFPV batch.

Section 6.3.3 illustrates, using a realistic example, the statistical methods presented in Section 4.3.5 for demonstrating that IHLW over an HLW waste type satisfies PCT limits.

Section 6.3.4 presents the results from the investigation described in Section 4.3.6 for assessing the effects of (1) the variations and uncertainties in PCT responses over an HLW waste type, and (2) the numbers of samples per MFPV batch and analyses per MFPV sample on the ability to demonstrate PCT compliance for IHLW over an HLW waste type. These results provide a basis for (1) assessing the sensitivity of PCT estimates to the ranges of possible variations and uncertainties over an HLW waste type and (2) the WTP Project to decide on the number of samples per MFPV batch and the number of chemical analyses per MFPV sample necessary to demonstrate PCT compliance for IHLW over an HLW waste type.

6.3.1 Illustration of Methods for Demonstrating PCT Compliance for IHLW from Each MFPV Batch

This section uses realistic simulated data to illustrate the use of Eqs. (4.3.4) to (4.3.7) presented in Section 4.3.3 for calculating CL% UCCIs to demonstrate that IHLW corresponding to a single MFPV batch meets PCT limits. For this illustration, it is assumed that an IHLW MFPV batch with HLW from AY-102 is sampled 8 times with each sample analyzed once. Tables I.7 and I.8 in Section I.3 of Appendix I list the simulated IHLW elemental (Table I.7) and radionuclide (Table I.8) concentrations corresponding to the single analyses of 8 samples selected from an MFPV batch. Table 6.9 lists the normalized mass fraction compositions for the 8 MFPV samples calculated using Eq. (4.3.3).

Table 6.9. Normalized IHLW Compositions, Model-Predicted PCT Results, and Model Uncertainties for Eight Simulated Samples with One Analysis Each from an IHLW MFPV Batch Corresponding to HLW Tank AY-102

Normalized Oxide	Normalized Mass Fraction Composition for IHLW MFPV Sample								Mean	SD
	1	2	3	4	5	6	7	8		
Al_2O_3	0.0501	0.0538	0.0532	0.0721	0.0691	0.0730	0.0609	0.0736	0.0632	
B_2O_3	0.0954	0.1162	0.1092	0.1046	0.1234	0.1636	0.1708	0.1278	0.1264	
Li_2O	0.0288	0.0269	0.0299	0.0314	0.0347	0.0308	0.0218	0.0333	0.0297	
MnO	0.0351	0.0294	0.0397	0.0377	0.0391	0.0403	0.0427	0.0541	0.0398	
Na_2O	0.1607	0.1325	0.1295	0.1571	0.1344	0.1417	0.1332	0.1704	0.1450	N/A[(a)]
SiO_2	0.6256	0.6360	0.6323	0.5933	0.5957	0.5449	0.5638	0.5324	0.5905	
ThO_2	0	0	0	0	0	0	0	0	0	
ZrO_2	0.0043	0.0052	0.0062	0.0039	0.0036	0.0057	0.0069	0.0083	0.0055	
Total	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	
Model-Predicted PCT Normalized Releases [ln(g/L)]										
$\hat{y}^{PCT\ B}$	-0.0454	-0.4372	-0.4006	-0.1937	-0.2461	0.1282	0.0006	0.3856	-0.1011	0.2765
$\hat{y}^{PCT\ Li}$	-0.0967	-0.3550	-0.3265	-0.2281	-0.2557	-0.0768	-0.1670	0.0962	-0.1762	0.1484
$\hat{y}^{PCT\ Na}$	-0.1048	-0.6012	-0.5415	-0.2529	-0.4167	-0.2036	-0.3894	0.2339	-0.2845	0.2682
Model Uncertainties of Predicted PCT Normalized Releases for the Mean Composition [ln(g/L)]										
$SD_M[\hat{y}^{PCT\ B}(\bar{\bar{x}})]$	0.0785	(b)								
$SD_M[\hat{y}^{PCT\ Li}(\bar{\bar{x}})]$	0.0615									
$SD_M[\hat{y}^{PCT\ Na}(\bar{\bar{x}})]$	0.0533									

95% UCCIs on PCT Normalized Releases						
PCT Normalized Elemental Release	$\bar{\hat{y}}$ [ln(g/L)]	$CHW_{95\%\ UCI}$ [ln(g/L)]	$MHW_{95\%\ SUCI}$ [ln(g/L)]	95% UCCI [ln(g/L)]	95% UCCI [g/L]	Limit [g/L]
PCT B	-0.1011	0.1852	0.2930	0.3771	1.4581	16.695
PCT Li	-0.1762	0.0994	0.2294	0.1526	1.1648	9.565
PCT Na	-0.2845	0.1796	0.1988	0.0939	1.0985	13.346

(a) These SDs are not relevant to the illustration of 95% UCCI calculations.
(b) This portion of the table is intended to be blank.

Substituting the normalized IHLW compositions from Table 6.9 and the PCT model coefficients from Table 4.1 into Eq. (4.3.2a) yields the predicted PCT results shown in Table 6.9. Also shown in Table 6.9 are the SDs of model predictions calculated using the $\sqrt{(\bar{x}_i^{MFPV})^T\ \Sigma_b^h\ \bar{x}_i^{MFPV}}$ portion of Eq. (4.3.7) for h = PCT B, PCT Li, and PCT Na. Finally, Table 6.9 presents the results of calculations using Eqs. (4.3.4) through (4.3.7) to obtain 95% UCCIs for PCT normalized B, Li, and Na releases. The 95% UCCI values are seen to be well below the WAPS 1.3 limiting values for each of these releases.

Detailed illustrations of calculations using Eqs. (4.3.4) through (4.3.7) to obtain the 95% UCCI for ln(PCT normalized B release) are now presented. Intermediate results from Table 6.9 are used in some cases to reduce what would otherwise be very long algebraic equations. Applying Eq. (4.3.5) yields

$$\bar{\hat{y}}_i^{PCT\,B} = \frac{\sum_{l=1}^{n_S^{MFPV}} \left(\sum_{k=1}^{n_{mc}} b_k^{PCT\,B}\, x_{ikl}^{MFPV} \right)}{n_S^{MFPV}} = \frac{(-0.0454) + (-0.4372) + \cdots + (0.3856)}{8} = -0.1011 \text{ ln(g/L)}.$$

Applying Eq. (4.3.6) yields

$$CHW_{i,95\%\,UCI}^{PCT\,B} = t_{0.95,7} \sqrt{\frac{\sum_{l=1}^{n_S^{MFPV}} \left(\hat{y}_{il}^{PCT\,B} - \bar{\hat{y}}_i^{PCT\,B} \right)^2 \Big/ \left(n_S^{MFPV} - 1 \right)}{n_S^{MFPV}}} = 1.8946 \sqrt{\frac{0.0765}{8}} = 0.1852.$$

Applying Eq. (4.3.7), where $n = 97$ and $p = 8$, yields

$$MHW_{i,95\%\,SUCI}^{PCT\,B} = \sqrt{p\, F_{0.95}(p, n-p)} \left[\sqrt{(\bar{\boldsymbol{x}}_i^{MFPV})^T\, \boldsymbol{\Sigma}_b^{PCT\,B}\, \bar{\boldsymbol{x}}_i^{MFPV}} \right] = \sqrt{8 F_{0.95}(8, 89)}\, [0.0785] = 0.2930.$$

Finally, combining the above results in Eq. (4.3.4) yields

$$95\%\ UCCI[\text{ln(PCT B)}] = \bar{\hat{y}}_{\text{i}}^{PCT\,B} + CHW_{i,95\%\,UCI}^{PCT\,B} + MHW_{i,CL\%\,SUCI}^{PCT\,B}$$
$$= -0.1011 + 0.1852 + 0.2930 = 0.3771 \text{ ln(g/L)}$$

The value can converted to units of g/L by exponentiating, yielding $e^{0.3771} = 1.4581$ g/L. The preceding two values for the 95% UCCI, in units of ln(g/L) and g/L, are the ones shown for PCT normalized B release in Table 6.9.

6.3.2 Results of Investigations to Assess the Effects of Process Uncertainties and Numbers of MFPV Samples and Analyses on PCT Uncertainties and Compliance for IHLW from a MFPV Batch

This section uses the methodology described in Section 4.3.4 to assess the numbers of samples per MFPV batch and analyses per MFPV sample necessary to demonstrate compliance with PCT limits for each IHLW MFPV batch. The methodology in Section 4.3.4 uses Eqs. (4.3.4), (4.3.5), (4.3.7), and (4.3.8) to calculate CL% UCCI values for PCT normalized releases of B, Li, and Na for various combinations of input factor values. If the CL% UCCI values (for PCT B, Li, and Na) for a given combination of factor values are less than the PCT specification limits, then compliance is demonstrated for that combination. Values of n_S^{MFPV}, n_A^{MFPV}, the mass fraction compositions of IHLW corresponding to the n_A^{MFPV} analyses of n_S^{MFPV} MFPV samples, the model coefficients and variance-covariance matrices, and the

desired statistical confidence level (CL%) are necessary in using Eqs. (4.3.4), (4.3.5), (4.3.7), and (4.3.8) to calculate the CL% UCCI values.

Table 6.10 shows how taking at least 3 samples per IHLW MFPV batch with 1 analysis of each sample will be sufficient to demonstrate compliance with PCT limits for each IHLW MFPV batch. The calculations in Table 6.10 used what are expected to be conservatively large MFPV mixing/sampling and analytical uncertainty estimates of $SD_S(\hat{y}^h_{ilm}) = 0.20$ and $SD_A(\hat{y}^h_{ilm}) = 0.50$. Table 6.10 shows the calculated 95% UCCI values for PCT B, Li, and Na for each of the three HLW tanks used for illustrations in this report. Comparing these values to the PCT limits [in ln(g/L)] shows that at least 3 samples per MFPV batch with 1 analysis per sample should be sufficient to demonstrate compliance with PCT limits for each MFPV batch.

Table 6.10. IHLW PCT Limits and Resulting 95% UCCI Values for Three HLW Tanks Using $n_S^{MFPV} = 3$, $n_A^{MFPV} = 1$, $SD_S(y^h_{ilm}) = 0.20$, and $SD_A(y^h_{ilm}) = 0.50$

Tank	Quantity	Units	PCT Normalized Release of h = B	Li	Na
	PCT Limit (untransformed)	g/L	16.695	9.565	13.346
	PCT Limit (transformed)	ln(g/L)	2.815	2.258	2.591
AY-102	$\bar{\hat{y}}^h_i = \bar{\ln}(r_i^{PCT\,h})$	ln(g/L)	0.179	0.007	-0.030
	$MHW^h_{i,95\%\ SUCI}$	ln(g/L)	0.293	0.229	0.199
	$CHW^h_{i,95\%\ UCI}$ ($n_S^{MFPV} = 3$)	ln(g/L)	0.908	0.908	0.908
	$95\%\,UCCI\,(y^h_i)$ (a)	ln(g/L)	1.380	1.144	1.077
AZ-102	$\bar{\hat{y}}^h_i = \bar{\ln}(r_i^{PCT\,h})$	ln(g/L)	-0.434	-0.263	-0.199
	$MHW^h_{i,95\%\ SUCI}$	ln(g/L)	0.399	0.312	0.207
	$CHW^h_{i,95\%\ UCI}$ ($n_S^{MFPV} = 3$)	ln(g/L)	0.908	0.908	0.908
	$95\%\,UCCI\,(y^h_i)$ (a)	ln(g/L)	0.873	0.957	0.916
C-104	$\bar{\hat{y}}^h_i = \bar{\ln}(r_i^{PCT\,h})$	ln(g/L)	0.259	0.159	-0.091
	$MHW^h_{i,95\%\ SUCI}$	ln(g/L)	0.293	0.230	0.199
	$CHW^h_{i,95\%\ UCI}$ ($n_S^{MFPV} = 3$)	ln(g/L)	0.908	0.908	0.908
	$95\%\,UCCI\,(y^h_i)$ (a)	ln(g/L)	1.460	1.297	1.198

(a) $95\%\,UCCI\,(y^h_i)$ is calculated using Eqs. (4.3.4), (4.3.5), (4.3.7), and (4.3.8).

Table 6.11 uses a range of process uncertainty values and 95% confidence level to determine the minimum number of samples per MFPV batch necessary to comply with PCT limits. Two to 10 samples per MFPV batch were explored, each with one analysis per sample. Values of 0.05, 0.10, and 0.20 were used for $SD_S(\hat{y}^h_{ilm})$ and values of 0.05, 0.20, and 0.50 were used for $SD_A(\hat{y}^h_{ilm})$. These values were judged to be representative of what might be seen in the data. Using nominal glass-composition data from three HLW tanks from Table C.6, the PCT test cases showed there would be at most 3 samples with 1 analysis per sample necessary to demonstrate compliance with PCT limits for each MFPV batch, and in some cases only 2 samples would be necessary.

Because the WTP Project has not yet produced final estimates of IHLW process uncertainties, it was necessary in the preceding results to consider conservative values (Table 6.10) and a range of values (Table 6.11) for process uncertainties. A future update of this report will use final estimates of $SD_S(\hat{y}^h_{ilm})$ and $SD_A(\hat{y}^h_{ilm})$ uncertainties to determine the final recommended number of MFPV samples and number of chemical analyses per sample to demonstrate compliance with WAPS 1.3 for each MFPV batch.

Table 6.11. Minimum Number of Samples per IHLW MFPV Batch (Assuming One Analysis per Sample) Necessary to Meet (for Each MFPV Batch from Each of Three HLW Tanks) with 95% Confidence the IHLW PCT Limits, Given MFPV Mixing/Sampling and Analytical Standard Deviations

$SD_S(\hat{y}^h_{ilm})$ [ln(g/L)]	$SD_A(\hat{y}^h_{ilm})$ [ln(g/L)]	AY-102			AZ-102			C-104		
		PCT B	PCT Li	PCT Na	PCT B	PCT Li	PCT Na	PCT B	PCT Li	PCT Na
0.05	0.05	2	2	2	2	2	2	2	2	2
	0.20	2	2	2	2	2	2	2	2	2
	0.50	2	3	2	2	3	2	2	3	2
0.10	0.05	2	2	2	2	2	2	2	2	2
	0.20	2	2	2	2	2	2	2	2	2
	0.50	2	3	2	2	3	2	3	3	2
0.20	0.05	2	2	2	2	2	2	2	2	2
	0.20	2	2	2	2	2	2	2	2	2
	0.50	3	3	2	2	3	2	3	3	2

6.3.3 Illustration of the Method for Demonstrating PCT Compliance for IHLW Corresponding to an HLW Waste Type

This section uses realistic simulated data to illustrate the use of Eqs. (4.3.9) to (4.3.15) presented in Section 4.3.5 for calculating X%/Y% UTIs to demonstrate that IHLW produced from an HLW waste type meets PCT limits. For this illustration, an AY-102/C-106 waste type yielding 18 MFPV batches is considered where each MFPV batch is sampled 8 times with each sample analyzed once. Table I.7 in Section I.3 of Appendix I lists the simulated IHLW chemical compositions (mass fractions of oxides or halogens) corresponding to the 8 samples (one analysis each) of the 18 MFPV batches. The mass fraction compositions in Table I.7 were then each renormalized using Eq. (4.3.3), including only those oxides

found in the PCT models in Table 4.1. Substituting the renormalized IHLW compositions and the PCT model coefficients from Table 4.1 into Eq. (4.3.2a) yields the predicted PCT results for each sample within each batch. Table 6.12 contains some of the intermediate results in the calculation of 95%/95% UTI for ln(PCT normalized B, Li, and Na releases).

Table 6.12. 95%/95% UTI Intermediate and Final Calculations for PCT Normalized Release of B, Li, and Na Using Eight Simulated Samples with One Analysis Each from 18 IHLW MFPV Batches Corresponding to HLW Tank AY-102/C-106

PCT B [ln(g/L)]	PCT Li [ln(g/L)]	PCT Na [ln(g/L)]
$\tilde{\mu} = \bar{\bar{\hat{y}}}^h = \frac{\sum_{i=1}^{I} \bar{\hat{y}}_i^h}{I} = \frac{1}{I}\sum_{i=1}^{I}\left[\frac{\sum_{l=1}^{n_S^{MFPV}}\left(\sum_{k=1}^{n_{mc}^h} b_k^h \, x_{ikl}^{MFPV}\right)}{n_S^{MFPV}}\right]$		
$\tilde{\mu} = \frac{1}{18}\left[\frac{89.430}{8}\right] = 0.62$	$\tilde{\mu} = \frac{1}{18}\left[\frac{38.168}{8}\right] = 0.27$	$\tilde{\mu} = \frac{1}{18}\left[\frac{113.701}{8}\right] = 0.79$
$k(X,Y) = \frac{t(X,Y,df_{\tilde{\sigma}},\delta)}{\sqrt{I}}$		
$k(X,Y) = \frac{t(95\%,95\%,20.6,6.56)}{\sqrt{18}}$ = 2.255	$k(X,Y) = \frac{t(95\%,95\%,22.9,6.15)}{\sqrt{18}}$ = 2.103	$k(X,Y) = \frac{t(95\%,95\%,19.5,6.50)}{\sqrt{18}}$ = 2.255
$\tilde{\sigma} = \left\{\left[(\bar{\bar{x}}_I^{MFPV})^T \, \Sigma_b^h \, \bar{\bar{x}}_I^{MFPV}\right] + \sum_{i=1}^{I}\left(\bar{\hat{y}}_i^h - \bar{\bar{\hat{y}}}^h\right)^2 \Big/ (I-1)\right\}^{0.5}$		
$\tilde{\sigma} = \left\{0.021 + \frac{3.41}{18-1}\right\}^{0.5} = 0.47$	$\tilde{\sigma} = \left\{0.013 + \frac{1.32}{18-1}\right\}^{0.5} = 0.30$	$\tilde{\sigma} = \left\{0.0095 + \frac{2.23}{18-1}\right\}^{0.5} = 0.38$
$95\%/95\%UTI = \tilde{\mu} + k(X,Y)\,\tilde{\sigma}$		
$0.62 + 2.255 \times 0.47 = 1.68$ ln(g/L) $e^{1.68} = 5.38$ g/L	$0.27 + 2.103 \times 0.30 = 0.90$ ln(g/L) $e^{0.90} = 2.45$ g/L	$0.79 + 2.255 \times 0.38 = 1.64$ ln(g/L) $e^{1.64} = 5.13$ g/L

Detailed illustrations of the calculations applying Eqs. (4.3.9) through (4.3.14) to the simulated data to obtain the 95%/95% UTI for ln(PCT normalized B release) are now presented. Applying Eq. (4.3.10) yields

$$\tilde{\mu} = \bar{\bar{\hat{y}}}^{PCT\,B} = \frac{\sum_{i=1}^{I} \bar{\hat{y}}_i^{PCT\,B}}{I} = \frac{1}{I}\sum_{i=1}^{I}\left[\frac{\sum_{l=1}^{n_S^{MFPV}}\left(\sum_{k=1}^{n_{mc}^{PCT\,B}} b_k^{PCT\,B}\, x_{ikl}^{MFPV}\right)}{n_S^{MFPV}}\right]$$

$$= \frac{1}{18}\left[\frac{(0.449 + ... + 0.163)}{8} + ... + \frac{(0.706 + ... + 0.856)}{8}\right] = 0.621 \text{ ln(g/L)}.$$

Note that 0.449 is the model-predicted PCT B normalized release value for the first sample from the first MFPV batch, 0.163 is the predicted PCT B value for the eighth sample from the first MFPV batch, 0.706 is the predicted PCT B value for the first sample from the 18th MFPV batch, and 0.856 is the predicted PCT B value for the eighth sample from the 18th MFPV batch.

Applying Eq. (4.3.12) yields

$$df_{\tilde{\sigma}} \approx \frac{\left\{\left[(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^{\mathrm{T}}\, \hat{\boldsymbol{\Sigma}}_b^{PCT\,B}\, \bar{\bar{\boldsymbol{x}}}_I^{MFPV}\right] + \sum_{i=1}^{I}(\bar{\hat{y}}_i^{PCT\,B} - \bar{\bar{\hat{y}}}^{PCT\,B})^2 \Big/ (I-1)\right\}^2}{\frac{\left[(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^{\mathrm{T}}\, \hat{\boldsymbol{\Sigma}}_b^{PCT\,B}\, \bar{\bar{\boldsymbol{x}}}_I^{MFPV}\right]^2}{df_m} + \frac{\left[\sum_{i=1}^{I}(\bar{\hat{y}}_i^{PCT\,B} - \bar{\bar{\hat{y}}}^{PCT\,B})^2 \Big/ (I-1)\right]^2}{I-1}}$$

$$= \frac{\left\{(0.021) + \left[(0.236 - 0.621)^2 + ... + (0.892 - 0.621)^2\right]/(18-1)\right\}^2}{\frac{(0.021)^2}{97-8} + \frac{\left\{\left[(0.236 - 0.621)^2 + ... + (0.892 - 0.621)^2\right]/(18-1)\right\}^2}{18-1}} = 20.6\,.$$

Note that $\bar{\hat{y}}_1^{PCT\,B} = 0.236$ and $\bar{\hat{y}}_{18}^{PCT\,B} = 0.892$, while $[(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^{\mathrm{T}}\, \hat{\boldsymbol{\Sigma}}_b^{PCT\,B}\, \bar{\bar{\boldsymbol{x}}}_I^{MFPV}] = 0.021$.

Applying Eq. (4.3.13) yields

$$\delta = z_{1-\beta}\sqrt{I}\,\frac{\sigma_g}{\sigma} = 1.645\sqrt{18} \times 0.94 = 6.56\,,$$

where the ratio σ_g / σ represents the ratio of the "true" to the "inflated" (by the nuisance uncertainties that are modeling, mixing/sampling, and analytical) standard deviations of ln(PCT B) values over an HLW waste type. The value of the ratio σ_g / σ is assumed known in the statistical theory (see Appendix H of Piepel and Cooley 2002). Before WTP IHLW production operations, it is expected that

this ratio will be well-estimated based on available testing data. For the illustration here, the ratio was estimated from the same simulated data that were used in the equations,[(a)] with the estimate of 0.94 resulting. The details of how the σ_g / σ ratio was estimated from the simulated data are presented in Section G.3 of Appendix G. The ratio of 0.94 suggests that the nuisance uncertainties are small relative to the variation in ln(PCT B) results over the 18 MFPV batches corresponding to an AY-102/C-106 waste type in this example. However, this may be a result of the large batch-to-batch variation in IHLW compositions estimated by the G2 run used to provide the basis for the simulated data used in this illustration.

Substituting the results of the previous calculations from Eqs. (4.3.12) and (4.3.13) into Eq. (4.3.11) yields

$$k(X,Y) = \frac{t(X,Y,df_{\tilde{\sigma}},\delta)}{\sqrt{I}} = \frac{t(95\%,95\%,20.6,6.56)}{\sqrt{18}} = \frac{9.568}{\sqrt{18}} = 2.255 .$$

Applying Eq. (4.3.14) yields

$$\tilde{\sigma} = \left\{ \left[(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^T \boldsymbol{\Sigma}_{\boldsymbol{b}}^{PCT\,B} \bar{\bar{\boldsymbol{x}}}_I^{MFPV} \right] + \sum_{i=1}^{I} \left(\hat{\bar{y}}_i^{PCT\,B} - \hat{\bar{\bar{y}}}^{PCT\,B} \right)^2 \Big/ (I-1) \right\}^{0.5}$$

$$= \left\{ (0.021) + \left[(0.236 - 0.621)^2 + \ldots + (0.892 - 0.621)^2 \right] / (18-1) \right\}^{0.5} = 0.47 .$$

Finally, combining the above results in Eq. (4.3.9) yields

$$95\%/95\%\ UTI[ln(r^{PCT\,B})] = \tilde{\mu} + k(X,Y)\,\tilde{\sigma} = 0.62 + 2.255 \times 0.47 = 1.68\ \ \ln(\text{g/L}).$$

This value can be converted to PCT normalized B release units of g/L by exponentiating, yielding $e^{1.68} = 5.38$ g/L.

Table 6.12 contains the resulting 95%/95% UTI values for PCT normalized release for B, Li, and Na for this illustrative simulation using AY-102 data. These results are 5.38 g/L for B (as shown above), 2.45 g/L for Li, and 5.13 g/L for Na. When comparing these values to the normalized release limits found in Eq. (4.3.1), it can be concluded that compliance is easily demonstrated in each case.

6.3.4 Results of Investigations to Assess the Effects of Batch-to-Batch Variations, Process Uncertainties, and Numbers of MFPV Samples, Analyses, and Volume Determinations on IHLW PCT Compliance over an HLW Waste Type

The methodology described in Section 4.3.6 can be used to investigate the impacts of the number of samples per MFPV batch, the number of chemical analyses per MFPV sample, and other factors on the

(a) Estimating this ratio using the same data used to calculate the X%/Y% UTI technically invalidates the statistical properties of the X%/Y% UTI. However, that practice was acceptable given the merely illustrative nature of the calculations here.

ability to demonstrate that IHLW produced from an HLW waste type complies with the PCT limits specified in WAPS 1.3. The methodology in Section 4.3.6 uses the formula for X%/Y% UTIs on PCT normalized releases (of B, Li, and Na) presented in Section 4.3.5. The general formula for an X%/Y% UTI is given by Eq. (4.3.9) in Section 4.3.5. However, in this section, the following simplified formula was used

$$\text{X\%/Y\% UTI} = \tilde{\mu} + k(X,Y)\,\tilde{\sigma} = \tilde{\mu} + \text{UTIHW} \qquad (6.3.1)$$

where $\tilde{\mu}$ is the mean ln(PCT normalized release) over IHLW produced from an HLW waste type, $k(X, Y)$ and $\tilde{\sigma}$ are as defined in Section 4.3.5, and UTIHW denotes the half-width of a X%/Y% UTI.

Piepel and Cooley (2002) previously investigated an X%/Y% UTI approach of the type described in Section 4.3.5 that is applicable to the current WTP IHLW compliance strategy (i.e., analyzing samples selected from the MFPV). They calculated UTIHWs for all combinations of the values of factors shown in Table 6.13.[(a)] The UTIHWs calculated by Piepel and Cooley that correspond to the X%/Y% UTI method presented in Section 4.3.5 are contained in their Table 4.4 (95%/95% UTIHWs) and Table 4.6 (99%/99% UTIHWs). The UTIHW values in those tables are in ln(PCT normalized release) units of ln(g/m^2). In this report, units of ln(g/L) are used for ln(PCT normalized release). Because, 1 g/m^2 = 2 g/L[(b)], we have ln(g/m^2) = 0.6931 + ln(g/L) and ln(g/L) = ln(g/m^2) – 0.6931.

Table 6.13. Factors and Values Used by Piepel and Cooley (2002) in Calculating UTIHWs of X%/Y% UTIs

Factor	Piepel and Cooley (2002) Notation	Values
$SD_{WT}(\hat{y}_i^h)$ [(a)]	$\hat{\sigma}_g$	0.10, 0.25, 0.50
I	n	10, 30, 50
$SD_S(\hat{y}_{ilm}^h)$ [(a)]	$\hat{\sigma}_s$	0.05, 0.10
n_S^{MFPV}	m	1, 3
$SD_A(\hat{y}_{ilm}^h)$ [(a)]	$\hat{\sigma}_a$	0.05, 0.20, 0.50
n_A^{MFPV}	r	1, 3
$SD_M\left[\hat{y}^h(\bar{\bar{\bar{x}}})\right]$ [(a)]	$\bar{\hat{\sigma}}_m$	0.20, 0.40
df_m [(b)]	df_m	20, 40
X%/Y%	X%/Y%	95/95, 99/99

(a) These SDs are for $\hat{y}_i^h = \hat{l}n(\text{PCT normalized release of element } h)$, which are approximately equal to RSDs of (PCT normalized release of element h).

(b) $df_m = n - p$, where n is the number of data points used to fit a model, and p is the number of model coefficients estimated from the data points.

(a) Table 6.13 is based on Table 4.1 of Piepel and Cooley (2002), but with notation modified to match that used in this report.

(b) Applying the standard assumption of a surface area-to-volume ratio of 2000 m^{-1}, the result is that 1 g/m^2 = 2 g/L.

The UTIHW values in Tables 4.4 and 4.6 of Piepel and Cooley (2002) can be used to determine the required numbers of samples per MFPV batch (n_S^{MFPV}) and analyses per MFPV sample (n_A^{MFPV}) by considering likely values of $\tilde{\mu}$, solving for the maximum acceptable value of UTIHW, and determining which entries of Tables 4.4 and 4.6 satisfy the solution. Thus, rewriting Eq. (6.3.1) when comparing to a PCT normalized release limit yields

$$\text{X\%/Y\% UTI} = \tilde{\mu} + \text{UTIHW} \le \ln(\text{limit}) \quad \Rightarrow \quad \text{UTIHW} \le \ln(\text{limit}) - \tilde{\mu} \, . \tag{6.3.2}$$

The UTIHW values in Tables 4.4 and 4.6 of Piepel and Cooley that are less than the maximum allowable per Eq. (6.3.2) then correspond to the required number of samples per MFPV batch and analyses per MFPV sample, which depend on the magnitudes of (1) the variation of IHLW over MFPV batches corresponding to an HLW waste type and (2) uncertainties for each IHLW MFPV batch.

The 95%/95% UTIHW results from Table 4.4 of Piepel and Cooley (2002) were utilized in another way to conservatively demonstrate that 3 samples per MFPV batch and 1 chemical analysis per MFPV sample are sufficient to easily demonstrate compliance with nominal HLW glass compositions for each of the three HLW tanks (AY-102, AZ-102, and C-104) used for investigations in this report. Specifically, the largest variation ($\hat{\sigma}_g = 0.50$) and uncertainties ($\hat{\sigma}_S = 0.10$, $\hat{\sigma}_A = 0.50$, and $\bar{\hat{\sigma}}_m = 0.40$) considered by Piepel and Cooley (2002) were used for conservatism. Also, $df_m = 40$ was used, which is conservative compared to the larger values of df_m values for current IHLW PCT models (see Table 4.1). The number of IHLW MFPV batches per HLW waste type (denoted *I* in this report, and *n* by Piepel and Cooley 2002) is expected to be 18. For this conservative investigation, the smallest number of batches (10) considered by Piepel and Cooley (2002) was used.

Table 6.14 shows the resulting 95%/95% UTI values on PCT normalized releases of B, Li, and Na for HLW glass corresponding to Tanks AY-102, AZ-102, and C-104 obtained using the conservative estimates discussed in the previous paragraph. Compliance was easily demonstrated in each case, despite the significant conservatism in the inputs for the calculations summarized in Table 6.14. This exercise shows that at least 3 samples per MFPV batch with 1 analysis per sample should be sufficient to demonstrate with 95% confidence that at least 95% of the IHLW produced over an HLW waste type will have PCT normalized releases of B, Li, and Na that meet the WAPS 1.3 limits. This conclusion is conditional on (1) the WTP IHLW having compositions similar to those for HLW Tanks AY-102, AZ-102, and C-104 and (2) the batch-to-batch variation and within-batch uncertainties are not larger than the conservative values assumed for the calculations.

Table 6.14. 95%/95% UTI Values for PCT Normalized Releases of B, Li, and Na from IHLW Corresponding to Three HLW Tanks Assuming $n_S^{MFPV} = 3$, $n_A^{MFPV} = 1$, and Conservative Values of Inputs Considered by Piepel and Cooley (2002)[a]

PCT	Limit[b]	AY-102			AZ-102			C-104		
		$\tilde{\mu}$ [c]	95%/95% UTIHW[d]	95%/95% UTI[e]	$\tilde{\mu}$ [c]	95%/95% UTIHW[d]	95%/95% UTI[e]	$\tilde{\mu}$ [c]	95%/95% UTIHW[d]	95%/95% UTI[e]
Results in ln(g/m^2)										
B	2.122	0.179	1.350	1.529	-0.434	1.350	0.916	0.259	1.350	1.609
Li	1.564	0.007	1.350	1.357	-0.263	1.350	1.087	0.159	1.350	1.509
Na	1.898	-0.030	1.350	1.320	-0.198	1.350	1.152	-0.091	1.350	1.259
Results in ln(g/L)[f]										
B	2.815	0.872	1.350	2.222	0.259	1.350	1.609	0.952	1.350	2.302
Li	2.258	0.700	1.350	2.050	0.430	1.350	1.780	0.852	1.350	2.202
Na	2.591	0.663	1.350	2.013	0.495	1.350	1.845	0.602	1.350	1.952
	Results in g/L									
B	16.695	2.392	6.835	9.227	1.296	3.703	4.999	2.591	7.405	9.996
Li	9.565	2.014	5.755	7.769	1.537	4.394	5.931	2.345	6.699	9.044
Na	13.346	1.941	5.546	7.487	1.641	4.688	6.329	1.826	5.218	7.044

(a) Using the notation of Piepel and Cooley (2002) as summarized in Table 6.13, the maximum variation and uncertainty SDs used were $\hat{\sigma}_g = 0.50$, $\hat{\sigma}_S = 0.10$, $\hat{\sigma}_A = 0.50$, and $\bar{\hat{\sigma}}_m = 0.40$. Conservative values of $df_m = 40$ and 10 MFPV batches per HLW waste type were also used.

(b) The limits for PCT normalized releases of B, Li, and Na are listed in units of g/m^2 and g/L in Eq. (4.3.1).

(c) $\tilde{\mu}$ denotes the predicted ln(PCT normalized release) values for B, Li, and Na calculated using the PCT models in Table 4.1 for the nominal AY-102, AZ-102, and C-104 IHLW compositions given in Table C.6 of Appendix C. Before applying the models in Table 4.1, the compositions in Table C.6 were normalized to mass fractions of the 8 components appearing in the models.

(d) 95%/95% UTIHW denotes the half-width of a 95%/95% UTI found in Table 4.4 of Piepel and Cooley (2002) for the combination of inputs listed in Footnote (a). The Piepel and Cooley (2002) UTIHWs are in ln(g/m^2) units. For the other units shown in the table, the UTIHWs were obtained via UTIHW = UTI - $\tilde{\mu}$ after converting UTI and $\tilde{\mu}$ to the new units.

(e) 95%/95% UTI is given by $\tilde{\mu}$ + UTIHW, according to Eq. (6.3.1).

(f) The relationship 1 g/L = 2 g/m^2 leads to the conversion ln(g/L) = ln(2) + ln(g/m^2) = 0.6931 + ln(g/m^2).

6.4 Compliance Results for IHLW WAPS Specification 1.5: Hazardous Waste

Relevant statistical methods and corresponding results for the statistical aspects of the WTP Project's compliance strategy for WAPS 1.5 described in Section 4.4.2 are discussed in the reports by Cook and Blumenkranz (2003), Kot et al. (2003), and Kot et al. (2004b).

If the HLW LDR treatment variance and delisting processes lead to future revisions in the IHLW compliance strategy that include "during production" aspects of compliance, any results associated with

statistical methods or equations presented in a future revision of Section 4.4.3 will be included in a future revision of this subsection.

6.5 Compliance Results for IHLW Contract Specification 1.2.2.1.5: Dangerous and Hazardous Waste Requirements

Relevant statistical methods and corresponding results for the statistical aspects of the WTP Project's compliance strategy for Contract Specification 1.2.2.1.5 described in Section 4.5.2 are discussed in the reports by Cook and Blumenkranz (2003), Kot et al. (2003), and Kot et al. (2004b).

If the HLW LDR treatment variance and delisting processes lead to future revisions in the IHLW compliance strategy that include "during production" aspects of compliance, any results associated with statistical methods or equations presented in a future revision of Section 4.5.3 will be included in a future revision of this subsection.

6.6 Compliance Results for IHLW WAPS Specification 1.6: IAEA Safeguards Reporting for HLW

This section is reserved for compliance method illustrations and results associated with WAPS Specification 1.6.

6.6.1 Illustration of the Statistical Method for Calculating Means and Standard Deviations of the Masses of Total and Fissile U and Pu in IHLW Canisters over an HLW Waste Type, Using Information from a Single MFPV Batch

This section is reserved for an illustration of the method to be developed and documented in a future revision of Section 4.6.3.

6.6.2 Illustration of the Statistical Method for Calculating the Mean and Standard Deviation of the Pu Concentration in IHLW Canisters over an HLW Waste Type

This section is reserved for an illustration of the method to be developed and documented in a future revision of Section 4.6.4.

6.6.3 Illustration of the Statistical Method for Estimating the Mass Isotopic Ratios of U and Pu and their Uncertainties in IHLW Canisters over an HLW Waste Type

This section is reserved for an illustration of the method to be developed and documented in a future revision of Section 4.6.5.

6.6.4 Results of Investigations to Assess the Effects of Numbers of MFPV Samples, Analyses, and Volume Determinations on WAPS 1.6 Compliance Quantities

This section is reserved for presenting the results of the investigations to be developed and documented in a future revision of Section 4.6.6.

6.7 Compliance Results for WAPS Specification 3.8.2: Heat Generation at Year of Shipment

As discussed in Section 4.7.3, the Statistical Analysis task of the WTPSP currently has no scope to address the statistical aspects of the WTP Project's compliance strategy for WAPS 3.8.2. Such scope was included in the past, but removed in subsequent re-planning efforts. Section 4.7.4 discusses some possible approaches should the WTP Project want to retain the statistical aspects of the compliance strategy for WAPS 3.8.2. If so, and scope to address these needs were added in the future, the results would be included in a future revision of this section.

6.8 Compliance Results for IHLW WAPS Specification 3.14: Concentration of Plutonium in Each Canister

This section is reserved for compliance method illustrations and results associated with WAPS Specification 3.14.

6.8.1 Illustration of Method for Demonstrating Compliance with Pu Concentration Limit for Each IHLW Canister Produced from an HLW Waste Type

This section is reserved for an illustration of the method to be developed and documented in a future revision of Section 4.8.3.

6.8.2 Results of Investigations Associated with the Compliance Method for WAPS 3.14

This section is reserved for any future results of investigations associated with the statistical compliance method to be developed in FY 2005 as discussed in Section 4.8.3. Any such investigations will be described in a new Section 4.8.4.

6.9 Compliance Results for IHLW Contract Specification 1.2.2.1.6: Product Loading

As discussed in Section 4.9.2, the current WTP Project's compliance strategy for Contract Specification 1.2.2.1.6 does not include any statistical aspects, and thus there are no illustrations of methods or results of investigations to report here. However, the report by Amidan et al. (2004) discusses statistical investigations performed for the previous WTP Project's IHLW compliance strategy (which

involved sampling and analyzing the HLW CRV). Although the CRV is no longer included in the IHLW vitrification process or compliance strategy, many aspects of the work by Amidan et al. (2004) are still at least partially relevant to the current WTP Project's compliance strategy for IHLW. Amidan et al. (2004) assessed the impacts of mixing/sampling random uncertainties and bias on meeting selected compliance and processing requirements, including IHLW waste loading (WL) requirements. They discuss and illustrate (1) key tradeoffs between IHLW waste loading and temperature at which HLW glass has 1 volume percent crystallinity ($T_{1\%}$) and (2) potentially narrow acceptable ranges of mixing and/or sampling bias allowable for meeting WL and $T_{1\%}$ requirements.

7.0 Results and Illustrations of Statistical Methods for ILAW Compliance

This section presents the results of statistical WFQ activities performed per the ILAW compliance strategies for applicable specifications, as discussed in Section 5.0. This section also presents for each specification an example illustrating the application of the statistically based compliance method(s) for that specification, as described in the corresponding subsection of Section 5.0. The examples are intended to illustrate (using realistic, simulated data) the statistical methods that will be used to demonstrate compliance with specifications during ILAW production.

7.1 Compliance Results for ILAW Contract Specification 2.2.2.6.2: Chemical Composition During Production

Section 7.1.1 presents the results of Monte Carlo simulations described in Section 5.1.3 to assess the effects of several factors (the number of samples per CRV batch, the number of analyses per CRV sample, the number of volume determinations per CRV and MFPV batch, mixing/sampling uncertainty, analytical uncertainty, uncertainties in GFC compositions, uncertainties of masses of GFCs added to the MFPV) on the uncertainty of the estimated chemical composition of ILAW from a single MFPV batch. These results provide a basis for (1) assessing the sensitivity of single-MFPV-batch chemical composition estimates to the range of possible uncertainties and (2) the WTP Project making decisions on the numbers of samples per CRV batch, chemical analyses per CRV sample, and other process measurements.

Section 7.1.2 illustrates, using realistic example data, the methodology presented in Section 5.1.4 for calculating means and SDs of ILAW chemical composition over MFPV batches corresponding to a given LAW waste type.

7.1.1 Results of Simulations to Assess the Effects of Process Uncertainties, Number of Samples per CRV Batch, and Number of Analyses per CRV Sample on Uncertainties in Chemical Composition of ILAW from an MFPV Batch

This section uses the Monte Carlo simulation results (see Section 3.4.2) and the methodology described in Section 5.1.3 to assess the numbers of samples per CRV batch and analyses per CRV sample necessary to estimate the ILAW composition corresponding to an ILAW MFPV batch with a given precision (i.e., within a specified percentage of the true value) and confidence. This section also uses the results from the Monte Carlo simulation investigation to assess the effects of the factors mentioned in Table 3.3 on the uncertainty of ILAW chemical composition for a single MFPV batch.

Each test case (see Table 3.4) of the Monte Carlo simulation investigation consisted of combinations of values for n_S^{CRV}, n_A^{CRV}, n_V^{CRV}, and n_V^{MFPV}, "low" and "high" values for $\%RSD_S(c_j^{CRV})$, $\%RSD_A(c_j^{CRV})$, $SD(G_{jk}^{GFC})$, $SD(a_k^{GFC})$, SD_V^{CRV}, and SD_V^{MFPV}, and the selected statistical confidence level (CL%). Mass fractions of ILAW components corresponding to a single MFPV batch were simulated 1000 times for each test case of the simulation. The simulation results and Eq. (5.1.1) were

then used to calculate $\%RHW_{CL\%}(g_j^{MFPV})$ from a 100(1-α)% two-sided ECI for each ILAW chemical composition component (oxide or halogen) for the s^{th} simulation test case. The $\%RHW_{CL\%}(g_{sj}^{MFPV})$ represents the precision for the s^{th} simulation test case of the estimated mass fraction of the j^{th} chemical composition component in ILAW corresponding to an MFPV batch.

The results of the Monte Carlo investigation were used to determine the numbers of LAW CRV samples and analyses per CRV sample that resulted in the minimal number of total analyses ($n_S^{CRV} \times n_A^{CRV}$) yielding %RHW = $\%RHW_{CL\%}(g_{sj}^{MFPV})$ values in specified ranges for each combination of uncertainty factors considered. This investigation was performed for each of the 16 reportable ILAW chemical composition components, with the results given in Tables H.1 to H.16 in Section H.1.1 of Appendix H. Table 7.1 summarizes these results across the 16 reportable ILAW chemical composition components. To illustrate using Table 7.1, consider LAW Tank AP-101 (Envelope A) when all uncertainties are at their low levels (see Appendix D). Then, 7 CRV samples with 2 analyses per sample would be necessary to have 90% confidence of estimating each of the 16 reportable ILAW components with precision (i.e., %RHW) ≤ 5%. If the estimates of the reportable components need only be within 10% of the true mean values, then 4 samples per CRV with 1 analysis each would suffice. Again for Tank AP-101 (Envelope A), if all uncertainties are at their high levels and 95% confidence is desired, then none of the tested number of samples or analyses would produce all reportable oxide %RHW values ≤ 5%, or even 10%. However, 8 samples per CRV batch and 1 analysis per sample would be sufficient to estimate with 95% confidence each of the 16 reportable ILAW chemical composition components with %RHW values ≤ 15%.

The Monte Carlo simulation data for single MFPV batches were also analyzed using analysis of variance (ANOVA) to determine which factors, and interactions between the factors, had significant effects on the %RHW values obtained from the simulation results. Main effects, as well as two-factor and three-factor interactions, were investigated. No interactions higher than three-factor were included due to the confounding of interactions occurring at those levels because of the fractional factorial design used (see Section 3.4.2). This was an acceptable analysis because (1) four-factor and higher interactions are usually not statistically significant and (2) when they are, they are usually too small to be practically significant. An ANOVA was performed for each ILAW chemical composition component, using a significance level (α) of 0.05 to assess whether a factor or interaction was significant. The ANOVA was performed for each of the three LAW tanks (one each from LAW waste Envelopes A, B, and C) used for the investigations in this report. There were 45 ILAW chemical composition components that were studied, with 15 of those designated as reportable components (as listed in Table 2.2).

Results from the ANOVAs for ILAW chemical composition components are summarized in Table 7.2. This table summarizes the percentage of chemical composition components (oxides) for which each factor and two-factor interaction was statistically significant for each of the three LAW tanks. The ANOVA results were summarized for all of the ILAW chemical composition oxides and just the 16 reportable chemical composition oxides. If an oxide was not present or not measured for a given LAW tank, then it was not included in the analysis. From Table 7.2, it can be seen that changes in the %RSD of both CRV mixing/sampling and CRV analytical usually affected the %RHW, as well as changes in the GFC uncertainties and GFC weights. As expected, changes in the number of samples per CRV batch, as

Table 7.1. Required Numbers of Samples per LAW CRV Batch (n_S^{CRV}) and Analyses per Sample (n_A^{CRV}) to Satisfy Certain %RHWs Across All Reportable Chemical Composition Components for a Waste Tank in Each of Three LAW Waste Envelopes[a]

Tank (Envelope)	$\%RSD_S(c_j^{CRV})$	$\%RSD_A(c_j^{CRV})$	Confidence (%)	Percent Relative Half-width (%RHW) on the Mass Fraction of an ILAW Chemical Composition Component															
				Other Uncertainties[b] at Low Values								Other Uncertainties[b] at High Values[c]							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	L[e]	L[f]	90	7	2	4	1	2	1	1	1	7	2	3	1	2	1	1	1
			95	-[d]	-	5	1	2	1	1	1	-	-	5	1	2	1	2	1
		H[f]	90	-	-	10	1	5	1	3	1	-	-	5	2	5	1	3	1
			95	-	-	-	-	8	1	4	1	-	-	-	-	8	1	4	1
	H[e]	L	90	-	-	5	1	3	1	1	1	-	-	4	1	2	1	2	1
			95	-	-	6	1	4	1	2	1	-	-	8	1	3	1	2	1
		H	90	-	-	-	-	5	1	3	1	-	-	7	2	6	1	4	1
			95	-	-	-	-	8	1	5	1	-	-	-	-	8	1	5	1
AZ-101 (Envelope B)	L	L	90	10	1	2	1	1	1	1	1	8	1	1	2	1	1	1	1
			95	-	-	3	1	2	1	1	1	7	2	1	3	2	1	1	1
		H	90	-	-	8	1	4	1	1	2	-	-	8	1	4	1	2	1
			95	-	-	10	1	5	1	3	1	-	-	7	2	5	1	3	1
	H	L	90	10	1	2	1	1	1	1	1	8	1	3	1	2	1	1	1
			95	-	-	4	1	2	1	1	1	5	2	3	1	2	1	1	1
		H	90	-	-	8	1	4	1	2	1	-	-	10	1	4	1	3	1
			95	-	-	7	2	5	1	3	1	-	-	7	2	5	1	3	1
AN-107 (Envelope C)	L	L	90	10	1	3	1	2	1	1	1	7	2	3	1	2	1	1	1
			95	-	-	2	2	2	1	1	1	-	-	4	1	2	1	1	1
		H	90	-	-	10	1	6	1	3	1	-	-	7	2	2	2	3	1
			95	-	-	7	2	2	3	4	1	-	-	-	-	8	1	4	1
	H	L	90	7	2	3	1	2	1	1	1	7	2	3	1	2	1	1	1
			95	-	-	4	1	2	1	2	1	-	-	5	1	2	1	2	1
		H	90	-	-	7	2	6	1	3	1	-	-	7	2	6	1	3	1
			95	-	-	7	2	8	1	2	2	-	-	7	2	8	1	4	1

(a) For space reasons, n_S is used to denote n_S^{CRV}, and n_A is used to denote n_A^{CRV}.

(b) Other uncertainties include GFC composition uncertainty, uncertainties in masses of GFCs added to the MFPV, and CRV and MFPV volume uncertainties. The low and high values of these uncertainties used for this work are listed in the tables of Appendix D.

(c) In some cases, the table shows lower number of samples for other uncertainties at high values than at low values. This can occur for two reasons. First, other uncertainties have little impact, and thus the simulation results may be close for low and high levels of other uncertainties. This can yield numbers of samples when other uncertainties are at high values that are slightly higher or lower than when other uncertainties are at low levels. Second, the results are ILAW component dependent, with the possibility of a different component providing the deciding results when other uncertainties are high versus low.

(d) A dash (-) means that no numbers of samples per CRV batch and analyses per CRV sample, as tested according to Table 3.3, satisfied that %RHW category.

(e) Low (L) and high (H) values of LAW CRV mixing/sampling uncertainties are listed in Table D.1 of Appendix D.

(f) Low (L) and high (H) values of LAW CRV analytical uncertainties are listed in Table D.1 of Appendix D.

Table 7.2. Percentage of ILAW Chemical Composition Components (Oxides) for which the Factor or Interaction was Significant in the ANOVAs (α = 0.05) for Each of Three LAW Tanks

Factor / Interaction[(a)]	All Chemical Composition Components (Oxides)			Reportable Chemical Composition Components (Oxides)		
	Envelope A (AP-101)	Envelope B (AZ-101)	Envelope C (AN-107)	Envelope A (AP-101)	Envelope B (AZ-101)	Envelope C (AN-107)
$\%RSD_S(c_j^{CRV})$ [(b)]	39.5	18.6	57.1	31.3	31.3	44.4
$\%RSD_A(c_j^{CRV})$ [(b)]	90.7	74.4	100.0	100.0	62.5	100.0
$SD(G_{jk}^{GFC})$ [(b)]	20.9	39.5	42.9	25.0	75.0	44.4
$SD(a_k^{GFC})$ [(b)]	18.6	23.3	21.4	43.8	62.5	33.3
SD_V [(c)]	0.0	2.3	0.0	0.0	6.3	0.0
n_S^{CRV}	90.7	67.4	78.6	100.0	43.8	77.8
n_A^{CRV}	81.4	65.1	78.6	87.5	37.5	88.9
n_V [(d)]	2.3	2.3	0.0	6.3	0.0	0.0
$\%RSD_S(c_j^{CRV}) \times \%RSD_A(c_j^{CRV})$	34.9	18.6	28.6	31.3	18.8	22.2
$\%RSD_S(c_j^{CRV}) \times SD(G_{jk}^{GFC})$	4.7	2.3	21.4	6.3	6.3	22.2
$\%RSD_A(c_j^{CRV}) \times SD(G_{jk}^{GFC})$	4.7	4.7	7.1	6.3	12.5	11.1
$\%RSD_S(c_j^{CRV}) \times SD(a_k^{GFC})$	0.0	2.3	0.0	0.0	6.3	0.0
$\%RSD_A(c_j^{CRV}) \times SD(a_k^{GFC})$	14.0	2.3	7.1	37.5	6.3	0.0
$SD(G_{jk}^{GFC}) \times SD(a_k^{GFC})$	14.0	20.9	21.4	31.3	56.3	33.3
$\%RSD_S(c_j^{CRV}) \times SD_V$	2.3	0.0	0.0	0.0	0.0	0.0
$\%RSD_A(c_j^{CRV}) \times SD_V$	0.0	4.7	0.0	0.0	6.3	0.0
$SD(G_{jk}^{GFC}) \times SD_V$	0.0	2.3	0.0	0.0	6.3	0.0
$SD(a_k^{GFC}) \times SD_V$	0.0	4.7	0.0	0.0	12.5	0.0
$\%RSD_S(c_j^{CRV}) \times n_S^{CRV}$	46.5	23.3	71.4	56.3	31.3	66.7
$\%RSD_A(c_j^{CRV}) \times n_S^{CRV}$	90.7	72.1	92.9	100.0	50.0	100.0
$SD(G_{jk}^{GFC}) \times n_S^{CRV}$	14.0	7.0	35.7	18.8	18.8	33.3

(a) Only two-factor interactions were included in the ANOVA model.

(b) This factor has a "low" case and a "high" case.

(c) The notation SD_V represents both SD_V^{CRV} and SD_V^{MFPV}. This factor has a "low" and "high" case, where both SD_V^{CRV} and SD_V^{MFPV} are varied at the same time.

(d) The notation n_V represents both n_V^{CRV} and n_V^{MFPV}, with each being varied at the same time.

Table 7.2. Percentage of Chemical Composition Components (Oxides) for which the Factor or Interaction was Significant in the ANOVAs (α = 0.05) for Each of Three LAW Tanks (cont.)

Factor / Interaction	All Chemical Composition Components (Oxides)			Reportable Chemical Composition Components (Oxides)		
	Envelope A (AP-101)	Envelope B (AZ-101)	Envelope C (AN-107)	Envelope A (AP-101)	Envelope B (AZ-101)	Envelope C (AN-107)
$SD(a_k^{GFC}) \times n_S^{CRV}$	14.0	2.3	7.1	37.5	0.0	11.1
$SD_V \times n_S^{CRV}$	2.3	0.0	7.1	0.0	0.0	11.1
$\%RSD_S(c_j^{CRV}) \times n_A^{CRV}$	32.6	16.3	28.6	25.0	18.8	22.2
$\%RSD_A(c_j^{CRV}) \times n_A^{CRV}$	90.7	69.8	85.7	100.0	50.0	88.9
$SD(G_{jk}^{GFC}) \times n_A^{CRV}$	0.0	2.3	14.3	0.0	6.3	22.2
$SD(a_k^{GFC}) \times n_A^{CRV}$	9.3	0.0	7.1	18.8	0.0	11.1
$SD_V \times n_A^{CRV}$	0.0	0.0	0.0	0.0	0.0	0.0
$n_S^{CRV} \times n_A^{CRV}$	81.4	67.4	85.7	68.8	43.8	77.8
$\%RSD_S(c_j^{CRV}) \times n_V$	0.0	2.3	0.0	0.0	6.3	0.0
$\%RSD_A(c_j^{CRV}) \times n_V$	2.3	0.0	0.0	0.0	0.0	0.0
$SD(G_{jk}^{GFC}) \times n_V$	2.3	2.3	0.0	0.0	0.0	0.0
$SD(a_k^{GFC}) \times n_V$	0.0	2.3	0.0	0.0	0.0	0.0
$SD_V \times n_V$	0.0	0.0	0.0	0.0	0.0	0.0
$n_S^{CRV} \times n_V$	0.0	4.7	0.0	0.0	0.0	0.0
$n_A^{CRV} \times n_V$	0.0	2.3	7.1	0.0	0.0	11.1

well as in the number of analyses per sample, also affected the %RHW. Changes in the CRV and MFPV volume uncertainties and the number of volume determinations per vessel did not have statistically significant effects on the %RHW. Most two-factor interactions were not significant, with a few exceptions. As expected, the $n_S^{CRV} \times n_A^{CRV}$ interaction was statistically significant. This is because as n_S^{CRV} was increased, n_A^{CRV} could be decreased to obtain a similar %RHW and vice versa. Other interactions that were often significant included: $SD(G_{jk}^{GFC}) \times SD(a_k^{GFC})$, $\%RSD_S(c_j^{CRV}) \times n_S^{CRV}$, $\%RSD_A(c_j^{CRV}) \times n_S^{CRV}$, and $\%RSD_A(c_j^{CRV}) \times n_A^{CRV}$. The first of these is the interaction between GFC uncertainties and GFC weight uncertainties. The remaining interactions that were often significant are between (1) number of CRV samples or number of analyses per CRV sample and (2) uncertainty in CRV sampling or uncertainty in analysis of CRV samples, which is to be expected.

The ANOVA results in Table 7.2 require an explanation relative to the results in Table 7.1. The results in Table 7.2 show that factors $\%RSD_A(c_j^{CRV})$ and n_A^{CRV}, and interaction $n_S^{CRV} \times n_A^{CRV}$ have

statistically significant effects, and yet Table 7.1 shows that generally one analysis per CRV sample ($n_A^{CRV} = 1$) is sufficient for compliance. The explanation for this seeming inconsistency is that increasing the number of samples per CRV batch n_S^{CRV} also increases the total number of analyses, even if each sample is only analyzed once. Thus, increasing the number of samples per batch effectively reduces (via averaging) $\%RSD_A(c_j^{CRV})$ as well as $\%RSD_S(c_j^{CRV})$. This "dual benefit" is better than the "single benefit" from increasing the number of analyses per sample, which only effectively reduces $\%RSD_A(c_j^{CRV})$. This explains why most of the results in Table 7.1 show that one analysis per CRV sample is sufficient despite $\%RSD_A(c_j^{CRV})$ and n_A^{CRV} having statistically significant effects.

7.1.2 Illustration of Calculating Means and Standard Deviations of ILAW Chemical Composition over an LAW Waste Type

This section uses realistic data to illustrate the equations presented in Section 5.1.4 for calculating means and SDs of ILAW chemical composition (mass fractions) over an LAW waste type. During ILAW production, there will be one "averaged" estimate of chemical composition per MFPV batch, and the compliance method consists of calculating and reporting the means and SDs of reportable ILAW components calculated over all MFPV batches associated with a given LAW waste type. Equations are presented in Section 5.1.4.1 for the case of balanced data (equal numbers of samples per CRV batch and equal numbers of analyses for each CRV sample) and in Section 5.1.4.2 for the case of unbalanced data (unequal numbers of samples per CRV batch and/or unequal numbers of analyses for each CRV sample). For a balanced data set, the means, SDs, and %RSDs of ILAW chemical composition components are, respectively, calculated using Eqs. (5.1.2), (5.1.5), and (5.1.6).

To illustrate this compliance method, simulated data were obtained (Vienna 2004b) from the WTP Project's Run 3.1vv of the G2 dynamic simulation flowsheet (Deng 2004; Vora 2004) corresponding to the LAW portion of waste Tank AP-101. Tables J.1 and J.2 in Appendix J, respectively, list the chemical and radionuclide compositions (mass fractions) of 25 MFPV batches associated with LAW from AP-101. The LAW corresponding to these 25 MFPV batches is assumed to be the "waste type" for purposes of this illustration.

Equations (5.1.2), (5.1.5), and (5.1.6) can be used to calculate means, SDs, and %RSDs of ILAW component mass fractions given the results of measurements to be made during operation of the LAW vitrification facility. However, the complete set of such data (derived from the G2 run outputs) needed for the application of these equations was not available at the time of writing of this section. Because the available data from the G2 simulation run consist of mass fractions of ILAW components for each of the 25 selected MFPV batches, simpler calculations were made for the current illustration. Mass fractions for each MFPV batch, representing average ILAW compositions over all samples and analyses for that batch, were employed to calculate means, SDs, and %RSDs of the ILAW chemical composition components for an LAW waste type. The means, SDs, and %RSDs of the mass fractions for the ILAW chemical composition components are summarized in Table 7.3. The results for the reportable chemical composition components are shown in boldface in Table 7.3.

Table 7.3. Means, SDs, and %RSDs of ILAW Chemical Composition Components (Mass Fractions) over 25 ILAW MFPV Batches Corresponding to Waste Tank AP-101

Chemical Composition Component	Mass Fraction			Chemical Composition Component	Mass Fraction		
	Mean	SD	%RSD		Mean	SD	%RSD
Ag_2O	9.28E-07	1.84E-08	1.98	NiO	3.34E-05	1.14E-06	3.42
Al_2O_3 [(a)]	**5.89E-02**	**2.37E-05**	**0.04**	**P_2O_5**	**1.82E-03**	**5.40E-05**	**2.97**
As_2O_5	3.40E-06	8.54E-08	2.51	PbO	3.26E-05	8.35E-07	2.56
B_2O_3	**9.28E-02**	**2.46E-05**	**0.03**	PdO	2.26E-07	1.09E-08	4.83
BaO	3.78E-07	7.58E-10	0.20	Pr_2O_3	3.77E-08	8.71E-10	2.31
BeO	3.09E-06	2.25E-08	0.73	Rb_2O	3.52E-06	3.31E-08	0.94
Bi_2O_3	1.86E-06	1.68E-08	0.90	Rh_2O_3	7.82E-07	3.76E-08	4.83
CaO	**4.98E-02**	**1.41E-05**	**0.03**	RuO_2	1.48E-05	7.13E-07	4.83
CdO	1.90E-06	1.09E-08	0.57	SiO_2	4.38E-01	1.38E-04	0.03
Ce_2O_3	8.40E-08	3.09E-10	0.37	Ta_2O_5	1.28E-07	1.13E-09	0.89
Cl	**1.56E-03**	**1.77E-05**	**1.14**	TeO_2	3.93E-07	1.90E-08	4.83
Cr_2O_3	2.50E-04	2.23E-06	0.89	TiO_2	1.53E-02	1.19E-05	0.08
Cs_2O	2.77E-10	2.72E-12	0.98	Tl_2O	1.13E-07	4.57E-09	4.05
CuO	1.96E-06	3.93E-09	0.20	**SO_3**	**3.21E-03**	**2.81E-06**	**0.09**
F	2.26E-03	2.71E-05	1.20	Sb_2O_3	7.23E-08	1.83E-09	2.53
Fe_2O_3	**5.83E-02**	**2.65E-05**	**0.05**	SeO_2	9.98E-06	3.30E-07	3.31
K_2O	**2.89E-02**	**3.75E-04**	**1.30**	**SiO_2**	**3.90E-04**	**5.05E-06**	**1.30**
La_2O_3	1.31E-06	7.25E-09	0.56	SrO	1.33E-05	6.31E-07	4.74
Li_2O	**1.20E-02**	**2.15E-05**	**0.18**	V_2O_5	1.57E-06	1.35E-08	0.86
MgO	**1.57E-02**	**2.03E-06**	**0.01**	WO_3	2.75E-05	3.69E-07	1.34
MnO	1.18E-06	1.58E-08	1.33	Y_2O_3	2.09E-06	1.01E-07	4.83
MoO_3	1.83E-05	1.36E-07	0.75	**ZnO**	**2.90E-02**	**9.77E-06**	**0.03**
Na_2O	**1.63E-01**	**1.51E-04**	**0.09**	**ZrO_2**	**2.90E-02**	**9.77E-06**	**0.03**
Nd_2O_3	6.33E-06	1.71E-07	2.70	**Total Mass Fraction**[(b)]	0.9996	(c)	
(c)							

(a) Results for reportable chemical composition components (per Table 2.2) are shown in boldface. Note that "Others" (the total of the remaining components) is also reportable per Table 2.2.

(b) This is the total sum of mean mass fractions of ILAW chemical composition components. The radionuclide composition portion (see Table 7.6) makes up the difference (aside from rounding error).

(c) This portion of the table is intentionally blank.

To illustrate the simpler calculations, individual MFPV batch averages for Na_2O were averaged to obtain the mean mass fraction composition over the 25 MFPV batches:

$$\bar{\bar{g}}^{MFPV}_{Na_2O} = \frac{0.1623 + 0.1624 + 0.1628 + \cdots + 0.1629}{25} = 0.1626 \ g_{Na_2O}/g_{glass} \qquad (7.1.1)$$

Given that MFPV batch averages and averages for a waste type are available, SDs and %RSDs for all reportable ILAW components can be calculated using Eqs. (5.1.5) and (5.1.6), respectively. Examples of the use of these two equations are now given. Plugging the appropriate quantities into Eq. (5.1.5), the standard deviation of Na_2O mass fractions over the 25 MFPV batches corresponding to an LAW waste type is obtained by

$$SD(\bar{g}_{Na_2O}^{MFPV}) = \sqrt{\frac{(0.1623-0.1626)^2 + (0.1624-0.1626)^2 + \cdots + (0.1629-0.1626)^2}{24}} \quad . \qquad (7.1.2)$$

$$= 0.00015 \ \ g_{Na_2O}/g_{glass}$$

The %RSD for Na_2O can be calculated by applying Eq. (5.1.6) to the results obtained from Eqs. (7.1.1) and (7.1.2).

$$\%RSD(\bar{\bar{g}}_{Na_2O}^{MFPV}) = 100\left(\frac{0.00015}{0.1626}\right) = 0.0928. \qquad (7.1.3)$$

The variation in Na_2O mass fractions of ILAW resulting from the 25 simulated MFPV batches in this example is quite small. This is directly explained by the small variability in the G2 results for these batches. However, because the G2 simulated data do not include mixing/sampling, analytical, and all of the other uncertainties affecting the estimate of ILAW composition for each MFPV batch, the results should be expected to be smaller than if all applicable uncertainties were included in the data. It should not be inferred from this one illustrative example that the variation in Na_2O over ILAW resulting from an LAW waste type will be that small during ILAW production.

For this AP-101 ILAW example, the variations of the ILAW chemical composition component mass fractions (over the 25 ILAW MFPV batches corresponding to an LAW waste type) summarized in Table 7.3 range from 0.01 to 4.83 %RSD. However, it should be kept in mind that this range of %RSDs reflects only batch-to-batch variation and not any of the within-batch uncertainties that will affect estimation of ILAW chemical (and radionuclide) compositions during WTP ILAW production.

When a full set of needed data is available, this section of the report will be revised to illustrate the use of Eqs. (5.1.2), (5.1.5), and (5.1.6) for calculating means, SDs, and %RSDs of ILAW chemical component compositions (mass fractions). The revisions will include taking the complete set of G2 data and augmenting it by random disturbances corresponding to the various uncertainties affecting the estimate of ILAW composition for an MFPV batch. The equations for means, SDs, and %RSDs will then be applied to this augmented data so that the effects of within-batch uncertainties as well as batch-to-batch variation will be reflected in the example results.

7.2 Compliance Results for ILAW Contract Specification 2.2.2.7.2: Radionuclide Composition During Production

Section 7.2.1 presents the results of Monte Carlo simulations as described in Section 5.2.3 to assess the effects of several factors, including (1) the magnitudes of mixing/sampling and analytical uncertainties, (2) the uncertainties pertaining to GFC weights and compositions, (3) the numbers of samples per CRV batch and analyses per CRV sample, and (4) the number of volume determinations per CRV and MFPV batch on the radionuclide composition of ILAW from a single MFPV batch. These results provide a basis for (1) assessing the sensitivity of single-MFPV-batch radionuclide composition estimates to the range of possible uncertainties, and (2) the WTP Project to decide on the number of samples per MFPV batch, the number of chemical analyses per sample, and the numbers of other process measurements.

Section 7.2.2 illustrates, using a realistic example, the methodology presented in Section 5.2.4 for calculating means and SDs of ILAW radionuclide compositions and inventories over MFPV batches and ILAW containers corresponding to a given LAW waste type.

7.2.1 Results of Simulations to Assess the Effects of Process Uncertainties, Number of Samples Per CRV Batch, and Number of Analyses per CRV Sample on Uncertainties in ILAW Radionuclide Composition from an MFPV Batch

This section uses the Monte Carlo simulation results (see Section 3.4.2) and the methodology described in Section 5.2.3 to assess the numbers of samples per CRV batch and analyses per CRV sample necessary to estimate the ILAW radionuclide composition corresponding to an ILAW MFPV batch with a given precision (i.e., within a specified percentage of the true value) and confidence. As noted at the start of Section 5.2.3, mass fractions of ILAW radionuclide components (oxides) may be of limited interest directly, but they play a key role in the equations developed to calculate ILAW radionuclide inventories (see Section B.2 of Appendix B). Hence, it is important to assess the numbers of LAW CRV samples, radiochemical analyses per sample, and other process determinations required to adequately estimate ILAW radionuclide compositions.

The methodology is the same as was used for ILAW chemical composition as described in Section 5.1.3 and illustrated in Section 7.1.1. This section also uses the results from the Monte Carlo simulation investigation to assess the effects of the factors mentioned in Table 3.3 on the uncertainty of ILAW radionuclide composition for a single MFPV batch.

Each test case (see Table 3.4) of the Monte Carlo simulation investigation consisted of combinations of values for n_S^{CRV}, n_A^{CRV}, n_V^{CRV}, and n_V^{MFPV}, "low" and "high" values for $\%RSD_S(c_j^{CRV})$, $\%RSD_A(c_j^{CRV})$, $SD(G_{jk}^{GFC})$, $SD(a_k^{GFC})$, SD_V^{CRV}, and SD_V^{MFPV}, and the selected statistical confidence level (CL%). Mass fractions of ILAW components corresponding to a single MFPV batch were simulated 1000 times for each test case of the simulation. The simulation results and Eq. (5.1.1) were then used to calculate $\%RHW_{CL\%}(g_{sj}^{MFPV})$ from a 100(1-α)% two-sided *empirical confidence interval* (ECI) for each radionuclide composition component (oxide) for the s^{th} simulation test case. The

$\%RHW_{CL\%}(g_{sj}^{MFPV})$ represents the precision for the s^{th} simulation test case of the estimated mass fraction of the j^{th} chemical composition component in ILAW corresponding to an MFPV batch.

The results of the Monte Carlo investigation were used to determine the numbers of LAW CRV samples and analyses per CRV sample that resulted in the minimal number of total analyses ($n_S^{CRV} \times n_A^{CRV}$) yielding %RHW = $\%RHW_{CL\%}(g_{sj}^{MFPV})$ values in specified ranges for each combination of uncertainty factors considered. This investigation was performed for each of the 14 reportable ILAW radionuclide composition components present in the three LAW tanks, with the results given in Tables H.17 to H.30 in Section H.2.1 of Appendix H. Table 7.4 summarizes these results across the 14 reportable ILAW radionuclide composition components present in the three LAW tank examples. To illustrate using Table 7.4, consider LAW Tank AP-101 (Envelope A) when all uncertainties are at their low levels (see Appendix D). Then 8 CRV samples with 1 analysis per sample would be necessary to have 95% confidence of estimating each of the 14 reportable ILAW radionuclide composition components with precision (i.e., %RHW) ≤10%. Again for Tank AP-101 (Envelope A), if all uncertainties are at their high levels, and 95% confidence is desired, then 7 samples per CRV batch with 2 analyses per sample would be needed to have all reportable radionuclide %RHW values ≤ 15%. However, all 14 reportable ILAW radionuclide composition components present in the three LAW tank examples would have %RHW values ≤ 20% with 95% confidence for 6 samples per CRV batch with 1 analysis per sample. Or, 8 samples per CRV batch with 1 analysis per sample would provide 90% confidence that all reportable radionuclides have %RHW values ≤ 15%.

The Monte Carlo simulation radionuclide data for single MFPV batches were also analyzed using ANOVA to determine which factors, and interactions between the factors, had significant effects on the %RHW values calculated during the simulations. This was done in the same manner as described for ILAW chemical compositions in Section 7.1.1. Main effects, as well as two-factor and three-factor interactions, were investigated. No interactions higher than three-factor were included due to the confounding of interactions occurring at those levels because of the fractional factorial design used (see Section 3.4.2). This was an acceptable analysis because (1) four-factor and higher interactions are usually not statistically significant and (2) when they are, they are usually too small to be practically significant. An ANOVA was performed for each ILAW radionuclide composition component, using a significance level (α) of 0.05 to assess whether a factor or interaction was significant. The ANOVA was performed for each of the three tanks (one each from LAW waste Envelopes A, B, and C) used for the investigations in this report. There were 30 ILAW radionuclide composition components that were studied, with 14 of the 30 designated in Table 2.1 as reportable radionuclides. The reportable radionuclides present in the three example LAW tanks include: $^{241}Am_2O_3$, $^{243+244}Cm_2O_3$, ^{60}CoO, $^{137}Cs_2O$, $^{154}Eu_2O_3$, $^{155}Eu_2O_3$, ^{63}NiO, $^{237}NpO_2$, $^{238}PuO_2$, $^{239}PuO_2$, $^{241}PuO_2$, $^{125}Sb_2O_3$, ^{90}SrO, and $^{99}Tc_2O_7$.

Results from the ANOVAs for ILAW radionuclide composition components are summarized in Table 7.5. This table summarizes the percentage of ILAW radionuclide composition components for which each factor and two-factor interaction was statistically significant for each of the three LAW tanks. The ANOVA results were summarized for all the ILAW radionuclide composition components and just the 14 reportable radionuclide components present in the three LAW tank examples. If a radionuclide was not present or not measured for a given LAW tank, then it was not included in the analysis. From Table 7.5, it can be seen that changes in the CRV analytical %RSD always affected the %RHW, with changes to CRV mixing/sampling %RSD occasionally affecting the %RHW. As expected, changes in the

Table 7.4. Required Number of Samples per LAW CRV Batch (n_S^{CRV}) and Analyses per Sample (n_A^{CRV}) to Satisfy Certain %RHWs Across All Reportable Radionuclide Composition Components for a Waste Tank in Each of Three LAW Waste Envelopes[a]

Tank (Envelope)	$\%RSD_S(c_j^{CRV})$	$\%RSD_A(c_j^{CRV})$	Confidence (%)	Percent Relative Half-width (%RHW) on the Mass Fraction of an ILAW Chemical Composition Component															
				Other Uncertainties[b] at Low Values								Other Uncertainties[b] at High Values[c]							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	L[e]	L[f]	90	-[d]	-	5	1	2	1	2	1	-	-	5	1	2	1	2	1
			95	-	-	8	1	3	1	2	1	-	-	8	1	3	1	2	1
		H[f]	90	-	-	-	-	8	1	2	2	-	-	-	-	8	1	5	1
			95	-	-	-	-	7	2	6	1	-	-	-	-	7	2	3	2
	H[e]	L	90	-	-	5	1	3	1	2	1	-	-	6	1	2	1	2	1
			95	-	-	8	1	4	1	2	1	-	-	8	1	4	1	2	1
		H	90	-	-	-	-	10	1	5	1	-	-	-	-	8	1	5	1
			95	-	-	-	-	10	1	6	1	-	-	-	-	7	2	6	1
AZ-101 (Envelope B)	L	L	90	7	2	4	1	2	1	1	1	7	2	4	1	2	1	1	1
			95	-	-	5	1	2	1	2	1	-	-	5	1	3	1	2	1
		H	90	-	-	7	2	5	1	1	3	-	-	7	2	6	1	3	1
			95	-	-	-	-	8	1	2	2	-	-	-	-	8	1	5	1
	H	L	90	-	-	4	1	2	1	1	1	7	2	4	1	2	1	1	1
			95	-	-	5	1	3	1	2	1	-	-	6	1	3	1	2	1
		H	90	-	-	7	2	6	1	4	1	-	-	7	2	6	1	4	1
			95	-	-	-	-	10	1	5	1	-	-	-	-	8	1	5	1
AN-107 (Envelope C)	L	L	90	-	-	5	1	2	1	1	1	-	-	5	1	2	1	2	1
			95	-	-	8	1	3	1	2	1	-	-	6	1	3	1	2	1
		H	90	-	-	-	-	8	1	5	1	-	-	7	2	8	1	2	2
			95	-	-	-	-	10	1	6	1	-	-	-	-	5	2	6	1
	H	L	90	-	-	5	1	2	1	2	1	-	-	4	1	2	1	2	1
			95	-	-	8	1	3	1	2	1	-	-	6	1	3	1	2	1
		H	90	-	-	-	-	6	1	2	2	-	-	-	-	8	1	2	2
			95	-	-	-	-	10	1	6	1	-	-	-	-	7	2	6	1

(a) For space reasons, n_S is used to denote n_S^{CRV}, and n_A is used to denote n_A^{CRV}.

(b) Other uncertainties include GFC composition uncertainty, uncertainties in masses of GFCs added to the MFPV, and CRV and MFPV volume uncertainties. Their low and high values of these uncertainties used for this work are listed in the tables of Appendix D.

(c) In some cases, the table shows lower number of samples for other uncertainties at high values than at low values. This can occur for two reasons. First, other uncertainties have little impact, and thus the simulation results may be close for low and high levels of other uncertainties. This can yield numbers of samples when other uncertainties are at high values that are slightly higher or lower than when other uncertainties are at low levels. Second, the results are ILAW component dependent, with the possibility of a different component providing the deciding results when other uncertainties are high versus low.

(d) A dash (-) means that no number of samples per CRV batch and analyses per sample, as tested according to Table 3.3, satisfied that %RHW category.

(e) Low (L) and high (H) values of LAW CRV mixing/sampling uncertainties are listed in Table D.2 of Appendix D.

(f) Low (L) and high (H) values of LAW CRV analytical uncertainties are listed in Table D.4 of Appendix D.

Table 7.5. Percentage of ILAW Radionuclide Composition Components (Oxides) for which the Factor or Interaction was Significant in the ANOVAs (α = 0.05) for Each of Three LAW Tanks

Factor / Interaction[a]	All Radionuclide Composition Components (Oxides)			Reportable Radionuclide Composition Components (Oxides)		
	Envelope A (AP-101)	Envelope B (AZ-101)	Envelope C (AN-107)	Envelope A (AP-101)	Envelope B (AZ-101)	Envelope C (AN-107)
$\%RSD_S(c_j^{CRV})$ [b]	7.4	9.1	33.3	15.4	16.7	50
$\%RSD_A(c_j^{CRV})$ [b]	100	100	100	100	100	100
$SD(G_{jk}^{GFC})$ [b]	0	0	0	0	0	0
$SD(a_k^{GFC})$ [b]	0	0	0	0	0	0
SD_V [c]	0	0	0	0	0	0
n_S^{CRV}	100	100	100	100	100	100
n_A^{CRV}	100	100	100	100	100	100
n_V [d]	0	0	0	0	0	0
$\%RSD_S(c_j^{CRV}) \times \%RSD_A(c_j^{CRV})$	7.4	9.1	33.3	15.4	16.7	50
$\%RSD_S(c_j^{CRV}) \times SD(G_{jk}^{GFC})$	0	0	0	0	0	0
$\%RSD_A(c_j^{CRV}) \times SD(G_{jk}^{GFC})$	0	0	0	0	0	0
$\%RSD_S(c_j^{CRV}) \times SD(a_k^{GFC})$	0	0	0	0	0	0
$\%RSD_A(c_j^{CRV}) \times SD(a_k^{GFC})$	0	0	0	0	0	0
$SD(G_{jk}^{GFC}) \times SD(a_k^{GFC})$	0	0	0	0	0	0
$\%RSD_S(c_j^{CRV}) \times SD_V$	0	0	0	0	0	0
$\%RSD_A(c_j^{CRV}) \times SD_V$	0	0	0	0	0	0
$SD(G_{jk}^{GFC}) \times SD_V$	0	0	0	0	0	0
$SD(a_k^{GFC}) \times SD_V$	0	0	0	0	0	0
$\%RSD_S(c_j^{CRV}) \times n_S^{CRV}$	7.4	9.1	33.3	100	100	100
$\%RSD_A(c_j^{CRV}) \times n_S^{CRV}$	100	100	100	0	0	0
$SD(G_{jk}^{GFC}) \times n_S^{CRV}$	0	0	0	0	0	0
$SD(a_k^{GFC}) \times n_S^{CRV}$	0	0	0	0	0	0
$SD_V \times n_S^{CRV}$	0	0	0	0	0	0
$\%RSD_S(c_j^{CRV}) \times n_A^{CRV}$	7.4	9.1	33.3	15.4	16.7	50
$\%RSD_A(c_j^{CRV}) \times n_A^{CRV}$	100	100	100	100	100	100
$SD(G_{jk}^{GFC}) \times n_A^{CRV}$	0	0	0	0	0	0
$SD(a_k^{GFC}) \times n_A^{CRV}$	0	0	0	0	0	0

Table 7.5. Percentage of Radionuclide Composition Components (Oxides) for which the Factor or Interaction was Significant in the ANOVAs (α = 0.05) for Each of Three LAW Tanks (cont.)

Factor / Interaction	All Radionuclide Composition Components (Oxides)			Reportable Radionuclide Composition Components (Oxides)		
	Envelope A (AP-101)	Envelope B (AZ-101)	Envelope C (AN-107)	Envelope A (AP-101)	Envelope B (AZ-101)	Envelope C (AN-107)
$SD_V \times n_A^{CRV}$	0	0	0	0	0	0
$n_S^{CRV} \times n_A^{CRV}$	100	100	100	100	100	100
$\%RSD_S(c_j^{CRV}) \times n_V$	0	0	0	0	0	0
$\%RSD_A(c_j^{CRV}) \times n_V$	0	0	0	0	0	0
$SD(G_{jk}^{GFC}) \times n_V$	0	0	0	0	0	0
$SD(a_k^{GFC}) \times n_V$	0	0	0	0	0	0
$SD_V \times n_V$	0	0	0	0	0	0
$n_S^{CRV} \times n_V$	0	0	0	0	0	0
$n_A^{CRV} \times n_V$	0	0	0	0	0	0

(a) Only two-factor interactions were included in the ANOVA model.
(b) This factor has a "low" case and a "high" case.
(c) The notation SD_V represents both SD_V^{CRV} and SD_V^{MFPV}. This factor has a "low" and "high" case, where both SD_V^{CRV} and SD_V^{MFPV} are varied at the same time.
(d) The notation n_V represents both n_V^{CRV} and n_V^{MFPV}, with each being varied at the same time.

number of samples per CRV batch, as well as in the number of analyses per sample, also affected the %RHW. Changes in the GFC uncertainties and GFC weight uncertainties did not have significant effects on the %RHW. This was expected because none of the GFCs included in ILAW contain radionuclides. Changes in the CRV and MFPV volume uncertainties and the number of volume determinations per vessel also did not have significant effects on the %RHW. Most two-factor interactions were not significant. As expected, the $n_S^{CRV} \times n_A^{CRV}$ interaction was statistically significant. This is because as n_S^{CRV} was increased, n_A^{CRV} could be decreased to obtain a similar %RHW, and vice versa. Also the $\%RSD_A(c_j^{CRV}) \times n_A^{CRV}$ interaction was always statistically significant. The only other interactions that were occasionally statistically significant included: $\%RSD_S(c_j^{CRV}) \times \%RSD_A(c_j^{CRV})$, $\%RSD_S(c_j^{CRV}) \times n_S^{CRV}$, $\%RSD_A(c_j^{CRV}) \times n_S^{CRV}$, and $\%RSD_S(c_j^{CRV}) \times n_A^{CRV}$, which were expected.

The ANOVA results in Table 7.5 require an explanation relative to the results in Table 7.4. The results in Table 7.5 show that factors $\%RSD_A(c_j^{CRV})$ and n_A^{CRV}, and interaction $n_S^{CRV} \times n_A^{CRV}$ have statistically significant effects, and yet Table 7.4 shows that generally one analysis per CRV sample

(n_A^{CRV} = 1) is sufficient for compliance. The explanation for this seeming inconsistency is that increasing the number of samples per CRV batch n_S^{CRV} also increases the total number of analyses, even if each sample is only analyzed once. Thus, increasing the number of samples per batch effectively reduces (via averaging) $\%RSD_A(c_j^{CRV})$ as well as $\%RSD_S(c_j^{CRV})$. This "dual benefit" is better than the "single benefit" from increasing the number of analyses per sample, which only effectively reduces $\%RSD_A(c_j^{CRV})$. This explains why most of the results in Table 7.4 show that one analysis per CRV sample is sufficient despite $\%RSD_A(c_j^{CRV})$ and n_A^{CRV} having statistically significant effects.

7.2.2 Illustration of Calculating Means and Standard Deviations of ILAW Radionuclide Compositions and Inventories over an LAW Waste Type for Radionuclides Analyzed in Every MFPV Batch

This section uses realistic data to illustrate the equations presented in Section 5.2.4 for calculating means and SDs of ILAW radionuclide component inventories per ILAW container (Ci/container) over an LAW waste type. During ILAW production, there will be one "averaged" estimate of radionuclide composition per MFPV batch, and the compliance method consists of reporting the means and SDs of reportable radionuclide inventories per ILAW container calculated over all MFPV batches and ILAW containers associated with a given LAW waste type. Equations for ILAW radionuclide inventories per ILAW container are presented in Section 5.2.4.1 for the case of balanced data (equal numbers of samples per CRV batch and equal numbers of analyses for each CRV sample), and in Section 5.2.4.2 for the case of unbalanced data (unequal numbers of samples per CRV batch and/or unequal numbers of analyses for each CRV sample). For a balanced data set, the means, SDs, and %RSDs of ILAW radionuclide inventories per ILAW container are respectively calculated using Eqs. (5.2.1), (5.2.2), and the usual formula for a %RSD. These equations make use of means and SDs for mass fractions of ILAW radionuclide composition components, which were presented and discussed for the AP-101 example data in Section 7.1.2.

The equations for calculating the means and SDs of radionuclide inventories per ILAW container have embedded in them equations for calculating the means and SDs of ILAW radionuclide compositions (mass fractions of radionuclide oxide components) per ILAW container. These equations are the same as presented in Section 5.1.4 and illustrated in Section 7.1.2 for chemical composition components.

A realistic balanced dataset to illustrate the use of Eqs. (5.1.2), (5.1.5), and (5.1.6) for the means, SDs, and %RSDs of ILAW radionuclide compositions (mass fractions) and Eqs. (5.2.1) and (5.2.2) for the means and SDs of radionuclide inventories per ILAW container was obtained as previously described in Section 7.1.2. Specifically, simulated data were obtained (Vienna 2004b) from the WTP Project's Run 3.1vv of the G2 dynamic simulation flowsheet (Deng 2004; Vora 2004) corresponding to the LAW portion of waste Tank AP-101 as discussed in Section 7.1.2. Table J.2 in Appendix J lists the radionuclide composition components (mass fractions) of 25 MFPV batches associated with LAW from AP-101. It is estimated that 41 ILAW containers will be produced from 25 ILAW MFPV batches.[(a)] The

(a) For ILAW, the MFPV is expected to contain the equivalent of approximately 10 MT of LAW glass, while an ILAW container is expected to contain 6 MT of LAW glass. Hence, an ILAW MFPV batch is expected to produce about one and two-thirds (i.e., 1.67) containers of ILAW.

LAW corresponding to the 25 ILAW MFPV batches and 41 ILAW containers is assumed to be the "waste type" for purposes of this illustration.

Table 7.6 contains the illustrative results of applying the previously mentioned equations for calculating the means, SDs, and %RSDs of ILAW radionuclide compositions over the 25 ILAW MFPV batches corresponding to an AP-101 waste type. The variations of the ILAW radionuclide composition component mass fractions (over the 25 ILAW MFPV batches corresponding to an LAW waste type) summarized in Table 7.6 range from 0.03 to 4.60 %RSD. However, it should be kept in mind that this range of %RSDs reflects only batch-to-batch variation and not any of the within-batch uncertainties that will affect estimation of ILAW radionuclide (and chemical) compositions during WTP ILAW production.

Table 7.6. Means, SDs, and %RSDs of ILAW Radionuclide Composition Components (Mass Fractions) over 25 ILAW MFPV Batches Corresponding to Waste Tank AP-101

Radionuclide Composition Component	Mass Fraction			Radionuclide Composition Component	Mass Fraction		
	Mean	SD	%RSD		Mean	SD	%RSD
$^{227}Ac_2O_3$	5.76E-15	7.68E-17	1.33	**$^{240}PuO_2$**	**6.94E-10**	**2.93E-11**	**4.22**
$^{241}Am_2O_3$[a]	**6.80E-11**	**7.12E-13**	**1.05**	**$^{241}PuO_2$**	**1.39E-11**	**5.99E-13**	**4.31**
$^{243}Am_2O_3$	6.29E-14	8.44E-16	1.34	$^{242}PuO_2$	4.57E-12	1.98E-13	4.34
^{113}CdO	8.22E-11	4.91E-13	0.60	^{226}RaO	5.72E-14	1.68E-16	0.29
$^{242}Cm_2O_3$	N/A	N/A	N/A	^{228}RaO	1.85E-13	2.49E-15	1.34
$^{243}Cm_2O_3$	**5.04E-16**	**8.52E-18**	**1.69**	$^{106}RuO_2$	N/A	N/A	N/A
$^{244}Cm_2O_3$	**5.60E-14**	**2.32E-15**	**4.14**	**$^{125}Sb_2O_3$**	**9.95E-12**	**1.22E-13**	**1.23**
^{60}CoO	**1.79E-12**	**1.48E-14**	**0.82**	$^{79}SeO_2$	1.30E-08	7.58E-11	0.58
$^{134}Cs_2O$	2.14E-16	4.04E-18	1.89	**$^{151}Sm_2O_3$**	**1.65E-07**	**4.33E-11**	**0.03**
$^{137}Cs_2O$	**7.91E-11**	**7.72E-13**	**0.98**	$^{126}SnO_2$	7.17E-08	6.21E-11	0.09
$^{152}Eu_2O_3$	9.00E-12	4.31E-15	0.05	**^{90}SrO**	**4.75E-09**	**1.99E-10**	**4.18**
$^{154}Eu_2O_3$	**7.78E-11**	**3.53E-12**	**4.53**	**$^{99}Tc_2O_7$**	**3.53E-06**	**2.39E-08**	**0.68**
$^{155}Eu_2O_3$	**2.20E-11**	**1.01E-12**	**4.59**	$^{229}ThO_2$	1.06E-11	1.42E-13	1.32
^{129}I	2.66E-07	1.62E-09	0.61	$^{232}ThO_2$	1.09E-04	1.40E-06	1.28
$^{93}Nb_2O_5$	2.85E-11	1.94E-14	0.07	$^{232}UO_3$	5.77E-13	7.75E-15	1.34
^{59}NiO	2.05E-08	7.86E-10	3.82	**$^{233}UO_3$**	**5.77E-09**	**7.75E-11**	**1.34**
^{63}NiO	**2.56E-09**	**9.78E-11**	**3.82**	$^{234}UO_3$	7.80E-09	1.90E-10	2.44
$^{237}NpO_2$	**1.72E-07**	**7.91E-09**	**4.60**	**$^{235}UO_3$**	**9.01E-07**	**2.06E-08**	**2.29**
$^{231}Pa_2O_5$	3.22E-11	9.47E-14	0.29	$^{236}UO_3$	4.34E-08	1.47E-09	3.39
$^{238}PuO_2$	**6.52E-12**	**2.71E-13**	**4.16**	**$^{238}UO_3$**	**1.17E-04**	**2.56E-06**	**2.18**
$^{239}PuO_2$	**1.22E-08**	**4.98E-10**	**4.07**	$^{93}ZrO_2$	3.10E-06	4.40E-09	0.14
(c)				**Total Mass Fraction**[b]	2.30E-04	(c)	

(a) Results for reportable radionuclide composition components (per Table 2.2) are shown in boldface.
(b) The total mass fraction adds the mean mass fractions of radionuclide composition components (oxides). Mass fractions of chemical composition components and their total are shown in Table 7.3.
(c) This portion of the table is intentionally blank.

To calculate ILAW radionuclide inventories, illustrative data for masses of glass in the assumed 41 containers for the AP-101 waste type were also required. The mean mass of glass in an ILAW container (5.911×10^6 g) and the SD for the mass of glass in an ILAW container (8.051×10^4g) were obtained using data from Andre (2004). Simulated masses of glass in the 41 ILAW containers generated by adding normally distributed random noise with SD = 8.051×10^4 g to the mean value of 5.911×10^6 g, are shown in Table J.3 in Appendix J. From these simulated values, a sample average glass container mass of 5.8926×10^6 g and a sample SD of 9.1923×10^4g were obtained.

Equations (5.2.1), (5.2.2), and the usual %RSD formula can be used to calculate means, SDs, and %RSDs of ILAW radionuclide inventories per ILAW container. The results of applying these equations to the simulated data for the 20 reportable ILAW radionuclides (see Table 2.1) are summarized in Table 7.7.

Table 7.7. Means, SDs, and %RSDs for Inventories per ILAW Container of Reportable Radionuclides over 25 ILAW MFPV Batches and 41 ILAW Containers Corresponding to LAW Waste Tank AP-101

Radionuclide	Radionuclide Inventories per ILAW Container[(a)]		
	Mean (Ci)	SD (Ci)	%RSD
^{60}Co	9.16E-03	1.62E-04	1.77
^{63}Ni	6.86E-01	2.83E-02	4.13
^{90}Sr	3.33E+00	1.49E-01	4.47
^{99}Tc	2.67E-01	4.54E-03	1.70
^{125}Sb	4.92E-02	9.76E-04	1.98
^{137}Cs	3.83E-02	7.05E-04	1.84
^{151}Sm	2.18E+01	3.40E-01	1.56
^{154}Eu	1.03E-01	4.95E-03	4.80
^{155}Eu	5.50E-02	2.67E-03	4.85
^{233}U	2.73E-04	5.63E-06	2.06
^{235}U	9.70E-06	2.68E-07	2.77
^{237}Np	6.34E-04	3.08E-05	4.86
^{238}U	1.95E-04	5.24E-06	2.69
^{238}Pu	5.76E-04	2.56E-05	4.44
^{239}Pu	3.93E-03	1.72E-04	4.37
^{240}Pu	8.30E-04	3.73E-05	4.50
^{241}Pu	7.23E-03	3.31E-04	4.58
^{241}Am	1.24E-03	2.33E-05	1.88
^{243}Cm	1.41E-07	3.23E-09	2.30
^{244}Cm	2.43E-05	1.08E-06	4.43

(a) Results obtained using data from Vienna (2004b).

To illustrate the use of Eqs. (5.2.1) and (5.2.2) in calculating the results in Table 7.7, consider the case of ^{60}Co. Plugging the appropriate quantities into Eq. (5.2.1), the mean inventory per ILAW container of ^{60}Co over the 25 MFPV batches and approximately 41 ILAW containers corresponding to the AP-101 LAW waste type is obtained by

$$\begin{aligned}
\overline{R}^{\text{Container}}_{\text{D}^{60}\text{Co}} &= \frac{\overline{\overline{g}}^{MFPV}_{^{60}\text{CoO}}\,\overline{m}_D^{Container}\,A_{^{60}\text{Co}}}{f_{^{60}\text{CoO}}} \\
&= \frac{(1.79\times10^{-12}\ \text{g}_{^{60}\text{CoO}}/\text{g}_{\text{glass}})\,(5.89\times10^{6}\ \text{g}_{\text{glass}})\,(1.10\times10^{3}\ \text{Ci}/\text{g}_{^{60}\text{Co}})}{1.2667\ \text{g}_{^{60}\text{CoO}}/\text{g}_{^{60}\text{Co}}} \qquad (7.2.1)\\
&= 9.16\times10^{-3}\ \text{Ci}\ ^{60}\text{Co/container}
\end{aligned}$$

Similarly, plugging the appropriate quantities into Eq. (5.2.2), the standard deviation of ^{60}Co inventory per container over the 25 MFPV batches and approximately 41 ILAW containers corresponding to the AP-101 LAW waste type is obtained by

$$\begin{aligned}
SD(R^{Container}_{d,^{60}\text{Co}}) &= \frac{A_q}{f_q}\left(\begin{array}{l}(\overline{\overline{g}}^{MFPV}_{^{60}\text{CoO}})^2\,SD(m_d^{Container})^2 + (\overline{m}_D^{Container})^2\,SD(\overline{g}^{MFPV}_{i,^{60}\text{CoO}})^2 \\ -\,SD(m_d^{Container})^2\ SD(\overline{g}^{MFPV}_{i,^{60}\text{CoO}})^2\end{array}\right)^{1/2} \\
&= \frac{1.10\times10^{3}\ \text{Ci}\ ^{60}\text{Co}/\text{g}_{^{60}\text{Co}}}{1.2667\ \text{g}_{^{60}\text{CoO}}/\text{g}_{^{60}\text{Co}}}\left(\begin{array}{l}(1.79\times10^{-12}\ \text{g}_{^{60}\text{CoO}}/\text{g}_{\text{glass}})^2\cdot(91923.27\ \text{g}_{\text{glass}})^2 \\ +(5.89\times10^{6}\ \text{g}_{\text{glass}})^2\cdot(1.48\times10^{-14}\ \text{g}_{^{60}\text{CoO}}/\text{g}_{\text{glass}})^2 \\ -(91923.27\ \text{g}_{\text{glass}})^2\cdot(1.48\times10^{-14}\ \text{g}_{^{60}\text{CoO}}/\text{g}_{\text{glass}})^2\end{array}\right)^{1/2} \qquad (7.2.2)\\
&= 1.62\times10^{-4}\ \text{Ci}\ ^{60}\text{Co/container}
\end{aligned}$$

Finally, the %RSD is calculated via the usual formula

$$\%RSD(R_{dq}^{Container}) = 100\left(\frac{1.62\times10^{-4}\ \text{Ci}}{9.16\times10^{-4}\ \text{Ci}}\right) = 1.77$$

making use of the results from Eqs. (7.2.1) and (7.2.2).

Means, SDs, and %RSDs for the inventories per ILAW container of other reportable radionuclides can be calculated in a similar way and are presented in Table 7.7. Note that even though a single number was used to represent the SD of the mass of glass in an ILAW container and another for each of the radionuclide inventories in this example, this should not be taken as an indication that a single source of variability is present in these SDs. The numbers used in this example only reflect the structure of the data available for the calculations. The total variability of the mass of glass determined to be present in a given ILAW container and of the radionuclide inventories may in fact be composed of several sources.

Project specifications call only for reporting means and SDs of radionuclide inventories per ILAW canister, so the results presented in Table 7.7 are representative of the way in which other radionuclide inventories per ILAW canister (obtained using different numbers of MFPV batches, ILAW containers, and/or a different LAW stream, for example) will be reported.

Finally, as discussed in Section 7.1.2, the data available for the illustrations of calculating means, SDs, and %RSDs of ILAW chemical composition, radionuclide composition, and radionuclide inventory per ILAW container only contain batch-to-batch variation and not any of the within-batch uncertainties that will affect estimation of ILAW chemical and radionuclide compositions, as well as radionuclide inventories per canister, during WTP ILAW production.

When a full set of needed data is available, this section of the report will be revised to illustrate the use of (1) Eqs. (5.1.2), (5.1.5), and (5.1.6) for calculating means, SDs, and %RSDs of ILAW radionuclide component compositions (mass fractions), and (2) Eqs. (5.2.1), (5.2.2), and the usual %RSD formula for calculating means, SDs, and %RSDs of ILAW radionuclide inventories per canister. The revisions will include taking the complete set of G2 data and augmenting it by random disturbances corresponding to the various uncertainties affecting the estimate of ILAW composition for an MFPV batch. The equations for means, SDs, and %RSDs will then be applied to this augmented data so that the effects of within-batch uncertainties as well as batch-to-batch variation will be reflected in the example results for radionuclide compositions and inventories.

7.3 Compliance Results for ILAW Contract Specification 2.2.2.8: Radionuclide Concentration Limits

Section 7.3.1 illustrates, using a realistic example, the methodology presented in Section 5.3.3 for demonstrating that ILAW radionuclide concentrations meet Class C limits in Tables 1 and 2 of 10 CFR 61.55. Section 7.3.2 presents results from the Monte Carlo simulations and uses the methodology in Section 5.3.4 to determine the numbers of samples per CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations necessary to demonstrate that ILAW radionuclide concentrations meet Class C limits. Section 7.3.3 illustrates, using a realistic example, the methodology presented in Section 5.3.5 for demonstrating that running-average concentrations of ^{137}Cs and ^{90}Sr meet specified limits. Section 7.3.4 presents results from the Monte Carlo simulations and uses the methodology in Section 5.3.6 to determine the numbers of samples per CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations necessary to demonstrate that the running-average concentrations of ^{137}Cs and ^{90}Sr meet specified limits.

7.3.1 Illustration of Statistical Methods to Demonstrate that ILAW Radionuclide Concentrations Meet Class C Limits

Section 7.3.1.1 illustrates, using a realistic example, the methodology presented in Section 5.3.3.1 for demonstrating that ILAW radionuclide concentrations over ILAW containers associated with an LAW waste type meet Class C limits. Section 7.3.1.2 illustrates the methodology presented in Section 5.3.3.2 to assess whether ILAW radionuclide concentrations for ILAW from each MFPV batch meet Class C limits.

7.3.1.1 Illustration of Statistical Method to Demonstrate that ILAW Radionuclide Concentrations over ILAW Containers Associated with an LAW Waste Type Meet Class C Limits

This section illustrates, using realistic example data, the methodology presented in Section 5.3.3.1 for demonstrating that ILAW radionuclide concentrations over ILAW containers associated with an LAW waste type meet Class C limits. The method presented in Section 5.3.3.1 is an X%/Y% UTI, applied to sum-of-fractions of ILAW Class C ILAW radionuclides in Table 1 (SF1) and Table 2 (SF2) of 10 CFR 61.55 as discussed in Section B.3.1.1 of Appendix B. The Class C limits for the radionuclides in Tables 1 and 2 of 10 CFR 61.55 are listed in Table B.1 of Appendix B.

Sum-of-Fractions of Radionuclides in 10 CFR 61.55 Table 1

The ILAW radionuclides involved in the sum-of-fractions calculations for 10 CRF 61.55 Table 1 are ^{99}Tc, alpha-emitting TRU (= ^{237}Np + ^{238}Pu + ^{239}Pu + ^{240}Pu + ^{241}Am + ^{244}Cm), ^{241}Pu, and ^{242}Cm. The Class C limits for these radionuclides are listed in Table B.1 of Appendix B.

Equation (5.3.1a) from Section 5.3.3.1, repeated here for convenience,

$$X\%/Y\%\ UTI(SF1_D^{Containers}) = \overline{SF1}_D^{Containers} + k(X,Y)\ SD(\overline{SF1}_d^{Container}) \qquad (7.3.1)$$

provides for calculating the desired X%/Y% UTI on SF1. The quantities $\overline{SF1}_D^{Containers}$ and $SD(\overline{SF1}_d^{Containers})$ in Eq. (7.3.1) are calculated using Eqs. (B.3.4) and (B.3.7) in Section B.3.1.1 of Appendix B. The applications of these equations are now illustrated using realistic values and simulated data corresponding to LAW waste from Tank AP-101.

First, the quantity $\overline{SF1}_D^{Containers}$ is calculated using Eq. (B.3.4) as follows

$$\overline{SF1}_D^{Containers} = \sum_{k=TRU,\,^{241}Pu,\,^{242}Cm}\left[\frac{1}{L_k^s}\left(\sum_{q=1}^{N_k}\frac{\left(10^9\right)\bar{\bar{g}}_q^{MFPV}A_q}{f_q}\right)\right] + \left[\frac{1}{L_q^r}\left(\frac{\bar{\bar{g}}_q^{MFPV}\bar{\rho}_D^{Container}A_q}{f_q}\right)\right]_{q=^{99}Tc}$$

$$= \frac{10^9}{100\times10^{-9}\ \text{Ci TRU/g}_{\text{glass}}}\left(\begin{array}{l}\dfrac{(1.72\times10^{-7})(0.00071)}{1.16877}+\dfrac{(6.52\times10^{-12})(17.0)}{1.13445}+\dfrac{(1.22\times10^{-8})(0.062)}{1.13389}\\ +\dfrac{(6.94\times10^{-10})(0.23)}{1.13333}+\dfrac{(6.80\times10^{-11})(3.4)}{1.09958}+\dfrac{(5.60\times10^{-14})(81.0)}{1.09836}\end{array}\right)$$

$$+\frac{1}{3500\times10^{-9}\ \text{Ci}\ ^{241}\text{Pu/g}_{\text{glass}}}\left(\frac{10^9(1.39\times10^{-11}\,\text{g}_{^{241}\text{PuO}_2}/\text{g}_{\text{glass}})(100\ \text{Ci}\ ^{241}\text{Pu/g}_{^{241}\text{Pu}})}{1.13278\,\text{g}_{^{241}\text{PuO}_2}/\text{g}_{^{241}\text{Pu}}}\right)$$

$$+\frac{1}{20000\times10^{-9}\ \text{Ci}\ ^{242}\text{Cm/g}_{\text{glass}}}\left(\frac{10^9(0.0\ \text{g}_{^{242}\text{Cm}_2\text{O}_3}/\text{g}_{\text{glass}})(3300\ \text{Ci}\ ^{242}\text{Cm/g}_{^{242}\text{Cm}})}{1.09917\,\text{g}_{^{242}\text{Cm}_2\text{O}_3}/\text{g}_{^{242}\text{Cm}}}\right)$$

$$+\frac{1}{3\ \text{Ci}\ ^{99}\text{Tc/m}^3\ \text{glass}}\left(\frac{(3.53\times10^{-6}\ \text{g}_{^{99}\text{Tc}_2\text{O}_7}/\text{g}_{\text{glass}})(2.65\times10^6\,\text{g}_{\text{glass}}/\text{m}^3\ \text{glass})(0.017\ \text{Ci}\ ^{99}\text{Tc/g}_{^{99}\text{Tc}})}{1.32323\,\text{g}_{^{99}\text{Tc}_2\text{O}_7}/\text{g}_{^{99}\text{Tc}}}\right)$$

$$= \frac{1}{100\times10^{-9}\ \text{Ci TRU/g}_{\text{glass}}}\left(3.3916\times10^{-10}\,\text{Ci TRU/g}_{\text{glass}}\right)$$

$$+\frac{1}{3500\times10^{-9}\ \text{Ci}^{241}\text{Pu/g}_{\text{glass}}}\left(1.8033\times10^{-10}\,\text{Ci}\ ^{241}\text{Pu/g}_{\text{glass}}\right) \qquad (7.3.2)$$

$$+\frac{1}{20000\times10^{-9}\ \text{Ci}^{242}\text{Cm/g}_{\text{glass}}}\left(0.0\,\text{Ci}^{242}\text{Cm/g}_{\text{glass}}\right)$$

$$+\frac{1}{3\,\text{Ci}^{99}\text{Tc/m}^3\ \text{glass}}\left(0.1311\,\text{Ci}^{99}\text{Tc/m}^3\ \text{glass}\right)$$

$$= 0.0034 + 0.0001 + 0.0 + 0.0437 = 0.0472$$

where the limiting values L_k^s and L_k^r are from Table B.1 in Appendix B, the $\bar{\bar{g}}_q^{MFPV}$ values are from Table 7.6, the A_q values are from Table A.2 in Appendix A, the f_q values are from Table A.1, and the mean density of glass in $D = 41$ ILAW containers ($\bar{\rho}_D^{Container}$) is 2.65×10^6 g/m^3. The resulting mean SF1 value of 0.0472 is well below the limiting value of 1, although the goal here is to have the X%/Y% UTI value below 1.

Equation (B.3.7) in Appendix B shows how to calculate the standard deviation of SF1. Starting with Eq. (B.3.7) and substituting values yields

$$SD(\overline{SF1}_d^{Container}) = \left\{ \sum_{k=TRU,\ ^{241}Pu,\ ^{242}Cm} \left(\frac{10^9}{L_k^s}\right)^2 \sum_{q=1}^{N_k} \left(\frac{A_q}{f_q}\right)^2 \left(SD(\overline{g}_{iq}^{MFPV})\right)^2 \right.$$

$$\left. + \left[\left[\frac{A_q}{L_q^r f_q}\right]^2 \left(\begin{array}{l} (\overline{\overline{g}}_q^{MFPV})^2 \left(SD(\rho_d^{Container})\right)^2 \\ + (\overline{\rho}_D^{Container})^2 \left(SD(\overline{g}_{iq}^{MFPV})\right)^2 - \left(SD(\rho_d^{Container})\right)^2 \left(SD(\overline{g}_{iq}^{MFPV})\right)^2 \end{array} \right)\right]_{q=^{99}Tc} \right\}^{1/2}$$

$$= \left\{ \left(\frac{1\times 10^9 \text{ nCi/Ci}}{100 \text{ nCi/g}}\right)^2 \left[1.2592\times 10^{-18} + 2.6554\times 10^{-21} + 1.1032\times 10^{-19} \right.\right.$$

$$\left. + 5.2029\times 10^{-21} + 3.2094\times 10^{-21} + 4.6016\times 10^{-24}\right] \text{Ci}^2/\text{g}^2 + 3.1959\times 10^{-8} + 4.3669\times 10^{-17} \qquad (7.3.3)$$

$$\left. + (1.8340\times 10^{-5})\left[0.005 + 0.3342 - 1.8751\times 10^{-5}\right]\right\}^{0.5} = (1.44\times 10^{-4})^{0.5} = 0.0120$$

To calculate a 95%/95% UTI, the results of Eqs. (7.3.2) and (7.3.3) are substituted into Eq. (7.3.1) along with the value $k(95, 95) = 2.2778$ obtained as described in Section F.2 of Appendix F. The result is

$$X\%/Y\%\ UTI(SF1_D^{Containers}) = \overline{SF1}_D^{Containers} + k(X,Y)\ SD(\overline{SF1}_d^{Container})$$

$$= 0.0472 + 2.2778\ (0.0120) = 0.0745$$

which is well below the limiting value of 1.

X%/Y% UTIs on the sum-of-fractions SF1 for other combinations of X and Y are listed in Table 7.8. Listed first in the table are X%/Y% UTIs corresponding to the preceding AP-101 illustration with 25 ILAW MFPV batches and 41 ILAW containers. Also included for comparison are X%/Y% UTIs for 125 MFPV batches and 208 ILAW containers. The latter case is included to illustrate the effect of increasing the number of MFPV batches on the values of the X%/Y% UTIs on SF1. For this investigation, the mean and SD for the sum-of-fractions SF1 remained unchanged at the values obtained earlier in this section for 25 MFPV batches. X%/Y% UTIs for several combinations of confidence levels (X) and population percentage (Y) are shown in Table 7.8.

Results in Table 7.8 show that the X%/Y% UTIs on SF1 are far below the limiting value of 1 for all cases. As expected, increasing the values of X and Y from 90 to 95 to 99 increases the value of the X%/Y% UTI. Although this nominally makes it more difficult for a X%/Y% UTI to be below its limit, even the 99%/99% UTI on SF1 is nowhere close to the limiting value of 1. Also, increasing the number of ILAW MFPV batches and containers associated with the LAW waste type yields smaller values of X%/Y% UTIs on SF1. However, if ILAW for other LAW tanks to be processed by the WTP also have ILAW radionuclide sum-of-fractions SF1 for Class C greatly below the limit of 1, the number of ILAW

MFPV batches and containers would likely have to be much lower than 25 before the X%/Y% UTI would have any chance of exceeding the limit.

Table 7.8. Parameter Values and X%/Y% UTIs on the Sum-of-Fractions of Radionuclides in Table 1 of 10 CFR 61.55 (SF1) over *D* ILAW Containers Associated with 25 or 125 ILAW MFPV Batches Corresponding to an AP-101 LAW Waste Type

I[(a)]	D[(a)]	X%	Y%	$\overline{SF1}_D^{Containers}$	$k(X, Y)$	$SD(\overline{SF1}_d^{Containers})$	X%/Y% UTI on SF1
25	41	0.90	0.90	0.0472	1.6851	0.0120	0.0674
25	41	0.90	0.95	0.0472	1.8257	0.0120	0.0691
25	41	0.90	0.99	0.0472	2.1367	0.0120	0.0728
25	41	0.95	0.90	0.0472	2.1121	0.0120	0.0725
25	41	0.95	0.95	0.0472	2.2778	0.0120	0.0745
25	41	0.95	0.99	0.0472	2.6485	0.0120	0.0790
25	41	0.99	0.90	0.0472	2.9251	0.0120	0.0823
25	41	0.99	0.95	0.0472	3.1415	0.0120	0.0849
25	41	0.99	0.99	0.0472	3.6315	0.0120	0.0908
125	208	0.90	0.90	0.0472	1.4458	0.0120	0.0645
125	208	0.90	0.95	0.0472	1.4962	0.0120	0.0652
125	208	0.90	0.99	0.0472	1.5960	0.0120	0.0664
125	208	0.95	0.90	0.0472	1.8330	0.0120	0.0692
125	208	0.95	0.95	0.0472	1.8911	0.0120	0.0699
125	208	0.95	0.99	0.0472	2.0071	0.0120	0.0713
125	208	0.99	0.90	0.0472	2.5644	0.0120	0.0780
125	208	0.99	0.95	0.0472	2.6388	0.0120	0.0789
125	208	0.99	0.99	0.0472	2.7877	0.0120	0.0807

(a) I and D, respectively, denote the number of ILAW MFPV batches and number of ILAW containers associated with an LAW waste type.

Sum-of-Fractions of Radionuclides in 10 CFR 61.55 Table 2

The ILAW radionuclides involved in the sum-of-fractions calculations for 10 CRF 61.55 Table 2 are ^{63}Ni, ^{90}Sr, and ^{137}Cs. The Class C limits for these radionuclides are listed in Table B.1 of Appendix B.

Equation (5.3.1b) from Section 5.3.3.1, repeated here for convenience,

$$X\%/Y\%\ UTI(SF2_D^{Containers}) = \overline{SF2}_D^{Containers} + k(X,Y)\ SD(\overline{SF2}_d^{Container}) \qquad (7.3.4)$$

provides for calculating the desired X%/Y% UTI on SF2. The quantities $\overline{SF2}_D^{Containers}$ and $SD(\overline{SF2}_d^{Containers})$ in Eq. (7.3.4) are calculated using Eqs. (B.3.5) and (B.3.9) in Section B.3.1.1 of

Appendix B. The applications of these equations are now illustrated using realistic values and simulated data corresponding to LAW waste from Tank AP-101.

First, the quantity $\overline{SF2}_D^{Containers}$ is calculated using Eq. (B.3.5) as follows

$$\begin{aligned}
\overline{SF2}_D^{Containers} &= \sum_{q={}^{63}Ni,\ {}^{90}Sr,\ {}^{137}Cs} \left[\frac{1}{L_q^r} \left(\frac{\bar{\bar{g}}_q^{MFPV}\, \bar{\rho}_D^{Container}\, A_q}{f_q} \right) \right] \\
&= \frac{1}{700\ \text{Ci}\ {}^{63}\text{Ni/m}^3{}_{\text{glass}}} \left(\frac{(2.56\times10^{-9}\ \text{g}_{63_{\text{NiO}}}/\text{g}_{\text{glass}})(2.65\times10^{6}\ \text{g}_{\text{glass}}/\text{m}^3\ \text{glass})(57\ \text{Ci}\ {}^{63}\text{Ni/g}_{63_{\text{Ni}}})}{1.25397\ \text{g}_{63_{\text{NiO}}}/\text{g}_{63_{\text{Ni}}}} \right) \\
&\quad + \frac{1}{7000\ \text{Ci}\ {}^{90}\text{Sr/m}^3\ \text{glass}} \left(\frac{(4.75\times10^{-9}\ \text{g}_{90_{\text{SrO}}}/\text{g}_{\text{glass}})(2.65\times10^{6}\ \text{g}_{\text{glass}}/\text{m}^3\ \text{glass})(140\ \text{Ci}\ {}^{90}\text{Sr/g}_{90_{\text{Sr}}})}{1.17778\ \text{g}_{90_{\text{SrO}}}/\text{g}_{90_{\text{Sr}}}} \right) \\
&\quad + \frac{1}{4600\ \text{Ci}\ {}^{137}\text{Cs/m}^3\ \text{glass}} \left(\frac{(7.91\times10^{-11}\ \text{g}_{137_{\text{Cs}_2\text{O}}}/\text{g}_{\text{glass}})(2.65\times10^{6}\ \text{g}_{\text{glass}}/\text{m}^3\ \text{glass})(87\ \text{Ci}\ {}^{137}\text{Cs/g}_{137_{\text{Cs}}})}{1.05839\ \text{g}_{137_{\text{Cs}_2\text{O}}}/\text{g}_{137_{\text{Cs}}}} \right) \\
&= \frac{1}{700\ \text{Ci}\ {}^{63}\text{Ni/m}^3{}_{\text{glass}}} \left(0.3048\ \text{Ci}\ {}^{63}\text{Ni/m}^3{}_{\text{glass}} \right) + \frac{1}{7000\ \text{Ci}\ {}^{90}\text{Sr/m}^3{}_{\text{glass}}} \left(1.4962\ \text{Ci}\ {}^{90}\text{Sr/m}^3{}_{\text{glass}} \right) \\
&\quad + \frac{1}{4600\ \text{Ci}\ {}^{137}\text{Cs/m}^3{}_{\text{glass}}} \left(0.0172\ \text{Ci}\ {}^{137}\text{Cs/m}^3{}_{\text{glass}} \right) \\
&= 4.4057\times10^{-4} + 2.1374\times10^{-4} + 3.7391\times10^{-6} = 6.5805\times10^{-4}
\end{aligned} \tag{7.3.5}$$

where the limiting values L_q^r are from Table B.1 in Appendix B, the $\bar{\bar{g}}_q^{MFPV}$ values are from Table 7.6, the A_q values are from Table A.2 in Appendix A, and the f_q values are from Table A.1. The resulting mean SF2 value of 6.5805×10^{-4} is well below the limiting value of 1, although the goal here is to have the X%/Y% UTI value below 1.

Equation (B.3.9) in Appendix B shows how to calculate the standard deviation of SF2. Starting with Eq. (B.3.9) and substituting values yields

$$SD(\overline{SF2}_d^{Container}) = \left[\sum_{q={}^{63}Ni+{}^{90}Sr+{}^{137}Cs} \left[\frac{A_q}{L_q^r f_q} \right]^2 \left(\begin{array}{l} (\bar{\bar{g}}_q^{MFPV})^2 \left(SD(\rho_d^{Container}) \right)^2 \\ + (\bar{\rho}_D^{Container})^2 \left(SD(\bar{g}_{iq}^{MFPV}) \right)^2 \\ - \left(SD(\rho_d^{Container}) \right)^2 \left(SD(\bar{g}_{iq}^{MFPV}) \right)^2 \end{array} \right) \right]^{1/2}$$

$$= \left[\begin{array}{l} \left[\frac{57\text{Ci}\,{}^{63}\text{Ni}/\text{g}_{{}^{63}\text{Ni}}}{700\text{Ci}\,{}^{63}\text{Ni}/\text{m}^3_{\text{glass}} \cdot 1.25397\ \text{g}_{{}^{63}\text{NiO}}/\text{g}_{{}^{63}\text{Ni}}} \right]^2 \bullet \\ \left[\begin{array}{l} (2.56\times10^{-9}\,\text{g}_{{}^{63}\text{NiO}}/\text{g}_{\text{glass}})^2\ (0.1\cdot 2.65\times10^{6}\,\text{g}_{\text{glass}}/\text{m}^3_{\text{glass}})^2 \\ +(2.65\times10^{6}\,\text{g}_{\text{glass}}/\text{m}^3_{\text{glass}})^2\ (9.78\times10^{-11}\,\text{g}_{{}^{63}\text{NiO}}/\text{g}_{\text{glass}})^2 \\ -(0.1\cdot 2.65\times10^{6}\,\text{g}_{\text{glass}}/\text{m}^3_{\text{glass}})^2\ (9.78\times10^{-11}\,\text{g}_{{}^{63}\text{NiO}}/\text{g}_{\text{glass}})^2 \end{array} \right] \\ + \left[\frac{140\text{Ci}\,{}^{90}\text{Sr}/\text{g}_{{}^{90}\text{Sr}}}{7000\text{Ci}\,{}^{90}\text{Sr}/\text{m}^3_{\text{glass}} \cdot 1.17778\ \text{g}_{{}^{90}\text{SrO}}/\text{g}_{{}^{90}\text{Sr}}} \right]^2 \bullet \\ \left[\begin{array}{l} (4.75\times10^{-9}\,\text{g}_{{}^{90}\text{SrO}}/\text{g}_{\text{glass}})^2\ (0.1\cdot 2.65\times10^{6}\,\text{g}_{\text{glass}}/\text{m}^3_{\text{glass}})^2 \\ +(2.65\times10^{6}\,\text{g}_{\text{glass}}/\text{m}^3_{\text{glass}})^2\ (1.99\times10^{-10}\,\text{g}_{{}^{90}\text{SrO}}/\text{g}_{\text{glass}})^2 \\ -(0.1\cdot 2.65\times10^{6}\,\text{g}_{\text{glass}}/\text{m}^3_{\text{glass}})^2\ (1.99\times10^{-10}\,\text{g}_{{}^{90}\text{SrO}}/\text{g}_{\text{glass}})^2 \end{array} \right] \\ + \left[\frac{87\text{Ci}\,{}^{137}\text{Cs}/\text{g}_{{}^{63}\text{Ni}}}{4600\text{Ci}\,{}^{137}\text{Cs}/\text{m}^3_{\text{glass}} \cdot 1.05839\ \text{g}_{{}^{137}\text{Cs}_2\text{O}}/\text{g}_{{}^{137}\text{Cs}}} \right]^2 \bullet \\ \left[\begin{array}{l} (7.91\times10^{-11}\,\text{g}_{{}^{137}\text{Cs}_2\text{O}}/\text{g}_{\text{glass}})^2\ (0.1\cdot 2.65\times10^{6}\,\text{g}_{\text{glass}}/\text{m}^3_{\text{glass}})^2 \\ +(2.65\times10^{6}\,\text{g}_{\text{glass}}/\text{m}^3_{\text{glass}})^2\ (7.72\times10^{-13}\,\text{g}_{{}^{137}\text{Cs}_2\text{O}}/\text{g}_{\text{glass}})^2 \\ -(0.1\cdot 2.65\times10^{6}\,\text{g}_{\text{glass}}/\text{m}^3_{\text{glass}})^2\ (7.72\times10^{-13}\,\text{g}_{{}^{137}\text{Cs}_2\text{O}}/\text{g}_{\text{glass}})^2 \end{array} \right] \end{array} \right]^{1/2}$$

$$= \left[\begin{array}{l} (4.2168\times10^{-3})\,(5.2672\times10^{-7}) + (2.8836\times10^{-4})\,(1.8598\times10^{-6}) \\ \quad + (3.1932\times10^{-4})\,(4.4353\times10^{-10}) \end{array} \right]^{1/2} \qquad (7.3.6)$$

$$= \left[2.2211\times10^{-9} + 5.3629\times10^{-10} + 1.4163\times10^{-13} \right]^{1/2}$$

$$= \left[2.7575\times10^{-9} \right]^{1/2} = 5.2512\times10^{-5}$$

To calculate a 95%/95% UTI, the results of Eqs. (7.3.5) and (7.3.6) are substituted into Eq. (7.3.4) along with the value $k(95, 95) = 2.2778$ obtained as described in Section F.2 of Appendix F. The result is

$$X\%/Y\%\ UTI(SF2_D^{Containers}) = \overline{SF2}_D^{Containers} + k(X,Y)\ SD(\overline{SF2}_d^{Containers}) \\ = 6.5805\times10^{-4} + 2.2778\,(5.2512\times10^{-5}) = 7.7766\times10^{-4} \tag{7.3.7}$$

which is well below the limiting value of 1.

X%/Y% UTIs on the sum-of-fractions SF2 for other combinations of X and Y are listed in Table 7.9. Listed first in the table are X%/Y% UTIs corresponding to the preceding AP-101 illustration with 25 ILAW MFPV batches and 41 ILAW containers. Also included for comparison are X%/Y% UTIs for 125 MFPV batches and 208 ILAW containers. The latter case is included to illustrate the effect of increasing the number of MFPV batches on the values of the X%/Y% UTIs on SF2. For this investigation, the mean and SD for the sum-of-fractions SF2 remained unchanged at the values obtained earlier in this section for 25 MFPV batches. X%/Y% UTIs for several combinations of confidence levels (X) and population percentage (Y) are shown in Table 7.9.

Table 7.9. Parameter Values and X%/Y% UTIs on the Sum-of-Fractions of Radionuclides in Table 1 of 10 CFR 61.55 (SF2) over *D* ILAW Containers Associated with 25 or 125 ILAW MFPV Batches Corresponding to an AP-101 LAW Waste Type

I[(a)]	D[(a)]	X%	Y%	$\overline{SF2}_D^{Containers}$	$k(X, Y)$	$SD(\overline{SF2}_d^{Containers})$	X%/Y% UTI on SF2
25	41	0.90	0.90	6.5805E-04	1.6851	5.2512E-05	7.47E-04
25	41	0.90	0.95	6.5805E-04	1.8257	5.2512E-05	7.54E-04
25	41	0.90	0.99	6.5805E-04	2.1367	5.2512E-05	7.70E-04
25	41	0.95	0.90	6.5805E-04	2.1121	5.2512E-05	7.69E-04
25	41	0.95	0.95	6.5805E-04	2.2778	5.2512E-05	7.78E-04
25	41	0.95	0.99	6.5805E-04	2.6485	5.2512E-05	7.97E-04
25	41	0.99	0.90	6.5805E-04	2.9251	5.2512E-05	8.12E-04
25	41	0.99	0.95	6.5805E-04	3.1415	5.2512E-05	8.23E-04
25	41	0.99	0.99	6.5805E-04	3.6315	5.2512E-05	8.49E-04
125	208	0.90	0.90	6.5805E-04	1.4458	5.2512E-05	7.34E-04
125	208	0.90	0.95	6.5805E-04	1.4962	5.2512E-05	7.37E-04
125	208	0.90	0.99	6.5805E-04	1.5960	5.2512E-05	7.42E-04
125	208	0.95	0.90	6.5805E-04	1.8330	5.2512E-05	7.54E-04
125	208	0.95	0.95	6.5805E-04	1.8911	5.2512E-05	7.57E-04
125	208	0.95	0.99	6.5805E-04	2.0071	5.2512E-05	7.63E-04
125	208	0.99	0.90	6.5805E-04	2.5644	5.2512E-05	7.93E-04
125	208	0.99	0.95	6.5805E-04	2.6388	5.2512E-05	7.97E-04
125	208	0.99	0.99	6.5805E-04	2.7877	5.2512E-05	8.04E-04

(a) I and D, respectively, denote the number of ILAW MFPV batches and number of ILAW containers associated with an LAW waste type.

Results in Table 7.9 show that the X%/Y% UTIs on SF2 are far below the limiting value of 1 for all cases. As expected, increasing the values of X and Y from 90 to 95 to 99 increases the value of the X%/Y% UTI. Although this nominally makes it more difficult for a X%/Y% UTI to be below its limit, even the 99%/99% UTI on SF2 is nowhere close to the limiting value of 1. Also, increasing the number of ILAW MFPV batches and containers associated with the LAW waste type yields smaller values of X%/Y% UTIs on SF2. However, if other ILAW for other LAW tanks to be processed by the WTP also have ILAW radionuclide sum-of-fractions SF2 for Class C greatly below the limit of 1, the number of ILAW MFPV batches and containers would likely have to be much lower than 25 before the X%/Y% UTI would have any chance of exceeding the limit.

7.3.1.2 Illustration of Statistical Method for Assessing Whether ILAW Radionuclide Concentrations for ILAW from Each MFPV Batch Meet Class C Limits

This section illustrates, using realistic example data, the methodology presented in Section 5.3.3.2 for demonstrating that ILAW radionuclide concentrations for ILAW from each MFPV batch meet Class C limits in Tables 1 and 2 of 10 CFR 61.55. The method presented in Section 5.3.3.2 is a CL% EUCI developed from Monte Carlo simulation calculations of the sum-of-fractions of ILAW radionuclides for Class C limits in Table 1 (SF1) and Table 2 (SF2) as discussed in Section B.3.1.2 of Appendix B.

The realistic example data used to illustrate the method for obtaining CL% EUCIs on $\overline{SF1}_i^{MFPV}$ and $\overline{SF2}_i^{MFPV}$ consists of results from the 1000 simulation runs for a test case with LAW Tank AP-101. The test case comprises the "high" case uncertainties for the factors listed in Table 3.3, three samples taken per CRV batch, and one analysis per sample. The 1000 simulated radionuclide compositions (1000 possibilities for a single MFPV batch given applicable uncertainties) for this test case were substituted in Eqs. (B.3.10) and (B.3.11) to calculate 1000 $\overline{SF1}_i^{MFPV}$ and $\overline{SF2}_i^{MFPV}$ values for a single MFPV batch. The density of glass produced from each of the 1000 simulated ILAW MFPV batches was assumed to be 2.65 g/cm^3 (= 2.65×10^6 g/m^3). Figure 7.1 shows a histogram of the 1000 $\overline{SF1}_i^{MFPV}$ values, while Figure 7.2 shows a histogram of the 1000 $\overline{SF2}_i^{MFPV}$ values.

The formula for the CL% EUCI on the sum-of-fractions for 10 CFR 61.55 Table 1 is given by Eq. (5.3.2a). As an illustration, a 99% EUCI on $\overline{SF1}_i^{MFPV}$ is shown using the data described in the previous paragraph. The result is

$$\text{CL\% EUCI}\left(\overline{SF1}_i^{MFPV}\right) = \overline{SF1}_i^{(1-\alpha)} = \overline{SF1}_i^{0.99} = 0.00215$$

where 0.00215 represents the 99th percentile of the 1000 simulated $\overline{SF1}_i^{MFPV}$ values (i.e., the 990th largest value out of the 1000 values). Table 7.10 summarizes the CL% EUCI $\overline{SF1}_i^{MFPV}$ values with 90%, 95%, 99%, and 99.9% confidence (relating to the percentiles) for the three LAW tanks.

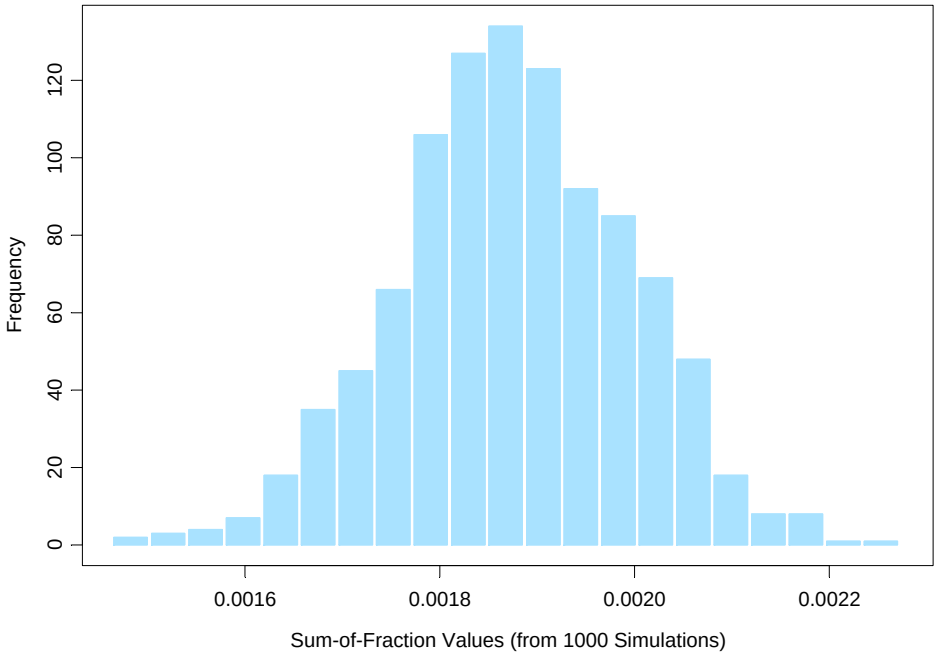

Figure 7.1. Histogram of the 1000 Simulated $\overline{SF1}_i^{MFPV}$ Values for ILAW from a Single MFPV Batch of AP-101 LAW

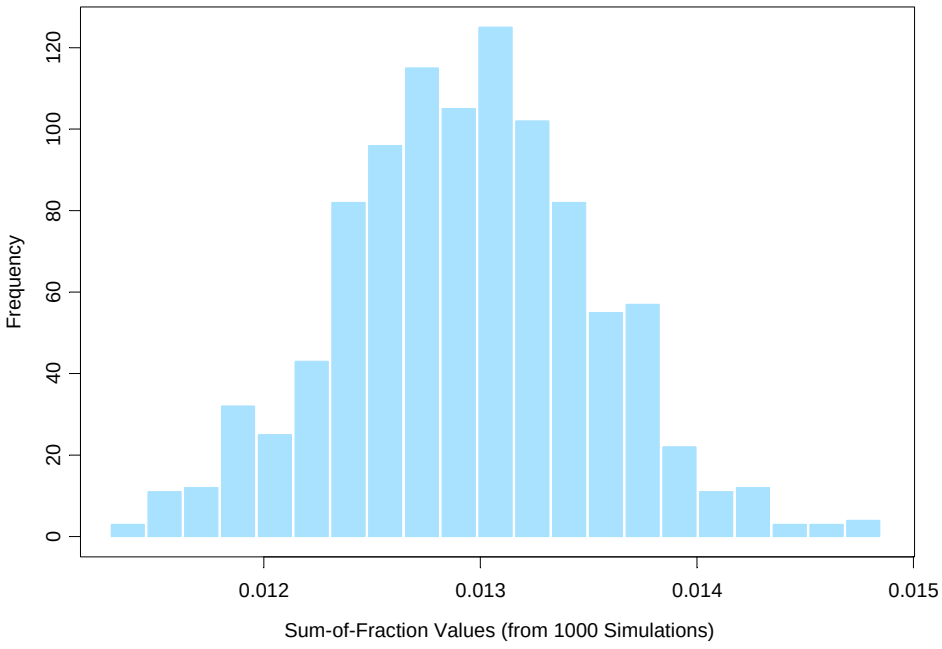

Figure 7.2. Histogram of the 1000 Simulated $\overline{SF2}_i^{MFPV}$ Values for ILAW from a Single MFPV Batch of AP-101 LAW

The formula for the CL% EUCI on the sum-of-fractions for 10 CFR 61.55 Table 2 is given by Eq. (5.3.2b). As an illustration, a 99% EUCI is shown using the data described previously. The result is

$$\text{CL\% EUCI}(\overline{SF2}_i^{MFPV}) = \overline{SF2}_i^{(1-\alpha)} = \overline{SF2}_i^{0.99} = 3.80\times10^{-5}$$

where 3.80×10^{-5} represents the 99th percentile of the 1000 simulated $\overline{SF2}_i^{MFPV}$ values (i.e., the 990th largest value out of the 1000 values). Table 7.10 summarizes the CL% EUCI $\overline{SF2}_i^{MFPV}$ values with 90%, 95%, 99%, and 99.9% confidence (relating to the percentiles) for the three LAW tanks.

Table 7.10. Resulting CL% EUCI ($\overline{SF1}_i^{MFPV}$) and CL% EUCI ($\overline{SF2}_i^{MFPV}$) Values for Three LAW Tanks Using $n_S^{CRV} = 3$, $n_A^{CRV} = 1$, and All Other Uncertainties at "High" Values

CL% EUCI ($\overline{SF}_i^{MFPV}$)	AP-101 (Envelope A)	AZ-101 (Envelope B)	AN-107 (Envelope C)
Sum-of-Fractions for ILAW Radionuclides in Table 1 of 10 CFR 61.55			
90% EUCI ($\overline{SF1}_i^{MFPV}$)	0.00203	0.000102	0.0720
95% EUCI ($\overline{SF1}_i^{MFPV}$)	0.00207	0.000104	0.0726
99% EUCI ($\overline{SF1}_i^{MFPV}$)	0.00215	0.000108	0.0737
99.9% EUCI ($\overline{SF1}_i^{MFPV}$)	0.00220	0.000113	0.0742
Sum-of-Fractions for ILAW Radionuclides in Table 2 of 10 CFR 61.55			
90% EUCI ($\overline{SF2}_i^{MFPV}$)	3.63×10^{-5}	3.35×10^{-5}	5.17×10^{-5}
95% EUCI ($\overline{SF2}_i^{MFPV}$)	3.68×10^{-5}	3.37×10^{-5}	5.24×10^{-5}
99% EUCI ($\overline{SF2}_i^{MFPV}$)	3.80×10^{-5}	3.41×10^{-5}	5.32×10^{-5}
99.9% EUCI ($\overline{SF2}_i^{MFPV}$)	3.91×10^{-5}	3.46×10^{-5}	5.43×10^{-5}

7.3.2 Results of Simulations to Determine the Numbers of Samples, Analyses, and Volume Determinations to Demonstrate that ILAW Radionuclide Concentrations for Each MFPV Batch Meet Class C Limits

This section presents results from the investigations described in Section 5.3.4 to determine the numbers of samples per CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations necessary to demonstrate that ILAW radionuclide concentrations for each MFPV batch meet Class C limits in Tables 1 and 2 of 10 CFR 61.55. The sum-of-fractions of the ILAW radionuclides for Table 1 and Table 2 (as described in Section 5.3.3) were calculated for each test case in the investigation described in Section 5.3.4. If the resulting calculations were below the limiting value of 1, then the numbers of samples per CRV batch, analyses per CRV sample, and CRV and MFPV volume

determinations associated with that test case would be sufficient to demonstrate that ILAW radionuclide concentrations met Class C limits.

Nominal values for the sum-of-fractions expressions for SF1 and SF2 are given by Eq. (B.3.6) and Eq. (B.3.8), respectively. The results are listed in Table 7.11. These values were calculated for each of the three LAW tanks used for the investigations in this report. ILAW simulation results were used to estimate the uncertainty around these nominal SF1 and SF2 values and to develop 95% EUCIs on SF1 and SF2 to compare to the sum-of-fractions limit of 1. For each LAW tank, two different 95% EUCI values were selected to summarize all of the 95% EUCI values for each of SF1 and SF2. The minimum 95% EUCI value represents the smallest total uncertainty across all the test cases for that particular LAW tank. This uncertainty is associated with simulation test cases that had (1) larger numbers of samples, analyses and volume determinations and (2) smaller processing uncertainties. The maximum 95% EUCI value represents the largest total uncertainty across all the test cases for that particular LAW tank. This uncertainty is associated with (1) smaller numbers of samples, analyses, and volume determinations and (2) larger processing uncertainties. The results in Table 7.11 show that the maximum 95% EUCI values are noticeably farther, on a relative basis, from the nominal values than the minimum 95% EUCI values. However, even the maximum 95% EUCI values are drastically below the sum-of-fractions limit of 1.

Table 7.11. Minimum and Maximum 95% EUCIs Showing the Impact of Various Factors[(a)] on Uncertainties of Sums-of-Fractions of ILAW Radionuclide Concentrations for Compliance with Class C Limits

LAW Tank (Envelope)	Value	SF1[(b)]	SF2[(c)]
AP-101 (Envelope A)	Nominal	0.00189	3.43×10^{-5}
	Minimum 95% EUCI	0.00193	3.50×10^{-5}
	Maximum 95% EUCI	0.00225	3.95×10^{-5}
AZ-101 (Envelope B)	Nominal	0.00009	3.25×10^{-5}
	Minimum 95% EUCI	0.00010	3.28×10^{-5}
	Maximum 95% EUCI	0.00011	3.46×10^{-5}
AN-107 (Envelope C)	Nominal	0.06975	4.95×10^{-5}
	Minimum 95% EUCI	0.07045	5.02×10^{-5}
	Maximum 95% EUCI	0.07483	5.45×10^{-5}

(a) These factors include the numbers of samples per CRV batch, analyses per CRV sample, and volume determinations as well as mixing/sampling, analytical, and other ILAW process uncertainties.
(b) Sum-of-fractions of radionuclides in Table 1 of 10 CFR 61.55.
(c) Sum-of-fractions of radionuclides in Table 2 of 10 CFR 61.55.

Figures 7.3 and 7.4 display boxplots[(a)] of the 95% EUCIs on SF1 and SF2, respectively, obtained for all combinations of factors investigated in the simulation test cases. Note that the overall minimum and maximum values for each LAW tank found in Table 7.11 correspond to the minimum and maximum values plotted in the Figure 7.3 and 7.4 boxplots for each LAW tank. The boxplots show the significant effect that the number of samples per CRV batch has on the sum-of-fraction 95% EUCI values. Figures 7.3 and 7.4 also show that each of the 95% EUCI values is well below the limiting value of 1. This means that each of the three example LAW tanks should be compliant for each of the simulation test

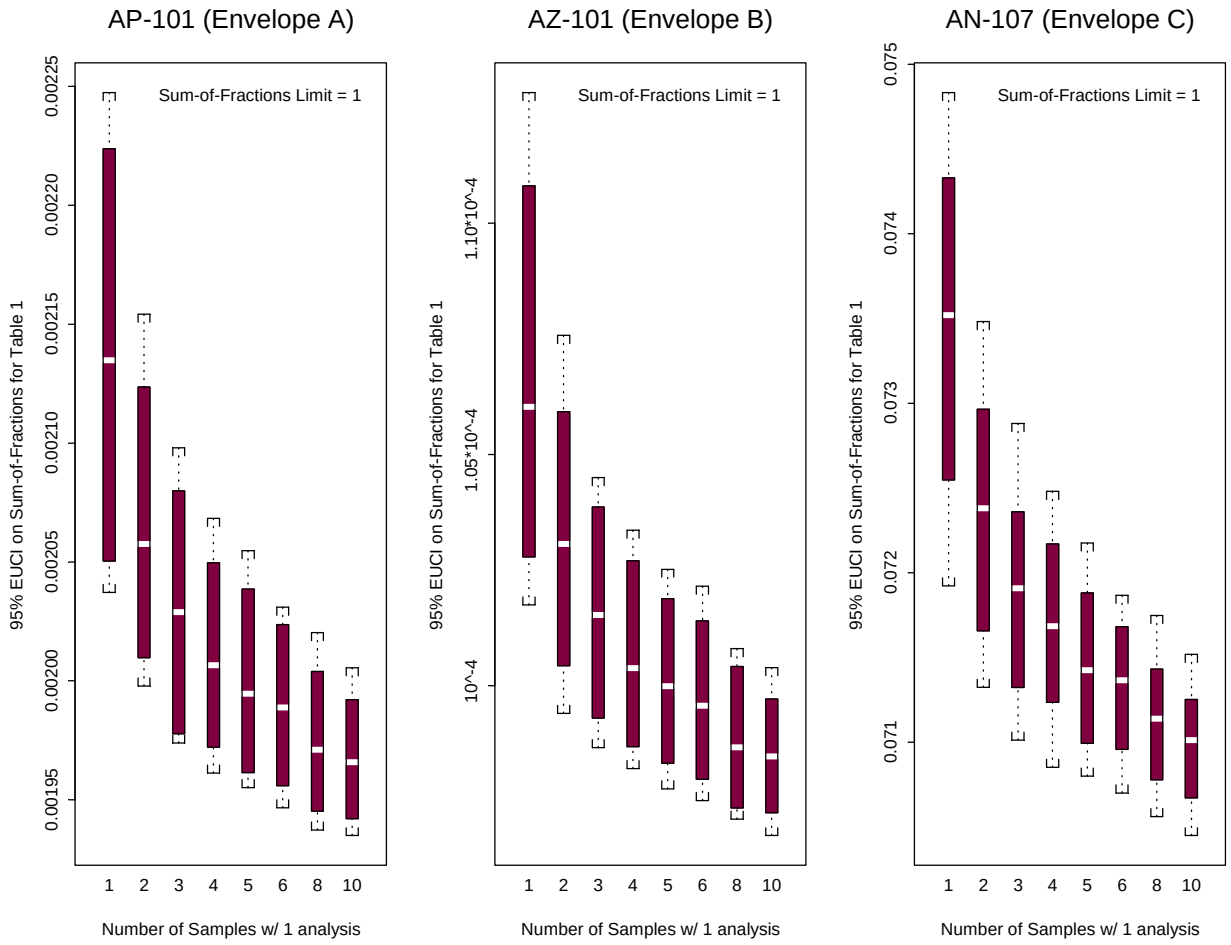

Figure 7.3. Boxplots of 95% EUCIs on ILAW Radionuclide Class C Sum-of-Fractions for 10 CFR 61.55 Table 1 from the ILAW Monte Carlo Simulations for Each of Three LAW Tanks and Various Number of Samples per CRV Batch with One Analysis per Sample

(a) A boxplot is a graphical display showing the distribution of data by quartiles. The first (bottom) line, or whisker, shows the range of the first quartile (up to the 25th percentile). The lower part of the box, below the box midline, shows the range of the second quartile (25th to 50th percentile). The upper part of the box, above the midline, shows the range of the third quartile (50th to 75th percentile). The top whisker shows the range of the last quartile (75th percentile to the maximum data point). See Appendix H.3 for a detailed discussion about interpreting boxplots.

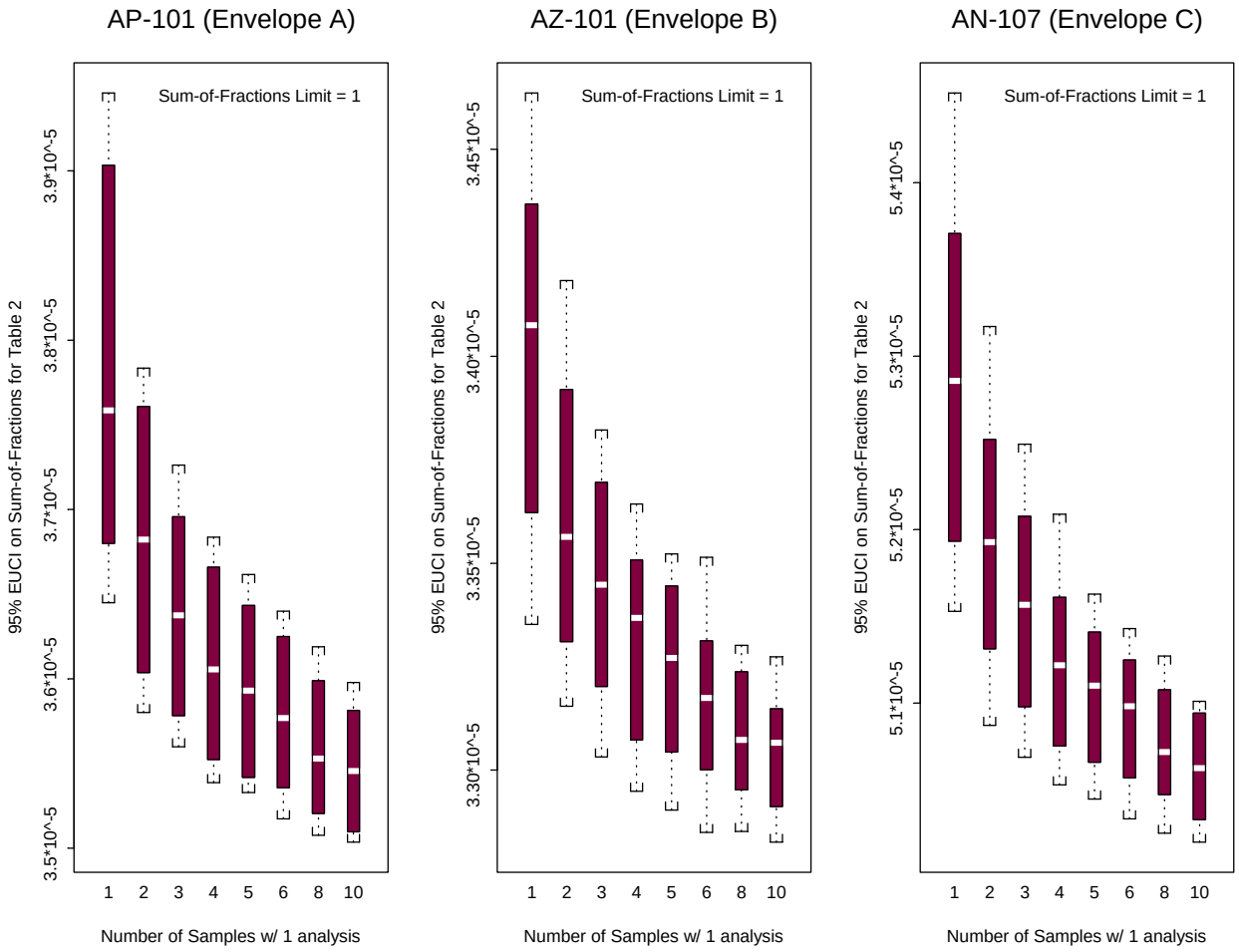

Figure 7.4. Boxplots of 95% EUCIs on ILAW Radionuclide Class C Sum-of-Fractions for 10 CFR 61.55 Table 2 from the ILAW Monte Carlo Simulations for Each of Three LAW Tanks and Various Number of Samples per CRV Batch with One Analysis per Sample

cases. The sum-of-fractions limit of 1 for SF1 and SF2 was satisfied for all test cases tested in the simulation, so taking one sample per CRV batch, one analysis per CRV sample, and one determination for each CRV and MFPV volume, or anything larger, should allow for radionuclide compliance for all three waste tanks. In usual situations, taking only one sample and one analysis per sample would not provide any basis for a statistical demonstration of compliance. However, in this case, a statistical demonstration of compliance is possible even for one sample per CRV batch and one analysis of that sample because the CL% EUCI is obtained from a Monte Carlo simulation. Whereas Monte Carlo simulations were performed for many test cases (combinations of factor values) in this investigation, during WTP ILAW operation for each ILAW MFPV batch, only one Monte Carlo simulation for the factor values applicable to that batch would need to be performed. The computing time for such a single Monte Carlo simulation would be negligible.

7.3.3 Illustration of Statistical Method to Demonstrate that Running-Average Concentrations of ^{137}Cs and ^{90}Sr Meet Specified Limits

This section illustrates, using realistic example data, the statistical method presented in Section 5.3.5 for demonstrating that running-average concentrations of ^{137}Cs and ^{90}Sr (over some specified period of ILAW production) meet Contract Specification 2.2.2.8 limits. The statistical method presented in Section 5.3.5 is to calculate CL% UCIs for the true, unknown running-average concentrations of ^{137}Cs and ^{90}Sr and then verify that the CL% UCI values are less than the specification limits.

The formula for calculating CL% UCIs on the running-average concentrations (Ci/m^3) of ^{137}Cs and ^{90}Sr over D ILAW containers corresponding to I ILAW MFPV batches is given by Eq. (5.3.3), which is repeated here for convenience

$$CL\%\ UCI = \bar{\bar{r}}_{Dq}^{Container} + t_{1-\alpha,df}\ SD(\bar{\bar{r}}_{Dq}^{Container})$$

In Eq. (5.3.3), the running-average $\bar{\bar{r}}_{Dq}^{Container}$ (q = ^{137}Cs and ^{90}Sr) is calculated using Eq. (B.3.9) in Section B.3.2.1 of Appendix B, and the standard deviation of the running-average $SD(\bar{\bar{r}}_{Dq}^{Container})$ is calculated using Eq. (F.3.3) in Section F.3 of Appendix F. A formula for calculating df in the Student's t-statistic $t_{1-\alpha,df}$ is given by Eq. (F.3.4) in Section F.3 of Appendix F.

The preceding equations are illustrated in this section using simulated data obtained (Vienna 2004b) from the WTP Project Run 3.1vv of the G2 dynamic simulation flowsheet (Deng 2004; Vora 2004) for 125 MFPV batches corresponding to LAW from Tank AP-101. Running averages over those 125 batches were calculated using the following form of Eq. (B.3.9)

$$\bar{\bar{r}}_{Dq}^{Container} = \frac{\bar{\bar{g}}_q^{MFPV}\,\bar{\rho}_D^{Container}\,A_q}{f_q} \tag{7.3.8}$$

where the $\bar{\bar{g}}_q^{MFPV}$ for q = $^{137}Cs_2O$ and ^{90}SrO are obtained from the G2 outputs via Eq. (B.2.7), $A_{^{137}Cs} = 87.0$ and $A_{^{90}Sr} = 140.0$ are from Table A.2 in Appendix A, and $f_{^{137}Cs_2O} = 1.0584$ and $f_{^{90}SrO} = 1.1778$ are from Table A.1. For this illustration, the glass density is assumed to be constant at 2.65 g/cm^3. Figure 7.5 and Figure 7.6 display the running-average concentrations (Ci/m^3) of ^{137}Cs and ^{90}Sr over the 125 simulated ILAW MFPV batches for AP-101. The running averages of ^{137}Cs concentrations (Ci/m^3) in Figure 7.5 are seen to be well below the Contract Specification 2.2.2.8 limit of 3 Ci/m^3. Similarly, the running averages of ^{90}Sr concentrations (Ci/m^3) in Figure 7.6 are seen to be well below the Contract Specification 2.2.2.8 limit of 20 Ci/m^3.

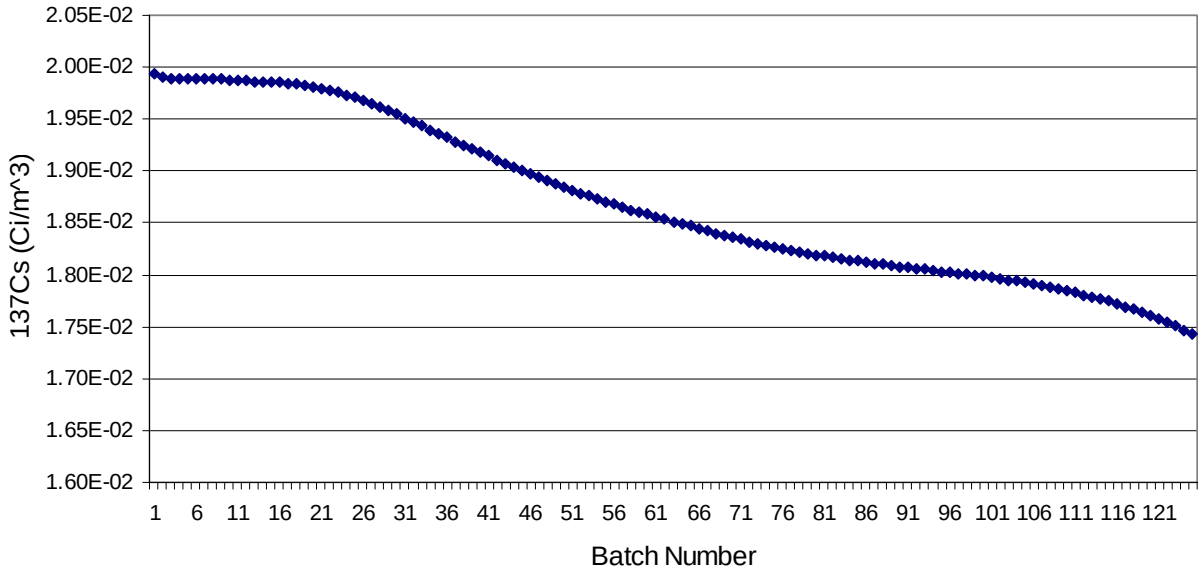

Figure 7.5. Running Averages of ^{137}Cs Concentrations (Ci/m^3) over 125 Simulated ILAW Batches for LAW from AP-101

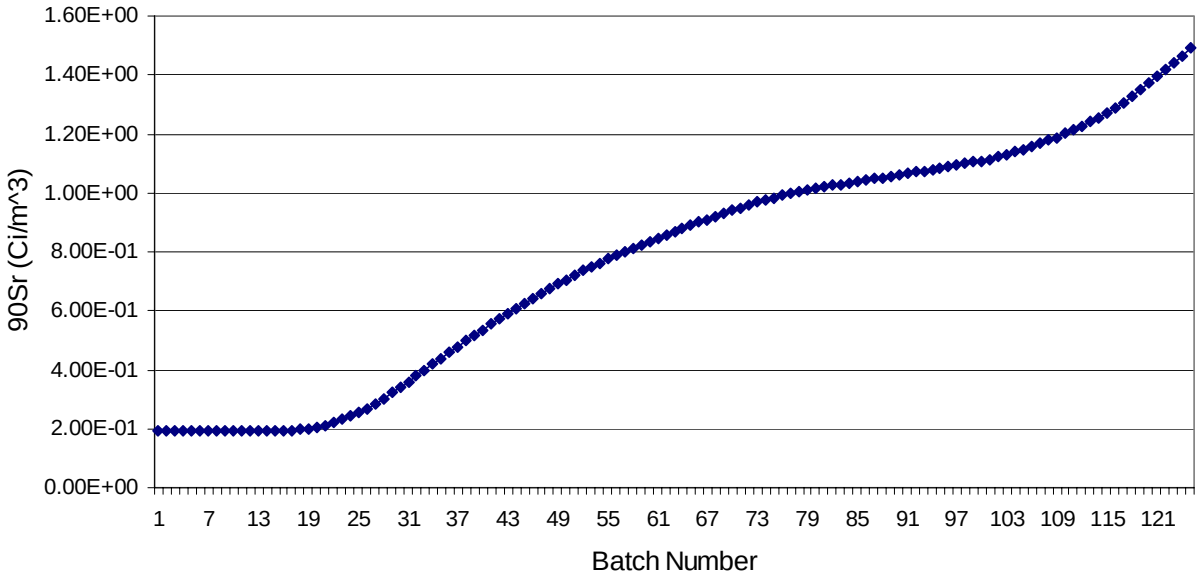

Figure 7.6. Running Averages of ^{90}Sr Concentrations (Ci/m^3) over 125 Simulated ILAW Batches for LAW from AP-101

To illustrate the calculation of CL% UCIs in Eq. (5.3.3) for ^{137}Cs and ^{90}Sr, it is necessary to calculate the running-average concentrations of both ^{137}Cs and ^{90}Sr and their respective SDs. For simplicity, running averages and SDs are illustrated after the first 25 ILAW MFPV batches. The running averages of ^{137}Cs and ^{90}Sr concentrations can be calculated by substituting data from Vienna (2004b) in Eq. (B.3.9), yielding

$$\begin{aligned}
\bar{\bar{r}}_{D^{137}\mathrm{Cs}}^{Container} &= \frac{\bar{\bar{g}}_{^{137}\mathrm{Cs_2O}}^{MFPV}\,\bar{\rho}_D^{Container}\,A_{^{137}\mathrm{Cs}}}{f_{^{137}\mathrm{Cs_2O}}} \\
&= \frac{(9.05\times10^{-11}\,\mathrm{g}_{^{137}\mathrm{Cs_2O}}/\mathrm{g}_{\mathrm{glass}})\,(2.65\times10^{6}\ \mathrm{g}_{\mathrm{glass}}/\mathrm{m}^3\ \mathrm{glass})\,(87\ \mathrm{Ci}\ ^{137}\mathrm{Cs}/\mathrm{g}_{^{137}\mathrm{Cs}})}{1.0584\,\mathrm{g}_{^{137}\mathrm{Cs_2O}}/\mathrm{g}_{^{137}\mathrm{Cs}}} \\
&= 0.0197\ \ \mathrm{Ci}\,^{137}\mathrm{Cs}/\mathrm{m}^3\ \mathrm{glass}
\end{aligned} \tag{7.3.9}$$

and

$$\begin{aligned}
\bar{\bar{r}}_{D^{90}\mathrm{Sr}}^{Container} &= \frac{\bar{\bar{g}}_{^{90}\mathrm{SrO}}^{MFPV}\,\bar{\rho}_D^{Container}\,A_{^{90}\mathrm{Sr}}}{f_{^{90}\mathrm{SrO}}} \\
&= \frac{(8.10\times10^{-10}\,\mathrm{g}_{\mathrm{SrO}}/\mathrm{g}_{\mathrm{glass}})\,(2.65\times10^{6}\ \mathrm{g}_{\mathrm{glass}}/\mathrm{m}^3\mathrm{glass})\,(140\ \mathrm{Ci}\ ^{90}\mathrm{Sr}/\mathrm{g}_{^{90}\mathrm{Sr}})}{1.1778\,\mathrm{g}_{^{90}\mathrm{SrO}}/\mathrm{g}_{^{90}\mathrm{Sr}}} \\
&= 0.2551\ \ \mathrm{Ci}/\mathrm{m}^3
\end{aligned} \tag{7.3.10}$$

Application of Eq. (5.3.3) also requires calculation of:

$$SD(\bar{\bar{r}}_{D^{137}Cs}^{Container}) = \left(\frac{A_{^{137}Cs}}{f_{^{137}Cs_2O}}\right)\left[\begin{array}{l}\left[\bar{\bar{g}}_{^{137}Cs}^{MFPV}\right]^2\left[SD(\bar{\rho}_d^{Container})\right]^2+\left[\bar{\rho}_D^{Container}\right]^2\left[SD(\bar{g}_{i^{137}Cs}^{MFPV})\Big/\sqrt{I}\right]^2 \\ -\left[SD(\bar{\rho}_d^{Container})\right]^2\left[SD(\bar{g}_{i^{137}Cs}^{MFPV})\Big/\sqrt{I}\right]^2\end{array}\right]^{1/2} \tag{7.3.11}$$

$$SD(\bar{\bar{r}}_{D^{90}Sr}^{Container}) = \left(\frac{A_{^{90}Sr}}{f_{^{90}SrO}}\right)\left[\begin{array}{l}\left[\bar{\bar{g}}_{^{90}Sr}^{MFPV}\right]^2\left[SD(\bar{\rho}_d^{Container})\right]^2+\left[\bar{\rho}_D^{Container}\right]^2\left[SD(\bar{g}_{i^{90}Sr}^{MFPV})\Big/\sqrt{I}\right]^2 \\ -\left[SD(\bar{\rho}_d^{Container})\right]^2\left[SD(\bar{g}_{i^{90}Sr}^{MFPV})\Big/\sqrt{I}\right]^2\end{array}\right]^{1/2} \tag{7.3.12}$$

However, the WTP Project currently has no basis to obtain an estimate of $SD(\bar{\rho}_d^{Container})$, the SD of the density of glass across the $d = 1, 2, \ldots, D = 41$ ILAW containers associated with the $I = 25$ MFPV batches. For the purposes of this illustration, a SD equal to 10% of the assumed mean density over all D

containers ($\overline{\rho}_D^{Container}$) was used. Under these conditions, the numerical values for the expressions shown in Eqs. (7.3.11) and (7.3.12) are:

$$SD(\overline{\overline{r}}_{D^{137}Cs}^{Container}) = \left(\frac{87\text{Ci/g}}{1.0584}\right)\left\{\begin{array}{l}\left[9.05\times10^{-11}\right]^2\left[0.1\cdot(2.65\times10^6\,\text{g/m}^3)\right]^2 + \left[2.65\times10^6\,\text{g/m}^3\right]^2\left[\frac{1.10\times10^{-12}}{5}\right]^2 \\ -\left[0.1\cdot(2.65\times10^6\,\text{g/m}^3)\right]^2\left[\frac{1.10\times10^{-12}}{5}\right]^2\end{array}\right\}^{1/2}$$

$$= 6.0820\times10^{-4}\ \ \text{Ci/m}^3$$

$$SD(\overline{\overline{r}}_{D^{90}Sr}^{Container}) = \left(\frac{140\text{Ci/g}}{1.1778}\right)\left\{\begin{array}{l}\left[8.10\times10^{-10}\right]^2\left[0.1\cdot(2.65\times10^6\,\text{g/m}^3)\right]^2 + \left[2.65\times10^6\,\text{g/m}^3\right]^2\left[\frac{3.55\times10^{-10}}{5}\right]^2 \\ -\left[0.1\cdot(2.65\times10^6\,\text{g/m}^3)\right]^2\left[\frac{3.55\times10^{-10}}{5}\right]^2\end{array}\right\}^{1/2}$$

$$= 0.0504\ \text{Ci/m}^3$$

Given the preceding results for averages and SDs of the averages, Eq. (5.3.3) can be applied to calculate 95% UCI values for ^{137}Cs and ^{90}Sr:

$$\begin{aligned}95\%\ \text{UCI} &= \overline{\overline{r}}_{D^{137}\text{Cs}}^{Container} + t_{1-\alpha,df}\ SD\left(\overline{\overline{r}}_{D^{137}\text{Cs}}^{Container}\right) = \overline{\overline{r}}_{D^{137}\text{Cs}}^{Container} + t_{1-0.05,25-1}\ SD\left(\overline{\overline{r}}_{D^{137}\text{Cs}}^{Container}\right) \\ &= \overline{\overline{r}}_{D^{137}\text{Cs}}^{Container} + t_{0.95,24}\ SD\left(\overline{\overline{r}}_{D^{137}\text{Cs}}^{Container}\right) \qquad (7.3.13) \\ &= 0.0197\ \ \text{Ci/m}^3 + 1.711\,(\,6.0820\times10^{-4}\ \text{Ci/m}^3) = 0.0207\ \ \text{Ci/m}^3\end{aligned}$$

$$\begin{aligned}95\%\ \text{UCI} &= \overline{\overline{r}}_{D^{90}\text{Sr}}^{Container} + t_{1-\alpha,df}\ SD\left(\overline{\overline{r}}_{D^{90}\text{Sr}}^{Container}\right) = \overline{\overline{r}}_{D^{90}\text{Sr}}^{Container} + t_{1-0.05,25-1}\ SD\left(\overline{\overline{r}}_{D^{90}\text{Sr}}^{Container}\right) \\ &= \overline{\overline{r}}_{D^{90}\text{Sr}}^{Container} + t_{0.95,24}\ SD\left(\overline{\overline{r}}_{D^{90}\text{Sr}}^{Container}\right) \qquad (7.3.14) \\ &= 0.2551\ \ \text{Ci/m}^3 + 1.711\,(\,0.0504\,\text{Ci/m}^3) = 0.3413\ \ \text{Ci/m}^3\end{aligned}$$

In the above equations, note that $df = I - 1 = 25 - 1 = 24$, where in this case I denotes the number of ILAW MFPV batches over which the running averages are being calculated. These 95% UCI values are seen to be well below their respective limits of 3 Ci/m^3 and 20 Ci/m^3.

7.3.4 Results of Simulations to Determine the Numbers of Samples, Analyses, and Volume Determinations to Demonstrate that Concentrations of ^{137}Cs and ^{90}Sr in ILAW for Each MFPV Batch Meet Specified Limits

This section presents results from the investigations described in Section 5.3.6 to determine the numbers of samples per CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations necessary to demonstrate that ILAW radionuclide concentrations of ^{137}Cs and ^{90}Sr for each MFPV batch meet specified limits. The concentrations of ^{137}Cs and ^{90}Sr (as described in Section 5.3.5) were calculated for each simulation test case in the investigation described in Section 5.3.6. If the resulting calculation was below the specified limits of $^{137}Cs \leq 3$ Ci/m^3 and $^{90}Sr \leq 20$ Ci/m^3 from Contract Specification 2.2.2.8, then the numbers of samples per CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations associated with that test case would be sufficient to demonstrate that ILAW radionuclide concentrations met the specified limits.

Nominal values for the concentrations of ^{137}Cs and ^{90}Sr for a single MFPV batch were calculated using Eq. (B.3.11), and the results are given in Table 7.12. These values were calculated for each of the three LAW tanks used for the investigations in this report. ILAW simulation results were used to estimate the uncertainty around these nominal values and to develop 95% EUCI values to compare to the specified limits of $^{137}Cs \leq 3$ Ci/m^3 and $^{90}Sr \leq 20$ Ci/m^3. For each LAW tank and each calculated concentration (i.e., ^{137}Cs and ^{90}Sr), two different 95% EUCI values were selected to summarize the 95% EUCI values across all of the test cases. The minimum 95% EUCI value represents the smallest total uncertainty across all the test cases for that particular LAW tank. This uncertainty is associated with simulation test cases that had (1) larger numbers of samples, analyses and volume determinations and (2) smaller processing uncertainties. The maximum 95% EUCI value represents the largest total

Table 7.12. Results of Investigation on the Impact of Factors[(a)] Giving Minimum and Maximum Total Uncertainties on Concentrations of ILAW ^{137}Cs and ^{90}Sr Complying with Specified Limits

LAW Tank (Envelope)	Value	$\bar{\bar{r}}^{MFPV}_{^{137}Cs}$ [(b)]	$\bar{\bar{r}}^{MFPV}_{^{90}Sr}$ [(c)]
AP-101 (Envelope A)	Nominal	0.00026	0.17333
	Minimum 95% EUCI	0.00027	0.17574
	Maximum 95% EUCI	0.00038	0.19195
AZ-101 (Envelope B)	Nominal	0.03827	0.16953
	Minimum 95% EUCI	0.03866	0.17145
	Maximum 95% EUCI	0.04151	0.18349
AN-107 (Envelope C)	Nominal	0.22289	0.00739
	Minimum 95% EUCI	0.22586	0.00781
	Maximum 95% EUCI	0.24569	0.01057

(a) These factors include the numbers of samples per CRV batch, analyses per CRV sample, and volume determinations as well as mixing/sampling, analytical, and other ILAW process uncertainties.
(b) This represents the running average of ^{137}Cs concentration.
(c) This represents the running average for ^{90}Sr concentration.

uncertainty across all the test cases for that particular LAW tank. This uncertainty is associated with (1) smaller numbers of samples, analyses, and volume determinations and (2) larger processing uncertainties. The results in Table 7.12 show that the maximum 95% EUCI values are noticeably farther, on a relative basis, from the nominal values than the minimum 95% EUCI values. However, even the maximum 95% EUCI values are drastically below the specified limits.

Figure 7.7 displays boxplots (see Section H.3 of Appendix H for help interpreting boxplots) of the 95% EUCIs on concentrations of ^{137}Cs and ^{90}Sr obtained for all combinations of factors investigated in the simulation test cases. Note that the overall minimum and maximum values for each LAW tank found in Table 7.12 correspond to the minimum and maximum values plotted in the boxplots in Figure 7.7 for each LAW tank. The boxplots show the significant effect that the number of samples per CRV batch has on the 95% EUCI values for ^{137}Cs and ^{90}Sr concentrations. Figure 7.7 also shows that each of the 95% EUCI values is well below the specified limits of $^{137}Cs \leq 3$ Ci/m^3 and $^{90}Sr \leq 20$ Ci/m^3. This means that each of the three example LAW tanks should be compliant for each of the simulation test cases. The specified limits of $^{137}Cs \leq 3$ Ci/m^3 and $^{90}Sr \leq 20$ Ci/m^3 were satisfied for all test cases assessed in the

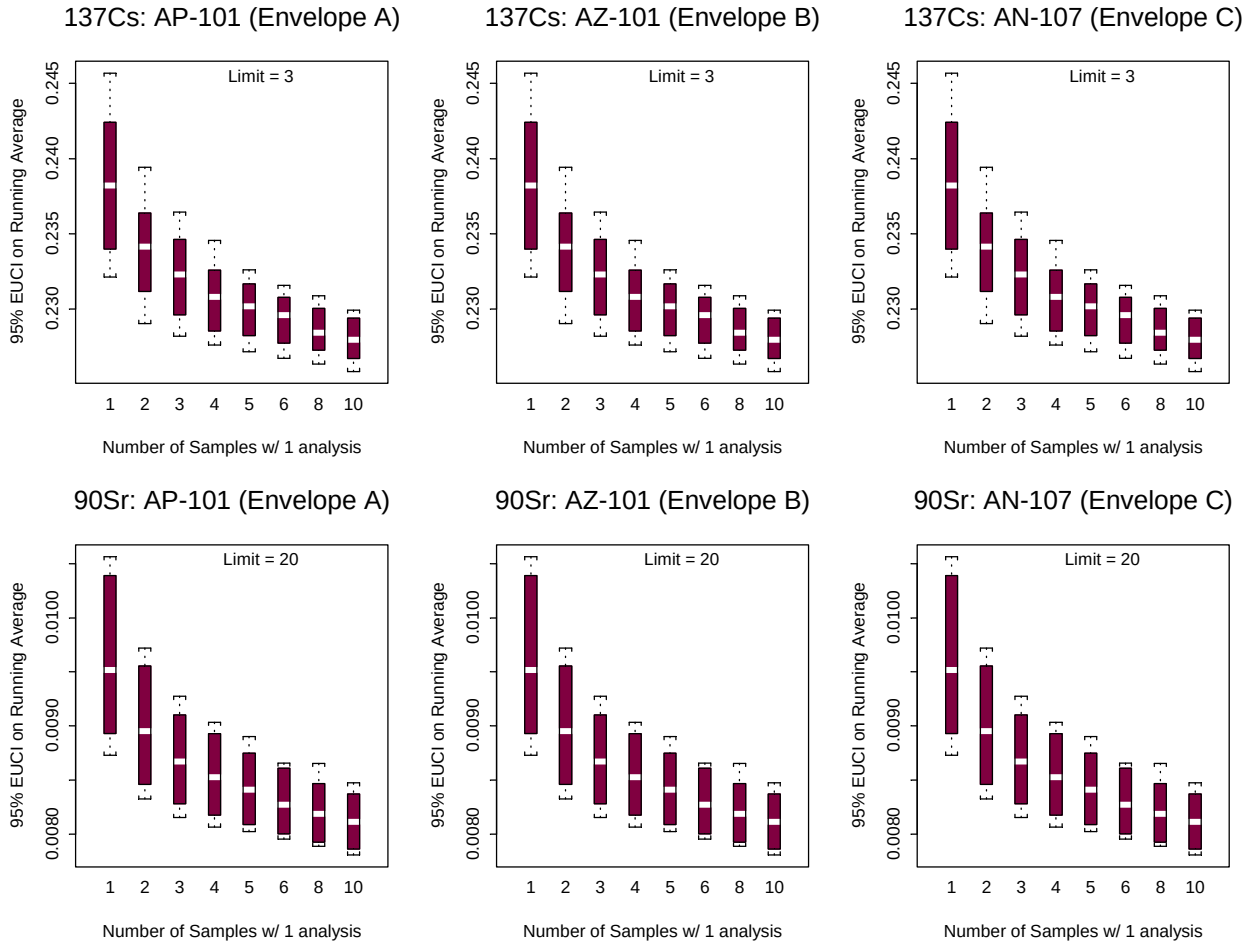

Figure 7.7. Boxplots of 95% EUCIs on ILAW Concentrations of ^{137}Cs and ^{90}Sr from the ILAW Monte Carlo Simulations for Each of Three LAW Tanks and Various Number of Samples per CRV Batch with One Analysis per Sample

simulation, so taking one sample per CRV batch, one analysis per CRV sample, and one determination for each CRV and MFPV volume, or anything larger, should allow for radionuclide compliance for all three waste tanks. In usual situations, taking only one sample and one analysis per sample would not provide any basis for a statistical demonstration of compliance. However, in this case, a statistical demonstration of compliance is possible even for one sample per CRV batch and one analysis of that sample because the CL% EUCI is obtained from a Monte Carlo simulation. Whereas Monte Carlo simulations were performed for many test cases (combinations of factor values) in this investigation, during WTP ILAW operation for each ILAW MFPV batch, only one Monte Carlo simulation for the factor values applicable to that batch would need to be performed. The computing time for such a single Monte Carlo simulation would be negligible.

As discussed in Section 5.3.6, the method applied in this section focused on assessing the required numbers of samples per CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations to demonstrate that each MFPV batch would yield ILAW satisfying the ^{137}Cs and ^{90}Sr concentration limits. The method accounted only for the various uncertainties affecting a single ILAW MFPV batch and did not account for variations across MFPV batches. Variations across MFPV batches are important in assessing whether running averages of ^{137}Cs and ^{90}Sr concentrations across MFPV batches satisfy the ^{137}Cs and ^{90}Sr concentration limits. When the details of a method to account for both variation and uncertainties are developed (see Section 5.3.6), the results of an investigation using that method will be reported in this section of a future revision of the report.

7.4 Compliance Results for ILAW Contract Specification 2.2.2.17.2: Product Consistency Test (PCT)

Section 7.4.1 illustrates, using a realistic example, the methodology presented in Section 5.4.3 for demonstrating that ILAW from a single MFPV batch satisfies PCT limits.

Section 7.4.2 presents results from the Monte Carlo simulations described in Section 5.4.4 for assessing the effects of (1) CRV mixing/sampling and analytical uncertainties, (2) the numbers of samples per CRV batch and analyses per CRV sample, and (3) the number of volume determinations of CRV and MFPV batches on the ability to demonstrate PCT compliance for ILAW from a single MFPV batch. These results provide a basis for (1) assessing the sensitivity of single-MFPV-batch PCT estimates to the range of possible uncertainties and (2) the WTP Project to decide on the number of samples per CRV batch, the number of chemical analyses per CRV sample, and the number of volume determinations of CRV and MRPV batches necessary to demonstrate PCT compliance for ILAW from a single MFPV batch.

Section 7.4.3 illustrates, using a realistic example, the methodology presented in Section 5.4.5 for demonstrating that ILAW over an LAW waste type satisfies PCT limits.

Section 7.4.4 presents the results from the simulation described in Section 5.4.6 for assessing the effects of (1) the variations and uncertainties in PCT responses over an LAW waste type and (2) the numbers of samples per CRV batch, number of analyses per CRV sample, and the number of volume determinations per CRV and MFPV batches on the ability to demonstrate PCT compliance for ILAW

over an LAW waste type. These results provide a basis for (1) assessing the sensitivity of PCT estimates to the ranges of possible variations and uncertainties over an LAW waste type and (2) the WTP Project to decide on the number of samples per CRV batch, the number of chemical analyses per CRV sample, and the number of CRV and MFPV volume determinations necessary to demonstrate PCT compliance for ILAW over an LAW waste type.

7.4.1 Illustration of Methods for Demonstrating PCT Compliance for ILAW Corresponding to an MFPV Batch

This section uses Monte Carlo simulation results to illustrate the use of Eqs. (5.4.3a), (5.4.5), (5.4.6), and (5.4.7) presented in Section 5.4.3 for calculating CL% UCCIs to demonstrate that ILAW corresponding to a single MFPV batch meets PCT limits.

For this illustration, the Monte Carlo simulation results from the AP-101 test case with (1) three CRV samples and each sample analyzed once, (2) one CRV and one MFPV volume determination, and (3) all uncertainties at the "high" case were used. Table 7.13 lists the normalized average mass composition (mass fractions) calculated using Eq. (4.3.3). These normalized ILAW composition values were calculated using the nominal AP-101 mass compositions as found in Table D.11 in Appendix D. For the final report, the illustration will be revised so that these normalized ILAW composition values will be calculated using CRV concentrations for three realistically simulated samples with single analyses, as well as realistically simulated values for all the other inputs found in Eq. (B.1.11) from Section B.1 of Appendix B. Substituting the normalized ILAW composition in Table 7.13 and the PCT model coefficients in Table 5.1 into Eq. (5.4.3a) yields the predicted PCT results shown in Table 7.13.

Table 7.13 also shows the SDs of model predictions calculated using the $\sqrt{(\bar{\boldsymbol{x}}_i^{MFPV})^T \boldsymbol{\Sigma}_b^h \bar{\boldsymbol{x}}_i^{MFPV}}$ portion of Eq. (5.4.7). These values are used in calculating the $MHW_{95\%\ SUCI}^{ih}$ quantity given by Eq. (5.4.7). Also listed in Table 7.13 are values of $CHW_{95\%\ UCI}^{ih}$ obtained by applying Eq. (5.4.6) to the results of a Monte Carlo simulation based on the simulated sampled and measured quantities. The Monte Carlo simulation used the high uncertainty values for all uncertain quantities in Eq. (B.1.11).

Finally, Table 7.13 presents the results of calculations using Eqs. (5.4.5) through (5.4.7) to obtain 95% UCCIs for PCT normalized B and Na releases. The 95% UCCI values are seen to be significantly below the Contract Specification 2.2.2.17.2 limiting value of 2 g/m^2 = 4 g/L = 1.386 ln(g/L) for each of these releases.

Table 7.13. Normalized ILAW Composition, Model-Predicted PCT Results, and Model Uncertainties for Simulated Data on an ILAW MFPV BatchCorresponding to LAW Tank AP-101

PCT B			PCT Na			
Model Term	$\bar{x}_{ik}^{MFPV}$ (a)	b_k^B (b)	**Model Term**	$\bar{x}_{ik}^{MFPV}$ (a)	b_k^{Na} (b)	
Al_2O_3	0.0634	-19.916	Al_2O_3	0.0634	-17.263	
B_2O_3	0.1037	1.672	B_2O_3	0.1037	2.262	
CaO	0.0208	-1.547	CaO	0.0208	3.924	
Fe_2O_3	0.0557	-0.829	Fe_2O_3	0.0557	2.160	
K_2O	0.0410	4.923	K_2O	0.0410	41.277	
Li_2O	8.06×10^{-7}	-6.972	Li_2O	8.06×10^{-7}	-5.476	
MgO	0.0156	-25.790	MgO	0.0156	-9.992	(d)
Na_2O	0.1914	15.233	Na_2O	0.1914	12.949	
SiO_2	0.4559	-3.199	SiO_2	0.4559	-3.417	
TiO_2	0.0209	-11.059	TiO_2	0.0209	-8.169	
ZrO_2	0.0312	-18.001	ZrO_2	0.0312	-19.810	
$B_2O_3 \times MgO$	0.0016	493.305	$B_2O_3 \times MgO$	0.0016	267.677	
$Li_2O \times ZrO_2$	2.51×10^{-8}	541.901	$Li_2O \times ZrO_2$	2.51×10^{-8}	526.316	
$Fe_2O_3 \times Li_2O$	4.49×10^{-8}	349.796	$Fe_2O_3 \times K_2O$	0.0023	-266.279	
(d)			$Fe_2O_3 \times Li_2O$	4.49×10^{-8}	201.497	
			$B_2O_3 \times K_2O$	0.0043	-199.268	
Model-Predicted PCT Normalized Releases: Nominal and 95th Percentiles [ln(g/L)]						
$\hat{\bar{y}}_i^h$	0.095		(d)	-0.011		(d)
$\hat{\bar{y}}_{i,95\%}^h$ (c)	0.311			0.200		
Model Uncertainties of Predicted PCT Normalized Releases for the Mean Composition [ln(g/L)]						
$SD_M[\hat{y}^{PCT\,B}(\bar{x})]$	0.092	(d)				
$SD_M[\hat{y}^{PCT\,Na}(\bar{x})]$	0.061					
95% UCCIs on PCT Normalized Releases						
PCT Normalized Elemental Release	$\hat{\bar{y}}$ [ln(g/L)]	$CHW_{95\%\ UCI}$ (c) [ln(g/L)]	$MHW_{95\%\ SUCI}$ [ln(g/L)]	95% UCCI [ln(g/L)]	95% UCCI [g/L]	Limit [g/L]
PCT B	0.095	0.216	0.440	0.751	2.119	4
PCT Na	-0.011	0.211	0.309	0.509	1.664	4

(a) The average ILAW composition for the MFPV batch is expressed in normalized mass fractions of the components in the model. Crossproduct terms are formed from these normalized mass fractions.
(b) The model coefficients for the ILAW PCT normalized B and Na releases are from Table 5.1.
(c) The Monte Carlo simulation results used were for (1) three CRV samples each analyzed once, (2) one CRV and one MFPV volume determination, and (3) all uncertainties at the "high" case.
(d) This portion of the table is intentionally blank.

Detailed illustrations of calculations using Eqs. (5.4.3a), (5.4.5), (5.4.6), and (5.4.7) to obtain the 95% UCCI for ln(PCT normalized B release) are now presented. Intermediate results from Table 7.13 are used in some cases to reduce what would otherwise be very long algebraic equations. Applying Eq. (5.4.3a) yields

$$\hat{\bar{y}}_i^{PCT\,B} = \sum_{k=1}^{n_{mc}^{PCT\,B}} b_k^{PCT\,B}\,\bar{x}_{ik}^{MFPV} + Selected\left\{\sum_{k=1}^{n_{mc}^{PCT\,B}} b_{kk}^{PCT\,B}\left(\bar{x}_{ik}^{MFPV}\right)^2 + \sum_{k=1}^{n_{mc}^{PCT\,B}-1}\sum_{l>k}^{n_{mc}^{PCT\,B}} b_{kl}^{PCT\,B}\,\bar{x}_{ik}^{MFPV}\,\bar{x}_{il}^{MFPV}\right\}$$

$$= (-19.9158)(0.0634) + \ldots + (-18.0010)(0.0312) \qquad \text{linear terms}$$

$$+ 493.3071(0.0016) + 349.796\left(4.49\times10^{-8}\right) + 541.9078\left(2.51\times10^{-8}\right) \qquad \text{crossproduct terms}$$

$$= 0.095 \text{ ln(g/L)}$$

Applying Eq. (5.4.6) to the results of a Monte Carlo simulation of 1000 runs using the high levels of uncertainty for all uncertain quantities yields

$$CHW_{i,95\%\,UCI}^{PCT\,B} = \hat{\bar{y}}_{i,95\%}^{PCT\,B} - \hat{\bar{y}}_i^{PCT\,B} = 0.311 - 0.095 = 0.216 \text{ ln(g/L)}.$$

Applying Eq. (5.4.7), where $n = 69$ and $p = 14$ per Table 5.1, yields

$$MHW_{i,95\%\,SUCI}^{PCT\,B} = \sqrt{p\,F_{1-\alpha}(p,n-p)}\left(\sqrt{(\bar{\boldsymbol{x}}_i^{MFPV})^{\mathrm{T}}\,\boldsymbol{\Sigma}_b^{PCT\,B}\,\bar{\boldsymbol{x}}_i^{MFPV}}\right) = \sqrt{14F_{0.95}(14,55)}(0.092) = 0.440 \text{ ln(g/L)}.$$

Finally, combining the above results in Eq. (5.4.5) yields

$$95\%\ UCCI\left[\ln(\text{PCT B})\right] = \hat{\bar{y}}_i^{PCT\,B} + CHW_{i,95\%\,UCI}^{PCT\,B} + MHW_{i,95\%\,SUCI}^{PCT\,B} = 0.095 + 0.216 + 0.440 = 0.751 \text{ ln(g/L)}.$$

This value can be converted to units of g/L by exponentiating, yielding $e^{0.751} = 2.119$ g/L. The preceding two values for the 95% UCCI, in units of ln(g/L) and g/L, are the ones shown for PCT normalized B release in Table 7.13. Table 7.13 also contains the steps of the 95% UCCI calculations for PCT normalized Na release. In both cases, these release rates are smaller than the compliance limit of 4 g/L. Therefore, with 3 samples and 1 analysis, the ILAW is compliant with PCT limits in this illustration.

7.4.2 Results of Simulations to Assess the Effects of Process Uncertainties and Numbers of Samples, Analyses, and Volume Determinations on ILAW PCT Uncertainties and Compliance Corresponding to an MFPV Batch

This section uses the methodology described in Section 5.4.4 to assess the numbers of samples per CRV batch, analyses per CRV sample, and number of CRV and MFPV volume determinations necessary to demonstrate compliance with PCT limits for each ILAW MFPV batch. The methodology in Section 5.4.4 uses Eqs. (5.4.3a), (5.4.5), (5.4.6), and (5.4.7) to calculate CL% UCCI values for PCT normalized releases of B and Na for various combinations of input factor values. If the CL% UCCI values (for PCT B and Na) for a given combination of factor values are less than the PCT specification limits, then compliance is demonstrated for that combination. Values of the mass fraction compositions

of ILAW resulting from the n_A^{CRV} analyses of n_S^{CRV} samples per CRV batch, the n_V volume determinations per CRV and MFPV batches, the model coefficients and variance-covariance matrices, and the selected statistical confidence level (CL%) and corresponding CL% percentile of the empirical distribution from the 1000 Monte Carlo simulations are necessary in using Eqs. (5.4.5), (5.4.6), and (5.4.7) to calculate the CL% UCCI values for PCT normalized B and Na releases.

Table 7.14 shows how taking at least 3 samples per LAW CRV batch with 1 analysis of each sample will be sufficient to demonstrate compliance with PCT limits for each ILAW MFPV batch. The calculations in Table 7.14 assumed all uncertainties to be at their highest levels. Table 7.14 shows the calculated 95% UCCI values (for PCT normalized B and Na releases) for each of the three LAW tanks used for illustrations in this report. Comparing these values to the PCT limits [in ln(g/L)] shows that a minimum of 3 samples per MFPV batch with one analysis per sample should be sufficient to demonstrate compliance with PCT limits for each MFPV batch.

In addition to the results described so far, we now summarize the results of the investigation described in Section 5.4.4. That investigation involved calculating CL% UCCI values on PCT normalized releases of B and Na for various combinations of factors (test runs) in the Monte Carlo simulation as described in Section 3.4.2. Typically, the results of such investigations would be summarized in a table (similar to ones presented in Section 6 and earlier in Section 7). However, no such table was necessary to display the numbers of samples per CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations necessary to comply with PCT limits because all test runs in the simulation were compliant. This means that when assuming the "high" case uncertainties, only one CRV sample with one analysis per sample was necessary to be compliant. Figure 7.8 shows boxplots (see Appendix H.3 for help interpreting boxplots) of the 95% UCCI values for PCT normalized B and Na releases across all combinations of input factors in the experimental design (see Section 3.4.2). As can be seen from the boxplots, the 95% UCCI values for PCT normalized B and Na releases for all of the simulation runs were well below the PCT limits, indicating that compliance was easily demonstrated.

ANOVA was performed for each PCT analyte (B and Na) and each of the three LAW tanks used for investigations in this report to help determine which factors from Table 3.3 and which two-factor interactions most affect %RHWs of CL% UCCIs. The resulting ANOVA p-values are summarized in Table 7.15. Those factors with p-values below 0.05 are considered to have statistically significant effects on %RHWs of CL% UCCIs for PCT normalized B and Na releases. Factors with statistically significant effects across both of the PCT analytes and the three LAW tanks included: $\%RSD_A(c_j^{CRV})$ and n_S^{CRV}. The $\%RSD_A(c_j^{CRV}) \times n_S^{CRV}$, $\%RSD_A(c_j^{CRV}) \times n_A^{CRV}$, and $n_S^{CRV} \times n_A^{CRV}$ interactions also had statistically significant effects. The $\%RSD_S(c_j^{CRV})$ factor and $\%RSD_S(c_j^{CRV}) \times n_S^{CRV}$ interaction had a statistically significant effect for LAW Tanks AZ-101 (Envelope B) and AN-107 (Envelope C). The n_A^{CRV} factor and $\%RSD_S(c_j^{CRV}) \times \%RSD_A(c_j^{CRV})$ interaction were statistically significant for LAW Tanks AP-101 (Envelope A) and AN-107 (Envelope C). The $SD(G_{jk}^{GFC})$ and $SD(a_k^{GFC})$ factors and the $SD(G_{jk}^{GFC}) \times SD(a_k^{GFC})$ and $n_S^{CRV} \times n_V$ interactions had statistically significant effects for only AZ-101 (Envelope B).

Table 7.14. ILAW PCT Limits and Resulting 95% UCCI Values for Three LAW Tanks Using $n_S^{CRV} = 3$, $n_A^{CRV} = 1$, and All Other Uncertainties at their "High" Cases

Tank (Envelope)	Quantity	Units	B	Na
	PCT Limit (untransformed)	g/L	4	4
	PCT Limit (transformed)	ln(g/L)	1.386	1.386
AP-101 (Envelope A)	$\bar{\hat{y}}_i^h = \overline{\ln}(r_i^{PCT\,h})$	ln(g/L)	0.095	-0.011
	$MHW_{i,95\%\ SUCI}^h$	ln(g/L)	0.440	0.309
	$CHW_{i,95\%\ UCI}^h\ (n_S^{CRV} = 3)$	ln(g/L)	0.216	0.211
	$95\%\,UCCI\,(y_i^h)$ (a)	ln(g/L)	0.751	0.509
AZ-101 (Envelope B)	$\bar{\hat{y}}_i^h = \overline{\ln}(r_i^{PCT\,h})$	ln(g/L)	-0.586	-0.620
	$MHW_{i,95\%\ SUCI}^h$	ln(g/L)	0.305	0.213
	$CHW_{i,95\%\ UCI}^h\ (n_S^{CRV} = 3)$	ln(g/L)	0.056	0.051
	$95\%\,UCCI\,(y_i^h)$ (a)	ln(g/L)	-0.225	-0.356
AN-107 (Envelope C)	$\bar{\hat{y}}_i^h = \overline{\ln}(r_i^{PCT\,h})$	ln(g/L)	-0.846	-0.746
	$MHW_{i,95\%\ SUCI}^h$	ln(g/L)	0.401	0.277
	$CHW_{i,95\%\ UCI}^h\ (n_S^{CRV} = 3)$	ln(g/L)	0.114	0.103
	$95\%\,UCCI\,(y_i^h)$ (a)	ln(g/L)	-0.331	-0.366

(a) $95\%\,UCCI\,(y_i^h)$ is calculated using Eqs. (5.4.3a), (5.4.5), (5.4.6), and (5.4.7).

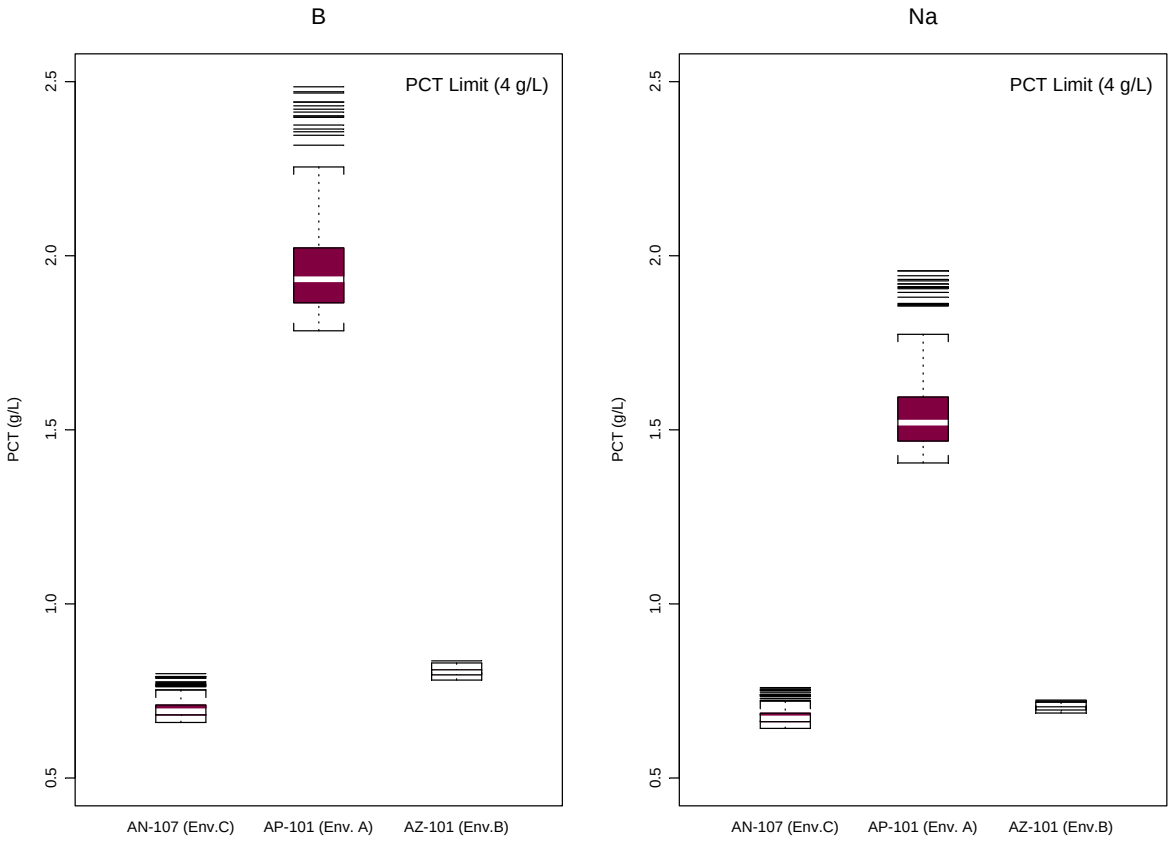

Figure 7.8. Boxplots Displaying 95% UCCIs for PCT Normalized B and Na Releases from Simulation Results Compared to the Compliance Limit

Table 7.15. Factors with Statistically Significant Effects (p-value ≤ 0.05 shaded gray) on %RHWs of ILAW PCT Normalized B and Na Releases for Three LAW Tanks

Factor / Interaction[a]	PCT B			PCT Na		
	AP-101 (Env. A)	AZ-101 (Env. B)	AN-107 (Env. C)	AP-101 (Env. A)	AZ-101 (Env. B)	AN-107 (Env. C)
$\%RSD_S(c_j^{CRV})$ [b]	0.15	<0.01	<0.01	0.19	<0.01	<0.01
$\%RSD_A(c_j^{CRV})$ [b]	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
$SD(G_{jk}^{GFC})$ [b]	0.98	<0.01	0.77	0.92	<0.01	0.60
$SD(a_k^{GFC})$ [b]	0.87	<0.01	0.98	0.87	<0.01	0.88
SD_V [c]	0.52	0.91	0.43	0.62	0.83	0.36
n_S^{CRV}	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
n_A^{CRV}	<0.01	0.33	<0.01	<0.01	0.08	<0.01
n_V [d]	0.98	0.02	0.96	0.98	0.08	0.92
$\%RSD_S(c_j^{CRV}) \times \%RSD_A(c_j^{CRV})$	0.03	0.48	<0.01	0.02	0.15	<0.01
$\%RSD_S(c_j^{CRV}) \times SD(G_{jk}^{GFC})$	0.69	0.12	0.37	0.65	0.11	0.35
$\%RSD_A(c_j^{CRV}) \times SD(G_{jk}^{GFC})$	0.43	0.60	0.16	0.50	0.23	0.12
$\%RSD_S(c_j^{CRV}) \times SD(a_k^{GFC})$	0.88	0.36	0.47	0.81	0.83	0.44
$\%RSD_A(c_j^{CRV}) \times SD(a_k^{GFC})$	0.62	0.03	0.30	0.74	0.07	0.36
$SD(G_{jk}^{GFC}) \times SD(a_k^{GFC})$	0.90	<0.01	0.92	0.87	<0.01	0.85
$\%RSD_S(c_j^{CRV}) \times SD_V$	0.90	0.70	0.92	0.98	0.89	0.97
$\%RSD_A(c_j^{CRV}) \times SD_V$	0.79	0.32	0.79	0.84	0.48	0.74
$SD(G_{jk}^{GFC}) \times SD_V$	0.62	0.80	0.79	0.70	0.66	0.80
$SD(a_k^{GFC}) \times SD_V$	0.99	0.23	0.92	0.87	0.49	0.82
$\%RSD_S(c_j^{CRV}) \times n_S^{CRV}$	0.05	<0.01	<0.01	0.06	<0.01	<0.01
$\%RSD_A(c_j^{CRV}) \times n_S^{CRV}$	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
$SD(G_{jk}^{GFC}) \times n_S^{CRV}$	0.57	0.16	0.06	0.66	0.11	0.10

(a) Only two-factor interactions were included in the ANOVA model.

(b) This factor has a "low" case and a "high" case.

(c) The notation SD_V represents both SD_V^{CRV} and SD_V^{MFPV}. This factor has a "low" and "high" case, where both SD_V^{CRV} and SD_V^{MFPV} are varied at the same time.

(d) The notation n_V represents both n_V^{CRV} and n_V^{MFPV}, with each being varied at the same time.

Table 7.15. Factors with Statistically Significant Effects (p-value ≤ 0.05 shaded gray) on %RHWs of ILAW PCT Normalized B and Na Releases for Three LAW Tanks (cont.)

Factor / Interaction	PCT B			PCT Na		
	AP-101 (Env. A)	AZ-101 (Env. B)	AN-107 (Env. C)	AP-101 (Env. A)	AZ-101 (Env. B)	AN-107 (Env. C)
$SD(a_k^{GFC}) \times n_S^{CRV}$	0.71	0.21	0.27	0.77	0.22	0.26
$SD_V \times n_S^{CRV}$	0.60	0.95	0.51	0.69	0.72	0.46
$\%RSD_S(c_j^{CRV}) \times n_A^{CRV}$	0.10	0.49	0.08	0.09	0.31	0.08
$\%RSD_A(c_j^{CRV}) \times n_A^{CRV}$	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
$SD(G_{jk}^{GFC}) \times n_A^{CRV}$	0.83	0.69	0.23	0.82	0.92	0.30
$SD(a_k^{GFC}) \times n_A^{CRV}$	0.77	0.27	0.55	0.80	0.50	0.52
$SD_V \times n_A^{CRV}$	0.47	1.00	0.48	0.55	0.69	0.45
$n_S^{CRV} \times n_A^{CRV}$	<0.01	0.01	<0.01	<0.01	<0.01	<0.01
$\%RSD_S(c_j^{CRV}) \times n_V$	0.89	0.62	0.94	0.93	0.83	0.95
$\%RSD_A(c_j^{CRV}) \times n_V$	0.71	0.23	0.97	0.62	0.54	0.93
$SD(G_{jk}^{GFC}) \times n_V$	0.91	0.42	0.85	0.92	0.78	0.78
$SD(a_k^{GFC}) \times n_V$	0.82	0.92	0.93	0.83	0.92	0.94
$SD_V \times n_V$	0.97	0.79	0.94	0.98	0.53	0.88
$n_S^{CRV} \times n_V$	0.98	0.03	0.82	0.94	0.03	0.98
$n_A^{CRV} \times n_V$	0.97	0.10	0.94	0.95	0.25	0.86

7.4.3 Illustration of the Method for Demonstrating PCT Compliance for ILAW Corresponding to a Waste Type

This section uses realistic simulated data and conservative uncertainty estimates to illustrate the use of Eqs. (5.4.8) to (5.4.14) presented in Section 5.4.5 for calculating X%/Y% UTIs to demonstrate that ILAW produced from an LAW waste type meets PCT limits. The general formula for an X%/Y% UTI is given by Eq. (5.4.8), but in this section, the following simplified form is used

$$\text{X\%/Y\% UTI} = \tilde{\mu} + k(X,Y)\,\tilde{\sigma} = \tilde{\mu} + \text{UTIHW} \tag{7.4.1}$$

where $\tilde{\mu}$ is the mean ln(PCT normalized release) of B or Na over ILAW produced from an LAW waste type, $k(X, Y)$ and $\tilde{\sigma}$ are as defined in Section 5.4.5, and UTIHW denotes the half-width of a X%/Y% UTI.

For this illustration, an AP-101 LAW waste type yielding 30 MFPV batches is considered, where each CRV batch is sampled 3 times with each sample analyzed once. Substituting the renormalized ILAW compositions from Table 7.13 and the PCT B and Na model coefficients in Table 5.1 into Eq. (5.4.9) yields the predicted ln(PCT) normalized B and Na releases. These values are used to represent the mean ($\tilde{\mu}$) of ln(PCT) normalized B and Na releases over ILAW produced from an LAW waste type.

Piepel and Cooley (2002) previously investigated an X%/Y% UTI approach of the type described in Section 5.4.5 that is not directly applicable to the current WTP ILAW compliance strategy (see Section 2.3), but can be adapted to it. They calculated UTIHWs for all combinations of the values of factors shown in Table 6.13.[(a)] The UTIHWs calculated by Piepel and Cooley that correspond to the X%/Y% UTI method presented in Section 5.4.5 are contained in their Table 4.4 (95%/95% UTIHWs) and Table 4.6 (99%/99% UTIHWs). The largest variation ($\hat{\sigma}_g = 0.50$) and uncertainties ($\hat{\sigma}_S = 0.10$, $\hat{\sigma}_A = 0.50$, and $\bar{\hat{\sigma}}_m = 0.40$) considered by Piepel and Cooley (2002) were used for conservatism. Also, $df_m = 40$ was used, which is conservative compared to the larger values of df_m values for current ILAW PCT models (see Table 5.1). The number of ILAW MFPV batches per LAW waste type (denoted I in this report, and n by Piepel and Cooley 2002) was assumed to be 30 for this illustration. UTIHWs from Table 4.4 of Piepel and Cooley (2002) for 30 batches are used to demonstrate compliance for the illustration in this section. The final report will use realistic simulated data and Eqs. (5.4.8) to (5.4.14) to calculate the 95%/95% UTI values to illustrate PCT compliance.

Using the conservative variation, uncertainties, and df_m values mentioned in the previous paragraph and assuming three samples per LAW CRV batch with one analysis per sample and 30 ILAW MFPV batches corresponding to an LAW waste type, Table 4.4 from Piepel and Cooley (2002) gives the 95%/95% UTIHW as 1.100. Note that the 95%/95% UTIHW value of 1.100 is for both ln(PCT normalized B release) and ln(PCT normalized Na release). Applying Eq. (5.4.9) yields

(a) Table 6.13 is based on Table 4.1 of Piepel and Cooley (2002), but with notation modified to match that used in this report.

$$\tilde{\mu} = \bar{\hat{y}}^{PCT\,B} = \frac{\sum_{i=1}^{I} \hat{y}_i^{PCT\,B}}{I} = \frac{1}{I}\sum_{i=1}^{I}\left[\begin{array}{l} \sum_{k=1}^{n_{mc}^{PCT\,B}} b_k^{PCT\,B}\,\bar{x}_{ik}^{MFPV} \\ + Selected\left\{\sum_{k=1}^{n_{mc}^{PCT\,B}} b_{kk}^{PCT\,B}\left(\bar{x}_{ik}^{MFPV}\right)^2 + \sum_{k=1}^{n_{mc}^{PCT\,B}-1}\ \sum_{l>k}^{n_{mc}^{PCT\,B}} b_{kl}^{PCT\,B}\,\bar{x}_{ik}^{MFPV}\,\bar{x}_{il}^{MFPV}\right\} \end{array}\right]$$

$$= \frac{1}{30}\sum_{i=1}^{30} \hat{y}_i^{PCT\,B} = 0.095 \ \ln(\text{g/L})$$

for ln(PCT normalized B release) and

$$\tilde{\mu} = \bar{\hat{y}}^{PCT\,Na} = \frac{\sum_{i=1}^{I} \hat{y}_i^{PCT\,Na}}{I} = \frac{1}{I}\sum_{i=1}^{I}\left[\begin{array}{l} \sum_{k=1}^{n_{mc}^{PCT\,Na}} b_k^{PCT\,Na}\,\bar{x}_{ik}^{MFPV} \\ + Selected\left\{\sum_{k=1}^{n_{mc}^{PCT\,Na}} b_{kk}^{PCT\,Na}\left(\bar{x}_{ik}^{MFPV}\right)^2 + \sum_{k=1}^{n_{mc}^{PCT\,Na}-1}\ \sum_{l>k}^{n_{mc}^{PCT\,Na}} b_{kl}^{PCT\,Na}\,\bar{x}_{ik}^{MFPV}\,\bar{x}_{il}^{MFPV}\right\} \end{array}\right]$$

$$= \frac{1}{30}\sum_{i=1}^{30} \hat{y}_i^{PCT\,Na} = -0.011 \ \ln(\text{g/L})$$

for ln(PCT normalized Na release).

Combining the above results in Eq. (7.4.1) yields

$$95\%/95\%\ \text{UTI} = \tilde{\mu} + k(95\%,95\%)\ \tilde{\sigma} = \tilde{\mu} + \text{UTIHW} = 0.095 + 1.100 = 1.195\ \ln(\text{g/L})$$

for ln(PCT normalized B release) and

$$95\%/95\%\ \text{UTI} = \tilde{\mu} + k(95\%,95\%)\ \tilde{\sigma} = \tilde{\mu} + \text{UTIHW} = -0.011 + 1.100 = 1.089\ \ln(\text{g/L})$$

for ln(PCT normalized Na release). These values can be converted to units of g/L by exponentiating, yielding $e^{1.195} = 3.304$ g/L for normalized B release and $e^{1.089} = 2.971$ g/L for normalized Na release. In both cases, these release rates are smaller than the compliance limit of 4 g/L. Therefore, even though conservative estimates of uncertainties were used for the illustration, 3 samples per LAW CRV batch with 1 analysis per sample was sufficient to demonstrate compliance with the PCT limits.

7.4.4 Results of Simulations to Assess the Effects of Batch-to-Batch Variations, Process Uncertainties, and Numbers of Samples, Analyses, and Volume Determinations on ILAW PCT Compliance over an LAW Waste Type

The methodology described in Section 5.4.6 can be used to investigate the impacts of the number of samples per CRV batch, the number of chemical analyses per CRV sample, the number of volume determinations per CRV and MFPV batch, and other factors on the ability to demonstrate that ILAW

produced from an LAW waste type complies with the PCT limits specified in Contract Specification 2.2.2.17.2. The methodology in Section 5.4.6 uses the formula for X%/Y% UTIs on PCT normalized releases (of B and Na) presented in Section 5.4.5. The general formula for an X%/Y% UTI is given by Eq. (5.4.8) in Section 5.4.5. However, the simplified formula given in Eq. (7.4.1) was used to produce the results in this section.

Piepel and Cooley (2002) previously investigated an X%/Y% UTI approach of the type described in Section 5.4.5 that is directly not directly applicable to the current WTP ILAW compliance strategy (see Section 2.3), but can be adapted to it. They calculated UTIHWs for all combinations of the values of factors shown in Table 6.13.[(a)] The UTIHWs calculated by Piepel and Cooley that correspond to the X%/Y% UTI method presented in Section 5.4.5 are contained in their Table 4.4 (95%/95% UTIHWs) and Table 4.6 (99%/99% UTIHWs). The UTIHW values in those tables for application to ln(PCT normalized release) are in units of ln(g/m^2). In this report, units of ln(g/L) are used for ln(PCT normalized release). Because 1 g/m^2 = 2 g/L[(b)], we have ln(g/m^2) = 0.6931 + ln(g/L) and ln(g/L) = ln(g/m^2) – 0.6931.

The UTIHW values in Tables 4.4 and 4.6 of Piepel and Cooley (2002) can be used to determine the required numbers of samples per CRV batch (n_S^{CRV}) and analyses per CRV sample (n_A^{CRV}) by considering likely values of $\tilde{\mu}$, solving for the maximum acceptable value of UTIHW, and determining which entries of Tables 4.4 and 4.6 satisfy the solution. Thus, rewriting Eq. (7.4.1) when comparing to a PCT normalized release limit yields

$$\text{X\%/Y\% UTI} = \tilde{\mu} + \text{UTIHW} \le \ln(\text{limit}) \quad \Rightarrow \quad \text{UTIHW} \le \ln(\text{limit}) - \tilde{\mu} \, . \tag{7.4.2}$$

The UTIHW values in Tables 4.4 and 4.6 of Piepel and Cooley that are less than the maximum allowable per Eq. (7.4.2) then correspond to the required number of samples per CRV batch and analyses per CRV sample, which depend on the magnitudes of (1) the variation of ILAW over MFPV batches corresponding to an LAW waste type and (2) uncertainties for each ILAW MFPV batch.

The 95%/95% UTIHW results from Table 4.4 of Piepel and Cooley (2002) were utilized in another way to conservatively demonstrate that 3 samples per CRV batch and 1 chemical analysis per CRV sample are sufficient to easily demonstrate compliance with nominal LAW glass compositions for each of the three LAW tanks (AP-101, AZ-101, and AN-107) used for investigations in this report. Specifically, the largest variation ($\hat{\sigma}_g = 0.50$) and uncertainties ($\hat{\sigma}_S = 0.10$, $\hat{\sigma}_A = 0.50$, and $\bar{\hat{\sigma}}_m = 0.40$) considered by Piepel and Cooley (2002) were used for conservatism. Also, $df_m = 40$ was used, which is conservative compared to the larger values of df_m values for current ILAW PCT models (see Table 5.1). The number of ILAW MFPV batches per LAW waste type (denoted I in this report, and n by Piepel and Cooley 2002) is expected to be at least 10, and potentially much larger for some LAW waste types. For this conservative investigation, the smallest number of batches (10) considered by Piepel and Cooley (2002) was used.

(a) Table 6.13 is based on Table 4.1 of Piepel and Cooley (2002), but with notation modified to match that used in this report.

(b) Applying the standard assumption of a surface area-to-volume ratio of 2000 m^{-1}, it results that 1 g/m^2 = 2 g/L.

Table 7.16 shows the resulting 95%/95% UTI values on PCT normalized releases of B and Na for LAW glass corresponding to Tanks AP-101, AZ-101, and AN-107 obtained using the conservative estimates discussed in the previous paragraph. Compliance was demonstrated in each case, except with PCT normalized release of B for AP-101. With this exception, compliance was achieved despite the significant conservatism in the inputs for the calculations summarized in Table 7.16. The illustration presented in Section 7.4.3 calculated the 95%/95% UTI value for PCT normalized release of B for AP-101 using 30 batches instead of 10 batches. This increase of 20 batches was enough to lower the 95%/95% UTI value from 4.242 g/L (see Table 7.16) to 3.304 g/L (see Section 7.4.3). This shows that compliance can be more easily demonstrated with a larger number of MFPV batches corresponding to an LAW waste type. This exercise shows that at least 3 samples per CRV batch with 1 analysis per sample should be sufficient to demonstrate with 95% confidence that at least 95% of the ILAW produced over an LAW waste type will have PCT normalized B and Na releases that meet the Contract Specification 2.2.2.17.2 limits. This conclusion is conditional on (1) the WTP ILAW having compositions similar to

Table 7.16. 95%/95% UTI Values for PCT Normalized Releases of B and Na from ILAW Corresponding to Three LAW Tanks Assuming $n_S^{CRV} = 3$, $n_A^{CRV} = 1$, and Conservative Values of Inputs Considered by Piepel and Cooley (2002)[a]

PCT	Limit[b]	AP-101			AZ-101			AN-107		
		$\tilde{\mu}$ [c]	95%/95% UTIHW[d]	95%/95% UTI[e]	$\tilde{\mu}$ [c]	95%/95% UTIHW[d]	95%/95% UTI[e]	$\tilde{\mu}$ [c]	95%/95% UTIHW[d]	95%/95% UTI[e]
Results in ln(g/m^2)										
B	0.693	-0.598	1.350	0.752	-1.278	1.350	0.071	-1.539	1.350	-0.189
Na	0.693	-0.704	1.350	0.646	-1.313	1.350	0.037	-1.440	1.350	-0.09
Results in ln(g/L)[f]										
B	1.386	0.095	1.350	1.445	-0.586	1.350	0.764	-0.846	1.350	0.504
Na	1.386	-0.011	1.350	1.339	-0.620	1.350	0.730	-0.746	1.350	0.604
	Results in g/L									
B	4	1.100	3.142	4.242	0.557	1.590	2.147	0.429	1.221	1.655
Na	4	0.989	2.826	3.815	0.538	1.537	2.075	0.474	1.355	1.829

(a) Using the notation of Piepel and Cooley (2002) as summarized in Table 6.13, the maximum variation and uncertainty SDs used were $\hat{\sigma}_g = 0.50$, $\hat{\sigma}_S = 0.10$, $\hat{\sigma}_A = 0.50$, and $\bar{\hat{\sigma}}_m = 0.40$. Conservative values of $df_m = 40$ and 10 MFPV batches per LAW waste type were also used.

(b) The limits for PCT normalized releases of B and Na are listed in units of g/m^2 and g/L in Eq. (5.4.1).

(c) $\tilde{\mu}$ denotes the predicted ln(PCT normalized release) values for B and Na calculated using the PCT models in Table 5.1 for the nominal AP-101, AZ-101, and AN-107 ILAW compositions given in Table D.11 of Appendix D. Before applying the models in Table 5.1, the compositions in Table D.11 were normalized to mass fractions of the 11 components appearing in the models.

(d) 95%/95% UTIHW denotes the half-width of a 95%/95% UTI found in Table 4.4 of Piepel and Cooley (2002) for the combination of inputs listed in footnote (a). The Piepel and Cooley (2002) UTIHWs for this application are in ln(g/m^2) units. For the other units shown in the table, the UTIHWs were obtained via UTIHW = UTI - $\tilde{\mu}$ after converting UTI and $\tilde{\mu}$ to the new units.

(e) 95%/95% UTI is given by $\tilde{\mu}$ + UTIHW, according to Eq. (7.4.1).

(f) One g/L is equal to 2 g/m^2. This leads to the conversion ln(g/L) = ln(2) + ln(g/m^2) = 0,6931+ ln(g/m^2).

those for LAW Tanks AP-101, AZ-101, and AN-107, (2) the number of MFPV batches corresponding to an LAW waste type not being too small, and (3) the batch-to-batch variation and within-batch uncertainties are not larger than the conservative values assumed for the calculations.

7.5 Compliance Results for ILAW Contract Specification 2.2.2.17.3: Vapor Hydration Test (VHT)

Section 7.5.1 illustrates, using a realistic example, the methodology presented in Section 5.4.3 for demonstrating that ILAW from a single MFPV batch satisfies the VHT limit.

Section 7.5.2 presents results from the Monte Carlo simulations described in Section 5.4.4 for assessing the effects of (1) CRV mixing/sampling and analytical uncertainties and (2) the numbers of samples per CRV batch, analyses per CRV sample, and volume determinations of CRV and MFPV batches on the ability to demonstrate VHT compliance for ILAW from a single MFPV batch. These results provide a basis for (1) assessing the sensitivity of single-MFPV-batch VHT estimates to the range of possible uncertainties and (2) the WTP Project to decide on the number of samples per CRV batch, the number of chemical analyses per CRV sample, and the number of volume determinations of CRV and MFPV batches necessary to demonstrate VHT compliance for ILAW from a single MFPV batch.

Section 7.5.3 illustrates, using a realistic example, the methodology presented in Section 5.4.5 for demonstrating that ILAW over an LAW waste type satisfies the VHT limit.

Section 7.5.4 presents the results from the simulation described in Section 5.4.6 for assessing the effects of (1) the variations and uncertainties in VHT responses over an LAW waste type and (2) the numbers of samples per CRV batch, number of analyses per CRV sample, and the number of volume determinations per CRV and MFPV batches on the ability to demonstrate VHT compliance for ILAW over an LAW waste type. These results provide a basis for (1) assessing the sensitivity of VHT estimates to the ranges of possible variations and uncertainties over an LAW waste type and (2) the WTP Project to decide on the number of samples per CRV batch, the number of chemical analyses per CRV sample, and the number of CRV and MFPV volume determinations necessary to demonstrate VHT compliance for ILAW over an LAW waste type.

7.5.1 Illustration of Methods for Demonstrating VHT Compliance for ILAW Corresponding to an MFPV Batch

This section uses Monte Carlo simulation results to illustrate the use of Eqs. (5.4.2), (5.4.3a), (5.4.5), (5.4.6), and (5.4.7) presented in Section 5.4.3 for calculating CL% UCCIs to demonstrate that ILAW corresponding to a single MFPV batch meets the VHT limit.

For this illustration, the Monte Carlo simulation results from the AP-101 test case with three CRV samples, each sample analyzed once, one CRV and one MFPV volume determination, and all uncertainties at the "high" case were used. Table 7.17 lists the normalized average mass composition (mass fractions) calculated using Eq. (4.3.3). These normalized ILAW composition values were calculated using the nominal AP-101 mass compositions as found in Table D.11 in Appendix D. For the final report, these normalized ILAW composition values will be calculated using CRV concentrations for

three realistically simulated samples as well as realistically simulated values for all the other inputs found in Eq. (B.1.11) from Section B.1 of Appendix B. Substituting the normalized ILAW composition in Table 7.17 and the VHT model coefficients in Table 5.1 into Eq. (5.4.3a) yields the predicted VHT results shown in Table 7.17.

Table 7.17 also shows the SDs of model predictions calculated using the $\sqrt{(\bar{\boldsymbol{x}}_i^{MFPV})^T \boldsymbol{\Sigma}_b^h \bar{\boldsymbol{x}}_i^{MFPV}}$ portion of Eq. (5.4.7). These values are used in calculating the $MHW_{i,95\%\ SUCI}^h$ quantity given by Eq. (5.4.7). Also listed in Table 7.17 are values of $CHW_{i,95\%\ UCI}^h$ obtained by applying Eq. (5.4.6) to the results of a Monte Carlo simulation based on the simulated sampled and measured quantities. The Monte Carlo simulation used the high uncertainty values for all uncertain quantities in Eq. (B.1.11).

Finally, Table 7.17 presents the results of calculations using Eqs. (5.4.5) through (5.4.7) to obtain 95% UCCIs for VHT alteration rate (g/m^{2}day). The 95% UCCI values are seen to be significantly below the Contract Specification 2.2.2.17.3 limiting value of 50 g/m^{2}day.

Detailed illustrations of calculations using Eqs. (5.4.2), (5.4.3a), (5.4.5), (5.4.6), and (5.4.7) to obtain the 95% UCCI for VHT alteration rate (g/m^{2}day) are now presented. Intermediate results from Table 7.17 are used in some cases to reduce what would otherwise be very long algebraic equations. Applying Eq. (5.4.3a) yields

$$\hat{\bar{y}}_i^{VHT} = \sum_{k=1}^{n_{mc}^{VHT}} b_k^{VHT}\, \bar{x}_{ik}^{MFPV} + Selected\left\{ \sum_{k=1}^{n_{mc}^{VHT}} b_{kk}^{VHT} \left(\bar{x}_{ik}^{MFPV}\right)^2 + \sum_{k<}^{n_{mc}^{VHT}-1} \sum_{l}^{n_{mc}^{VHT}} b_{kl}^{VHT}\, \bar{x}_{ik}^{MFPV}\, \bar{x}_{il}^{MFPV} \right\}$$

$$= (49.861)(0.0608) + \ldots + (-83.534)(0.0072) \quad \text{linear terms}$$

$$+ (1430.328)\left(3.00 \times 10^{-4}\right) + \ldots + (304.468)(0.0087) \quad \text{crossproduct terms}$$

$$= 2.590 \text{ ln(μm)}.$$

Applying Eq. (5.4.6) to the results of a Monte Carlo simulation of 1000 runs using the high levels of uncertainty for all uncertain quantities yields

$$CHW_{i,95\%\ UCI}^{VHT} = \hat{\bar{y}}_{i,95\%}^{VHT} - \hat{\bar{y}}_i^{VHT} = 3.028 - 2.590 = 0.438 \text{ ln(μm)}.$$

Applying Eq. (5.4.7), where $n = 70$ and $p = 22$ per Table 5.1, yields

$$MHW_{i,95\%\ SUCI}^h = \sqrt{p\, F_{1-\alpha}(p, n-p)}\left(\sqrt{(\bar{\boldsymbol{x}}_i^{MFPV})^{\mathrm{T}} \boldsymbol{\Sigma}_b^{VHT} \bar{\boldsymbol{x}}_i^{MFPV}}\right) = \sqrt{22 F_{0.95}(22,48)}(0.261) = 1.529 \text{ ln(μm)}.$$

Finally, combining the above results in Eq. (5.4.5) yields

$$95\%\ UCCI[D^{VHT}] = \hat{\bar{y}}_i^{VHT} + CHW_{i,95\%\ UCI}^{VHT} + MHW_{i,95\%\ SUCI}^{VHT} = 2.590 + 0.438 + 1.529 = 4.556 \text{ ln(μm)}.$$

Table 7.17. Normalized ILAW Composition, Model-Predicted VHT Results, and Model Uncertainties for Simulated Data on an ILAW MFPV Batch Corresponding to LAW Tank AP-101

Model Term	VHT		
	$\bar{x}_{ik}^{MFPV}$ (a)	b_k^{VHT} (b)	
Al_2O_3	0.0608	49.861	
B_2O_3	0.0995	8.581	
CaO	0.0200	-21.469	
Fe_2O_3	0.0535	18.324	
K_2O	0.0400	137.663	
Li_2O	$7.74\ E^{-7}$	113.437	
MgO	0.0150	-31.398	
Na_2O	0.1837	35.203	
SO_3	0.0036	-707.506	
SiO_2	0.4375	-15.589	(c)
TiO_2	0.0201	-20.149	
ZnO	0.0295	1.849	
ZrO_2	0.0299	-73.697	
Others	0.0072	-83.534	
MgO × TiO_2	3.00×10^{-4}	1430.328	
Al_2O_3 × K_2O	0.0024	-1206.846	
CaO × Fe_2O_3	0.0011	-486.322	
K_2O × ZnO	0.0012	-1288.199	
B_2O_3 × CaO	0.0020	-731.607	
B_2O_3 × SO_3	3.58×10^{-4}	6505.983	
MgO × Others	1.07×10^{-4}	1733.193	
CaO × SiO_2	0.0087	304.468	
Model-Predicted VHT Alteration Depth: Nominal and 95th Percentile [ln(µm)]			
$\hat{\bar{y}}_i^{VHT}$	2.590		(c)
$\hat{\bar{y}}_{i,95\%}^{VHT}$	3.028		
Model Uncertainties of Predicted VHT Alteration Depth [ln(µm)]			
$SD_M[\hat{y}^{VHT}(\bar{\bar{x}})]$	0.261	(c)	

95% UCCIs on VHT						
	$\hat{\bar{y}}$ Alteration Depth [ln(µm)]	$CHW_{95\%\ UCI}$ [ln(µm)]	$MHW_{95\%\ SUCI}$ [ln(µm)]	95% UCCI Alteration Depth [ln(µm)]	95% UCCI Alteration Rate [g/m^2day]	Limit [g/m^2day]
VHT	2.590	0.438	1.529	4.556	10.516	50

(a) The average ILAW composition for the MFPV batch is expressed in normalized mass fractions of the components in the model. Crossproduct terms are formed from these normalized mass fractions.
(b) The model coefficients for the ILAW VHT alteration depth are from Table 5.1.
(c) This portion of the table is intentionally blank.

This VHT alteration depth [ln(μm)] can be converted to alteration rate (g/m^{2}day) by applying Eq. (5.4.2)

$$R^{VHT} = e^{\ln(D^{VHT})} \times \frac{2.65}{24} = e^{4.556} \times \frac{2.65}{24} = 10.516 \text{ g/m}^2\text{day}.$$

This 95% UCCI on R^{VHT} of 10.516 g/m^2/day is much smaller than the compliance limit of 50 g/m^2/day. Therefore, with 3 samples and 1 analysis, the ILAW is shown to be compliant with the VHT limit in this illustration.

7.5.2 Results of Simulations to Assess the Effects of Process Uncertainties, Numbers of Samples, Analyses, and Volume Determinations on ILAW VHT Uncertainties and Compliance Corresponding to an MFPV Batch

This section uses the methodology described in Section 5.4.4 to assess the numbers of samples per CRV batch, analyses per CRV sample, and number of CRV and MFPV volume determinations necessary to demonstrate compliance with VHT limits for each ILAW MFPV batch. The methodology in Section 5.4.4 uses Eqs. (5.4.2), (5.4.3a), (5.4.5), (5.4.6), and (5.4.7) to calculate CL% UCCI values for VHT alteration rates (g/m^{2}day) for various combinations of input factor values. If the CL% UCCI values for a given combination of factor values are less than the VHT specification limits, then compliance is demonstrated for that combination. Values of the mass fraction compositions of ILAW calculated using several inputs are necessary in using Eqs. (5.4.5), (5.4.6), and (5.4.7) to calculate the CL% UCCI values for VHT alteration rates. These inputs include (1) the n_A^{CRV} analyses of n_S^{CRV} samples per CRV batch, (2) the n_V volume determinations per CRV and MFPV batches, (3) the model coefficients and variance-covariance matrices, and (4) the selected statistical confidence level (CL%) and corresponding CL% percentile of the empirical distribution from the 1000 Monte Carlo simulations.

Table 7.18 shows how taking at least 3 samples per LAW CRV batch with 1 analysis of each sample will be sufficient to demonstrate compliance with the VHT limit for each ILAW MFPV batch. The calculations in Table 7.18 assumed all uncertainties to be at their highest levels. Table 7.18 shows the calculated 95% UCCI values (for VHT alteration rates) for each of the three LAW tanks used for illustrations in this report. Comparing these values to the VHT limit of 50 g/m^{2}day shows that at least 3 samples per MFPV batch with 1 analysis per sample should be sufficient to demonstrate compliance with the VHT limit for each MFPV batch.

In addition to the results described so far, we now summarize the results of the investigation described in Section 5.4.4. That investigation involved calculating CL% UCCI values of VHT alteration rate for various combinations of factors (test runs) in the Monte Carlo simulation as described in Section 3.4.2. Typically, the results of such investigations would be summarized in a table (similar to ones presented in Section 6 and earlier in Section 7). However, no such table was necessary to display the numbers of samples per CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations necessary to comply with VHT because all test runs in the simulation were compliant. This means that when assuming the "high" case uncertainties, only one CRV sample with one analysis per sample was necessary to be compliant. Figure 7.9 shows boxplots (see Appendix H.3 for help interpreting boxplots) of the 95% UCCI values for VHT alteration rates across all combinations of input factors in the experimental design (see Section 3.4.2). As can be seen from the boxplots, the 95% UCCI

values for VHT alteration rates for all of the simulation runs were well below the VHT limit, indicating that compliance was easily demonstrated.

Table 7.18. ILAW VHT Limits, and Resulting 95% UCCI Values for Three LAW Tanks Using $n_S^{CRV} = 3$, $n_A^{CRV} = 1$, and All Other Uncertainties at the "High" Cases

Tank (Envelope)	Quantity	Units	VHT
	VHT Limit	g/m^{2}day	50
AP-101 (Envelope A)	$\hat{\bar{y}}_i^{VHT} = \hat{\ln}(D^{VHT})$	ln(μm)	2.590
	$MHW_{i,95\%\,SUCI}^{h}$	ln(μm)	1.529
	$CHW_{i,95\%\,UCI}^{h}$ ($n_S^{CRV} = 3$)	ln(μm)	0.438
	$95\%\,UCCI(\ln[D^{VHT}])$ (a)	ln(μm)	4.556
	$95\%\,UCCI(R^{VHT})$ (b)	g/m^{2}day	10.516
AZ-101 (Envelope B)	$\hat{\bar{y}}_i^{VHT} = \hat{\ln}(D^{VHT})$	ln(μm)	2.805
	$MHW_{i,95\%\,SUCI}^{h}$	ln(μm)	1.046
	$CHW_{i,95\%\,UCI}^{h}$ ($n_S^{CRV} = 3$)	ln(μm)	0.157
	$95\%\,UCCI(\ln[D^{VHT}])$ (a)	ln(μm)	4.007
	$95\%\,UCCI(R^{VHT})$ (b)	g/m^{2}day	6.071
AN-107 (Envelope C)	$\hat{\bar{y}}_i^{VHT} = \hat{\ln}(D^{VHT})$	ln(μm)	0.662
	$MHW_{i,95\%\,SUCI}^{h}$	ln(μm)	1.447
	$CHW_{i,95\%\,UCI}^{h}$ ($n_S^{CRV} = 3$)	ln(μm)	0.443
	$95\%\,UCCI(\ln[D^{VHT}])$ (a)	ln(μm)	2.552
	$95\%\,UCCI(R^{VHT})$ (b)	g/m^{2}day	1.417

(a) $95\%\,UCCI(\ln[D^{VHT}])$ is calculated using Eqs. (5.4.3a), (5.4.5), (5.4.6), and (5.4.7).

(b) $95\%\,UCCI(\ln[D^{VHT}])$ is converted to $95\%\,UCCI(R^{VHT})$ using Eq. (5.4.2).

ANOVA was performed for VHT results on each of the three LAW tanks used for investigations in this report to help determine which factors from Table 3.3 and which interactions most affect %RHWs of CL% UCCIs on VHT alteration rates. The resulting ANOVA p-values are summarized in Table 7.19. Those factors with p-values below 0.05 are considered to have statistically significant effects on %RHWs for VHT alteration rates. Factors with statistically significant effects across each of the three LAW tanks included $\%RSD_A(c_j^{CRV})$, n_S^{CRV}, and n_A^{CRV}. The $\%RSD_A(c_j^{CRV}) \times n_S^{CRV}$ and $\%RSD_A(c_j^{CRV}) \times n_A^{CRV}$

interactions also had statistically significant effects. The $\%RSD_S(c_j^{CRV})$, $SD(G_{jk}^{GFC})$, and $SD(a_k^{GFC})$ factors and the $\%RSD_S(c_j^{CRV}) \times n_S^{CRV}$ interaction had statistically significant effects for LAW Tanks AZ-101 (Envelope B) and AN-107 (Envelope C). The $\%RSD_S(c_j^{CRV}) \times SD(a_k^{GFC})$, $\%RSD_A(c_j^{CRV}) \times SD(a_k^{GFC})$, $SD(G_{jk}^{GFC}) \times SD(a_k^{GFC})$, and $SD(a_k^{GFC}) \times n_A^{CRV}$ interactions had statistically significant effects for LAW Tank AZ-101 (Envelope B). The $SD(G_{jk}^{GFC}) \times n_S^{CRV}$ and $n_S^{CRV} \times n_A^{CRV}$ interactions had statistically significant effects only for LAW Tank AN-107 (Envelope C).

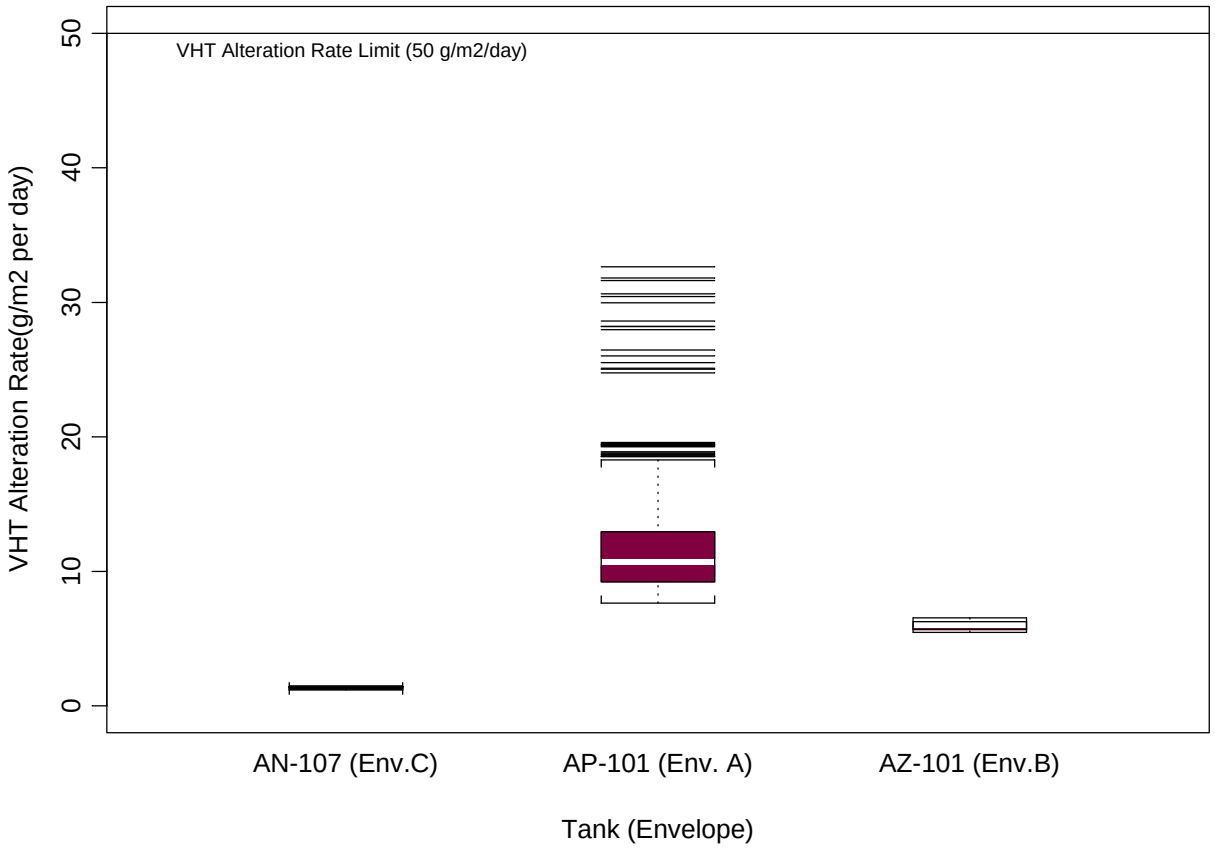

Figure 7.9. Boxplots Displaying 95% UCCIs for VHT Alteration Rate from Simulation Results Compared to the Compliance Limit

Table 7.19. Factors with Statistically Significant Effects (p-value ≤ 0.05 shaded gray) on %RHWs of ILAW VHT Alteration Rates for Three LAW Tanks

Factor / Interaction[a]	AP-101 (Env. A)	AZ-101 (Env. B)	AN-107 (Env. C)
$\%RSD_S(c_j^{CRV})$ [b]	0.94	0.01	<0.01
$\%RSD_A(c_j^{CRV})$ [b]	<0.01	<0.01	<0.01
$SD(G_{jk}^{GFC})$ [b]	0.89	<0.01	<0.01
$SD(a_k^{GFC})$ [b]	0.81	<0.01	0.06
SD_V [c]	0.73	0.65	0.75
n_S^{CRV}	<0.01	<0.01	<0.01
n_A^{CRV}	<0.01	0.01	0.01
n_V [d]	0.71	0.26	0.70
$\%RSD_S(c_j^{CRV}) \times \%RSD_A(c_j^{CRV})$	0.32	0.97	0.30
$\%RSD_S(c_j^{CRV}) \times SD(G_{jk}^{GFC})$	0.70	0.69	0.39
$\%RSD_A(c_j^{CRV}) \times SD(G_{jk}^{GFC})$	0.90	0.13	0.20
$\%RSD_S(c_j^{CRV}) \times SD(a_k^{GFC})$	0.89	0.02	0.47
$\%RSD_A(c_j^{CRV}) \times SD(a_k^{GFC})$	0.90	0.02	0.39
$SD(G_{jk}^{GFC}) \times SD(a_k^{GFC})$	0.69	0.01	0.08
$\%RSD_S(c_j^{CRV}) \times SD_V$	0.84	0.99	0.86
$\%RSD_A(c_j^{CRV}) \times SD_V$	0.85	0.08	0.71
$SD(G_{jk}^{GFC}) \times SD_V$	0.59	0.77	0.84
$SD(a_k^{GFC}) \times SD_V$	0.54	0.46	0.88
$\%RSD_S(c_j^{CRV}) \times n_S^{CRV}$	0.90	<0.01	<0.01
$\%RSD_A(c_j^{CRV}) \times n_S^{CRV}$	<0.01	<0.01	<0.01
$SD(G_{jk}^{GFC}) \times n_S^{CRV}$	0.85	0.70	0.01

(a) Only two-factor interactions were included in the ANOVA model.
(b) This factor has a "low" case and a "high" case.
(c) The notation SD_V represents both SD_V^{CRV} and SD_V^{MFPV}. This factor has a "low" and "high" case, where both SD_V^{CRV} and SD_V^{MFPV} are varied at the same time.
(d) The notation n_V represents both n_V^{CRV} and n_V^{MFPV}, with each being varied at the same time.

Table 7.19. Factors with Statistically Significant Effects (p-value ≤ 0.05 shaded gray) on %RHWs of ILAW VHT Alteration Rates for Three LAW Tanks (cont.)

Factor / Interaction	AP-101 (Env. A)	AZ-101 (Env. B)	AN-107 (Env. C)
$SD(a_k^{GFC}) \times n_S^{CRV}$	0.90	0.04	0.74
$SD_V \times n_S^{CRV}$	0.71	0.97	0.54
$\%RSD_S(c_j^{CRV}) \times n_A^{CRV}$	0.18	0.93	0.74
$\%RSD_A(c_j^{CRV}) \times n_A^{CRV}$	<0.01	<0.01	<0.01
$SD(G_{jk}^{GFC}) \times n_A^{CRV}$	0.96	0.65	0.09
$SD(a_k^{GFC}) \times n_A^{CRV}$	0.93	0.04	0.70
$SD_V \times n_A^{CRV}$	0.87	0.79	0.79
$n_S^{CRV} \times n_A^{CRV}$	0.24	0.08	<0.01
$\%RSD_S(c_j^{CRV}) \times n_V$	0.78	1.00	0.77
$\%RSD_A(c_j^{CRV}) \times n_V$	0.70	0.55	0.67
$SD(G_{jk}^{GFC}) \times n_V$	0.70	0.29	0.44
$SD(a_k^{GFC}) \times n_V$	0.98	0.23	0.72
$SD_V \times n_V$	0.84	0.45	0.61
$n_S^{CRV} \times n_V$	0.84	0.28	0.91
$n_A^{CRV} \times n_V$	0.62	0.44	0.60

7.5.3 Illustration of the Method for Demonstrating VHT Compliance for ILAW Corresponding to a Waste Type

This section uses realistic simulated data and conservative uncertainty estimates to illustrate the use of Eqs. (5.4.8) to (5.4.14) presented in Section 5.4.5 for calculating X%/Y% UTIs to demonstrate that ILAW produced from an LAW waste type meets the VHT limit. The general formula for an X%/Y% UTI is given by Eq. (5.4.8), but in this section the following simplified form is used

$$\text{X\%/Y\% UTI} = \tilde{\mu} + k(X,Y)\,\tilde{\sigma} = \tilde{\mu} + \text{UTIHW} \qquad (7.5.1)$$

where $\tilde{\mu}$ is the mean $\ln(D^{VHT})$ over ILAW produced from an LAW waste type, $k(X, Y)$ and $\tilde{\sigma}$ are as defined in Section 5.4.5, and UTIHW denotes the half-width of a X%/Y% UTI.

For this illustration, an AP-101 LAW waste type yielding 30 MFPV batches is considered where each CRV batch is sampled 3 times with each sample analyzed once. Substituting the renormalized ILAW compositions from Table 7.17 and the VHT model coefficients in Table 5.1 into Eq. (5.4.9) yields the predicted $\ln(D^{VHT})$ results used to represent the mean ($\tilde{\mu}$) $\ln(D^{VHT})$ over ILAW produced from an LAW waste type.

Piepel and Cooley (2002) previously investigated an X%/Y% UTI approach of the type described in Section 5.4.5 that is not directly applicable to the current WTP ILAW compliance strategy (see Section 2.3), but can be adapted to it. They calculated UTIHWs for all combinations of the values of factors shown in Table 6.13.[(a)] The UTIHWs calculated by Piepel and Cooley that correspond to the X%/Y% UTI method presented in Section 5.4.5 are contained in their Table 4.4 (95%/95% UTIHWs) and Table 4.6 (99%/99% UTIHWs). The largest variation ($\hat{\sigma}_g = 0.50$) and uncertainties ($\hat{\sigma}_S = 0.10$, $\hat{\sigma}_A = 0.50$, and $\bar{\hat{\sigma}}_m = 0.40$) considered by Piepel and Cooley (2002) were used for conservatism. Also, $df_m = 40$ was used, which is conservative compared to the larger values of df_m values for the current ILAW VHT model (see Table 5.1). The number of ILAW MFPV batches per LAW waste type (denoted I in this report and n by Piepel and Cooley 2002) was assumed to be 30 for this illustration. UTIHWs from Table 4.4 of Piepel and Cooley (2002) are used to demonstrate compliance for the illustration in this section. The final report will use realistic simulated data and Eqs. (5.4.8) to (5.4.14) to calculate the 95%/95% UTI values to illustrate VHT compliance.

Using the conservative variation, uncertainties, and df_m values mentioned in the previous paragraph and assuming three samples per LAW CRV batch with one analysis per sample and 30 batches, Table 4.4 from Piepel and Cooley (2002) gives the 95%/95% UTIHW as 1.100. Applying Eq. (5.4.9) yields

$$\tilde{\mu} = \bar{\hat{y}}^{VHT} = \frac{\sum_{i=1}^{I} \hat{y}_i^{VHT}}{I} = \frac{1}{I}\sum_{i=1}^{I}\left[\begin{array}{l} \sum_{k=1}^{n_{mc}^{VHT}} b_k^{VHT}\, \bar{x}_{ik}^{MFPV} \\ + \mathit{Selected}\left\{ \sum_{k=1}^{n_{mc}^{VHT}} b_{kk}^{VHT}\left(\bar{x}_{ik}^{MFPV}\right)^2 + \sum_{k=1}^{n_{mc}^{VHT}-1}\sum_{l>k}^{n_{mc}^{VHT}} b_{kl}^{VHT}\, \bar{x}_{ik}^{MFPV}\, \bar{x}_{il}^{MFPV} \right\} \end{array}\right]$$

$$= \frac{1}{30}\sum_{i=1}^{30} \hat{y}_i^{VHT} = 2.590 \ \ \ln(\mu\text{m})$$

Combining the above results in Eq. (7.5.1) yields

$$95\%/95\%\ \text{UTI} = \tilde{\mu} + k(95\%,95\%)\ \tilde{\sigma} = \tilde{\mu} + \text{UTIHW} = 2.590 + 1.100 = 3.690\ \ln(\mu\text{m}).$$

The 95%/95% UTI on alteration depth [ln(μm)] can be converted to alteration rate (g/m^2day) by applying Eq. (5.4.2)

$$95\%/95\%\ \text{UTI on}\ R^{VHT} = e^{ln(D^{VHT})} \times \frac{2.65}{24} = e^{3.690} \times \frac{2.65}{24} = 4.422\ \ g/m^2day.$$

(a) Table 6.13 is based on Table 4.1 of Piepel and Cooley (2002), but with notation modified to match that used in this report.

This 95% UCCI on R^{VHT} of 4.422 g/m^{2}day is much smaller than the compliance limit of 50 g/m^{2}day. Therefore, even though conservative estimates of uncertainties were used for the illustration, 3 samples per LAW CRV batch with 1 analysis per sample was sufficient to demonstrate compliance with the VHT limit.

7.5.4 Results of Simulations to Assess the Effects of Batch-to-Batch Variations, Process Uncertainties, and Numbers of Samples, Analyses, and Volume Determinations on ILAW VHT Compliance over an LAW Waste Type

The methodology described in Section 5.4.6 can be used to investigate the impacts of the number of samples per CRV batch, the number of chemical analyses per CRV sample, the number of volume determinations per CRV and MFPV batch, and other factors on the ability to demonstrate that ILAW produced from an LAW waste type complies with the VHT limits specified in Contract Specification 2.2.2.17.3. The methodology in Section 5.4.6 uses the formula for X%/Y% UTIs on VHT alteration rate presented in Section 5.4.5. The general formula for an X%/Y% UTI is given by Eq. (5.4.8) in Section 5.4.5. However, the simplified formula given in Eq. (7.5.1) was used to produce the results in this section.

Piepel and Cooley (2002) previously investigated an X%/Y% UTI approach of the type described in Section 5.4.5 that is not directly applicable to the current WTP ILAW compliance strategy (see Section 2.3), but can be adapted to it. They calculated UTIHWs for all combinations of the values of factors shown in Table 6.13.[(a)] The UTIHWs calculated by Piepel and Cooley that correspond to the X%/Y% UTI method presented in Section 5.4.5 are contained in their Table 4.4 (95%/95% UTIHWs) and Table 4.6 (99%/99% UTIHWs). The UTIHW values in those tables for application to ln(D^{VHT}) are in units of ln(μm).

The UTIHW values in Tables 4.4 and 4.6 of Piepel and Cooley (2002) can be used to determine the required numbers of samples per CRV batch (n_S^{CRV}) and analyses per CRV sample (n_A^{CRV}) by considering likely values of $\tilde{\mu}$, solving for the maximum acceptable value of UTIHW, and determining which entries of Tables 4.4 and 4.6 satisfy the solution. Thus, rewriting Eq. (7.5.1) when comparing to a VHT limit yields

$$\text{X\%/Y\% UTI} = \tilde{\mu} + \text{UTIHW} \le \ln(\text{limit}) \quad \Rightarrow \quad \text{UTIHW} \le \ln(\text{limit}) - \tilde{\mu} \, . \tag{7.5.2}$$

The UTIHW values in Tables 4.4 and 4.6 of Piepel and Cooley that are less than the maximum allowable per Eq. (7.5.2) then correspond to the required number of samples per CRV batch and analyses per CRV sample, which depend on the magnitudes of (1) the variation of ILAW over MFPV batches corresponding to an LAW waste type and (2) uncertainties for each ILAW MFPV batch.

The 95%/95% UTIHW results from Table 4.4 of Piepel and Cooley (2002) were utilized in another way to conservatively demonstrate that 3 samples per CRV batch and 1 chemical analysis per CRV sample are sufficient to easily demonstrate compliance with nominal LAW glass compositions for each of

(a) Table 6.13 is based on Table 4.1 of Piepel and Cooley (2002), but with notation modified to match that used in this report.

the three LAW tanks (AP-101, AZ-101, and AN-107) used for investigations in this report. Specifically, the largest variation ($\hat{\sigma}_g = 0.50$) and uncertainties ($\hat{\sigma}_S = 0.10$, $\hat{\sigma}_A = 0.50$, and $\bar{\hat{\sigma}}_m = 0.40$) considered by Piepel and Cooley (2002) were used for conservatism. Also, $df_m = 40$ was used, which is conservative compared to the larger values of df_m values for the current ILAW VHT model (see Table 5.1). The number of ILAW MFPV batches per LAW waste type (denoted I in this report, and n by Piepel and Cooley 2002) is expected to be at least 10 and potentially much larger for some LAW waste types. For this conservative investigation, the smallest number of batches (10) considered by Piepel and Cooley (2002) was used.

Table 7.20 shows the resulting 95%/95% UTI values on VHT alteration depth and rate for LAW glass corresponding to Tanks AP-101, AZ-101, and AN-107 obtained using the conservative estimates discussed in the previous paragraph. Compliance was easily demonstrated in each case, despite the significant conservatism in the inputs for the calculations summarized in Table 7.20. This exercise shows that at least 3 samples per CRV batch with 1 analysis per sample should be sufficient to demonstrate with 95% confidence that at least 95% of the ILAW produced over an LAW waste type will have the VHT alteration rate that meets the Contract Specification 2.2.2.17.3 limit. This conclusion is conditional on (1) the WTP ILAW having compositions similar to those for LAW Tanks AP-101, AZ-101, and AN-107 and (2) the batch-to-batch variation and within-batch uncertainties are not larger than the conservative values assumed for the calculations.

Table 7.20. 95%/95% UTI Values for VHT Alteration Depth and Rate (D^{VHT} and R^{VHT}) from ILAW Corresponding to Three LAW Tanks Assuming $n_S^{CRV} = 3$, $n_A^{CRV} = 1$, and Conservative Values of Inputs Considered by Piepel and Cooley (2002)[a]

Limit[b]	AP-101			AZ-101			AN-107		
	$\tilde{\mu}$ [c]	95%/95% UTIHW[d]	95%/95% UTI[e]	$\tilde{\mu}$ [c]	95%/95% UTIHW[d]	95%/95% UTI[e]	$\tilde{\mu}$ [c]	95%/95% UTIHW[d]	95%/95% UTI[e]
Results in Alteration Depth [ln(μm)]									
6.116	2.590	1.350	3.940	2.805	1.350	4.155	0.662	1.350	2.012
Results in Alteration Rate [g/m^{2}day]									
50	1.472	4.205	5.677	1.825	5.214	7.039	0.214	0.612	0.826

(a) Using the notation of Piepel and Cooley (2002) as summarized in Table 6.13, the maximum variation and uncertainty SDs used were $\hat{\sigma}_g = 0.50$, $\hat{\sigma}_S = 0.10$, $\hat{\sigma}_A = 0.50$, and $\bar{\hat{\sigma}}_m = 0.40$. Conservative values of $df_m = 40$ and 10 MFPV batches per LAW waste type were also used.

(b) The limits for VHT alteration rate are listed in units of g/m^{2}day and μm in Eq. (5.4.1).

(c) $\tilde{\mu}$ denotes the predicted ln(D^{VHT}) values calculated using the VHT model in Table 5.1 for the nominal AP-101, AZ-101, and AN-107 ILAW compositions given in Table D.11 of Appendix D. Before applying the model in Table 5.1, the compositions in Table D.11 were normalized to mass fractions of the 14 components appearing in the model.

(d) 95%/95% UTIHW denotes the half-width of a 95%/95% UTI found in Table 4.4 of Piepel and Cooley (2002) for the combination of inputs listed in footnote (a). The Piepel and Cooley (2002) UTIHWs for this application are in ln(μm) units. For the other units shown in the table, the UTIHWs were obtained via UTIHW = UTI - $\tilde{\mu}$ after converting UTI and $\tilde{\mu}$ to the new units.

(e) 95%/95% UTI is given by $\tilde{\mu}$ + UTIHW, according to Eq. (7.5.1).

7.6 Compliance Results for ILAW Contract Specification 2.2.2.20: Dangerous Waste Limitations

Relevant statistical methods and corresponding results for the statistical aspects of the WTP Project's compliance strategy for ILAW Contract Specification 2.2.2.20 described in Section 5.5.2 are discussed in the reports by Cook and Blumenkranz (2003) and Kot et al. (2003).

If the LAW LDR treatment variance process leads to future revisions in the ILAW compliance strategy that include "during production" aspects of compliance, any results associated with statistical methods or equations presented in a future revision of Section 5.5.3 will be included in a future revision of this subsection.

7.7 Compliance Results for ILAW Contract Specification 2.2.2.2: Waste Loading

As discussed in Section 5.6.3, the Statistical Analysis task scope associated with the WTP Project's Rev. 0 compliance strategy (Nelson et al. 2003) for ILAW Contract Specification 2.2.2.2 addressed in this report[(a)] was removed part way through developing the methods and performing the investigations. The partial results obtained before the scope cut are briefly discussed in this section.

Related to Item 1 in Section 5.6.2, mass-balance equations for calculating waste Na_2O loading in ILAW were developed and are presented in Section B.6 of Appendix B.

Related to Item 2 in Section 5.6.2, equations for waste Na_2O loading in ILAW (from Section B.6 of Appendix B) were implemented in the ILAW single-MFPV-batch Monte Carlo simulation work described in Section 3.4.2. Specifically, the equations were included in the final simulation runs. The data from those simulation runs were saved and could be accessed in the future to provide guidance to the WTP Project on numbers of samples per LAW CRV batch, analyses per CRV sample, and volume determinations required to demonstrate (with high confidence) compliance with the waste Na_2O limits for each MFPV batch.

Investigations to assess the numbers of samples, analyses per sample, and other process measurements needed to demonstrate compliance, with high confidence, over an LAW waste type were also planned, but not started before the scope reduction. Such work, if needed in the future, would account for variation in ILAW composition and waste Na_2O loading over MFPV batches corresponding to a waste type. The results on required numbers of samples, analyses per sample, and other process measurements from such work may differ from those presented in this report that consider only uncertainties affecting a single MFPV batch.

(a) See Section 1.0 for a discussion of why this report addresses ILAW PCP Rev. 0 (Nelson et al. 2003) rather than ILAW PCP Rev. 1 (Westsik et al. 2004).

As discussed in Section 5.6.3 in relation to Item 3 in Section 5.6.2:

- A statistical CI would be appropriate to account for process uncertainties and demonstrate compliance with waste Na_2O limits for each MFPV batch.
- A statistical TI would be appropriate to account for process uncertainties (affecting each MFPV batch) and variations (over MFPV batches associated with an LAW waste type) in demonstrating compliance with waste Na_2O limits for LAW waste types.

Equations for CIs and TIs applicable for demonstrating ILAW waste loading compliance could be developed and illustrated in the future if desired by the WTP Project.

Finally, there are some results in the report by Amidan et al. (2004) that are partially applicable to waste loading compliance for ILAW. The investigations reported by Amidan et al. (2004) nominally assessed the ability to satisfy several IHLW compliance and processing conditions, based on the previous IHLW process and compliance strategy that still included the HLW CRV (Nelson 2003). However, that work also considered applying the current ILAW compliance strategy to the IHLW process with a CRV. Thus, that portion of the work was essentially an investigation of the ILAW compliance strategy. The interested reader should refer to the "ILAW strategy" portion of the Amidan et al. (2004) results having to do with meeting the ILAW waste loading requirements.

8.0 Summary of Statistical Methods and Investigations for IHLW and ILAW Compliance

Section 8.1 summarizes the methods developed and results obtained to implement the statistical aspects of the WTP IHLW compliance strategy. Section 8.2 summarizes the methods developed and results obtained to implement the statistical aspects of the WTP ILAW compliance strategy.

In both Sections 8.1 and 8.2, some of the methods and results that are summarized relate to estimating radionuclide compositions, expressed as mass fractions of oxides. Although mass fractions of radionuclide components may be of limited interest directly, they play a key role in the equations developed to calculate radionuclide inventories.

8.1 Summary of Statistical Methods and Results for IHLW Compliance

Section 8.1.1 summarizes the statistical methods developed in this report to implement the statistical aspects of the WTP Project's IHLW compliance strategy. Section 8.1.2 summarizes the statistical investigations regarding the number of samples per IHLW MFPV batch and the number of chemical and/or radiochemical analyses per MFPV sample required to demonstrate compliance with various IHLW specifications. Section 8.1.3 summarizes the results of these investigations.

8.1.1 Summary of Statistical Methods for IHLW Compliance

Table 8.1 lists the statistical methods developed in this report to implement the statistical aspects of the WTP Project's IHLW compliance strategy. Table 8.1 lists in successive columns (i) the relevant WAPS (DOE-EM 1996) or WTP contract (DOE-ORP 2003) specification, (ii) the statistical aspect of the compliance strategy for the specification, (iii) the statistical method developed to address that aspect of the compliance strategy, (iv) the section of the report where the method is described, (v) the section of the report where the method is illustrated using realistic, simulated data, and (vi) the section(s) of the report where the compliance equations and/or any derivations or details of the method are presented.

The methods to implement the statistical aspects of the WTP IHLW compliance strategy for various specifications fall into three categories:

- Methods to calculate CL% statistical confidence intervals for demonstrating that the true mean values of compliance quantities for IHLW corresponding to each IHLW MFPV batch satisfy specification limits
- Methods to calculate means and standard deviations representing the averages and variabilities of compliance quantities (e.g., chemical and radionuclide compositions) over the IHLW MFPV batches and/or IHLW canisters corresponding to an HLW waste type

Table 8.1. Statistical Methods for IHLW Compliance

IHLW Specification	Statistical Aspect of IHLW Compliance Strategy	Statistical Method	Report Section Method Described	Report Section Method Illustrated	Report Section(s) of Compliance Equations and Method Derivation or Details
WAPS 1.1.2, Chemical Composition During Production	Develop equations for calculating the means and SDs of IHLW chemical composition of reportable glass components over an HLW waste type.	Equations for mass-weighted averages, SDs, and %RSDs of IHLW chemical composition (mass fractions) over a waste type. Balanced and unbalanced data cases.	4.1.4	6.1.2	A.1 E.1
WAPS 1.2.2, Radionuclide Inventory During Production	Develop equations for calculating the means and SDs of radionuclide inventories in IHLW canisters from an HLW waste type for radionuclides analyzed in every MFPV batch.	Equations for mass-weighted averages, SDs, and %RSDs of IHLW radionuclide composition (mass fractions) over a waste type. Balanced and unbalanced data cases.	4.2.4	6.2.2	A.2 E.1
WAPS 1.2.2, Radionuclide Inventory During Production	Develop statistical methods to quantify the variations and uncertainties of radionuclide inventories in IHLW canisters from an HLW waste type for radionuclides analyzed in the first MFPV batch only.	Not yet developed. Requires discussion with the WTP Project on viable approaches given the new IHLW compliance strategy.	4.2.5	N/A[(a)]	A.2
WAPS 1.3, Product Consistency	Develop a statistical interval method to demonstrate that each MFPV batch would produce IHLW compliant with PCT limits, after accounting for applicable uncertainties.	CL% upper combined confidence interval, which accounts for IHLW composition uncertainty and model uncertainty, each with CL% confidence.	4.3.3.2	6.3.1	A.1 A.3 E.2

Table 8.1. Statistical Methods for IHLW Compliance (cont.)

IHLW Specification	Statistical Aspect of IHLW Compliance Strategy	Statistical Method	Report Section Method Described	Report Section Method Illustrated	Report Section(s) of Compliance Equations and Method Derivation or Details
WAPS 1.3, Product Consistency	Develop a statistical interval method to demonstrate that IHLW corresponding to an HLW waste type complies with the PCT limits of WAPS 1.3, after accounting for applicable variations and uncertainties.	X%/Y% upper tolerance interval, which provides X% confidence that at least Y% of the IHLW produced from an HLW waste type individually meets the PCT B, Li, and Na limits	4.3.5	6.3.3	A.1 A.3 E.3
WAPS 1.5, Hazardous Waste Specification	See Section 4.4.2 and Cook and Blumenkranz (2003).	See Section 4.4.3, Kot et al. (2003), and Kot et al. (2004b).	4.4.3	N/A[(b)]	N/A[(b)]
Contract Specification 1.2.2.1.5, Dangerous and Hazardous Waste Requirements	See Section 4.5.2 and Cook and Blumenkranz (2003).	See Section 4.5.3, Kot et al. (2003), and Kot et al. (2004b).	4.5.3	N/A[(b)]	N/A[(b)]
WAPS 1.6, IAEA Safeguards Reporting for IHLW	Develop formulas for calculating the means and SDs of the total and fissile uranium and plutonium mass in IHLW canisters corresponding to an HLW waste type.	Scheduled for completion in FY 2005.	4.6.3	Future revision of 6.6.1	A.5.1
WAPS 1.6, IAEA Safeguards Reporting for IHLW	Develop a statistical method for estimating the concentration of plutonium in IHLW canisters during production.	Scheduled for completion in FY 2005.	4.6.4	Future revision of 6.6.2	A.5.2
WAPS 1.6, IAEA Safeguards Reporting for IHLW	Develop a statistical method for estimating the isotopic ratios of uranium and plutonium in IHLW canisters during production.	Scheduled for completion in FY 2005.	4.6.5	Future revision of 6.6.3	A.5.3

Table 8.1. Statistical Methods for IHLW Compliance (cont.)

IHLW Specification	Statistical Aspect of IHLW Compliance Strategy	Statistical Method	Report Section Method Described	Report Section Method Illustrated	Report Section(s) of Compliance Equations and Method Derivation or Details
WAPS Specification 3.8.2: Heat Generation at Year of Shipment	Calculate the mean and standard deviation for heat generation rates over the course of a given waste type.	Not developed because the corresponding work scope was deleted. Possible approaches are discussed in Section 4.7.4.	4.7.4	N/A	A.6
WAPS Specification 3.14: Concentration of Plutonium in Each Canister	Develop statistical methods to account for variations and uncertainties in per canister plutonium concentrations to demonstrate with high confidence that the limits of this specification will be satisfied for each canister produced from a given HLW waste type.	Scheduled for completion in FY 2005. It is envisioned that a statistical X%/Y% UTI formula will be developed using the mean and SD equations from Section A.7.	4.8.3	Future revision of 6.8.1	A.7
IHLW Contract Specification 1.2.2.1.6: Product Loading	The WTP IHLW compliance strategy changed from demonstrating compliance via a statistical interval approach to a non-statistical approach of comparing average product loadings (over a batch transfer of an HLW waste type) to the minimum values given in Table TS-1.1.	None, because the current WTP IHLW compliance strategy does not involve accounting for variation and uncertainty in demonstrating compliance with the product loading specification.	N/A[(c)]	N/A[(c)]	N/A[(c)]

(a) The method has not yet been developed and thus cannot yet be illustrated.
(b) Applicable methods are discussed and illustrated in reports by Kot et al. (2003) and Kot et al. (2004b).
(c) Waste loading was removed from the scope of the work covered by this report, and hence no methods, details, or illustrations are provided.

- Methods to calculate X%/Y% statistical tolerance intervals over the IHLW MFPV batches and/or IHLW canisters corresponding to an HLW waste type. A statistical tolerance interval provides for demonstrating with high (X%) confidence that at least a high percentage (Y%) of the distribution of a compliance quantity for IHLW corresponding to an HLW waste type satisfies the specification limit(s).

As summarized in Table 8.1, each of the methods is illustrated using simulated data that are realistic of the data that will be obtained by sampling, chemical analysis, and other process measurements during IHLW production operations.

8.1.2 Summary of Statistical Investigations on the Numbers of Samples per MFPV Batch and Analyses per Sample for IHLW Compliance

Table 8.2 lists the statistical investigations of the number of samples per IHLW MFPV batch, the number of chemical and/or radiochemical analyses per MFPV sample, and in some cases, the number of volume determinations per MFPV batch required to demonstrate compliance with various specifications. Table 8.2 lists in successive columns (i) the relevant WAPS (DOE-EM 1996) or WTP contract (DOE-ORP 2003) specification, (ii) the statistical aspect of the compliance strategy for the specification, (iii) the investigation performed to address that aspect of the compliance strategy, (iv) the section of the report where the investigation is described, (v) the section of the report where the results of the investigation are presented, and (vi) the section(s) of the report where the compliance equations and/or any details of the investigation are presented.

Table 8.2 shows that there were four investigations performed to assess the required numbers of samples per IHLW MFPV batch and analyses per IHLW MFPV sample to (1) estimate IHLW chemical composition for each MFPV batch, (2) estimate IHLW radionuclide composition for each MFPV batch, (3) demonstrate that IHLW from each MFPV batch meets PCT limits, and (4) demonstrate that IHLW corresponding to an HLW waste type meets PCT limits. It remains to compare the required numbers of samples per MFPV batch and analyses per MFPV sample resulting from these investigations to obtain an overall recommendation. However, note that Items (1) and (2) are related to process control and reporting where there are no specific requirements about how well chemical and radionuclide composition must be estimated. This decision belongs to the WTP Project, with the summary of results here intended to provide input for that decision. On the other hand, Items (3) and (4) involve demonstrating that IHLW has PCT responses less than specification limits. The WTP Project has some flexibility in choosing the minimum values of CL% for CL% UCIs, and X and Y for X%/Y% UTIs. However, it is recommended that CL%, X%, and Y% should be at least 90%.

Table 8.2. Statistical Investigations of Numbers of Samples, Analyses, and Volume Determinations for IHLW Compliance

IHLW Specification	Statistical Aspect of IHLW Compliance Strategy	Statistical Investigation	Report Section Investigation Described	Report Section Containing Investigation Results	Report Section(s) of Compliance Equations and Investigation Details
WAPS 1.1.2, Chemical Composition During Production	Determine the numbers of samples per MFPV batch and analyses per MFPV sample necessary to estimate IHLW chemical composition from an MFPV batch.	Calculate required numbers of samples per MFPV batch and analyses per MFPV sample for combinations of values of factors (including applicable uncertainties) that affect IHLW chemical composition estimates and uncertainties for an IHLW MFPV batch.	4.1.3	6.1.1	A.1 3.4.1
WAPS 1.2.2, Radionuclide Inventory During Production	Determine the numbers of samples per MFPV batch, analyses per MFPV sample, and other process measurements required to estimate IHLW radionuclide compositions for an MFPV batch, which are in turn used to estimate IHLW radionuclide inventories.	Calculate required numbers of samples per MFPV batch and analyses per MFPV sample for combinations of values of factors (including applicable uncertainties) that affect IHLW radionuclide composition estimates and uncertainties for an IHLW MFPV batch.	4.2.3	6.2.1	A.2 3.4.1
WAPS 1.3, Product Consistency	Determine the numbers of samples per MFPV batch, analyses per MFPV sample, and other process measurements required to demonstrate that the PCT B, Li, and Na releases for IHLW from an MFPV batch will satisfy their respective limits.	Calculate required numbers of samples per MFPV batch and analyses per MFPV sample for combinations of values of factors (including applicable uncertainties) that affect PCT normalized B, Li, and Na release estimates and uncertainties for IHLW from a single MFPV batch.	4.3.4	6.3.2	A.1 A.3
WAPS 1.3, Product Consistency	Determine the numbers of samples per MFPV batch, analyses per MFPV sample, and other process measurements required to demonstrate that the PCT B, Li, and Na releases for IHLW from an HLW waste type will satisfy their respective limits.	Calculate required numbers of samples per MFPV batch and analyses per MFPV sample for combinations of values of factors (including applicable uncertainties) that affect PCT normalized B, Li, and Na release estimates and uncertainties for IHLW from an HLW waste type.	4.3.6	6.3.4	A.1 A.3

Table 8.2. Statistical Investigations of Numbers of Samples, Analyses, and Volume Determinations for IHLW Compliance (cont.)

IHLW Specification	Statistical Aspect of IHLW Compliance Strategy	Statistical Investigation	Report Section Investigation Described	Report Section Containing Investigation Results	Report Section(s) of Compliance Equations and Investigation Details
WAPS 1.6, IAEA Safeguards Reporting for IHLW	Determine the numbers of samples, analyses per sample, and other process measurements required to adequately estimate the compliance quantities described in WAPS 1.6.	Scheduled for completion in FY 2005.	4.6.6	Future revision of 6.6.4	A.5.1 A.5.2 A.5.3 3.4.1
IHLW Contract Specification 1.2.2.1.6: Product Loading	WTP Project strategy changed from demonstrating compliance via a statistical approach that accounts for variations and uncertainties to one that compares average product loadings (over a batch transfer of an HLW waste type) to the minimum values given in Table TS-1.1.	None, because the current WTP IHLW compliance strategy does not involve accounting for variation and uncertainty in demonstrating compliance with the product loading specification.	N/A[(a)]	N/A[(a)]	N/A[(a)]

(a) Waste loading was removed from the scope of the work covered by this report, and hence no methods, details, or illustrations are provided.

8.1.3 Summary of Statistical Results on the Numbers of Samples per MFPV Batch and Analyses per Sample for IHLW Compliance

Discussion in Sections 6.1.1 and 6.2.1 explain that it is not necessary to make more than one chemical or radiochemical analysis of an MFPV sample given the IHLW compliance strategy. Thus, it remains to summarize the results on how many samples per IHLW MFPV batch are required to satisfy goals and specifications related to Items (1) to (4) discussed in Section 8.1.2. Sections 8.1.3.1 and 8.1.3.2, respectively, summarize the number of samples per MFPV batch needed to estimate IHLW chemical composition [Item (1)] and radionuclide composition [Item (2)] for selected values of confidence and precision. Section 8.1.3.3 summarizes the number of samples per MFPV batch required for PCT compliance [Items (3) and (4)].

8.1.3.1 Number of Samples per IHLW MFPV Batch to Estimate IHLW Chemical Composition

Table 6.1 summarizes the number of samples per IHLW MFPV batch (with one chemical analysis per sample) required to estimate the mass fraction of any given chemical composition component (oxide or halogen) with precisions (%RHWs) of <5%, <10%, <15%, and <20%) and confidence of 90% or 95%. The number of samples depends not only on the selected values of precision and confidence, but also on the values of IHLW MFPV mixing/sampling uncertainty [$\%RSD_S(g_j^{MFPV})$] and chemical analysis uncertainty [$\%RSD_A(g_j^{MFPV})$][(a)]. All combinations of % confidence = 90, 95; $\%RSD_S(g_j^{MFPV})$ = 1, 5 and 15%; $\%RSD_A(g_j^{MFPV})$ = 5, 10, 20, 25, 40, and 50%; and the four categories of precision (%RHW) mentioned previously were investigated. Several conclusions based on Table 6.1 follow.

For $\%RSD_S(g_j^{MFPV})$ = 5, taking 8 samples per MFPV batch (with one chemical analysis each) supports estimating the mass fraction of any IHLW component "*j*" within:

- 10% of its true value with 95% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 10$
- 15% of its true value with 90% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 20$
- 20% of its true value with at least 90% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 25$.

Any IHLW chemical composition components with analytical uncertainties greater than 40 %RSD require 13 or more samples per IHLW MFPV batch to be estimated within 20% precision with 90% confidence.

If $\%RSD_S(g_j^{MFPV})$ is as small as 1%, taking 7 samples per MFPV batch (with one analysis each) supports estimating the mass fraction of any IHLW component "*j*" within:

(a) Note that performing only one analysis per sample is an option, and in fact ultimately recommended in nearly all cases.

- 10% of its true value with 95% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 10$
- 15% of its true value with 90% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 20$
- 20% of its true value with 95% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 20$
  or with 90% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 25$.

Any IHLW components with analytical uncertainties greater than 40 %RSD again require 13 or more samples per IHLW MFPV batch to be estimated within 25% precision with 90% confidence, despite the smaller assumed value for mixing/sampling uncertainty of 1 %RSD.

If $\%RSD_S(g_j^{MFPV})$ is as large as 15%, taking 8 samples per MFPV batch (with one analysis each) supports estimating the mass fraction of any IHLW component "*j*" within 20% of its true value with 90% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 25$. In this case, any IHLW components with analytical uncertainties greater than 40 %RSD would require 15 or more samples per IHLW MFPV batch to be estimated within 25% precision with 90% confidence.

Tables 6.2 and 6.3 provide 90 and 95% confidence results, respectively, for the required numbers of samples per MFPV batch (with one chemical analysis per sample) to estimate within specified precision ranges (%RHWs) the mass fractions of reportable IHLW chemical composition components (as listed in Table 2.2) for IHLW corresponding to three HLW tanks (AY-102, AZ-102, and C-104). Tables 6.2 and 6.3 provide results for low and high estimates of mixing/sampling and analytical uncertainties for IHLW corresponding to each of the three HLW tanks, which are listed in Appendix C. A summary of the results in the last two columns of Table 6.2 for 90% confidence is given in Table 8.3.

Table 8.3 summarizes (for each combination of mixing/sampling uncertainty, chemical analysis uncertainty, and selected precision [%RHW]) the maximum number of samples per IHLW MFPV batch (n_S^{MFPV}) over reportable IHLW components (oxides or halogens) with mass fractions greater than 0.005 (0.5 wt%) and greater than 0.02 (2 wt%). The maximum n_S^{MFPV} values are given for IHLW corresponding to each of the three HLW tanks, with maximum values across the three tanks also listed. For the subset of reportable IHLW components with mass fractions > 0.005, the maximum n_S^{MFPV} values for tank AY-102 are the maximums across the three tanks. The maximum n_S^{MFPV} values for AY-102 are

Table 8.3. Summary of Numbers of IHLW MFPV Samples (with One Chemical Analysis per Sample) to Satisfy Certain Precisions (%RHWs) with 90% Confidence for Reportable IHLW Chemical Composition Components (Oxides) for Low and High Combinations of Mixing/Sampling and Analytical Uncertainties for Each of Three HLW Tanks

$\%RSD_S\,(g_j^{MFPV})$ [b]	$\%RSD_A\,(g_j^{MFPV})$ [b]	%RHW	Reportable IHLW Chemical Composition Components, MF > 0.005[a]				Reportable IHLW Chemical Composition Components, MF > 0.02 and MF > 0.005 Except U_3O_8[a]			
			AY-102	AZ-102	C-104	Max Over 3 Tanks	AY-102	AZ-102	C-104	Max Over 3 Tanks
L	L	10	14	6	4	14	5	4	4	5
		15	8	4	3	8	4	3	3	4
		20	5	3	3	5	3	3	3	3
	H	10	-[c]	14	6	-	13	6	6	13
		15	22	8	4	22	7	4	4	7
		20	13	5	3	13	5	3	3	5
H	L	10	19	11	9	19	6	9	9	9
		15	10	6	6	10	4	6	6	6
		20	7	5	4	7	3	4	4	4
	H	10	-	19	11	-	14	11	11	14
		15	24	10	6	24	8	6	6	8
		20	15	7	5	15	5	5	5	5

(a) Maximum values of n_S^{MFPV} are given across reportable chemical composition components with mass fraction (MF) values > 0.005 and 0.02. Because U_3O_8 is the only component with 0.005 < MF < 0.02, the results for MF > 0.02 also apply to the case of MF > 0.005 excluding U_3O_8.

(b) Low (L) and High (H) levels of mixing/sampling and analytical uncertainties associated with reportable elements for each of the three HLW tanks are given in Table C.1 of Appendix C.

(c) A dash (–) indicates that over 30 samples per MFPV batch would be necessary to satisfy the %RHW category.

substantially larger than the values for AZ-102 and C-104. This occurs because of the relatively large estimates of analytical uncertainty for uranium (U) in AY-102, namely a low estimate of 20 %RSD and a high estimate of 40 %RSD (see Table C.1 in Appendix C). However, the results for the subset of reportable IHLW components with mass fractions > 0.02 shown in Table 8.3 are the same as those with mass fractions > 0.005 but excluding uranium (U_3O_8). Hence, the last column in Table 8.3 shows that to estimate with 90% confidence all IHLW chemical composition components with mass fractions > 0.005 (except U_3O_8 in AY-102):

- within 10% of their true values requires from 5 to 14 samples per MFPV
- within 15% of their true values requires from 4 to 8 samples per MFPV
- within 20% of their true values requires from 3 to 5 samples per MFPV

depending on the values of MFPV mixing/sampling and analytical uncertainties. These conclusions may be applicable to IHLW for other HLW tanks to be processed by the WTP to the extent that the ranges of MFPV mixing/sampling and analytical uncertainties for IHLW corresponding to Tanks AY-102, AZ-102, and C-104 (see Appendix C) are representative.

8.1.3.2 Number of Samples per IHLW MFPV Batch to Estimate IHLW Radionuclide Composition

Table 6.5 summarizes the number of samples per IHLW MFPV batch (with one radiochemical analysis per sample) required to estimate the mass fraction of any given radionuclide composition component with precisions (%RHWs) of < 10%, < 15%, < 20%, and < 50%) and confidence of 90% or 95%. The number of samples depends not only on the selected values of precision and confidence, but also on the values of IHLW MFPV mixing/sampling uncertainty [$\%RSD_S(g_j^{MFPV})$] and radiochemical analysis uncertainty [$\%RSD_A(g_j^{MFPV})$][(a)]. All combinations of % confidence = 90, 95; $\%RSD_S(g_j^{MFPV})$ = 1 and 5%; $\%RSD_A(g_j^{MFPV})$ = 5, 10, 15, 20, 25, 30, 40, 50, and 60%; and the four categories of precision (%RHW) mentioned previously were investigated. Several conclusions based on Table 6.5 follow.

For $\%RSD_S(g_j^{MFPV})$ = 5, taking 8 samples per MFPV batch (with one radiochemical analysis each) supports estimating the mass fraction of any IHLW component "*j*" within:

- 10% of its true value with 95% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 10$
- 15% of its true value with 90% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 20$
- 20% of its true value with at least 90% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 25$
- 50% of its true value with at least 95% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 50$.

Any IHLW radionuclide composition components with analytical uncertainties greater than 40 %RSD require 13 or more samples per IHLW MFPV batch to be estimated within 20% precision with 90% confidence.

If $\%RSD_S(g_j^{MFPV})$ is as small as 1%, taking 7 samples per MFPV batch (with one analysis each) supports estimating the mass fraction of any IHLW radionuclide composition component "*j*" within:

- 10% of its true value with 95% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 10$
- 15% of its true value with 90% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 20$

(a) Note that performing only one analysis per sample is an option, and in fact ultimately recommended in nearly all cases.

- 20% of its true value with 95% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 20$

  or with 90% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 25$
- 50% of its true value with 95% confidence provided $\%RSD_A(g_j^{MFPV}) \leq 50$.

Any IHLW radionuclide composition components with analytical uncertainties greater than 40 %RSD again require 13 or more samples per IHLW MFPV batch to be estimated within 20% precision with 90% confidence, despite the smaller assumed value for mixing/sampling uncertainty of 1 %RSD.

Tables 6.6 and 6.7 provide 90 and 95% confidence results, respectively, for the required numbers of samples per MFPV batch (with one radiochemical analysis per sample) to estimate within specified precision ranges (%RHWs) the mass fractions of reportable IHLW radionuclide composition components (as listed in Table 2.1) for IHLW corresponding to three HLW tanks (AY-102, AZ-102, and C-104). Tables 6.6 and 6.7 provide results for low and high estimates of mixing/sampling and analytical uncertainties for IHLW corresponding to each of the three HLW tanks, which are listed in Appendix C. A summary of the results in the last two columns of Table 6.6 for 90% confidence is given in Table 8.4.

Table 8.4 summarizes (for each combination of mixing/sampling uncertainty, radiochemical analysis uncertainty, and selected precision [%RHW]) the maximum number of samples per IHLW MFPV batch (n_S^{MFPV}) over reportable IHLW radionuclide components with mass fractions greater than 0.00001 (0.001 wt%) and greater than 0.001 (0.1 wt%). The maximum n_S^{MFPV} values are given for IHLW corresponding to each of the three HLW tanks, with maximum values across the three tanks also listed. For the subset of reportable radionuclide IHLW components with mass fractions > 0.00001, the maximum n_S^{MFPV} values for tanks AZ-102 and C-104 provide the maximums across the three tanks. Table 8.4 shows that to estimate with 90% confidence all IHLW radionuclide composition components with mass fractions > 0.00001:

- within 15% of their true values requires from 7 to 22 samples per MFPV
- within 20% of their true values requires from 5 to 13 samples per MFPV
- within 50% of their true values requires from 3 to 4 samples per MFPV

depending on the values of MFPV mixing/sampling and analytical uncertainties. For the subset of reportable radionuclide IHLW components with mass fractions > 0.001, the maximum n_S^{MFPV} values for Tank AZ-102 and C-104 provide the maximums across the three tanks because AY-102 does not have any radionuclide components with mass fractions > 0.001. The last column in Table 8.4 shows that to estimate with 90% confidence all IHLW radionuclide composition components with mass fractions > 0.001:

- within 10% of their true values requires from 3 to 6 samples per MFPV
- within 15% of their true values requires from 3 to 4 samples per MFPV
- within 20% of their true values requires 3 samples per MFPV

- within 50% of their true values requires from 1 to 2 samples per MFPV

depending on the values of MFPV mixing/sampling and analytical uncertainties. These conclusions may be applicable to IHLW for other HLW tanks to be processed by the WTP to the extent that the ranges of mixing/sampling and analytical uncertainties for HLW from Tanks AY-102, AZ-102, and C-104 (see Appendix C) are representative.

Table 8.4. Summary of Numbers of IHLW MFPV Samples (with One Radiochemical Analysis per Sample) to Satisfy Certain Precisions (%RHWs) with 90% Confidence for Reportable IHLW Radionuclide Composition Components (Oxides) for Low and High Combinations of Mixing/Sampling and Analytical Uncertainties for Each of Three HLW Tanks

$\%RSD_S(g_j^{MFPV})$ [b]	$\%RSD_A(g_j^{MFPV})$ [b]	%RHW	Reportable IHLW Radionuclide Composition Components, MF > 0.00001[a]				Reportable IHLW Radionuclide Composition Components, MF > 0.001 [a]			
			AY-102	AZ-102	C-104	Max Over 3 Tanks	AY-102	AZ-102	C-104	Max Over 2 Tanks
L	L	10	5	13	13	13	(c)	3	3	3
		15	4	7	7	7		3	3	3
		20	3	5	5	5		3	3	3
		50	2	3	3	3		1	1	1
	H	10	13	-[d]	-	-		5	5	5
		15	7	22	22	22		4	4	4
		20	5	13	13	13		3	3	3
		50	3	4	4	4		2	2	2
H	L	10	6	14	14	14		4	4	4
		15	4	8	8	8		3	3	3
		20	3	5	5	5		3	3	3
		50	2	3	3	3		1	1	1
	H	10	14	-	-	-		6	6	6
		15	8	22	22	22		4	4	4
		20	5	13	13	13		3	3	3
		50	3	4	4	4		2	2	2

(a) Maximum values of n_S^{MFPV} are given across reportable radionuclide composition components with mass fractions (MFs) > 0.00001 and 0.001.

(b) Low (L) and High (H) levels of mixing/sampling and analytical uncertainties associated with reportable radionuclides for each of the three HLW tanks are given in Tables C.2 and C.4 of Appendix C.

(c) Empty cells indicate that no radionuclide composition component had a nominal wt% greater than 0.1% for AY-102.

(d) A dash (–) indicates that over 30 samples per MFPV batch would be necessary to satisfy the %RHW category.

8.1.3.3 Number of Samples per IHLW MFPV Batch and over an HLW Waste Type to Demonstrate PCT Compliance

The number of samples per IHLW MFPV batch required to demonstrate PCT compliance for each MFPV batch [Item (3) in Section 8.1.2] and over an HLW waste type [Item (4) in Section 8.1.2] are the easiest to summarize. Specifically, investigations in Section 6.3.2 for single-MFPV-batch compliance and in Section 6.3.4 for HLW waste type compliance showed that 3 samples per IHLW MFPV batch with 1 chemical analysis per sample was sufficient for demonstrating PCT compliance using the relevant statistical methods. This conclusion was reached using ranges of reasonable estimates of mixing/sampling and analytical uncertainties for IHLW MFPV batches corresponding to each of three HLW waste tanks (AY-102, AZ-102, and C-104) used for investigations. The conclusion was also confirmed in an investigation using wider ranges of mixing/sampling uncertainty (5 to 20 %RSD) and analytical uncertainty (5 to 50 %RSD).[(a)] The explanation for why 3 samples per IHLW MFPV batch with 1 chemical analysis per sample is expected to be sufficient for demonstrating PCT compliance (for each MFPV batch as well as over a collection of batches corresponding to an HLW waste type) is as follows. It is relatively easy to formulate HLW glasses with PCT responses significantly below (e.g., a factor of 5 to 10 lower than) the specification limits. Further, the combination of PCT model uncertainty, chemical composition uncertainty, and chemical composition variation over an HLW waste type do not overcome this large margin even for 3 samples per IHLW MFPV batch with 1 chemical analysis per sample.

8.2 Summary of Statistical Methods and Results for ILAW Compliance

Section 8.2.1 summarizes the statistical methods developed in this report to implement the statistical aspects of the WTP Project's ILAW compliance strategy. Section 8.2.2 summarizes the statistical investigations regarding the number of samples per ILAW CRV batch, the number of chemical and/or radiochemical analyses per CRV sample, and the numbers of volume determinations per CRV and MFPV batches required to demonstrate compliance with various ILAW specifications. Section 8.2.3 summarizes the results of these investigations.

8.2.1 Summary of Statistical Methods for ILAW Compliance

Table 8.5 lists the statistical methods developed in this report to implement the statistical aspects of the WTP Project's ILAW compliance strategy. Table 8.5 lists in successive columns (i) the relevant WTP contract (DOE-ORP 2003) specification, (ii) the statistical aspect of the compliance strategy for the specification, (iii) the statistical method developed to address that aspect of the compliance strategy, (iv) the section of the report where the method is described, (v) the section of the report where the method is illustrated using realistic, simulated data, and (vi) the section(s) of the report where the compliance equations and/or any derivations or details of the method are presented.

[(a)] These %RSDs represent uncertainties in PCT responses after propagating IHLW chemical-composition uncertainties through IHLW PCT property-composition models.

The methods to implement the statistical aspects of the WTP ILAW compliance strategy for various specifications fall into three categories:

- Methods to calculate CL% statistical confidence intervals for demonstrating that the true mean values of compliance quantities for ILAW corresponding to each ILAW MFPV batch satisfy specification limits.
- Methods to calculate means and SDs representing the averages and variabilities of compliance quantities (e.g., chemical and radionuclide compositions) over the ILAW MFPV batches and/or ILAW canisters corresponding to an LAW waste type
- Methods to calculate X%/Y% statistical tolerance intervals over the ILAW MFPV batches and/or ILAW canisters corresponding to an LAW waste type. A statistical tolerance interval provides for demonstrating with high (X%) confidence that at least a high percentage (Y%) of the distribution of a compliance quantity for ILAW corresponding to an LAW waste type satisfies the specification limit(s).

As summarized in Table 8.5, each of the methods is illustrated using simulated data that is realistic of the data that will be obtained by sampling, chemical analysis, and other process measurements during ILAW production operations.

Table 8.5. Statistical Methods for ILAW Compliance

ILAW Contract Specification	Statistical Aspect of ILAW Compliance Strategy	Statistical Method	Report Section Method Described	Report Section Method Illustrated	Report Section(s) of Compliance Equations and Method Derivation or Details
2.2.2.6.2: Chemical Composition During Production	Develop equations for calculating the means and SDs of ILAW chemical composition of reportable glass components over an LAW waste type	Equations for mass-weighted averages, SDs, and %RSDs of ILAW chemical composition (mass fractions) over a waste type. Balanced and unbalanced data cases.	5.1.4	7.1.2	B.1 F.1
2.2.2.7.2: Radionuclide Composition During Production	Develop equations for calculating the means and SDs of radionuclide inventories in ILAW containers from an LAW waste type for radionuclides analyzed in every CRV batch.	Equations for mass-weighted averages, SDs, and %RSDs of ILAW radionuclide composition (mass fractions) over a waste type. Balanced and unbalanced data cases.	5.2.4	7.2.2	B.2 F.1
2.2.2.8: Radionuclide Concentration Limits	Develop a statistical method to demonstrate that ILAW radionuclide concentrations over a waste type are below Class C limits.	X%/Y% upper tolerance interval on the sum-of-fractions (SF) of ILAW Class C radionuclides. This interval provides X% confidence that at least Y% of the ILAW produced from an LAW waste has SF meeting the required limit.	5.3.3.1	7.3.3.1	B.3.1 F.2
	Develop a statistical method to demonstrate that ILAW radionuclide concentrations corresponding to an MFPV batch are below Class C limits.	CL% empirical upper confidence interval on the SF of ILAW Class C radionuclides, which accounts for ILAW composition uncertainty with CL% confidence	5.3.3.2	7.3.3.2	B.3.1

Table 8.5. Statistical Methods for ILAW Compliance (cont.)

ILAW Contract Specification	Statistical Aspect of ILAW Compliance Strategy	Statistical Method	Report Section Method Described	Report Section Method Illustrated	Report Section(s) of Compliance Equations and Method Derivation or Details
2.2.2.8: Radionuclide Concentration Limits	Develop a statistical method to demonstrate that running averages of ^{137}Cs and ^{90}Sr concentrations (over all ILAW containers presented to date for acceptance on a waste type basis) are below the specified limits.	CL% upper confidence intervals on running average concentrations of ^{137}Cs and ^{90}Sr	5.3.5	7.3.3	B.3.2 F.3
2.2.2.17.2: PCT and 2.2.2.17.3: VHT	Develop a statistical interval method to demonstrate that each MFPV batch would produce ILAW compliant with PCT and VHT limits, after accounting for applicable uncertainties	CL% upper combined confidence interval, which accounts for ILAW composition uncertainty and model uncertainty, each with CL% confidence	5.4.3.2	7.4.1 (PCT) 7.5.1 (VHT)	B.1 B.4 F.4
2.2.2.17.2: PCT and 2.2.2.17.3: VHT	Develop a statistical interval method to demonstrate that ILAW corresponding to an LAW waste type complies with PCT and VHT limits, after accounting for applicable variations and uncertainties	X%/Y% upper tolerance interval, which provides X% confidence that at least Y% of the ILAW produced from an LAW waste type individually meets the PCT and VHT limits	5.4.5	7.4.3 (PCT) 7.5.3 (VHT)	B.1 B.4 F.4
2.2.2.20: Dangerous Waste Limitations	See Section 5.5.2 and Cook and Blumenkranz (2003)	See Section 5.5.3 and Kot et al. (2003)	5.5.3[(a)]	N/A[(a)]	N/A[(a)]
2.2.2.2: Waste Loading	Develop a method for determining waste Na_2O loading through sampling and analyses of pretreated LAW feed, measurements of GFCs added during processing, including effects of heel mixing, and accounting for volatilization during the vitrification process.	Mass-balance equations were developed to calculate the mass fractions of non-volatile oxides and waste Na_2O expected to be produced by vitrifying pretreated LAW feed and added GFCs.	5.6.3	N/A[(b)]	B.6
2.2.2.2: Waste Loading	Develop a statistical interval method to provide high confidence that ILAW	None, because the current WTP ILAW compliance strategy does not involve a	5.6.3	N/A[(b)]	N/A[(b)]

Table 8.5. Statistical Methods for ILAW Compliance (cont.)

ILAW Contract Specification	Statistical Aspect of ILAW Compliance Strategy	Statistical Method	Report Section Method Described	Report Section Method Illustrated	Report Section(s) of Compliance Equations and Method Derivation or Details
	produced from an LAW waste type will have waste Na_2O loading that meets the applicable envelope-specific minimums (Nelson 2003). The WTP ILAW compliance strategy has changed (Westsik et al. 2004) to comparing average waste Na_2O loading (over an ILAW production lot) to the LAW envelope minimum values given in Specification 2.2.2.2.	statistical approach that accounts for variation and uncertainty in demonstrating compliance with the waste loading specification. However, a CL% empirical confidence interval approach for demonstrating that each ILAW MFPV batch meets waste loading requirements was developed and implemented in the final ILAW Monte Carlo simulation runs before the change in compliance strategy. Also, an X%/Y% lower tolerance interval approach would be applicable to demonstrating that ILAW corresponding to an LAW waste type satisfies the waste loading limits.			

(a) Brief discussion is given in Section 5.5.3, but all applicable methods are discussed and illustrated in the report by Kot et al. (2003).
(b) No statistical methods for demonstrating compliance with waste loading requirements were developed or illustrated because the scope for that portion of the work was removed by the WTP Project in anticipation of a revised compliance strategy that would not require a statistically based compliance approach.

8.2.2 Summary of Statistical Investigations on the Numbers of Samples per CRV Batch, Analyses per CRV Sample, and Volume Determinations per CRV and MFPV Batches for ILAW Compliance

Table 8.6 lists the statistical investigations of the number of samples per ILAW CRV batch, the number of chemical and/or radiochemical analyses per CRV sample, and the number of volume determinations per CRV and MFPV batches required to demonstrate compliance with various specifications. Table 8.6 lists in successive columns (i) the relevant WTP contract (DOE-ORP 2003) specification, (ii) the statistical aspect of the compliance strategy for the specification, (iii) the investigation performed to address that aspect of the compliance strategy, (iv) the section of the report where the investigation is described, (v) the section of the report where the results of the investigation are presented, and (vi) the section(s) of the report where the compliance equations and/or any details of the investigation are presented.

Table 8.6 shows that there were six investigations performed to assess the required numbers of samples per LAW CRV batch and analyses per CRV sample to (1) estimate ILAW chemical composition for each MFPV batch, (2) estimate ILAW radionuclide composition for each MFPV batch, (3) demonstrate that ILAW radionuclide concentrations over a waste type are below Class C limits, (4) demonstrate that running averages of ^{137}Cs and ^{90}Sr concentrations in ILAW are below their specification limits, (5) demonstrate ILAW from each MFPV batch meets PCT and VHT limits, and (6) demonstrate that ILAW corresponding to an LAW waste type meets PCT and VHT limits. It remains to compare the required numbers of samples per LAW CRV batch and analyses per CRV sample resulting from these investigations to obtain an overall recommendation. However, note that Items (1) and (2) are related to process control and reporting where there are no specific requirements about how well chemical and radionuclide composition must be estimated. This decision belongs to the WTP Project, with the summary of results here intended to provide input for that decision. On the other hand, Items (3) to (6) involve demonstrating that ILAW satisfies radionuclide, PCT, and VHT specification limits. The WTP Project has some flexibility in choosing the minimum values of CL% for CL% UCIs, and X and Y for X%/Y% UTIs. However, it is recommended that CL%, X%, and Y% should be at least 90%.

8.2.3 Summary of Statistical Results on the Numbers of Samples per CRV Batch, Analyses per CRV Sample, and Volume Determinations per CRV and MFPV Batches for ILAW Compliance

This section summarizes the results on how many samples per ILAW CRV batch and how many analyses per CRV sample are required to satisfy goals and specifications related to Items (1) to (6) discussed in Section 8.2.2. Sections 8.2.3.1 and 8.2.3.2, respectively, summarize the numbers of samples per CRV batch, analyses per CRV sample, and volume determinations per CRV and MFPV batches needed to estimate ILAW chemical composition [Item (1)] and radionuclide composition [Item (2)] for selected values of confidence and precision. Section 8.2.3.3 summarizes the numbers of samples per CRV batch, analyses per CRV sample, and volume determinations per CRV and MFPV batches required for radionuclide concentration and running average compliance [Items (3) and (4)]. Section 8.2.3.4 summarizes the numbers of samples per CRV batch, analyses per CRV sample, and volume determinations per CRV and MFPV batches required for PCT and VHT compliance [Items (5) and (6)].

Table 8.6. Statistical Investigations of Numbers of Samples, Analyses, and Other Process Measurements for ILAW Compliance

ILAW Specification	Statistical Aspect of ILAW Compliance Strategy	Statistical Investigation	Report Section Investigation Described	Report Section Containing Investigation Results	Report Section(s) of Compliance Equations and Investigation Details
2.2.2.6.2: Chemical Composition During Production	Determine the numbers of samples per CRV batch and analyses per CRV sample necessary to estimate ILAW chemical composition from an MFPV batch.	Calculate required numbers of samples per CRV batch and analyses per CRV sample for combinations of values of factors (including applicable uncertainties) that affect ILAW chemical composition estimates and uncertainties for an ILAW MFPV batch.	5.1.3	7.1.1	B.1 3.4.2
2.2.2.7.2: Radionuclide Composition During Production	Determine the numbers of samples per CRV batch, analyses per CRV sample, and other process measurements required to estimate ILAW radionuclide compositions for an MFPV batch, which are in turn used to estimate ILAW radionuclide inventories.	Calculate required numbers of samples per CRV batch and analyses per CRV sample for combinations of values of factors (including applicable uncertainties) that affect ILAW radionuclide composition estimates and uncertainties for an ILAW MFPV batch.	5.2.3	7.2.1	B.2 3.4.2
2.2.2.8: Radionuclide Concentration Limits	Determine the numbers of samples per CRV batch, analyses per CRV sample, and other process measurements required to demonstrate that ILAW radionuclide concentrations over a waste type are below Class C limits.	Calculate required numbers of samples per CRV batch and analyses per CRV sample for combinations of values of factors (including applicable uncertainties) that affect the estimate and uncertainty of the ILAW radionuclide sum-of-fractions for an ILAW MFPV batch.	5.3.4	7.3.2	B.3.1 3.4.2 F.2
2.2.2.8: Radionuclide Concentration Limits	Determine the numbers of samples per CRV batch, analyses per CRV sample, and other process measurements required to demonstrate that running averages of ^{137}Cs and ^{90}Sr concentrations in ILAW are below their specified limits.	Calculate required numbers of samples per CRV batch and analyses per CRV sample for combinations of values of factors (including applicable uncertainties) that affect the estimates and uncertainties of running averages of ^{137}Cs and ^{90}Sr concentrations.	5.3.6	7.3.4	B.3.2 3.4.2 F.3

Table 8.6. Statistical Investigations of Numbers of Samples, Analyses, and Other Process Measurements for ILAW Compliance (cont.)

ILAW Specification	Statistical Aspect of ILAW Compliance Strategy	Statistical Investigation	Report Section Investigation Described	Report Section Containing Investigation Results	Report Section(s) of Compliance Equations and Investigation Details
2.2.2.17.2: PCT and 2.2.2.17.3: VHT	Determine the numbers of samples per CRV batch, analyses per CRV sample, and other process measurements required to demonstrate that the PCT and VHT responses for ILAW from an MFPV batch will satisfy their respective limits.	Calculate required numbers of samples per CRV batch and analyses per CRV sample for combinations of values of factors (including applicable uncertainties) that affect the estimates of PCT and VHT responses and their uncertainties for ILAW from a single MFPV batch	5.4.4	7.4.2 (PCT) 7.5.2 (VHT)	B.1 B.4 F.4
2.2.2.17.2: PCT and 2.2.2.17.3: VHT	Determine the numbers of samples per CRV batch, analyses per CRV sample, and other process measurements required to demonstrate that the PCT and VHT responses for ILAW from an LAW waste type will satisfy their respective limits.	Calculate required numbers of samples per CRV batch and analyses per CRV sample for combinations of values of factors (including applicable uncertainties) that affect the estimates of PCT and VHT responses and their uncertainties for ILAW from an LAW waste type	5.4.6	7.4.4 (PCT) 7.5.4 (VHT)	B.1 B.4 F.4
2.2.2.2: Waste Loading	Determine the numbers of samples per CRV batch, analyses per CRV sample, and other process measurements required to meet the envelope-specific minimums for waste Na_2O loading (Nelson 2003). The WTP ILAW compliance strategy has changed (Westsik et al. 2004) to comparing average waste Na_2O loading (over an ILAW production lot) to the LAW envelope minimum values in Specification 2.2.2.2.	None, because the current WTP ILAW compliance strategy does not involve a statistical approach that accounts for variation and uncertainty in demonstrating compliance with the waste loading specification.	N/A[(a)]	N/A[(a)]	N/A[(a)]

(a) No statistical methods for demonstrating compliance with waste loading requirements were developed or illustrated because the scope for that portion of the work was removed by the WTP Project in anticipation of a revised compliance strategy that would not require a statistically based compliance approach.

8.2.3.1 Number of Samples per ILAW CRV Batch, Analyses per CRV Sample, and Numbers of Volume Determinations per CRV and MFPV Batches to Estimate ILAW Chemical Composition

Table 7.1 provides the numbers of samples per CRV batch and analyses per sample required to estimate, within specified precision ranges (%RHWs) at 90% and 95% confidence, the mass fractions of reportable ILAW chemical composition components (as listed in Table 2.2) for ILAW corresponding to three LAW tanks (AP-101, AZ-101, and AN-107). Table 7.1 provides results for low and high estimates of mixing/sampling and analytical uncertainties in the CRV concentrations, as well as low and high estimates of all the other uncertainties as shown in Table 3.3, for ILAW corresponding to each of the three LAW tanks. These other uncertainties include GFC composition uncertainty, GFC batching uncertainty, and volume uncertainty. The low and high values of the uncertainties are listed in Appendix D. A summary of the results in Table 7.1 are given in Table 8.7. The number of volume determinations for each CRV and MFPV batch was also a factor varied in the simulation as shown in Table 3.3. ANOVA results determined that there was no statistically significant difference in %RHW between taking 1 volume determination and 3 volume determinations for each CRV and MFPV batch. For this reason only 1 volume determination for each CRV and MFPV batch is necessary, and so the number of CRV and MFPV volume determinations are not listed in Table 8.7.

Table 8.7 summarizes (for the "low" and "high" cases for all uncertainties [as defined in Table 3.3] and selected precision [%RHW]) the maximum number of samples per ILAW CRV batch (n_S^{CRV}) and number of analyses per sample (n_A^{CRV}) over all reportable ILAW components (oxides or halogens). When only the "low" estimates for all the uncertainties are considered, Table 8.7 shows that to estimate with 95% confidence all ILAW chemical composition components:

- within 10% of their true values requires from 2 to 5 samples per CRV with 1 analysis per sample
- within 15% of their true values requires 2 samples per CRV with 1 analysis per sample
- within 20% of their true values requires 1 sample per CRV with 1 analysis per sample.

When only the "high" estimates for all the uncertainties are considered, Table 8.7 shows that to estimate with 95% confidence all ILAW chemical composition components:

- within 10% of their true values requires at least 7 samples per CRV with 2 analyses per sample
- within 15% of their true values requires from 5 to 8 samples per CRV with 1 analysis per sample
- within 20% of their true values requires from 3 to 5 samples per CRV with 1 analysis per sample.

These conclusions may be applicable to ILAW for other LAW tanks to be processed by the WTP to the extent that the ranges of CRV mixing/sampling and analytical uncertainties, as well as the other uncertainties, for ILAW corresponding to Tanks AP-101, AZ-101, and AN-107 (see Appendix D) are representative.

Table 8.7. Summary of Numbers of ILAW CRV Samples and Analyses per CRV Sample to Satisfy Certain Precisions (%RHWs) with 90% and 95% Confidence for Reportable ILAW Chemical Composition Components (Oxides) for Low and High Estimates of All Uncertainties[a] for Each of Three LAW Tanks

All Uncertainties[b]	Confidence (%)	%RHW	AP-101 (Envelope A)	AZ-101 (Envelope B)	AN-107 (Envelope C)	Max Over 3 Tanks
L	90	5	7(2)[c]	10(1)	10(1)	7(2)
		10	4(1)	2(1)	3(1)	4(1)
		15	2(1)	1(1)	2(1)	2(1)
		20	1(1)	1(1)	1(1)	1(1)
	95	5	-[d]	-	-	-
		10	5(1)	3(1)	2(2)	5(1)
		15	2(1)	2(1)	2(1)	2(1)
		20	1(1)	1(1)	1(1)	1(1)
H	90	5	-	-	-	-
		10	7(2)	10(1)	7(2)	7(2)
		15	6(1)	4(1)	6(1)	6(1)
		20	4(1)	3(1)	3(1)	4(1)
	95	5	-	-	-	-
		10	-	7(2)	7(2)	-
		15	8(1)	5(1)	8(1)	8(1)
		20	5(1)	3(1)	4(1)	5(1)

(a) All uncertainties include CRV mixing/sampling %RSD, CRV analytical %RSD, GFC composition uncertainty, GFC batching uncertainty, and volume uncertainty.
(b) Low (L) and High (H) levels of all uncertainties associated with reportable elements for each of the three LAW tanks are given in Tables D.1, D.6, D.7, and D.9 of Appendix D.
(c) Each cell in the table lists the number of samples followed by the number of analyses per sample in parenthesis.
(d) A dash (–) indicates that more than the number of samples/analyses used in the Monte Carlo simulation (see Table 3.3) were necessary to satisfy the %RHW category.

8.2.3.2 Numbers of Samples per ILAW CRV Batch, Analyses per CRV Sample, and Volume Determinations per CRV and MFPV Batches to Estimate ILAW Radionuclide Composition

Table 7.5 provides the numbers of samples per CRV batch and analyses per sample required to estimate, within specified precision ranges (%RHWs) at 90% and 95% confidence, the mass fractions of reportable ILAW radionuclide composition components (as listed in Table 2.1) for ILAW corresponding to three LAW tanks (AP-101, AZ-101, and AN-107). Table 7.5 provides results for low and high

estimates of mixing/sampling and analytical uncertainties in the CRV concentrations, as well as low and high estimates of all the other uncertainties as shown in Table 3.3, for ILAW corresponding to each of the three LAW tanks. These other uncertainties include GFC composition uncertainty, GFC batching uncertainty, and volume uncertainty. The low and high values of the uncertainties are listed in Appendix D. A summary of the results in Table 7.5 are given in Table 8.8. The number of volume determinations for each CRV and MFPV batch was also a factor varied in the simulation as shown in Table 3.3. ANOVA results determined that there was no significant difference in %RHW between taking 1 volume determination and 3 volume determinations for each CRV and MFPV batch. For this reason only 1 volume determination for each CRV and MFPV batch is necessary, and so the number of volume determination is not listed in Table 8.8.

Table 8.8 summarizes (for the "low" and "high" cases for all uncertainties [as defined in Table 3.3] and selected precision [%RHW]) the maximum number of samples per ILAW CRV batch (n_S^{CRV}) and number of analyses per sample (n_A^{CRV}) over all reportable ILAW radionuclide components. When only the "low" estimates for all the uncertainties are considered, Table 8.7 shows that to estimate with 95% confidence all ILAW chemical composition components:

- within 10% of their true values requires from 2 to 5 samples per CRV with 1 analysis per sample
- within 15% of their true values requires 2 samples per CRV with 1 analysis per sample
- within 20% of their true values requires 1 sample per CRV with 1 analysis per sample.

When only the "high" estimates for all the uncertainties are considered, Table 8.7 shows that to estimate with 95% confidence all ILAW chemical composition components:

- within 10% of their true values requires at least 7 samples per CRV with 2 analyses per sample
- within 15% of their true values requires from 5 to 8 samples per CRV with 1 analysis per sample
- within 20% of their true values requires from 3 to 5 samples per CRV with 1 analysis per sample.

These conclusions may be applicable to ILAW for other LAW tanks to be processed by the WTP to the extent that the ranges of mixing/sampling and analytical uncertainties, as well as the other uncertainties, for LAW from Tanks AP-101, AZ-101, and AN-107 (see Appendix D) are representative.

8.2.3.3 Numbers of Samples per LAW CRV Batch, Analyses per CRV Sample, and Volume Determinations per CRV and MFPV Batches to Demonstrate Compliance with Radionuclide Concentration Requirements

Investigations in Section 7.3.2 for single-MFPV-batch radionuclide concentration compliance with Class C limits and in Section 7.3.4 for single-MFPV-batch compliance with ^{137}Cs and ^{90}Sr concentration limits showed that all 95% EUCI values in the Monte Carlo simulation were easily below the specified limits. This means that 1 sample per CRV batch with 1 chemical analysis per sample and 1 volume determination per each CRV and MFPV batch was sufficient for demonstrating compliance using the single-CRV-batch statistical methods. The Monte Carlo simulation 95% EUCI results are illustrated in Figures 7.3 and 7.4 for radionuclide concentration compliance with Class C limits and Figure 7.7 for

compliance with ^{137}Cs and ^{90}Sr concentration limits. These conclusions were reached using ranges of reasonable estimates of mixing/sampling and analytical uncertainties for ILAW CRV batches, as well as other process uncertainties, corresponding to each of three ILAW waste tanks (AP-101, AZ-101, and AN-107) used for investigations.

Table 8.8. Summary of Numbers of ILAW CRV Samples and Analyses per CRV Sample to Satisfy Certain Precisions (%RHWs) with 90% and 95% Confidence for Reportable ILAW Radionuclide Composition Components for Low and High Estimates of All Uncertainties[(a)] for Each of Three LAW Tanks

All Uncertainties[(b)]	Confidence (%)	%RHW	AP-101 (Envelope A)	AZ-101 (Envelope B)	AN-107 (Envelope C)	Max Over 3 Tanks
L	90	5	-[(c)]	7(2)[(d)]	-	-
		10	5(1)	4(1)	5(1)	5(1)
		15	2(1)	2(1)	2(1)	2(1)
		20	2(1)	1(1)	1(1)	2(1)
	95	5	-	-	-	-
		10	8(1)	5(1)	8(1)	8(1)
		15	3(1)	2(1)	3(1)	3(1)
		20	2(1)	2(1)	2(1)	2(1)
H	90	5	-	-	-	-
		10	-	7(2)	-	-
		15	8(1)	6(1)	8(1)	8(1)
		20	5(1)	4(1)	2(2)	5(1)
	95	5	-	-	-	-
		10	-	-	-	-
		15	7(2)	8(1)	7(2)	7(2)
		20	6(1)	5(1)	6(1)	6(1)

(a) All uncertainties include CRV mixing/sampling %RSD, CRV analytical %RSD, GFC composition uncertainty, GFC batching uncertainty, and volume uncertainty.

(b) Low (L) and High (H) levels of all uncertainties associated with reportable elements for each of the three LAW tanks are given in Tables D.2, D.4, D.6, D.7, and D.9 of Appendix D.

(c) A dash (–) indicates that more than the number of samples / analyses used in the Monte Carlo simulation (see Table 3.3) were necessary to satisfy the %RHW category.

(d) Each cell in the table lists the number of samples followed by the number of analyses per sample in parenthesis.

8.2.3.4 Number of Samples per ILAW CRV Batch, Analyses per CRV Sample, and Numbers of Volume Determinations per CRV and MFPV Batches and over an LAW Waste Type to Demonstrate PCT and VHT Compliance

The numbers of samples per ILAW CRV, analyses per CRV sample, and volume determinations per CRV and MFPV batches required to demonstrate PCT and VHT compliance for each MFPV batch [Item (5) in Section 8.2.2] and over an LAW waste type [Item (6) in Section 8.1.2] are the easiest to summarize. Specifically, investigations in Section 7.4.2 for single-CRV-batch PCT compliance and Section 7.5.2 for single-CRV-batch VHT compliance showed that all 95% UCCI values in the Monte Carlo simulation were compliant, meaning that 1 sample per CRV batch with 1 chemical analysis per sample and 1 volume determination per each CRV and MFPV batch was sufficient for demonstrating compliance using the single-CRV-batch statistical methods. Investigations in (1) Section 7.4.4 for demonstrating PCT compliance over an LAW waste type and (2) Section 7.5.4 for demonstrating VHT compliance over an LAW waste type showed that 3 samples per ILAW CRV batch with 1 chemical analysis per sample was sufficient for demonstrating compliance in all cases except one. Using highly conservative estimates for the uncertainties and variation between batches and assuming a conservative 10 batches per LAW waste type resulted in the 95%/95% UTI for PCT normalized B release of 4.244 g/L being slightly higher than the limit of 4 g/L. Compliance can be obtained by having slightly lower uncertainties or variation, increasing the number of MFPV batches per LAW waste type from 10, or increasing the number of samples per ILAW CRV batch from 3. The final report will use better estimates in each case to obtain the final recommendation of the numbers of samples, analyses, and volume determinations.

These conclusions were reached using ranges of reasonable estimates of mixing/sampling and analytical uncertainties for ILAW CRV batches, as well as other process uncertainties, corresponding to each of three ILAW waste tanks (AP-101, AZ-101, and AN-107) used for investigations. The conclusion was also confirmed in an investigation using wider ranges of mixing/sampling uncertainty (5 to 20 %RSD) and analytical uncertainty (5 to 50 %RSD).[(a)] The explanation for why 3 samples per ILAW CRV batch with 1 chemical analysis per sample is expected to be sufficient for demonstrating PCT and VHT compliance (for each CRV batch as well as over a collection of batches corresponding to an LAW waste type) is as follows. It is relatively easy to formulate LAW glasses with PCT and VHT responses significantly below the specification limits. Further, the combination of PCT and VHT model uncertainty, chemical composition uncertainty, and chemical composition variation over an LAW waste type do not overcome (except the one exception noted) this margin even for 3 samples per ILAW CRV batch, 1 chemical analysis per sample, and 1 determination for each CRV and MFPV volume.

(a) These %RSDs represent uncertainties in PCT and VHT responses after propagating ILAW chemical composition uncertainties through ILAW PCT and VHT property-composition models.

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Appendix A

Compliance Equations for IHLW Specifications

Appendix A: Compliance Equations for IHLW Specifications

This appendix contains derivations and descriptions of equations for calculating immobilized high-level waste (IHLW) compliance quantities during IHLW production. The compliance equations are functions of process samples, analyses per sample, and measurements that will be available for demonstrating compliance with IHLW specifications during production, according to the IHLW compliance strategy. Compliance equations are presented in this appendix for IHLW specifications where the compliance strategy has statistical aspects. Compliance equations are also provided for IHLW specifications where the Waste Treatment and Immobilization Plant (WTP) compliance strategy previously had statistical aspects but was changed, and the equations had been developed before the strategy change. Such equations may still play roles in process control and revised WTP compliance strategies, and these are presented in this appendix.

Many aspects of the WTP IHLW compliance strategy are associated with reporting or demonstrating compliance for glass from a series of IHLW Melter Feed Preparation Vessel (MFPV) batches corresponding to a *high-level waste* (*HLW*) *type.* The WTP Project's IHLW compliance strategy (Nelson 2003; Nelson et al. 2004) identifies an HLW waste type as corresponding to the contents of an HLW Blend Vessel (HBV). An HBV is planned to yield 18 MFPV batches. Hence, according to the current IHLW compliance strategy, an HLW waste type will correspond to 18 MFPV batches. However, the equations presented in this appendix are applicable to waste types defined as any series of MFPV batches, and thus the more general term "waste type" is subsequently used in most cases rather than "HBV." The number of IHLW MFPV batches produced from an HLW waste type is denoted I, and the number of IHLW canisters associated with that HLW waste type is denoted D. The D IHLW canisters produced from the I IHLW MFPV batches will be those produced starting after the mean melter residence time plus the time of transfer from the IHLW MFPV to the melter. The total mass of glass oxides per IHLW MFPV batch will be summed for the I batches and divided by the mass of glass per canister to determine the number of IHLW canisters D represented by the I IHLW MFPV batches.

The majority of results presented in this appendix are based on the IHLW compliance strategy as described in Rev. 0 of the *IHLW Product Compliance Plan* (IHLW PCP) by Nelson (2003). During the latter part of the work leading to this report, the WTP Project made significant changes in the IHLW compliance strategy. Some of the results in this appendix (identified as such in the following sections) are based on informal descriptions of the new compliance strategy provided by the WTP Project. As this report was being completed, Rev. 1 of the IHLW PCP was issued (Nelson et al. 2004). The IHLW PCP Rev. 1 ultimately reflects direction from the DOE-ORP to implement WASRD (DOE-RW 2002) requirements in place of the WAPS (DOE-EM 1996). Any revisions to results in this appendix necessitated by revisions to the compliance strategies in the Rev. 1 IHLW PCP (including those related to the change from WASRD to WAPS requirements) will be made in a future revision of this report.

A.1 Compliance Equations for IHLW WAPS Specification 1.1.2: Chemical Composition During Production

IHLW Waste Acceptance Preliminary Specifications (WAPS) Specification 1.1.2 is listed verbatim to provide the context for the IHLW chemical compliance equations presented in this section.

WAPS Specification 1.1.2: Chemical Composition During Production

> *In the Production Records, the Producer shall report the oxide composition of the waste form. The reported composition shall include all elements, excluding oxygen, present in concentrations greater than 0.5 percent by weight of the glass, for each waste type. The Producer shall describe the method to be used for compliance in the WCP. An estimate of the error of the reported composition and the basis for the estimate shall be reported in the WQR.*

In WAPS 1.1.2, WCP is the acronym for Waste Compliance Plan, and WQR is the acronym for Waste Form Qualification Report. For the WTP Project, the IHLW PCP serves as the WCP, and the IHLW Product Qualification Report (PQR) serves as the WQR.

This section documents the equations for calculating the chemical composition of IHLW based on the results of chemical analyses of IHLW MFPV process samples to be taken during production operations of the WTP IHLW facility. The equations presented are based on informal descriptions and early revisions to the Rev. 0 IHLW PCP (Nelson 2003), which have since been documented in Rev. 1 of the IHLW PCP (Nelson et al. 2004). The IHLW PCP Rev. 0, and subsequent early revisions leading to Rev. 1, document the WTP strategy for complying with IHLW specifications in the WAPS (DOE-EM 1996) and the WTP contract (DOE-ORP 2003).

The IHLW chemical-composition equations presented in this section are based on work by (1) John Vienna, representing the Waste Form Qualification (WFQ) area of the Research and Technology (R&T) organization within the WTP Project, and (2) Greg Piepel, Scott Cooley, and Brett Amidan of Battelle—Pacific Northwest Division (PNWD).

The IHLW operating strategy for IHLW chemical composition described in the IHLW PCP (Nelson et al. 2004) involves (1) transferring a portion of the HLW in the HBV to the MFPV and mixing it with the heel of the previous MFPV batch, (2) sampling and analyzing the contents of the MFPV to determine component concentrations, (3) calculating and weighing required amounts of glass forming chemicals (GFCs) to add to the MFPV to yield the desired IHLW glass composition, and (4) transferring the GFCs to the MFPV and mixing the contents. For compliance and reporting purposes, the chemical composition of IHLW corresponding to an MFPV batch will be calculated based on chemical analyses of MFPV samples after GFCs have been added. Additional details of the process control and compliance strategies are described in the IHLW PCP (Nelson et al. 2004).

An important topic involves the list of glass components that will be used to represent the chemical composition of IHLW. The IHLW chemical-composition equations in this document treat this topic in a general way, with the total number of glass components denoted J and individual components indexed by j. However, to obtain accurate mass-fraction estimates of glass composition, the components used must comprise almost all of the mass that will end up in glass. This includes chemical composition components (oxides or halogens) and radionuclide composition components (oxides). Otherwise, mass fractions of glass components will be biased high. For example, suppose that the number of components chosen to represent IHLW composition corresponds to 98 wt% of the true composition for a given IHLW glass. Then, the mass-balance-based equations in this document would yield, on average, mass fractions that are biased high by the factor 1.0/0.98 = 1.0204 (i.e., slightly over a 2% positive bias). Hence, it is

important that a sufficient number of components be included (e.g., in chemical and radiochemical analyses) to avoid obtaining biased estimates of the mass fractions of those glass components.

The IHLW chemical-composition equations do not at this time (per WTP Project R&T direction) account for possible volatility of components in the melter. If needed based on further consideration by the WTP Project, melter volatility aspects could be accounted for in future updates of the IHLW chemical-composition equations and related statistical compliance activities.

The IHLW chemical-composition equations presented in this appendix assume there are no biases in sampling, chemical analysis, and measurements that yield inputs for the equations. It is assumed that any significant long-term systematic biases in MFPV mixing, sampling, and chemical analysis will be detected and corrected before operation of the WTP IHLW facility. If intermittent biases were to occur during WTP IHLW production, it is assumed the WTP will have methods for detecting and correcting such biases or rejecting the biased results. For example, Piepel and Weier (2003) present methods for accepting/rejecting, bias detection/correction, and weighted normalization of analyzed slurry and glass compositions. These methods could be included in the IHLW chemical-composition compliance equations in the future if desired by the WTP Project.

In summary, the IHLW chemical-composition equations presented in this section are intended for use during WTP IHLW production operations to calculate the chemical composition of IHLW that would result from vitrifying the contents of a given IHLW MFPV batch. The contents of an IHLW MFPV batch are formed by adding (1) waste from the HBV to the MFPV (and its heel from the previous batch), and (2) calculated and weighed amounts of GFCs. The composition of a completed MFPV batch will be calculated based on chemical analyses of samples from the MFPV. The current equations for calculating IHLW composition corresponding to an MFPV batch do not (1) account for any biases in MFPV mixing, sampling, or chemical analyses yielding inputs for the equations, (2) account for volatility in the melter, and (3) implement the adjustment methods for analyzed compositions discussed by Weier and Piepel (2003).

Section A.1.1 presents general equations for calculating masses and mass fractions of IHLW components given a single MFPV sample, analysis per sample, and volume determination. Section A.1.2 extends these equations for calculating masses and mass fractions to accommodate averages over multiple IHLW MFPV samples, analyses per sample, and volume determinations.

A.1.1 Development of Compliance Equations for IHLW Chemical Composition

Composition of waste glass is typically expressed as mass fractions (summing to one) or mass percents (summing to 100) of the components in the glass. In this report, mass fractions are used. The general equation for the chemical composition (mass fractions) of IHLW formed from the i^{th} MFPV batch is

$$g_{ij}^{MFPV} = \frac{m_{ij}^{MFPV}}{M_i^{MFPV}} = \frac{m_{ij}^{MFPV}}{\sum_{j=1}^{J} m_{ij}^{MFPV}} \qquad \text{(A.1.1)}$$

where

g_{ij}^{MFPV} = mass fraction of the j^{th} glass oxide[(a)] component in the i^{th} MFPV batch (g_{oxide}/g_{oxides})

m_{ij}^{MFPV} = mass of the j^{th} glass oxide component in the i^{th} MFPV batch (g)

I = total number of MFPV batches per reporting or compliance period

J = total number of glass oxide components

M_i^{MFPV} = $\sum_{j=1}^{J} m_{ij}^{MFPV}$ = total mass of glass oxide components $j = 1, 2, \ldots, J$ in the i^{th} MFPV batch (g)

The masses m_{ij}^{MFPV} appearing in Eq. (A.1.1) are not measured directly. Instead, they are calculated using information such as analyzed concentrations and measured volumes. The mass of the j^{th} glass oxide component in the i^{th} MFPV batch m_{ij}^{MFPV} is calculated by

$$m_{ij}^{MFPV} = c_{ij}^{MFPV} f_j u V_i^{MFPV} \quad \text{for} \quad j = 1, 2, \ldots, J \tag{A.1.2}$$

where

c_{ij}^{MFPV} = analyzed concentration of analyte j in the i^{th} MFPV batch (μg/mL = mg/L)

f_j = $\frac{MW_j^{oxide}}{MW_j^{analyte}} R_j$ where MW_j^{oxide} and $MW_j^{analyte}$ are the molecular weights of oxide j and analyte j, respectively, and R_j is the ratio of moles of oxide per mole of analyte for oxide j. Hence, f_j is the factor for converting the concentration of analyte j (μg analyte j/mL = mg analyte j/L) to the concentration of oxide j (μg oxide j/mL = mg oxide/L). The quantity f_i is called the oxide factor for oxide j.

u = $\frac{1\,(g)}{1000\,(mg)}$, a units conversion factor for converting mg to g

V_i^{MFPV} = volume of the i^{th} MFPV batch (L).

Table A.1 lists the values of f_j for elements, radionuclides, and the expected prevalent oxide form for each in waste glass. Table A.1 applies to LAW glass as well as HLW glass.

(a) A few glass components (e.g., F and Cl) are not expressed as oxides. However, for simplicity in the presentation, the term oxides will be used to differentiate from situations where elements are the focus.

Table A.1. Element and Radionuclide to Oxide Conversion Factors (f_j)

Element	Oxide	Oxide Factor
Ag	Ag_2O	1.074162
Al	Al_2O_3	1.889464
As	As_2O_5	1.533871
B	B_2O_3	3.219878
Ba	BaO	1.116506
Be	BeO	2.775308
Bi	Bi_2O_3	1.114839
Ca	CaO	1.399207
Cd	CdO	1.142329
Ce	Ce_2O_3	1.171281
Cl	Cl	1
Co	CoO	1.271484
Cr	Cr_2O_3	1.461556
Cs	Cs_2O	1.060191
Cu	CuO	1.251777
Dy	Dy_2O_3	1.147687
Eu	Eu_2O_3	1.157925
F	F	1
Fe	Fe_2O_3	1.429729
K	K2O	1.204605
La	La_2O_3	1.172773
Li	Li_2O	2.152528
Mg	MgO	1.658276
Mn	MnO	1.291226
Mo	MoO_3	1.500294
Na	Na_2O	1.347968
Nd	Nd_2O_3	1.166383
Ni	NiO	1.272593
P	P_2O_5	2.291367
Pb	PbO	1.077217
Pd	PdO	1.150342
Pr	Pr_2O_3	1.170318
Rh	Rh_2O_3	1.233215
Ru	RuO_2	1.3166
S	SO_3	2.496856
Sb	Sb_2O_3	1.197107
Se	SeO_2	1.405253
Si	SiO_2	2.139335
Sn	SnO_2	1.269554

Element	Oxide	Oxide Factor
SO_4	SO_3	0.83345
Sr	SrO	1.1826
Th	ThO_2	1.137903
Ti	TiO_2	1.668312
Tl	Tl_2O	1.039141
U	UO_3	1.201649
V	V_2O_5	1.785185
W	WO_3	1.261073
Y	Y_2O_3	1.269938
Zn	ZnO	1.244677
Zr	ZrO_2	1.350772

Radionuclide	Oxide	Oxide Factor
^{241}Am	$^{241}Am_2O_3$	1.099581
^{243}Am	$^{243}Am_2O_3$	1.098762
^{144}Ce	$^{144}Ce_2O_3$	1.16666
^{242}Cm	$^{242}Cm_2O_3$	1.09917
$^{243+244}Cm2$	$^{243+244}Cm_2O_3$	1.098559
^{60}Co	^{60}CoO	1.266657
$^{51}Cr2$	$^{51}Cr_2O_3$	1.470571
^{134}Cs	$^{134}Cs_2O$	1.059699
^{135}Cs	$^{135}Cs_2O$	1.059257
^{137}Cs	$^{137}Cs_2O$	1.058392
^{152}Eu	$^{152}Eu_2O_3$	1.157889
^{154}Eu	$^{154}Eu_2O_3$	1.155838
^{155}Eu	$^{155}Eu_2O_3$	1.154833
$^{59}Fe2$	$^{59}Fe2O_3$	1.406764
Nb93	$^{93}Nb_2O_5$	1.430091
Nb95	$^{95}Nb_2O_5$	1.421037
Ni59	^{59}NiO	1.271176
Ni63	^{63}NiO	1.253959
Np237	$^{237}NpO_2$	1.135021
Pu236	$^{236}PuO_2$	1.135588
Pu238	$^{238}PuO_2$	1.134449
Pu239	$^{239}PuO_2$	1.133886
Pu240	$^{240}PuO_2$	1.133328
Pu241	$^{241}PuO_2$	1.132775
Pu242	$^{242}PuO_2$	1.132226

Radionuclide	Oxide	Oxide Factor
^{106}Rh	$^{106}Rh_2O_3$	1.226407
^{103}Ru	$^{103}RuO_2$	1.310668
^{106}Ru	$^{106}RuO_2$	1.301875
^{125}Sb	$^{125}Sb_2O_3$	1.192
^{79}Se	$^{79}SeO_2$	1.405048
^{151}Sm	$^{151}Sm_2O_3$	1.158934
^{113}Sn	$^{113}SnO_2$	1.283175
^{126}Sn	$^{126}SnO_2$	1.253959
^{90}Sr	^{90}SrO	1.177771
^{99}Tc	$^{99}Tc_2O_7$	1.565657
^{232}Th	$^{232}ThO_2$	1.137926
^{233}U	$^{233}U_3O_8$	1.206009
^{234}U	$^{234}U_3O_8$	1.205128
^{235}U	$^{235}U_3O_8$	1.204255
^{236}U	$^{236}U_3O_8$	1.203390
^{238}U	$^{238}U_3O_8$	1.201681
^{88}Y	$^{88}Y_2O_3$	1.272717
^{93}Zr	$^{93}ZrO_2$	1.344073

Substituting Eq. (A.1.2) into Eq. (A.1.1) yields the formula for calculating the chemical composition (in mass fractions of oxide components) of the IHLW that would result from the i^{th} MFPV batch:

$$g_{ij}^{MFPV} = \frac{m_{ij}^{MFPV}}{\sum_{j=1}^{J} m_{ij}^{MFPV}} = \frac{c_{ij}^{MFPV} f_j u V_i^{MFPV}}{\sum_{j=1}^{J} c_{ij}^{MFPV} f_j u V_i^{MFPV}} = \frac{c_{ij}^{MFPV} f_j}{\sum_{j=1}^{J} c_{ij}^{MFPV} f_j} \quad \text{(A.1.3)}$$

where all notation is as previously defined following Eq. (A.1.1) and Eq. (A.1.2). Note in Eq. (A.1.3) that the units conversion factor (u) cancels because it is constant for all $i = 1, 2, \ldots, I$ and $j = 1, 2, \ldots, J$. Further, note that the MFPV volume (V_i^{MFPV}) cancels because it depends only on i and is the same for all $j = 1, 2, \ldots, J$. The cancellation of V_i^{MFPV} is important when it comes to calculating the uncertainties of the g_{ij}^{MFPV}, because then the uncertainty in V_i^{MFPV} can be ignored.

A.1.2 Equations for Calculating the IHLW Chemical Composition Corresponding to an MFPV Batch Based on Averages over Multiple Samples, Analyses, and Volume Determinations

The analyte concentrations c_{ij}^{MFPV} in Eqs. (A.1.2) and (A.1.3) and the volume determinations V_i^{MFPV} in Eq. (A.1.2) are subject to various random uncertainties. Some of these random uncertainties can be effectively reduced by making and averaging multiple determinations of a variable. In general, averages over two or more determinations of a variable have smaller uncertainties than single determinations, with the uncertainty reducing as the number of determinations increases.

The analyte concentrations c_{ij}^{MFPV} in Eqs. (A.1.2) and (A.1.3) are subject to the following random uncertainties: random mixing inhomogeneity in the MFPV contents, sampling from the MFPV, and chemical analyses of MFPV samples. In practice when collecting multiple samples from a MFPV batch, it is not possible to separately quantify mixing and sampling uncertainties. Hence, the term mixing/sampling will be used to reflect this situation. MFPV mixing/sampling and analytical uncertainties can be effectively reduced by (1) taking more than one MFPV sample, (2) analyzing each MFPV sample more than once, and (3) averaging the resulting multiple determinations of the concentrations c_{ij}^{MFPV}.

The volume determinations V_i^{MFPV} in Eq. (A.1.2) will also be subject to random uncertainty during WTP IHLW operation. In the WTP IHLW facility, MFPV volumes will be determined by a device for measuring the level of the MFPV contents and then using a level-to-volume calibration equation to calculate the volume of the MFPV contents. Hence, there will be random uncertainties in measuring MFPV levels and uncertainties in the calibration equation (e.g., in the estimated coefficients). Uncertainties in MFPV level-volume calibration equations can be reduced by the way and amount in which data are obtained to develop the calibration equation. It is beyond the scope of this work to address such issues at this time. However, it is within scope to consider reducing the uncertainty in MFPV volume determinations by making multiple level determinations and averaging them. Because level-

volume calibration equations have not yet been developed by the WTP Project, we consider multiple volume determinations directly in this section.

The re-expression of Eq. (A.1.2) to include (1) averages of analyte concentrations over multiple MFPV samples and analyses, and (2) averages over multiple volume determinations is given by:

$$\begin{aligned} \overline{m}_{ij}^{MFPV} &= \overline{c}_{ij}^{MFPV} f_j u \overline{V}_i^{MFPV} \\ &= \left(\frac{1}{n_S^{MFPV} n_A^{MFPV}} \sum_{l=1}^{n_S^{MFPV}} \sum_{m=1}^{n_A^{MFPV}} c_{ijlm}^{MFPV} \right) f_j u \left(\frac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV} \right) \end{aligned} \qquad \text{(A.1.4)}$$

where

$\overline{m}_{ij}^{MFPV}$ = mass of the j^{th} IHLW component for the i^{th} MFPV batch averaged over n_S^{MFPV} samples per MFPV batch, n_A^{MFPV} analyses per sample, and n_V^{MFPV} volume determinations per MFPV batch (g_{oxide})

n_S^{MFPV} = number of samples per MFPV batch

n_A^{MFPV} = number of chemical analyses per MFPV sample

n_V^{MFPV} = number of volume measurements per MFPV batch

$\overline{c}_{ij}^{MFPV}$ = average concentration of the j^{th} analyte over n_A^{MFPV} analyses on each of n_S^{MFPV} samples from the i^{th} MFPV batch (μg/mL = mg/L)

$\overline{V}_i^{MFPV}$ = average volume over n_V^{MFPV} volume determinations of the i^{th} MFPV batch (L)

c_{ijlm}^{MFPV} = analyzed concentration of the j^{th} analyte from the m^{th} analysis of the l^{th} sample from the i^{th} MFPV batch (μg/mL = mg/L)

V_{ih}^{MFPV} = the h^{th} volume determination of the i^{th} MFPV batch (L).

and f_j and u are as previously defined following Eq. (A.1.2).

The re-expression of Eq. (A.1.3) to include averages of analyte concentrations over multiple MFPV samples and analyses is given by:

$$\bar{g}_{ij}^{MFPV} = \frac{\bar{c}_{ij}^{MFPV} f_j}{\sum_{j=1}^{J} \bar{c}_{ij}^{MFPV} f_j} = \frac{\left(\frac{1}{n_S^{MFPV} n_A^{MFPV}} \sum_{l=1}^{n_S^{MFPV}} \sum_{m=1}^{n_A^{MFPV}} c_{ijlm}^{MFPV} \right) f_j}{\sum_{j=1}^{J} \left(\frac{1}{n_S^{MFPV} n_A^{MFPV}} \sum_{l=1}^{n_S^{MFPV}} \sum_{m=1}^{n_A^{MFPV}} c_{ijlm}^{MFPV} \right) f_j} \tag{A.1.5}$$

where

$\bar{g}_{ij}^{MFPV}$ = mass fraction of the j^{th} glass oxide component resulting from averaging concentrations over n_A^{MFPV} analyses each of n_S^{MFPV} samples from the i^{th} MFPV batch (g_{oxide}/g_{oxides})

c_{ijlm}^{MFPV} = analyzed concentration of the j^{th} analyte from the m^{th} analysis of the l^{th} sample from the i^{th} MFPV batch (μg/mL = mg/L)

n_S^{MFPV} = number of samples per MFPV batch

n_A^{MFPV} = number of chemical analyses per MFPV sample

$\bar{c}_{ij}^{MFPV}$ = average concentration of the j^{th} analyte over n_A^{MFPV} analyses each of n_S^{MFPV} samples from the i^{th} MFPV batch (μg/mL = mg/L).

and f_j is as previously defined following Eq. (A.1.2). Note that n_A^{MFPV} is assumed to be the same for every MFPV sample. An extension of this equation to the case of unequal numbers of analyses per sample is given by Eq. (4.1.5) in Section 4.1.4.2.

Alternately, mass-fraction compositions can be calculated for every analysis of every sample of an MFPV batch and averaged, yielding

$$\tilde{g}_{ij}^{MFPV} = \frac{\sum_{l=1}^{n_S^{MFPV}} \sum_{m=1}^{n_A^{MFPV}} g_{ijlm}^{MFPV}}{n_S^{MFPV} n_A^{MFPV}} = \frac{\sum_{l=1}^{n_S^{MFPV}} \sum_{m=1}^{n_A^{MFPV}} \frac{c_{ijlm}^{MFPV} f_j}{\sum_{j=1}^{J} c_{ijlm}^{MFPV} f_j}}{n_S^{MFPV} n_A^{MFPV}} \tag{A.1.6}$$

where

$\tilde{g}_{ij}^{MFPV}$ = average mass fraction of the j^{th} glass oxide component resulting from n_A^{MFPV} analyses of each of n_S^{MFPV} samples from the i^{th} MFPV batch (g_{oxide}/g_{oxides})

g_{ijlm}^{MFPV} = mass fraction of the j^{th} glass-oxide component corresponding to the m^{th} analysis of the l^{th} sample from the i^{th} MFPV batch (g_{oxide}/g_{oxides})

and the remaining notation is as previously defined following Eq. (A.1.4).

A.2 Compliance Equations for IHLW WAPS Specification 1.2.2: Radionuclide Inventory During Production

IHLW WAPS Specification 1.2 and Sub-Specification 1.2.2 are listed verbatim to provide the context for the IHLW radionuclide inventory equations corresponding to WAPS 1.2.2, which are presented in this section.

WAPS Specification 1.2: Radionuclide Inventory During Production

The Producer shall report the inventory of radionuclides (in Curies) that have half-lives longer than 10 years and that are, or will be, present in concentrations greater than 0.05 percent of the total radioactive inventory for each waste type, indexed to the years 2015 and 3115.

1.2.2 Radionuclide Inventory During Production

The Producer shall provide in the Production Records estimates of the inventories of individual reportable radionuclides for each canister and for each waste type. The Producer shall also report the estimated error of these estimates in the WQR.

To address WAPS Specification 1.2.2, the WTP Project will determine which radionuclides (1) have half-lives longer than 10 years, and (2) are or will be present in concentrations greater than 0.05 percent of the total radioactive inventory for each waste type, indexed to the years 2015 and 3115. The IHLW radionuclides currently determined by the WTP Project as satisfying these conditions or as reportable for other reasons are summarized in Table 2.1 of Section 2. The equations to calculate required concentrations and inventories of the "reportable" radionuclides are discussed in the following subsections.

Section A.2.1 presents the equations for calculating masses and mass fractions of radionuclide oxide components in IHLW corresponding to an MFPV batch, which is the initial basis for compliance in the WTP IHLW compliance strategy. These results are then used to derive results per canister and results per waste type. Section A.2.2 presents equations for calculating radionuclide inventories in IHLW canisters. Section A.2.3 presents equations for calculating the total inventories of radionuclides in IHLW canisters corresponding to an HLW waste type.

A.2.1 Equations for Calculating Masses and Mass Fractions of Radionuclide Oxide Components in IHLW Corresponding to an MFPV Batch

During IHLW production, the concentrations of all reportable radionuclides (see Table 2.1 in Section 2) will be measured in the first[(a)] HLW MFPV batch per HBV (waste type). In the subsequent HLW MFPV batches, only the concentrations of selected radionuclides will be measured (see Table 2.1). Radionuclides whose concentrations will be measured in only the first HLW MFPV batch per waste type will have their concentrations reported as the same values for the remaining HLW MFPV batches of a given waste type. Efforts before IHLW production will be required to quantify the variation in these radionuclides over the course of a waste type.

The measured radionuclide concentrations in an MFPV batch will be reported as activity-per-volume concentrations in units of μCi/mL = mCi/L. These radionuclide concentrations will be at the time of analysis. However, WAPS Specification 1.2 requires reporting inventories indexed to the years 2015 and 3115. Hence, the activity-per-volume concentrations at the time of analysis will be indexed to the years 2015 and 3115. These indexed concentrations (still in units of μCi/mL) are assumed to be the inputs to all of the radionuclide compliance equations presented subsequently.

During IHLW production, radiochemical analyses of MFPV samples will yield radionuclide concentrations in units of μCi/mL (= mCi/L). Such an activity-per-volume concentration of a radionuclide in the HLW MFPV can be converted to a mass-per-volume concentration by

$$c_{iq}^{MFPV} = \frac{r_{iq}^{MFPV}}{A_q} \tag{A.2.1}$$

where

c_{iq}^{MFPV} = mass-per-volume concentration of the q^{th} radionuclide in the i^{th} MFPV batch (μg/mL = mg/L)

r_{iq}^{MFPV} = activity-per-volume concentration of the q^{th} radionuclide in the i^{th} MFPV batch (μCi/mL = mCi/L)

A_q = specific activity of the q^{th} radionuclide (Ci/g = mCi/mg).

Values of A_q for a large number of radionuclides q are listed in Table A.2. Table A.2 contains values for far more radionuclides than are reportable for IHLW (or immobilized low-activity waste [ILAW]), but the complete list is retained because the lists of reportable radionuclides are not yet finalized.

(a) At the time of this writing, the WTP Project had not decided whether it would be the first MFPV batch per waste type, one of the middle MFPV batches of a waste type, or possibly even an analysis of a composite sample formed by combining samples from each of the MFPV batches. In what follows, the first batch is assumed, but the equations apply or can be adapted to the other options.

Table A.2. List of Specific Activities A_q for Selected Isotopes q[(a)]

Isotope, q	A_q (Ci/g)	Isotope, q	A_q (Ci/g)	Isotope, q	A_q (Ci/g)	Isotope, q	A_q (Ci/g)	Isotope, q	A_q (Ci/g)
Ac-225	5.80E+04	Ce-139	8.00E+02	F-18	9.50E+07	Kr-87	2.80E+07	Pm-145	1.40E+02
Ac-227	7.20E+01	Ce-141	2.80E+04	Fe-52	7.30E+06	La-137	4.40E-02	Pm-147	9.30E+02
Ac-228	2.20E+06	Ce-143	6.60E+05	Fe-55	2.40E+03	La-140	5.60E+05	Pm-148m	2.10E+04
Ag-105	3.00E+04	Ce-144	3.20E+03	Fe-59	5.00E+04	Lu-172	1.10E+05	Pm-149	4.00E+05
Ag-108m	2.60E+01	Cf-248	1.60E+03	Fe-60	2.00E-02	Lu-173	1.50E+03	Pm-151	7.30E+05
Ag-110m	4.70E+03	Cf-249	4.10E+00	Ga-67	6.00E+05	Lu-174m	5.30E+03	Po-208	5.90E+02
Ag-111	1.60E+05	Cf-250	1.10E+02	Ga-68	4.10E+07	Lu-177	1.10E+05	Po-209	1.70E+01
Al-26	1.90E-02	Cf-251	1.60E+00	Ga-72	3.10E+06	Lu-74	6.20E+02	Po-210	4.50E+03
Am-241	3.40E+00	Cf-252	5.40E+02	Gd-146	1.90E+04	Mg-28	5.40E+06	Pr-142	1.20E+06
Am-242m	1.00E+01	Cf-253	2.90E+04	Gd-148	3.20E+01	Mn-52	4.40E+05	Pr-143	6.70E+04
Am-243	2.00E-01	Cf-254	8.50E+03	Gd-153	3.50E+03	Mn-53	1.80E-03	Pt-188	6.80E+04
Ar-37	9.90E+04	Cl-36	3.30E-02	Gd-159	1.10E+06	Mn-54	7.70E+03	Pt-191	2.40E+05
Ar-39	3.40E+01	Cl-38	1.30E+08	Ge-68	7.10E+03	Mn-56	2.20E+07	Pt-193	3.70E+01
Ar-41	4.20E+07	Cm-240	2.00E+04	Ge-71	1.60E+05	Mo-93	1.10E+00	Pt-193m	1.60E+05
Ar-42	2.60E+02	Cm-241	1.70E+04	Ge-77	3.60E+06	Mo-99	4.80E+05	Pt-195m	1.70E+05
As-72	1.70E+06	Cm-242	3.30E+03	H-3	9.70E+03	N-13	1.50E+09	Pt-197	8.70E+05
As-73	2.20E+04	Cm-243	5.20E+01	Hf-172	1.10E+03	Na-22	6.30E+03	Pt-197m	1.00E+07
As-74	9.90E+04	Cm-244	8.10E+01	Hf-175	1.10E+04	Na-24	8.70E+06	Pu-236	5.30E+02
As-76	1.60E+06	Cm-245	1.70E-01	Hf-181	1.70E+04	Nb-92m	1.40E+05	Pu-237	1.20E+04
As-77	1.00E+06	Cm-246	3.10E-01	Hf-182	2.20E-04	Nb-93m	2.40E+02	Pu-238	1.70E+01
At-211	2.10E+06	Cm-247	9.30E-05	Hg-194	3.50E+00	Nb-94	1.90E-01	Pu-239	6.20E-02
Au-193	9.20E+05	Cm-248	4.20E-03	Hg-195m	4.00E+05	Nb-95	3.90E+04	Pu-240	2.30E-01
Au-194	4.10E+05	Co-55	3.10E+06	Hg-197	2.50E+05	Nb-97	2.70E+07	Pu-241	1.00E+02
Au-195	3.70E+03	Co-56	3.00E+04	Hg-197m	6.70E+05	Nd-147	8.10E+04	Pu-242	3.90E-03
Au-196	1.10E+05	Co-57	8.40E+03	Hg-203	1.40E+04	Nd-149	1.20E+07	Pu-244	1.80E-05
Au-198	2.40E+05	Co-58	3.20E+04	Ho-163	7.60E+01	Ni-59	8.00E-02	Ra-223	5.10E+04
Au-199	2.10E+05	Co-58m	5.90E+06	Ho-166	7.00E+05	Ni-63	5.70E+01	Ra-224	1.60E+05
Ba-131	8.40E+04	Co-60	1.10E+03	Ho-166m	1.80E+00	Ni-65	1.90E+07	Ra-225	3.90E+04
Ba-133	2.60E+02	Cr-51	9.20E+04	I-123	1.90E+06	Np-235	1.40E+03	Ra-226	1.00E+00
Ba-133m	6.10E+05	Cs-129	7.60E+05	I-124	2.50E+05	Np-236	1.30E-02	Ra-228	2.70E+02
Ba-140	7.30E+04	Cs-131	1.00E+05	I-125	1.70E+04	Np-237	7.10E-04	Rb-nat	1.80E+08
Be-10	2.20E-02	Cs-132	1.50E+05	I-126	8.00E+04	Np-239	2.30E+05	Rb-81	8.40E+06
Be-7	3.50E+05	Cs-134	1.30E+03	I-129	1.80E-04	Os-185	7.50E+03	Rb-83	1.80E+04
Bi-205	4.20E+04	Cs-134m	8.00E+06	I-131	1.20E+05	Os-191	4.40E+04	Rb-84	4.70E+04
Bi-206	1.00E+05	Cs-135	1.20E-03	I-132	1.00E+07	Os-191m	1.30E+06	Rb-86	8.10E+04
Bi-207	5.20E+01	Cs-136	7.30E+04	I-133	1.10E+06	Os-193	5.30E+05	Rb-87	8.60E-08
Bi-210	1.20E+05	Cs-137	8.70E+01	I-134	2.70E+07	Os-194	3.10E+02	Re-nat	2.40E+08
Bi-210m	5.70E-04	Cu-64	3.90E+06	I-135	3.50E+06	P-32	2.90E+05	Re-183	1.00E+04
Bi-212	1.50E+07	Cu-67	7.60E+05	In-111	4.20E+05	P-33	1.60E+05	Re-184	1.90E+04
Bk-247	1.00E+00	Dy-159	5.70E+03	In-113m	1.70E+07	Pa-230	3.30E+04	Re-184m	4.30E+03
Bk-249	1.60E+03	Dy-165	8.20E+06	In-114m	2.30E+04	Pa-231	4.70E-02	Re-186	1.90E+05
Br-76	2.50E+06	Dy-166	2.30E+05	In-115m	6.10E+06	Pa-233	2.10E+04	Re-187	3.80E-08
Br-77	7.10E+05	Er-169	8.30E+04	Ir-189	5.20E+04	Pb-201	1.70E+06	Re-188	9.80E+05
Br-82	1.10E+06	Er-171	2.40E+06	Ir-190	6.20E+04	Pb-202	3.40E-03	Re-189	6.80E+05
C-11	8.40E+08	Eu-147	3.70E+04	Ir-192	9.20E+03	Pb-203	3.00E+05	Rh-101	1.10E+03
C-14	4.50E+00	Eu-148	1.60E+04	Ir-193m	6.40E+04	Pb-205	1.20E-04	Rh-102	1.20E+03
Ca-41	8.50E-02	Eu-149	9.40E+03	Ir-194	8.40E+05	Pb-210	7.60E+01	Rh-102m	6.20E+03
Ca-45	1.80E+04	Eu-150	1.60E+06	K-40	6.40E-06	Pb-212	1.40E+06	Rh-103m	3.30E+07
Ca-47	6.10E+05	Eu-152	1.80E+02	K-42	6.00E+06	Pd-103	7.50E+04	Rh-105	8.40E+05
Cd-109	2.60E+03	Eu-152m	2.20E+06	K-43	3.30E+06	Pd-107	5.10E-04	Rh-99	8.20E+04
Cd-113m	2.20E+02	Eu-154	2.60E+02	Kr-81	2.10E-02	Pd-109	2.10E+06	Rn-222	1.50E+05
Cd-115	5.10E+05	Eu-155	4.90E+02	Kr-85	3.90E+02	Pm-143	3.40E+03	Ru-103	3.20E+04
Cd-115m	2.50E+04	Eu-156	5.50E+04	Kr-85m	8.20E+06	Pm-144	2.50E+03	Ru-105	6.70E+06

(a) From 49CFR173.435, Rev. 10/1/2002.

Table A.2. List of Specific Activities A_q for Selected Isotopes q[(a)] (cont.)

Isotope, q	A_q (Ci/g)	Isotope, q	A_q (Ci/g)	Isotope, q	A_q (Ci/g)	Isotope, q	A_q (Ci/g)	Isotope, q	A_q (Ci/g)
Ru-106	3.30E+03	Sn-123	8.20E+03	Tc-99	1.70E-02	Tl-201	2.10E+05	Xe-123	1.20E+07
Ru-97	4.60E+05	Sn-125	1.10E+05	Tc-99m	5.30E+06	Tl-202	5.30E+04	Xe-127	2.80E+04
S-35	4.30E+04	Sn-126	2.80E-02	Te-118	1.80E+05	Tl-204	4.60E+02	Xe-131m	8.40E+04
Sb-122	4.00E+05	Sr-82	6.20E+04	Te-121	6.40E+04	Tm-167	8.50E+04	Xe-133	1.90E+05
Sb-124	1.70E+04	Sr-85	2.40E+04	Te-121m	7.00E+03	Tm-168	8.30E+03	Xe-135	2.60E+06
Sb-125	1.00E+03	Sr-85m	3.30E+07	Te-123m	8.90E+03	Tm-170	6.00E+03	Y-87	4.50E+05
Sb-126	8.40E+04	Sr-87m	1.30E+07	Te-125m	1.80E+04	Tm-171	1.10E+03	Y-88	1.40E+04
Sc-44	1.80E+07	Sr-89	2.90E+04	Te-127	2.60E+06	U-nat	7.10E-07	Y-90	5.40E+05
Sc-46	3.40E+04	Sr-90	1.40E+02	Te-127m	9.40E+03	U-230	2.70E+04	Y-91	2.50E+04
Sc-47	8.30E+05	Sr-91	3.60E+06	Te-129	2.10E+07	U-232	2.20E+01	Y-91m	4.20E+07
Sc-48	1.50E+06	Sr-92	1.30E+07	Te-129m	3.00E+04	U-233	9.70E-03	Y-92	9.60E+06
Se-75	1.50E+04	Ta-178	1.10E+08	Te-131m	8.00E+05	U-234	6.20E-03	Y-93	3.30E+06
Se-79	7.00E-02	Ta-179	1.10E+03	Te-132	3.00E+05	U-235	2.20E-06	Yb-169	2.40E+04
Si-31	3.90E+07	Ta-182	6.20E+03	Th-nat	2.20E-07	U-236	6.50E-05	Yb-175	1.80E+05
Si-32	1.10E+02	Tb-157	1.50E+01	Th-227	3.10E+04	U-238	3.40E-07	Zn-65	8.20E+03
Sm-145	2.60E+03	Tb-158	1.50E+01	Th-228	8.20E+02	V-48	1.70E+05	Zn-69	4.90E+07
Sm-147	2.30E-08	Tb-160	1.10E+04	Th-229	2.10E-01	V-49	8.10E+03	Zn-69m	3.30E+06
Sm-151	2.60E+01	Tc-95m	2.20E+04	Th-230	2.10E-02	W-178	3.40E+04	Zr-88	1.80E+04
Sm-153	4.40E+05	Tc-96	3.20E+05	Th-231	5.30E+05	W-181	6.00E+03	Zr-93	2.50E-03
Sn-113	1.00E+04	Tc-96m	3.80E+07	Th-232	1.10E-07	W-185	9.40E+03	Zr-95	2.10E+04
Sn-117m	8.20E+04	Tc-97	1.40E-03	Th-234	2.30E+04	W-187	7.00E+05	Zr-97	1.90E+06
Sn-119m	3.70E+03	Tc-97m	1.50E+04	Ti-44	1.70E+02	W-188	1.00E+04		
Sn-121m	5.40E+01	Tc-98	8.70E-04	Tl-200	6.00E+05	Xe-122	1.30E+06		

(a) From 49CFR173.435, Rev. 10/1/2002.

During operation of the WTP HLW vitrification facility, the measurements of activity-per-volume concentrations r_{iq}^{MFPV} in Eq. (A.2.1) will be subject to uncertainties from (1) multiple samples taken from every MFPV batch selected for analysis, and (2) possibly multiple radiochemical analyses made on every sample. Averaging over multiple samples and multiple analyses per sample will reduce the uncertainty due to these sources. Rewriting Eq. (A.2.1) with means (averages) yields

$$\bar{c}_{iq}^{MFPV} = \frac{\bar{r}_{iq}^{MFPV}}{A_q} = \frac{1}{A_q}\left(\frac{1}{n_S^{MFPV}\, n_A^{MFPV}} \sum_{l=1}^{n_S^{MFPV}} \sum_{m=1}^{n_A^{MFPV}} r_{iqlm}^{MFPV} \right) \tag{A.2.2}$$

where

$\bar{c}_{iq}^{MFPV}$ = mean mass-per-volume concentration of the q^{th} radionuclide in the i^{th} MFPV batch (μg/mL = mg/L)

$\bar{r}_{iq}^{MFPV}$ = mean activity-per-volume concentration of the q^{th} radionuclide in the i^{th} MFPV batch (μCi/mL = mCi/L)

n_S^{MFPV} = number of samples per MFPV batch, assuming all samples are analyzed for the q^{th} radionuclide[(a)]

n_A^{MFPV} = number of radionuclide analyses per MFPV sample, assuming this number is the same for all radionuclides[(a)]

r_{iqlm}^{MFPV} = activity-per-volume concentration of the q^{th} radionuclide in the i^{th} MFPV batch, based on the m^{th} radionuclide analysis of the l^{th} MFPV sample (μCi/mL = mCi/L).

The mean mass-per-volume concentrations $\overline{c}_{iq}^{MFPV}$ from Eq. (A.2.2) can be used to calculate the average masses ($\overline{m}_{iq}^{MFPV}$) and mass fractions ($\overline{g}_{iq}^{MFPV}$) of radionuclide oxides in the glass that would be made from the i^{th} MFPV batch using the equations for IHLW chemical composition in Section A.1.2. Specifically, masses of radionuclide oxides would be calculated with Eq. (A.1.4), and mass fractions of radionuclide oxides would be calculated with Eq. (A.1.5). The IHLW radionuclides indexed by q in this Section A.2 are treated as a subset of the components indexed by j in these IHLW chemical-composition compliance equations for masses and mass fractions in Section A.1.2. Hence, the mass fraction compositions of IHLW are with respect to the total mass of "chemical composition" as well as "radionuclide composition" components. In the few cases where chemical analyses of selected radionuclides are performed in addition to radiochemical analyses, the masses must only be included once to avoid double-counting such radionuclides. See footnotes (b) and (c) of Table C.6 for information on how this issue was handled in this report based on input from the WTP Project.

Adaptations to the equations for masses and mass fractions of radionuclide components are needed to account for the revised IHLW compliance strategy, which was provided informally by the WTP Project during the course of this work and formally in Rev. 1 of the IHLW PCT (Nelson et al. 2004) as this report was being completed. In the new IHLW compliance strategy, all reportable radionuclides will only be analyzed in the first MFPV batch of an HLW waste type. Ratio methods will not be used to calculate concentrations (and thus masses and mass fractions) of radionuclides not measured in the second through last MFPV batches of an HLW waste type (as had been the strategy in Rev. 0 of the IHLW PCP (Nelson 2003). Thus, it will be necessary to use the analyzed radionuclide concentrations from the first MFPV batch of an HLW waste type for the second through last MFPV batches as well. This is problematic in that the production data then provide no basis for quantifying the variations in the concentrations, masses, mass fractions, and inventories of such radionuclides over the waste type. Thus, other methods will have to be developed to quantify the batch-to-batch variations of these radionuclides over an HLW waste type so that they can be reported in the Production Records. There is also the issue of bias in the single estimate, which will have to be addressed in future work.

The IHLW compliance equations for mass and mass fraction of the q^{th} radionuclide oxide in the i^{th} IHLW MFPV batch [Eqs. (A.1.4) and (A.1.5)] in turn provide inputs for calculating the inventories of the

(a) The number of samples (n_S^{MFPV}) and number of radionuclide analyses per sample (n_A^{MFPV}) need not be the same for each of the radionuclides. In such a case, these notations could be modified to include a q in the subscript to denote the dependence on the q^{th} radionuclide.

q^{th} radionuclide in IHLW canisters, as discussed in Section A.2.2 and over waste types as discussed in Section A.2.3.

A.2.2 Equations for Calculating Inventories of Radionuclides in IHLW Canisters

To report the inventories of radionuclides in each IHLW canister, the relationship between contents of individual IHLW MFPV batches and contents of individual canisters would have to be estimated. Because of (1) the time to process each IHLW MFPV batch through the melter, (2) the volume of glass melt in the melter, and (3) the mixing of MFPV batches that occurs, it is impossible to directly calculate, and difficult to estimate, the composition of a specific IHLW canister based on compositions of IHLW MFPV batches. Hence, the WTP IHLW compliance strategy, as described in Rev. 0 of the IHLW PCP (Nelson 2003) was to report means and standard deviations (SDs) of radionuclide inventories per canister over canisters of glass estimated to be produced from a series of IHLW MFPV batches. This strategy provided for (1) measuring all reportable radionuclides in the first MFPV batch from an HLW waste type, (2) measuring a limited number of radionuclides for the second through last MFPV batches from an HLW waste type, and (3) calculating by ratio methods the concentrations (and thus ultimately inventories) of the unmeasured radionuclides for the second through last MFPV batches of an HLW waste type. This strategy would have provided for calculating and reporting means and SDs of radionuclide inventories for every reportable radionuclide.

Subsequent to Rev. 0 of the IHLW PCP (Nelson 2003) and during the course of work documented in this section, the WTP Project substantially changed the IHLW compliance strategy for WAPS 1.2.2 as discussed at the end of Section A.2.1. The change in strategy means that adaptations to the results in this section will be needed. Specifically, for those radionuclides only measured in one MFPV batch corresponding to an HLW waste type, it will be necessary to develop other methods to quantify batch-to-batch variations in the inventories of these radionuclides over an HLW waste type so that they can be reported in the Production Records.

A.2.2.1 Equation for a Mean Radionuclide Inventory per Canister over *D* IHLW Canisters

A general equation for the mean radionuclide inventory over *D* IHLW canisters is first developed. Then this general equation is extended to include averages over multiple samples, analyses per sample, and volume determinations of an MFPV batch.

General Equation for a Mean Radionuclide Inventory per Canister over D IHLW Canisters

The mean inventory per canister of the q^{th} radionuclide over *D* IHLW canisters associated with the *I* MFPV batches from an HLW waste type is calculated in three steps.

Step 1: The mean mass fraction of radionuclide oxide q in glass estimated to be produced from the I MFPV batches corresponding to an HLW waste type is calculated by

$$\bar{g}_q^{MFPV} = \frac{\sum_{i=1}^{I}\left(\sum_{j=1}^{J} m_{ij}^{MFPV}\right) g_{iq}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J} m_{ij}^{MFPV}} = \frac{\sum_{i=1}^{I} m_{iq}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J} m_{ij}^{MFPV}}$$

$$= \frac{\sum_{i=1}^{I} c_{iq}^{MFPV} f_q u V_i^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J} c_{ij}^{MFPV} f_j u V_i^{MFPV}} = \frac{\sum_{i=1}^{I} \frac{r_{iq}^{MFPV} f_q V_i^{MFPV}}{A_q}}{\sum_{i=1}^{I}\left[\sum_{j\in CHEM}^{J} c_{ij}^{MFPV} f_j + \sum_{j\in RAD}^{J} \frac{r_{ij}^{MFPV} f_j}{A_j}\right] V_i^{MFPV}} \quad \text{(A.2.3)}$$

where

$\bar{g}_q^{MFPV}$ = mean (mass-weighted-average) mass fraction of the q^{th} radionuclide oxide over I MFPV batches (g_{oxide}/g_{oxides})

m_{ij}^{MFPV} = mass of the j^{th} oxide (non-radionuclides as well as radionuclides) from the i^{th} MFPV batch (g_{oxide})

g_{iq}^{MFPV} = mass fraction of the q^{th} radionuclide oxide for glass that would be made from the i^{th} MFPV batch (g_{oxide}/g_{oxides})

I = number of MFPV batches corresponding to an HLW waste type

m_{iq}^{MFPV} = mass of the q^{th} radionuclide oxide from the i^{th} MFPV batch (g)

J = number of non-radionuclide oxides and radionuclide oxides estimated for the composition of each MFPV batch

c_{iq}^{MFPV} = mass-per-volume concentration of the q^{th} radionuclide in the i^{th} MFPV batch (μg/mL = mg/L)

c_{ij}^{MFPV} = mass-per-volume concentration of the j^{th} analyte in the i^{th} MFPV batch (μg/mL = mg/L)

V_i^{MFPV} = volume of the i^{th} MFPV batch (L)

r_{iq}^{MFPV} = activity-per-volume concentration of the q^{th} radionuclide in the i^{th} MFPV batch (μCi/mL = mCi/L)

A_q = specific activity of the q^{th} radionuclide (Ci/g = mCi/mg)

$j \in CHEM$ = chemical composition components of IHLW

$j \in RAD$ = radionuclide composition components of IHLW

$CHEM$ = set of chemical composition components in IHLW

RAD = set of radionuclide components in IHLW

and f_j and f_q are as previously defined following Eq. (A.1.2). The equation for calculating m_{ij}^{MFPV} (where j denotes non-radionuclide oxides as well as radionuclide oxides) is given by Eq. (A.1.2) in Section A.1. After substituting this equation in the development, the unit conversion terms (u) in the numerator and denominator cancel. Substituting the expression in Eq. (A.2.1) for c_{iq}^{MFPV} and c_{ij}^{MFPV}, $j \in RAD$ yields the final form of Eq. (A.2.3).

Step 2: The mean mass of the q^{th} radionuclide oxide over the D IHLW canisters associated with an HLW waste type is calculated by multiplying the mean mass fraction of the q^{th} radionuclide oxide ($\overline{g}_q^{MFPV}$) from Eq. (A.2.3) times the mean mass of glass over the D IHLW canisters estimated to correspond to the I MFPV batches:

$$\overline{m}_{Dq}^{Canister} = \overline{g}_q^{MFPV} \overline{m}_D^{Canister} \tag{A.2.4}$$

where

$\overline{m}_{Dq}^{Canister}$ = mean mass of the q^{th} radionuclide oxide over the D IHLW canisters associated with the I MFPV batches corresponding to an HLW waste type (g_{oxide})

$\overline{m}_D^{Canister}$ = mean mass of glass in the D IHLW canisters associated with an HLW waste type (g_{glass})

and $\overline{g}_q^{MFPV}$ is as previously defined and calculated by Eq. (A.2.3).

Step 3: The mean inventory per canister of the q^{th} radionuclide over D IHLW canisters associated with the I MFPV batches from an HLW waste type is given by the following general equation:

$$\overline{R}_{Dq}^{Canister} = \frac{\overline{m}_{Dq}^{Canister} A_q}{f_q} = \frac{\overline{g}_q^{MFPV} \overline{m}_D^{Canister} A_q}{f_q}$$

$$= \frac{\left(\dfrac{\sum_{i=1}^{I} \dfrac{r_{iq}^{MFPV} f_q V_i^{MFPV}}{A_q}}{\sum_{i=1}^{I} \left[\sum_{j \in CHEM}^{J} c_{ij}^{MFPV} f_j + \sum_{j \in RAD}^{J} \dfrac{r_{ij}^{MFPV} f_j}{A_j} \right] V_i^{MFPV}} \right) \left(\dfrac{1}{D} \sum_{d=1}^{D} m_d^{Canister} \right) A_q}{f_q}$$

$$= \left(\frac{\sum_{i=1}^{I} r_{iq}^{MFPV} V_i^{MFPV}}{\sum_{i=1}^{I} \left[\sum_{j \in CHEM}^{J} c_{ij}^{MFPV} f_j + \sum_{j \in RAD}^{J} \dfrac{r_{ij}^{MFPV} f_j}{A_j} \right] V_i^{MFPV}} \right) \left(\frac{1}{D} \sum_{d=1}^{D} m_d^{Canister} \right) \qquad \text{(A.2.5)}$$

where

$\overline{R}_{Dq}^{Canister}$ = mean inventory per canister of the q^{th} radionuclide over the D IHLW canisters associated with an HLW waste type (Ci)

$\overline{m}_{Dq}^{Canister}$ = mean mass of the q^{th} radionuclide oxide over the D IHLW canisters associated with the I MFPV batches comprising an HLW waste type (g_{oxide})

A_q = specific activity of the q^{th} radionuclide ($Ci/g_{radionuclide}$)

f_q = $\dfrac{MW_q^{oxide}}{MW_q^{radionuclide}} K_q$ where MW_q^{oxide} and $MW_q^{radionuclide}$ are the molecular weights of radionuclide oxide q and radionuclide q, respectively, and K_q is the ratio of moles of radionuclide oxide q per mole of radionuclide q. Hence, f_j is the factor for converting the concentration of analyte j (µg analyte j/mL = mg analyte j/L) to the concentration of oxide j (µg oxide j/mL = mg oxide/L). The quantity f_q is called the oxide factor for oxide q ($g_{oxide}/g_{radionuclide}$).

$\overline{g}_q^{MFPV}$ = mean (mass-weighted-average) mass fraction of the q^{th} radionuclide oxide over I MFPV batches (g_{oxide}/g_{oxides})

D = number of IHLW canisters associated with an HLW waste type

$\overline{m}_D^{Canister}$ = mean mass of glass in the D IHLW canisters associated with an HLW waste type (g_{glass})

$m_d^{Canister}$ = measured mass of glass in the d^{th} IHLW canister, $d = 1, 2, \ldots, D$ (g_{glass})

I = number of MFPV batches corresponding to an HLW waste type

J = number of non-radionuclide oxides and radionuclide oxides estimated for the composition of each MFPV batch.

and the remaining notation is as previously defined following Eq. (A.2.3). In the second line of the derivation, Eq. (A.2.5) is used to substitute for $\overline{g}_q^{MFPV}$ and $\overline{m}_D^{Canister}$ is expanded using the usual formula for a mean. The final form is obtained in the third line of Eq. (A.2.5) after canceling pairs of f_q and A_q terms.

Equation for the Mean Radionuclide Inventory per Canister over *D* IHLW Canisters Based on Averages of Multiple Samples, Analyses, and Volume Determinations for Each MFPV Batch

Equation (A.2.5) provides the general formula for calculating the mean inventory per canister of each reportable radionuclide q over the D IHLW canisters associated with the I IHLW MFPV batches corresponding to a given HLW waste type. The variables in Eq. (A.2.5) are subject to several within-batch sources of uncertainty. These include MFPV mixing/sampling uncertainty, MFPV analytical uncertainty, uncertainty in MFPV level/volume determinations, and uncertainty in the mass of IHLW in canisters. The first three of these four uncertainties can be effectively reduced by averaging results over multiple MFPV samples per IHLW batch (n_A^{MFPV}), multiple chemical or radiochemical analyses per MFPV sample (n_A^{MFPV}), and multiple vessel level/volume determinations (n_V^{MFPV}). It is assumed that the mass of IHLW per canister ($m_d^{Canister}$) will be determined only once, and thus that the uncertainty associated with it will not be eligible for reduction by averaging. This assumption was made because the uncertainty in determining this mass is expected to be fairly small, and thus not much would be gained by averaging multiple determinations.

The re-expression of Eq. (A.2.5) to include (1) the average analyte concentrations over multiple MFPV samples and analyses, and (2) the average MFPV volume over multiple volume determinations is given by:

$$\overline{\overline{R}}_{Dq}^{Canister} = \frac{\overline{\overline{g}}_q^{MFPV}\,\overline{m}_D^{Canister}\,A_q}{f_q} = \frac{\left(\dfrac{\sum_{i=1}^{I}\overline{m}_{iq}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J}\overline{m}_{ij}^{MFPV}}\right)\left(\dfrac{1}{D}\sum_{d=1}^{D}m_d^{Canister}\right)A_q}{f_q}$$

$$= \frac{\left(\dfrac{\sum_{i=1}^{I}\left(\dfrac{1}{n_S^{MFPV}\,n_A^{MFPV}}\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}}c_{iqlm}^{MFPV}\right)\left(\dfrac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}}V_{ih}^{MFPV}\right)f_q u}{\sum_{i=1}^{I}\sum_{j=1}^{J}\left(\dfrac{1}{n_S^{MFPV}\,n_A^{MFPV}}\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}}c_{ijlm}^{MFPV}\right)\left(\dfrac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}}V_{ih}^{MFPV}\right)f_j u}\right)\left(\dfrac{1}{D}\sum_{d=1}^{D}m_d^{Canister}\right)A_q}{f_q}$$

$$= \left(\frac{\sum_{i=1}^{I}\left(\dfrac{1}{n_S^{MFPV}\,n_A^{MFPV}}\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}}c_{iqlm}^{MFPV}\right)\left(\dfrac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}}V_{ih}^{MFPV}\right)}{\sum_{i=1}^{I}\sum_{j=1}^{J}\left(\dfrac{1}{n_S^{MFPV}\,n_A^{MFPV}}\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}}c_{ijlm}^{MFPV}f_j\right)\left(\dfrac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}}V_{ih}^{MFPV}\right)}\right)\left(\frac{1}{D}\sum_{d=1}^{D}m_d^{Canister}\right)A_q$$

$$= \left(\frac{\left[\sum_{i=1}^{I}\left(\dfrac{\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}}r_{iqlm}^{MFPV}/A_q}{n_S^{MFPV}\,n_A^{MFPV}}\right)\left(\dfrac{\sum_{h=1}^{n_V^{MFPV}}V_{ih}^{MFPV}}{n_V^{MFPV}}\right)\right]\left[\left(\dfrac{1}{D}\sum_{d=1}^{D}m_d^{Canister}\right)A_q\right]}{\sum_{i=1}^{I}\left(\sum_{j\in CHEM}^{J}\dfrac{\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}}c_{ijlm}^{MFPV}f_j}{n_S^{MFPV}\,n_A^{MFPV}}+\sum_{j\in RAD}^{J}\dfrac{\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}}r_{ijlm}^{MFPV}f_j/A_j}{n_S^{MFPV}\,n_A^{MFPV}}\right)\left(\dfrac{\sum_{h=1}^{n_V^{MFPV}}V_{ih}^{MFPV}}{n_V^{MFPV}}\right)}\right)$$

$$= \left(\frac{\left[\sum_{i=1}^{I}\left(\dfrac{\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}}r_{iqlm}^{MFPV}}{n_S^{MFPV}\,n_A^{MFPV}}\right)\left(\dfrac{\sum_{h=1}^{n_V^{MFPV}}V_{ih}^{MFPV}}{n_V^{MFPV}}\right)\right]\left[\dfrac{1}{D}\sum_{d=1}^{D}m_d^{Canister}\right]}{\sum_{i=1}^{I}\left(\sum_{j\in CHEM}^{J}\dfrac{\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}}c_{ijlm}^{MFPV}f_j}{n_S^{MFPV}\,n_A^{MFPV}}+\sum_{j\in RAD}^{J}\dfrac{\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}}r_{ijlm}^{MFPV}f_j/A_j}{n_S^{MFPV}\,n_A^{MFPV}}\right)\left(\dfrac{\sum_{h=1}^{n_V^{MFPV}}V_{ih}^{MFPV}}{n_V^{MFPV}}\right)}\right) \qquad \text{(A.2.6)}$$

where

$\overline{\overline{R}}_{Dq}^{Canister}$ = mean inventory per canister of the q^{th} radionuclide over the D IHLW canisters associated with an HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (Ci)

$$\overline{\overline{g}}_{q}^{MFPV} = \frac{\sum_{i=1}^{I} \overline{m}_{iq}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J} \overline{m}_{ij}^{MFPV}} = \text{mass weighted average of the mass fractions of the} \quad \text{(A.2.7)}$$

q^{th} radionuclide oxide over the I IHLW canisters associated with an HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch ($g_{oxide\ q}/g_{oxides}$)

and the remaining notation is as previously defined following Eq. (A.2.3) and Eq. (A.2.4). From the second to third lines of the development, $\overline{m}_{iq}^{MFPV}$ and $\overline{m}_{ij}^{MFPV}$ are substituted using Eq. (A.1.4). In the fourth line, pairs of f_q and u terms cancel. In the fifth line, Eq. (A.2.2) is applied for the subset of IHLW components determined by radiochemical analysis (denoted *RAD*). In the final line of Eq. (A.2.6), the pair of A_q terms cancel.

Despite the effective reductions of some within-batch uncertainties due to averaging, it should be recognized that values of $\overline{\overline{R}}_{Dq}^{Canister}$ calculated via Eq. (A.2.6) will still be subject to reduced within-MFPV-batch uncertainty as well as MFPV batch-to-batch variations.

A.2.2.2 Equation for the SD of a Radionuclide Inventory per Canister over *D* IHLW Canisters

The standard deviation of the inventory per canister of radionuclide q over the D IHLW canisters associated with the I IHLW MFPV batches corresponding to an HLW waste type can be obtained by applying variance propagation methods to a conceptual equation for the inventory of radionuclide q in a single IHLW canister. First, a general equation for the inventory of radionuclide q in a single IHLW canister is presented. Then this general equation is extended to include averages over multiple samples, analyses per sample, and volume determinations of an MFPV batch.

General Equation for the SD of a Radionuclide Inventory per Canister over *D* IHLW Canisters

A general, conceptual equation for the inventory of radionuclide q in a single IHLW canister is given by:

$$R_{dq}^{Canister} = \frac{g_{iq}^{MFPV}\, m_{d}^{Canister}\, A_q}{f_q} \quad \text{(A.2.8)}$$

where

$R_{dq}^{Canister}$ = inventory of radionuclide q for the d^{th} IHLW canister (Ci)

g_{iq}^{MFPV} = mass fraction of the q^{th} radionuclide oxide in the i^{th} MFPV batch (g_{oxide}/g_{oxides})

$m_d^{Canister}$ = measured mass of glass in the d^{th} IHLW canister (g_{glass})

and A_q and f_q are as previously defined following Eq. (A.1.2) and Eq. (A.2.3). The quantity f_q is a known constant for each radionuclide q and hence is not subject to uncertainty. The A_q are subject to uncertainty corresponding to uncertainties in radionuclide half-lives. However, there is no compiled, complete table of such uncertainties, and so for now the A_q values will be treated as being known with minimal uncertainty.

Equation (A.2.8) for $R_{dq}^{Canister}$ provides a general, conceptual formula for calculating the inventory of each reportable radionuclide q for the d^{th} IHLW canister associated with the i^{th} MFPV batch corresponding to a given HLW waste type. The formula is conceptual because it is not possible to directly calculate an IHLW radionuclide inventory for a given IHLW canister as represented in the equation. The impossibility stems from the inability to easily relate the composition of the i^{th} IHLW MFPV batch to that of the d^{th} IHLW canister. However, a subsequent variation of Eq. (A.2.7) is useful for calculating the standard deviation of a radionuclide inventory per canister over the D canisters of IHLW and corresponding I MFPV batches corresponding to a given waste type.

Equation for the SD of Radionuclide Inventory per Canister over *D* IHLW Canisters Based on Averages of Multiple Samples, Analyses, and Volume Determinations for Each MFPV Batch

The variables in Eq. (A.2.8) are subject to several within-batch sources of uncertainty. These include MFPV mixing/sampling uncertainty, MFPV analytical uncertainty, uncertainty in MFPV level/volume determinations, and uncertainty in the mass of IHLW in canisters. The first three of these four uncertainties can be effectively reduced by averaging results over multiple MFPV samples per IHLW batch (n_A^{MFPV}), multiple chemical or radiochemical analyses per MFPV sample (n_A^{MFPV}), and multiple vessel level/volume determinations (n_V^{MFPV}). It is assumed that the mass of IHLW per canister ($m_d^{Canister}$) will be determined only once, and thus that the uncertainty associated with it will not be eligible for reduction by averaging. This assumption was made because the uncertainty in determining this mass is expected to be fairly small, and thus not much would be gained by averaging multiple determinations.

The re-expression of Eq. (A.2.8) to include (1) the average analyte concentrations over multiple MFPV samples and analyses, and (2) the average MFPV volume over multiple volume determinations is given by:

$$\overline{R}_{dq}^{Canister} = \frac{\overline{g}_{iq}^{MFPV} m_d^{Canister} A_q}{f_q} \tag{A.2.9}$$

where

$\overline{R}_{dq}^{Canister}$ = inventory of radionuclide q for the d^{th} IHLW canister based on averages over multiple samples, analyses per sample, and volume determinations of the corresponding i^{th} MFPV batch (Ci),

$\overline{g}_{iq}^{MFPV}$ is given by Eq. (A.1.5) with "q" in place of "j," and the other notation is as previously defined following Eq. (A.1.2), Eq. (A.2.3), and Eq. (A.2.8). Note that $\overline{g}_{iq}^{MFPV}$ incorporates averages of analyte concentrations over multiple samples, analyses per sample, and averages of multiple volume determinations for each MFPV batch.

The equation for the standard deviation of $\overline{R}_{dq}^{Canister}$ over D canisters associated with I IHLW MFPV batches was obtained by applying the variance propagation method of Goodman (1960) to Eq. (A.2.9) and assuming statistical independence among the radionuclide oxide mass fractions in an IHLW MFPV batch and the measured mass of glass in an IHLW canister.[(a)] The standard-deviation equation is:

$$SD(\overline{R}_{dq}^{Canister}) = \left(\frac{A_q}{f_q}\right)\left[\begin{array}{l}\left[\overline{\overline{g}}_q^{MFPV}\right]^2\left[SD(m_d^{Canister})\right]^2 + \left[\overline{m}_D^{Canister}\right]^2\left[SD(\overline{g}_{iq}^{MFPV})\right]^2 \\ -\left[SD(m_d^{Canister})\right]^2\left[SD(\overline{g}_{iq}^{MFPV})\right]^2\end{array}\right]^{1/2} \tag{A.2.10}$$

where

$SD(\overline{R}_{dq}^{Canister})$ = standard deviation of the average inventory of radionuclide q for the d^{th} IHLW canister, where the average is based on multiple samples, analyses per sample, and volume determinations of the corresponding i^{th} MFPV batch (Ci)

$SD(m_d^{Canister})$ = standard deviation of the measured mass of glass in the d^{th} IHLW canister (g_{glass})

(a) The assumption of statistical independence between radionuclide oxide mass fractions in the MFPV and mass of glass in an IHLW canister is clearly reasonable as the process of filling canisters is independent of the glass composition. It is not clear the extent to which the assumption of statistical independence among mass fractions of radionuclide oxides in the MFPV is appropriate, but from a practical standpoint, it would be very difficult to estimate the many within-batch and batch-to-batch covariances between pairs of radionuclide oxide mass fractions. However, treating the radionuclide covariances as negligible is probably justified given the relatively tiny fractions of glass made up by radionuclides.

$SD(\bar{g}_{iq}^{MFPV})$ = standard deviation of the average mass fraction of the q^{th} radionuclide oxide in the i^{th} MFPV batch, where the average is based on multiple samples, analyses per sample, and volume determinations of the corresponding i^{th} MFPV batch (g_{oxide}/g_{oxides})

and the remaining notation is as previously defined following Eq. (A.1.2), Eq. (A.2.3), and Eq. (A.2.4). In Eq. (A.2.10), $\bar{\bar{g}}_{q}^{MFPV}$ is given by Eq. (A.2.7). Note that the minus sign in front of the third term in the square-bracketed portion of Eq. (A.2.10) is correct for estimating the standard deviation, as discussed by Goodman (1960).

The term $SD(\bar{g}_{iq}^{MFPV})$ includes variation in mass fractions of the q^{th} radionuclide oxide across all I MFPV batches associated with an HLW waste type, as well as uncertainties in determining mass fractions of radionuclide oxides for each MFPV batch. These uncertainties include random inhomogeneities in mixing the MFPV contents, random sampling uncertainties associated with the MFPV sampling system, random irreproducibility of the chemical-analysis techniques employed, and random uncertainties in making MFPV volume determinations. The first three of these are effectively reduced by averaging when multiple samples, analyses per sample, and volume determinations per MFPV batch are made. A value of $SD(\bar{g}_{iq}^{MFPV})$ is calculated from the $\bar{g}_{iq}^{MFPV}$ (i = 1, 2, … , I) values using the usual standard deviation formula.

In a similar way, the term $SD(m_d^{Canister})$ includes uncertainties associated with measuring the mass of glass in an IHLW canister as well as the variation in the masses of glass that occur across canisters associated with an HLW waste type. A value of $SD(m_d^{Canister})$ is calculated from the $m_d^{Canister}$ (d = 1, 2, … , D) values using the usual standard deviation formula.

A.2.3 Total Inventory of a Radionuclide in Canisters Corresponding to an HLW Waste Type

The total inventory of the q^{th} radionuclide in D IHLW canisters corresponding to an HLW waste type could be obtained by summing the inventories over the D canisters. However, as discussed previously, it is not feasible to accurately determine the exact glass composition and radionuclide inventory of each IHLW canister as a function of glass compositions and radionuclide inventories of IHLW MFPV batches. Rather, the WTP Project compliance strategy, as describe in Rev. 0 of the IHLW PCP (Nelson 2003), is to report means and SDs of radionuclide inventories over the D IHLW canisters corresponding to a waste type. As described at the end of Section A.2.2, the IHLW compliance strategy has been revised, as presented in Rev. 1 of the IHLW PCP (Nelson et al. 2004). The equations for compliance quantities presented in this section will be revised as needed in a future revision of this report.

Based on the WTP Project's strategy, the total inventory of the q^{th} radionuclide in D IHLW canisters corresponding to an HLW waste type can be calculated by multiplying the mean inventory per canister over the D canisters times the number of canisters:

$$R_{Dq}^{Canisters} = D\,\overline{\overline{R}}_{Dq}^{Canister} = D\left(\frac{\overline{\overline{g}}_q^{MFPV}\,\overline{m}_D^{Canister}\,A_q}{f_q}\right) \tag{A.2.11}$$

where

$R_{Dq}^{Canisters}$ = total inventory of the q^{th} radionuclide in D IHLW canisters associated with an HLW waste type (Ci)

D = number of IHLW canisters corresponding to an HLW waste type

$\overline{\overline{R}}_{Dq}^{Canister}$ = mean inventory per canister of the q^{th} radionuclide over the D IHLW canisters associated with an HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (Ci)

and the remaining notation is as previously defined following Eq. (A.1.2) and Eq. (A.2.3). The equation for calculating $\overline{\overline{R}}_{Dq}^{Canister}$ is given by Eq. (A.2.7). Note that Eq. (A.2.11) uses averages over multiple samples, analyses per sample, and volume determination for each MFPV batch to effectively reduce the uncertainty in the total inventory $R_{Dq}^{Canisters}$.

The standard deviation of the total inventory in Eq. (A.2.11) is given by

$$SD(R_{Dq}^{Canisters}) = D\left[SD(\overline{\overline{R}}_{Dq}^{Canister})\right] = D\left(\frac{A_q}{f_q}\right)\left[\begin{array}{l}\left(\overline{\overline{g}}_q^{MFPV}\right)^2\left[SD(\overline{m}_D^{Canister})\right]^2 + \left(\overline{m}_D^{Canister}\right)^2\left[SD(\overline{\overline{g}}_q^{MFPV})\right]^2 \\ -\left[SD(\overline{m}_D^{Canister})\right]^2\left[SD(\overline{\overline{g}}_q^{MFPV})\right]^2\end{array}\right]^{1/2} \tag{A.2.12}$$

where

$SD(R_{Dq}^{Canisters})$ = standard deviation of the total inventory of the q^{th} radionuclide in D IHLW canisters associated with an HLW waste type (Ci)

$SD(\overline{\overline{R}}_{Dq}^{Canisters})$ = standard deviation of the mean inventory per canister of the q^{th} radionuclide in D IHLW canisters associated with an HLW waste type (Ci)

$SD(\overline{m}_D^{Canister})$ = standard deviation of the mean mass of glass in the D IHLW canisters associated with an HLW waste type (g_{glass})

$SD(\overline{\overline{g}}_q^{MFPV})$ = standard deviation of the mean (mass-weighted-average) mass fraction of the q^{th} radionuclide oxide over D IHLW canisters associated with an HLW waste type (g_{oxide}/g_{oxides})

and other terms are as previously defined following Eq. (A.1.2), Eq. (A.2.3), and Eq. (A.2.4). In this equation, $\overline{\overline{R}}_{Dq}^{Canisters}$ is calculated using Eq. (A.2.6) while $\overline{\overline{g}}_{q}^{MFPV}$ is calculated according to Eq. (A.2.7). Note that the minus sign in front of the third term in the square-bracketed portion of Eq. (A.2.12) is correct for estimating the standard deviation, as discussed by Goodman (1960).

The term $SD(\overline{\overline{g}}_{q}^{MFPV})$ includes variation in mass fractions of the q^{th} radionuclide oxide across all I MFPV batches associated with an HLW waste type, as well as uncertainties in determining mass fractions of radionuclide oxides for each MFPV batch. These uncertainties include random inhomogeneities in mixing the MFPV contents, random sampling uncertainties associated with the MFPV sampling system, random irreproducibility of the chemical-analysis techniques employed, and random uncertainties in making MFPV volume determinations. The first three of these are effectively reduced by averaging when multiple samples, analyses per sample, and volume determinations per MFPV batch are made. An equation for $SD(\overline{\overline{g}}_{q}^{MFPV})$ is given by

$$SD(\overline{\overline{g}}_{q}^{MFPV}) = \frac{SD(\overline{g}_{iq}^{MFPV})}{\sqrt{I}} \tag{A.2.13}$$

where $SD(\overline{g}_{iq}^{MFPV})$ is calculated from the $\overline{g}_{iq}^{MFPV}$ (i = 1, 2, …, I) values using the usual standard deviation formula.

In a similar way, the term $SD(\overline{m}_{D}^{Canister})$ includes uncertainties associated with measuring the mass of glass in an IHLW canister as well as the variation in the mass of glass that occurs across canisters associated with an HLW waste type. An equation for $SD(\overline{m}_{D}^{Canister})$ is given by

$$SD(\overline{m}_{D}^{Canister}) = \frac{SD(m_{d}^{Canister})}{\sqrt{D}} \tag{A.2.14}$$

where $SD(\overline{m}_{D}^{Canister})$ is calculated from the $m_{d}^{Canister}$ (d = 1, 2, …, D) values using the usual standard deviation formula.

A.3 Compliance Equations for IHLW WAPS Specification 1.3: Product Consistency

IHLW WAPS Specification 1.3 is listed verbatim to provide the context for the IHLW product consistency equations presented in this section.

WAPS Specification 1.3: Product Consistency

The Producer shall demonstrate control of waste form production by comparing, either directly or indirectly, production samples to the Environmental Assessment (EA) benchmark glass. The Producer shall describe the method for demonstrating compliance in the WCP and shall provide verification in the Production Records. The Producer shall demonstrate the ability to comply with the specification in the WQR.

This section documents the general form of equations for calculating predicted property values for IHLW as well as the uncertainties associated with the predicted property values.

For a particular glass property *P* of interest (e.g., PCT response), predicted property values $\hat{y} = \hat{f}(P)$ are nominally calculated using a model of the general form

$$\hat{y} = \hat{f}(P) = \boldsymbol{x}^T \boldsymbol{b} \tag{A.3.1}$$

where $\hat{y} = \hat{f}(P)$ denotes the predicted value of a possibly mathematically transformed property (such as a logarithmic transformation), $\boldsymbol{x}^T$ is a row-vector containing the composition for a particular glass formulation for which a predicted property value is to be calculated, and $\boldsymbol{b}$ is a $p \times 1$ column-vector of model coefficients. The model coefficients in the $\boldsymbol{b}$ vector are uncertain because the model is an approximation to the real property-composition relationship and because the model form is fitted to experimental property-composition data subject to uncertainty. During operation of the WTP IHLW facility, estimated glass compositions $\boldsymbol{x}$ will be subject to several sources of uncertainty. Because the model uncertainty and glass composition uncertainty are statistically independent, the variance of $\hat{y}$ is given by

$$\text{var}(\hat{y}) = \text{var}(\boldsymbol{b}^T \boldsymbol{x}) = \boldsymbol{b}^T \boldsymbol{\Sigma}_{\boldsymbol{x}} \boldsymbol{b} + \boldsymbol{x}^T \boldsymbol{\Sigma}_{\boldsymbol{b}} \boldsymbol{x} \tag{A.3.2}$$

where $\boldsymbol{b}^T$ and $\boldsymbol{x}^T$ are transposes of $\boldsymbol{b}$ and $\boldsymbol{x}$, respectively, $\boldsymbol{\Sigma}_{\boldsymbol{x}}$, is the composition variance-covariance matrix, and $\boldsymbol{\Sigma}_{\boldsymbol{b}}$ is the variance-covariance matrix for the model coefficients. The first term of Eq. (A.3.2) represents compositional uncertainty, while the second term represents model uncertainty.

When a model is fitted to property-composition data using unweighted least squares (ULS) regression, an algebraic expression to estimate $\boldsymbol{\Sigma}_{\boldsymbol{b}}$ is given by

$$\hat{\boldsymbol{\Sigma}}_b = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \hat{\sigma}_U^2 \tag{A.3.3}$$

where $\boldsymbol{X}$ is the design matrix used to generate the property-composition model, $\boldsymbol{X}^T$ is the matrix transpose of $\boldsymbol{X}$, and $\hat{\sigma}_U^2$ is the estimated mean square for error associated with the ULS fit of the model. In the ULS case, the second term in Eq. (A.3.2) representing model uncertainty can be written as

$$\boldsymbol{x}^T (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{x} \, \hat{\sigma}_U^2 \, . \tag{A.3.4}$$

When a model is fitted to property-composition data using weighted least squares (WLS) regression, an algebraic expression to estimate $\boldsymbol{\Sigma_b}$ is given by

$$\hat{\boldsymbol{\Sigma}}_b = (\boldsymbol{X}^T \boldsymbol{W} \boldsymbol{X})^{-1} \hat{\sigma}^2_W \tag{A.3.5}$$

where $\boldsymbol{W}$ is a diagonal matrix of weights associated with the data points used to fit the property-composition model, $\hat{\sigma}^2_W$ is the estimated mean square for error associated with the WLS fit of the model, and the remaining notation is as previously defined. In the WLS case, the second term in Eq. (A.3.2) representing model uncertainty can be written as

$$\boldsymbol{x}^T (\boldsymbol{X}^T \boldsymbol{W} \boldsymbol{X})^{-1} \boldsymbol{x}\, \hat{\sigma}^2_W \,. \tag{A.3.6}$$

In Eq. (A.3.2), the variance-covariance matrix $\boldsymbol{\Sigma_x}$ associated with a glass composition $\boldsymbol{x}$ must be estimated from replicate experimental data rather than via a formula as in the case of model uncertainty. Because the number of glass components appearing in IHLW property-composition models is expected to be at least 8 to 12, an extremely large number of replicate compositions would be needed to adequately estimate $\boldsymbol{\Sigma_x}$. Further, variance-covariance matrices can have several sources of uncertainty (e.g., sampling, chemical analysis) associated with an estimate of glass composition associated with an IHLW MFPV batch. Batch-to-batch variation in IHLW composition can also be written as a variance-covariance matrix. Hence, because IHLW composition is multivariate, coupled with the presence of batch-to-batch variation and within-batch uncertainty (with several contributing sources of uncertainty), it is essentially impossible to collect sufficient replicate data to estimate composition variance-covariance matrices. However, there are practical alternatives that allow for quantifying the second term in Eq. (A.3.2).

For the IHLW compliance strategy, IHLW composition estimates will be associated with multiple samples per MFPV batch and possibly multiple analyses per sample. A property-composition model can be applied to these multiple estimates of composition, resulting in multiple corresponding predicted property values. These univariate property values can then be used with statistical variance estimation or propagation methods to quantify composition uncertainty in property units (corresponding to the second term in Eq. (A.3.2).

Similarly, during WTP IHLW facility operations, estimated compositions for multiple MFPV batches can be substituted into a property-composition model, yielding multiple property values. The usual standard deviation (or variance) formulas can be used to calculate batch-to-batch variation of IHLW composition in property units.

A.4 Compliance Equations for IHLW WAPS Specification 1.5: Hazardous Waste and Contract Specification 1.2.2.1.5: Dangerous and Hazardous Waste Requirements

IHLW WAPS Specification 1.5 and Contract Specification 1.2.2.1.5 are listed verbatim to provide the context for the following discussion.

WAPS Specification 1.5: Hazardous Waste Specification

> *The Producer shall determine and report to DOE/RW the presence or absence of any hazardous waste listed in 40 CFR 261.31 through 40 CFR 261.33, in the waste or in any feed stream proposed for storage or disposal. Any RCRA-listed component in a waste shall require the Producer to petition EPA and receive exemption to delist the waste.*
>
> *The Producer shall perform the appropriate tests and procedures, as described in 40 CFR 261.20 through 40 CFR 261.24 using samples from production runs or prototypical specimens to determine if the waste that will be received by DOE/RW for transportation and disposal has hazardous characteristics. Any waste that is shown to have hazardous characteristics shall be treated to remove such characteristics.*
>
> *The Producer shall certify in the WQR that the waste is not hazardous, including the absence of any listed components. The characteristic testing methods to be used shall be described in the WCP and the results documented in the WQR. Any modification to these methods needs prior approval from DOE/RW.*

Contract Specification 1.2.2.1.5: Dangerous and Hazardous Waste Requirements

> *The WTP shall be designed, constructed, and operated so that the IHLW product does not designate as characteristic or criteria for dangerous waste or extremely hazardous waste pursuant to WAC 173-303-070, and is not restricted from land disposal pursuant to WAC 173-303-140 and 40CFR268, Land Disposal Restrictions.*

Currently, the Statistical Analysis task of the WTPSP does not have any scope to develop compliance equations or statistical methods for demonstrating compliance with WAPS 1.5 and Contract Specification 1.2.2.1.5 during IHLW production. The reason for this is that any activities to demonstrate compliance during IHLW production will be determined as part of the delisting petition process. Hence, a placeholder section has been left here in case compliance equations and methods are developed in the future. In that case, any equations for calculating associated compliance quantities would be included here.

A.5 Compliance Equations for IHLW WAPS Specification 1.6: IAEA Safeguards Reporting for HLW

IHLW WAPS Specification 1.6 is listed verbatim to provide the context for the IHLW IAEA safeguards equations presented in this section.

WAPS Specification 1.6: IAEA Safeguards Reporting

The Producer shall report the following in the production records:
(1) The total and fissile uranium and plutonium content of each canister in grams.
(2) The concentration of plutonium in grams per cubic meter for each canister.
(3) The ratio by weight of the total element of the following isotopes: U-233, U-234, U-235, U-236, U-238, Pu-238, Pu-239, Pu-240, Pu-241, and Pu-242.

The compliance equations for the three aspects of this specification are addressed in Sections A.5.1, A.5.2, and A.5.3, respectively.

Subsequent to the completion of the work presented in this section, Rev. 1 of the IHLW PCP (Nelson et al. 2004) was issued with revisions to the compliance strategy. A significant revision was that only selected radionuclides would be measured for every MFPV batch (see Table 2.1 in Section 2). Revisions to the compliance quantity equations necessary to implement the IHLW PCP Rev. 1 compliance strategy for WAPS 1.6 will be addressed in a future revision of this report.

A.5.1 Total and Fissile U and Pu Mass Per Canister

The WTP IHLW compliance strategy for Part (1) of this specification, as described in Rev. 0 of the IHLW PCP (Nelson 2003), is to calculate the means and SDs of total U, fissile U, total Pu, and fissile Pu masses per canister and report them for each canister produced from a given waste type. The U isotopes to be included in total U are ^{233}U, ^{234}U, ^{235}U, ^{236}U, and ^{238}U. The fissile U isotopes are ^{233}U and ^{235}U. The Pu isotopes to be included in total Pu are ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, and ^{242}Pu. The fissile Pu isotopes are ^{239}Pu and ^{241}Pu.

Section A.5.1.1 presents the equation for calculating the means of total and fissile U and Pu mass over D IHLW canisters associated with an HLW waste type. Section A.5.1.2 presents the equation for the SDs of the same quantities. These equations assume that the isotopes of U and Pu will be estimated for every MFPV batch corresponding to an HLW waste type. That was the WTP compliance strategy according to Rev. 0 of the IHLW PCP (Nelson 2003).

A.5.1.1 Equation for the Means of Total and Fissile U and Pu Mass over *D* IHLW Canisters, Based on Averages of Multiple Samples, Analyses, and Volume Determinations for Each MFPV Batch

The mean mass (in g) of total or fissile U or Pu in IHLW canisters corresponding to an HLW waste type can be calculated by an equation of the form

$$\overline{\overline{m}}_{D,Nk}^{Canister} = \left(\sum_{q \in Nk} \frac{\overline{\overline{g}}_q^{MFPV}}{f_q} \right) \overline{m}_D^{Canister} = \left(\frac{\sum_{q \in Nk} \sum_{i=1}^{I} \left(\overline{m}_{iq}^{MFPV} / f_q \right)}{\sum_{i=1}^{I} \sum_{j=1}^{J} \overline{m}_{ij}^{MFPV}} \right) \left(\frac{1}{D} \sum_{d=1}^{D} m_d^{Canister} \right) \qquad \text{(A.5.1)}$$

where

$\overline{\overline{m}}_{D,Nk}^{Canister}$ = mean mass of radionuclide k for the set N_k of isotopes of k = U or Pu over the D IHLW canisters associated with the I MFPV batches comprising an HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch ($g_{radionuclide}$)

Nk = Tk, the set of all isotopes of k = U or Pu, or

= Fk, the set of fissile isotopes of k = U or Pu

$\overline{\overline{g}}_q^{MFPV}$ = mean (mass-weighted-average) mass fraction of the q^{th} isotope oxide of U or Pu over the I MFPV batches corresponding to an HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (g_{oxide}/g_{oxides})

f_q = $\frac{MW_q^{oxide}}{MW_q^{radionuclide}} K_q$ where MW_q^{oxide} and $MW_q^{radionuclide}$ are the molecular weights of radionuclide oxide q and radionuclide q, respectively, and K_q is the ratio of moles of radionuclide oxide q per mole of radionuclide q. Hence, f_j is the factor for converting the concentration of analyte j (μg analyte j/mL = mg analyte j/L) to the concentration of oxide j (μg oxide j/mL = mg oxide/L). The quantity f_q is called the oxide factor for oxide q ($g_{oxide}/g_{radionuclide}$)

$\overline{m}_D^{Canister}$ = mean mass of glass in the D IHLW canisters associated with an HLW waste type (g_{glass})

$\overline{m}_{iq}^{MFPV}$ = mass of the q^{th} isotope oxide for U or Pu from the i^{th} MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (g_{oxide})

I = number of MFPV batches corresponding to a given HLW waste type

$\overline{m}_{ij}^{MFPV}$ = mass of the j^{th} oxide (non-radionuclides as well as radionuclides) from the i^{th} MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (g_{oxide})

J = number of non-radionuclide oxides and radionuclide oxides estimated for the composition of each MFPV batch

$m_d^{Canister}$ = mass of glass in canister d (d = 1, 2, … , D), where D is the number of canisters produced from a given waste type (g_{glass}).

The masses $\overline{m}_{iq}^{MFPV}$ and $\overline{m}_{ij}^{MFPV}$ in Eq. (A.5.1) are calculated using Eq. (A.1.4) from Section A.1. The averages over multiple samples, analyses per sample, and volume determinations per MFPV batch are seen in Eq. (A.1.4). On the other hand, $m_d^{Canister}$ is a single determination of the mass of IHLW in the d^{th} canister. It is assumed the mass of glass in a canister ($m_d^{Canister}$) will be determined with relatively small uncertainty during IHLW production operations and thus that it is not worthwhile to make and average multiple determinations as a way to effectively reduce that uncertainty.

A.5.1.2 Equation for the SDs of Total and Fissile U and Pu Mass over *D* IHLW Canisters, Based on Averages of Multiple Samples, Analyses, and Volume Determinations for Each MFPV Batch

To derive an equation for the standard deviation of the mass of total or fissile U or Pu over the D IHLW canisters associated with a waste type, it is necessary to introduce an equation for the mass of total or fissile U or Pu for a single canister (Equation A.5.1 represents the mean mass of U or Pu over the D canisters associated with an HLW waste type). Because it is not possible to easily relate the composition of waste in one or several MFPV batches to that in individual canisters, the equation for the mass of total fissile U or Pu in a canister is a conceptual quantity and presented simply as a way to compute the standard deviation. The mass (in g) of total or fissile U or Pu in an IHLW canister can be expressed as:

$$\overline{m}_{d,Nk}^{Canister} = \left(\sum_{q \in Nk} \frac{\overline{g}_{iq}^{MFPV}}{f_q} \right) m_d^{Canister} \qquad \text{(A.5.2)}$$

where

$\overline{m}_{d,Nk}^{Canister}$ = mass in the d^{th} canister of radionuclide k for the set N_k of isotopes of k = U or Pu, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch ($g_{radionuclide}$)

Nk = Tk, the set of all isotopes of k = U or Pu, or

= Fk, the set of fissile isotopes of k = U or Pu

$\overline{g}_{iq}^{MFPV}$ = mass fraction of the q^{th} isotope oxide of U or Pu in the i^{th} MFPV batch corresponding to an HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (g_{oxide}/g_{oxides})

f_q = $\frac{MW_q^{oxide}}{MW_q^{radionuclide}} K_q$ where MW_q^{oxide} and $MW_q^{radionuclide}$ are the molecular weights of radionuclide oxide q and radionuclide q, respectively, and K_q is the ratio of moles of radionuclide oxide q per mole of radionuclide q. Hence, f_j is the factor for converting the concentration of analyte j (μg analyte j/mL = mg analyte j/L) to the concentration of oxide j (μg oxide j/mL = mg oxide/L). The quantity f_q is called the oxide factor for oxide q ($g_{oxide}/g_{radionuclide}$)

$m_d^{Canister}$ = mass of glass in the d^{th} canister associated with an HLW waste type (g_{glass}).

Note that $\overline{g}_{iq}^{MFPV}$ is given by Eq. (A.1.5), which depends on averages of multiple samples, analyses per sample, and volume determinations for each MFPV sample.

The standard deviation of the mass (in g) of total or fissile k = U or Pu over the D IHLW canisters corresponding to an HLW waste type is given by the following equation based on the variance propagation work of Hines et al. (2003) and Goodman (1960), and assuming statistical independence among the $\overline{g}_q^{MFPV}, q \in Nk$ and $m_d^{Canister}$

$$SD(\overline{m}_{d,Nk}^{Canister}) = \sum_{q \in Nk} \left[\begin{array}{l} \left(\frac{\overline{\overline{g}}_q^{MFPV}}{f_q} \right)^2 \left[SD(m_d^{Canister}) \right]^2 + \left(\overline{m}_D^{Canister} \right)^2 \left(\frac{1}{f_q} \right)^2 \left[SD(\overline{g}_{iq}^{MFPV}) \right]^2 \\ \\ - \left(\frac{1}{f_q} \right)^2 \left[SD(m_d^{Canister}) \right]^2 \left[SD(\overline{g}_{iq}^{MFPV}) \right]^2 \end{array} \right]^{1/2} \quad \text{(A.5.3)}$$

where

$SD(\overline{m}_{d,Nk}^{Canister})$ = standard deviation of the mass of radionuclide k for the set N_k of isotopes of k = U or Pu in an individual IHLW canister across the D canisters associated with the I MFPV batches comprising an HLW waste type ($g_{radionuclide}$)

$\overline{\overline{g}}_q^{MFPV}$ = mean (mass-weighted-average) oxide mass fraction of the q^{th} isotope of

U or Pu over the I MFPV batches corresponding to an HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (g_{oxide}/g_{oxides})

$SD(m_d^{Canister})$ = standard deviation of the mass of glass in the d^{th} canister associated with an HLW waste type. During production, this standard deviation will be calculated from the measured values $m_d^{Canister}$, $d = 1, 2, \ldots, D$ (g_{glass})

$\overline{m}_D^{Canister}$ = mean mass of glass over the D IHLW canisters associated with an HLW waste type (g_{glass})

$SD(\overline{g}_{iq}^{MFPV})$ = standard deviation of the mass fraction of the q^{th} isotope oxide of U or Pu in the i^{th} MFPV batch corresponding to an HLW waste type (g_{oxide}/g_{oxides}). During production, this standard deviation will be calculated from the calculated values $\overline{g}_{iq}^{MFPV}$, $i = 1, 2, \ldots, I$ over the MFPV batches corresponding to the HLW waste type (g_{oxide}/g_{oxides})

and all other terms are as previously defined following Eq. (A.5.1). The quantity $\overline{\overline{g}}_q^{MFPV}$ can be calculated using Eqs. (A.2.7) and (A.1.4), while the quantity $\overline{m}_D^{Canister}$ can be calculated using the equation implicit in Eq. (A.5.1). Finally, note that the minus sign in front of the third term in the square-bracketed portion of Eq. (A.5.3) is correct for estimating the standard deviation, as discussed by Goodman (1960).

The standard deviation in Eq. (A.5.3) includes (1) variation in $\overline{g}_{iq}^{MFPV}$ values over MFPV batches $i = 1, 2, \ldots, I$ from a given waste type, (2) uncertainty in determining $\overline{g}_{iq}^{MFPV}$ for each MFPV batch, (3) variation in $m_d^{Canister}$ values over canisters $d = 1, 2, \ldots, D$ corresponding to a given waste type, and (4) uncertainty in estimating $m_d^{Canister}$ (the mass of glass in a canister). The uncertainty in $\overline{g}_{iq}^{MFPV}$ [i.e., $SD(\overline{g}_{iq}^{MFPV})$] is effectively reduced because of averaging over multiple samples, analyses per sample, and volume determinations for each MFPV batch.

In summary, Eqs. (A.5.1) and (A.5.3) give the mean and SD of the mass of total k = U or Pu when $Nk = Tk$, while the same equations give the mean and SD of the mass of fissile k = U or Pu when $Nk = Fk$.

A.5.2 Concentration of Pu (g/m^3) Per Canister

The WTP IHLW compliance strategy for Part (2) of this specification, as described in Rev. 0 of the IHLW PCP (Nelson 2003), is to calculate the mean and SD of Pu concentration per canister and report them for each canister produced from a given waste type. Section A.5.2.1 presents the equation for calculating the mean Pu concentration per canister over *D* IHLW canisters associated with an HLW waste type. Section A.5.2.2 presents the equation for the standard deviation of the same quantity. These equations assume that the isotopes of Pu will be estimated in every MFPV batch corresponding to an HLW waste type. That was the WTP compliance strategy according to Rev. 0 of the IHLW PCP (Nelson 2003).

A.5.2.1 Equation for the Mean Concentration of Pu Per Canister over *D* IHLW Canisters, Based on Averages of Multiple Samples, Analyses, and Volume Determinations for Each MFPV Batch

The mean concentration of Pu (g/m^3) in glass over the *D* IHLW canisters corresponding to the *I* IHLW MFPV batches from an HLW waste type is calculated using:

$$\overline{\overline{c}}_{D,Pu}^{Canister} = \left(\sum_{q \in Pu} \frac{\overline{\overline{g}}_q^{MFPV}}{f_q} \right) \overline{\rho}_D^{Canister} = \left(\frac{\sum_{q \in Pu} \sum_{i=1}^{I} \left(\overline{m}_{iq}^{MFPV} \Big/ f_q \right)}{\sum_{i=1}^{I} \sum_{j=1}^{J} \overline{m}_{ij}^{MFPV}} \right) \overline{\rho}_D^{Canister} \qquad \text{(A.5.4)}$$

where

$\overline{\overline{c}}_{D,Pu}^{Canister}$ = mean mass-per-volume concentration of Pu isotopes in glass from the *D* IHLW canisters corresponding to the *I* MFPV batches for a given HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (g/m^3)

$\overline{\rho}_D^{Canister}$ = mean density of glass in the *D* IHLW canisters corresponding to the *I* MFPV batches for a given HLW waste type (g_{glass}/m^3_{glass})

and f_q, $\overline{m}_{iq}^{MFPV}$, and $\overline{m}_{ij}^{MFPV}$ are as previously defined following Eq. (A.5.1). The masses $\overline{m}_{iq}^{MFPV}$ and $\overline{m}_{ij}^{MFPV}$ in Eq. (A.5.4) are calculated using Eq. (A.1.4) from Section A.1. The averages over multiple samples, analyses per sample, and volume determinations per MFPV batch are seen in Eq. (A.1.4).

A.5.2.2 Equation for the SD of Pu Concentration per Canister over *D* IHLW Canisters, Based on Averages of Multiple Samples, Analyses, and Volume Determinations for Each MFPV Batch

To derive an equation for the standard deviation of the mass-per-volume concentration of Pu isotopes in glass in an IHLW canister over the *D* canisters associated with a waste type, it is necessary to introduce an equation for the mass-per-volume concentration of a single canister (Equation A.5.4 represents the mean concentration of these Pu isotopes over the *D* canisters). Because it is not possible to easily relate the composition of waste in one or several MFPV batches to that in specific canisters, the equation for the mass-per-volume concentration of Pu isotopes in a canister is a conceptual quantity and presented simply as a way to calculate the standard deviation. The mass-per-volume concentration (in g/m^3) of Pu isotopes in an IHLW canister can be expressed as:

$$\bar{c}_{d,Pu}^{Canister} = \left(\sum_{q \in Pu} \frac{\bar{g}_{iq}^{MFPV}}{f_q} \right) \rho_d^{Canister} \tag{A.5.5}$$

where

$\bar{c}_{d,Pu}^{Canister}$ = mass-per-volume concentration of Pu isotopes in glass from the *D* IHLW canisters corresponding to the *I* MFPV batches for a given HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (g/m^3)

and all other notation is as previously defined following Eq. (A.5.1) and Eq. (A.5.4). The quantity $\bar{g}_{iq}^{MFPV}$ is given by Eq. (A.1.5) with "*q*" in place of "*j*".

The standard deviation of the Pu concentration (in g/m^3) over the *D* individual IHLW canisters corresponding to an HLW waste type is given by the following equation. The equation was developed using the conceptual Eq. (A.5.5), based on the variance propagation work of Hines et al. (2003) and Goodman (1960), assuming statistical independence between the $\bar{g}_{iq}^{MFPV}$, $q \in Pu$ and $\rho_d^{Canister}$.

$$SD(\bar{c}_{d,Pu}^{Canister}) = \sum_{q \in Pu} \left[\begin{array}{l} \left(\dfrac{\bar{\bar{g}}_q^{MFPV}}{f_q} \right)^2 \left[SD(\rho_d^{Canister}) \right]^2 + \left(\bar{\rho}_D^{Canister} \right)^2 \left(\dfrac{1}{f_q} \right)^2 \left[SD(\bar{g}_{iq}^{MFPV}) \right]^2 \\ - \left(\dfrac{1}{f_q} \right)^2 \left[SD(\rho_d^{Canister}) \right]^2 \left[SD(\bar{g}_{iq}^{MFPV}) \right]^2 \end{array} \right]^{1/2} \tag{A.5.6}$$

where

$SD(\bar{c}_{d,Pu}^{Canister})$ = standard deviation of the mass-per-volume concentration of Pu isotopes in glass from the D IHLW canisters corresponding to the I MFPV batches for a given HLW waste type (g/m^3)

$\bar{\bar{g}}_q^{MFPV}$ = mean (mass-weighted-average) oxide mass fraction of the q^{th} Pu isotope over the I MFPV batches corresponding to an HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (g_{oxide}/g_{oxides})

$SD(\rho_d^{Canister})$ = standard deviation of the density of glass in the D IHLW canisters corresponding to the I MFPV batches for a given HLW waste type. During production, this standard deviation will be calculated from the measured values $\rho_d^{Canister}$, $d = 1, 2, \ldots, D$ (g_{glass}/m^3_{glass})

$\bar{\rho}_D^{Canister}$ = mean density of glass over the D IHLW canisters associated with an HLW waste type. During production, this mean will be calculated from the measured values $\rho_d^{Canister}$, $d = 1, 2, \ldots, D$ (g_{glass}/m^3_{glass})

$SD(\bar{g}_{iq}^{MFPV})$ = standard deviation of the oxide mass fraction of the q^{th} Pu isotope over the I MFPV batches corresponding to an HLW waste type. During production, this standard deviation will be calculated from the calculated values $\bar{g}_{iq}^{MFPV}$, $i = 1, 2, \ldots, I$ over the MFPV batches corresponding to the HLW waste type (g_{roxide}/g_{oxides})

and the other quantities are as previously defined following Eq. (A.5.1) and Eq. (A.5.4). The quantity $\bar{\bar{g}}_q^{MFPV}$ can be calculated using Eqs. (A.2.7) and (A.1.4). Finally, note that the minus sign in front of the third term in the square-bracketed portion of Eq. (A.5.6) is correct for estimating the standard deviation, as discussed by Goodman (1960).

The variability in Eq. (A.5.6) includes (1) variation in $\bar{g}_{iq}^{MFPV}$ values over the MFPV batches $i = 1, 2, \ldots, I$ from a given waste type, (2) uncertainty in determining $\bar{g}_{iq}^{MFPV}$ for each MFPV batch, (3) variation in $\rho_d^{Canister}$ values over canisters $d = 1, 2, \ldots, D$ corresponding to a given waste type, and (4) uncertainty in estimating $\rho_d^{Canister}$ (the density of glass in a canister). The uncertainty in $\bar{g}_{iq}^{MFPV}$ (i.e., $SD\left(\bar{g}_{iq}^{MFPV}\right)$ is effectively reduced because of averaging over multiple samples, analyses per sample, and volume determinations for each MFPV batch.

A.5.3 Masses of U and Pu Isotopes per Total Masses of U and Pu

The WTP IHLW compliance strategy for Part (3) of this specification, as described in Rev. 0 of the IHLW PCP (Nelson 2003), is to calculate the means and SDs of U and Pu mass isotopic ratios and report them for each canister produced from a given waste type. However, that portion of this work had not yet been completed before notification by the WTP Project that the IHLW compliance strategy was undergoing major revisions. Based on that notification, the equation for calculating isotopic ratios presented in this section was developed based on the strategy that all isotopes of U and Pu would only be measured on the first MFPV batch corresponding to a waste type. Hence, the equation presented in this section is for that strategy.

The equation to calculate mass isotopic ratios (of U and Pu isotopes to total U and Pu, respectively) based on multiple samples and analyses of the first IHLW MFPV batch (out of 18 batches) per HBV (HLW waste type) is given by:

$$\overline{IR}_{kq} = \frac{\bar{c}_{1kq}^{MFPV}}{\sum_{q \in Tk} \bar{c}_{1kq}^{MFPV}} = \frac{\bar{r}_{1kq}^{MFPV} \Big/ A_q}{\sum_{q \in Tk} \left(\bar{r}_{1kq}^{MFPV} \Big/ A_q \right)} \tag{A.5.7}$$

where

$\overline{IR}_{kq}$ = isotopic ratio by mass of the q^{th} isotope of k = U or Pu, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (unitless)

$\bar{c}_{1kq}^{MFPV}$ = mass-per-volume concentration of the q^{th} isotope of k = U or Pu in the first MFPV batch of an HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (μg/mL = mg/L)

$\bar{r}_{1kq}^{MFPV}$ = activity-per-volume concentration of the q^{th} isotope of k = U or Pu in the first MFPV batch of an HLW waste type, based on averages over multiple samples, analyses per sample, and volume determinations for each MFPV batch (μCi/mL = mCi/L)

A_q = specific activity of the q^{th} radionuclide (Ci/g).

The ratios calculated by Eq. (A.5.7) for the first MFPV batch of an HLW waste type also apply to the remaining MFPV batches of the waste type, as described in Section 4.6.5.

A.6 Compliance Equations for IHLW WAPS Specification 3.8: Heat Generation at Year of Shipment

IHLW WAPS Specification 3.8 is listed verbatim to provide the context for the IHLW heat generation equations presented in this section.

WAPS Specification 3.8: Heat Generation Specification

The heat generation rate for each canistered waste form shall not exceed 1500 watts per canister at the year of shipment.

WAPS Specification 3.8.2: Heat Generation at Year of Shipment

The Producer shall report in the Storage and Shipping Records the estimated heat generation rate for each canistered waste form. The Producer shall describe the method for compliance in the WCP.

The RPP-WTP Project strategy for demonstrating compliance with this specification (Nelson 2003; Nelson et al. 2004) has some statistical aspects (see Section 4.7.2), but the scope of the Statistical Analysis task to address them was cut in anticipation of revising the compliance strategy to remove the statistical aspects. The anticipated strategy is based on the expectation that the limit will be easily met and thus a statistical demonstration of compliance (by accounting for applicable uncertainties) will not be needed. However, a statistically based compliance strategy was planned at one time, and so the following work that had been completed is presented.

The heat output of HLW glass in a canister accounted for by radionuclides can be conservatively estimated during WTP IHLW production by the following general equation:

$$H_{i,max}^{Canister} = \left(\sum_{q=1}^{N} r_{iq}^{MFPV} T_q \right) V_{max}^{Canister} = \left(\sum_{q=1}^{N} \frac{g_{iq}^{MFPV} \rho_i^{MFPV} A_q T_q}{f_q} \right) V_{max}^{Canister}$$
$$= \sum_{q=1}^{N} \frac{g_{iq}^{MFPV} m_{i,max}^{Canister} A_q T_q}{f_q} \qquad \text{(A.6.1)}$$

where

$H_{i,max}^{Canister}$ = maximum heat per canister if 100% filled with glass that would be made from the i^{th} IHLW MFPV batch (W)

N = the number of radionuclides contributing to heat generation

r_{iq}^{MFPV} = activity-per-volume concentration of the q^{th} radionuclide in glass that would be produced from the i^{th} IHLW MFPV batch (Ci/m^3)

T_q = specific thermal output of the q^{th} radionuclide (W/Ci)

$V_{max}^{Canister}$ = the glass volume that would result from a 100% fill of an IHLW canister (m^3).

g_{iq}^{MFPV} = mass fraction of the q^{th} radionuclide oxide in glass that would be made from the i^{th} IHLW MFPV batch (g_{oxide}/g_{oxides})

ρ_i^{MFPV} = density of glass that would be made from the i^{th} IHLW MFPV batch (g_{glass}/m^3_{glass}), assumed to be 2.65×10^6 g/m^3

$m_{i,max}^{Canister}$ = maximum mass of glass per canister if 100% filled with glass that would be made from the i^{th} IHLW MFPV batch (g_{glass})

and A_q and f_q are as previously defined following Eq. (A.2.3) and Eq. (A.1.2). The quantity g_{iq}^{MFPV} can be calculated using Eq. (A.1.3) with "q" in place of "j".

The T_q values are listed in Table A-1 of Appendix A in Fluor Hanford (2004). Equation (A.6.1) provides a conservative estimate because of the use of $V_{max}^{Canister}$ and $m_{i,max}^{Canister}$.

Note that Eq. (A.6.1) could be expanded to account for the use of averages over multiple determinations of uncertain measured quantities, as was done in previous sections of this appendix. For example, r_{iq}^{MFPV} could be substituted by $\bar{r}_{iq}^{MFPV}$ (calculated by averaging over multiple MFPV samples and analyses per sample) g_{iq}^{MFPV} could be substituted by $\bar{g}_{iq}^{MFPV}$ [calculated by (A.1.5)], and ρ_i^{MFPV} could be substituted by $\bar{\rho}_i^{MFPV}$ (calculated by averaging multiple density determinations per MFPV batch, if such were possible). Presumably $V_{max}^{Canister}$ and $m_{i,max}^{Canister}$ can be determined without uncertainty.

A.7 Compliance Equations for IHLW WAPS Specification 3.14: Concentration of Plutonium in Each Canister

IHLW WAPS Specification 3.14 is listed verbatim to provide the context for the equations to calculate the concentration of plutonium in an IHLW canister presented in this section.

WAPS Specification 3.14: Concentration of Plutonium in each Canister

The concentration of plutonium in each HLW standard canister shall be less than 2,500 grams/m^3.

The WTP IHLW compliance strategy for this specification is discussed in Rev. 0 of the IHLW PCP by Nelson (2003). The strategy involves (1) demonstrating before production that the maximum concentration of Pu in any IHLW canister will be less than 2500 g/m^3 and (2) confirming this with limited radionuclide analyses during production. A previous version of the strategy called for demonstrating compliance with the specification during IHLW production, based on the use of the mean and SD of Pu concentration over IHLW canisters corresponding to a HLW waste type. Because that work had been completed, it is presented in this section.

The equations for calculating the mean and SD of the concentration of Pu in each canister are discussed in Section A.7.1. The general equation for calculating Pu concentration for a single MFPV batch is given in Section A.7.2. This equation is extended in Section A.7.3 to incorporate averages over multiple samples, analyses per sample, and volume determination per MFPV batch.

Subsequent to the completion of the work presented in this section, Rev. 1 of the IHLW PCP (Nelson et al. 2004) was issued with revisions to the compliance strategy. Revisions to the compliance quantity equations necessary to implement the IHLW PCP Rev. 1 compliance strategy for WAPS 3.14 will be addressed in a future revision of this report. The equations for calculating Pu concentration per canister presented in this section should also be useful for use in Waste Form Qualification (pre-production) and Waste Form Compliance (during production) work to implement the compliance strategy in Rev. 1 of the IHLW PCP.

A.7.1 Mean and SD of Pu Concentrations over a Waste Type

The equations for calculating the mean and SD of Pu concentration (g/m^3) across the D IHLW canisters corresponding to an HLW waste type were presented in Section A.5.2. Specifically, the mean is calculated via Eq. (A.5.4), and the SD is calculated via Eq. (A.5.6).

A.7.2 A General Equation for the Concentration of Pu in each MFPV Batch

It is also desirable to assess compliance with WAPS 3.14 for the glass that would be made from each MFPV batch. A general equation for the concentration of Pu (g/m^3) in glass that would be made from the i^{th} MFPV batch from an HLW waste type is calculated using:

$$c_{i,Pu}^{MFPV} = \left(\sum_{q \in Pu} \frac{g_{iq}^{MFPV}}{f_q} \right) \rho_i^{MFPV} = \left(\frac{\sum_{q \in Pu} \sum_{i=1}^{I} \left(m_{iq}^{MFPV} / f_q \right)}{\sum_{i=1}^{I} \sum_{j=1}^{J} m_{ij}^{MFPV}} \right) \rho_i^{MFPV} \qquad \text{(A.7.1)}$$

where

$c_{i,Pu}^{MFPV}$ = mass-per-volume concentration of Pu isotopes in glass that would be made from the i^{th} MFPV batch from a given HLW waste type (g/m^3)

g_{iq}^{MFPV} = oxide mass fraction of the q^{th} isotope of Pu in glass that would be made from the i^{th} MFPV batch from a given HLW waste type (g_{oxide}/g_{oxides})

$q \in Pu$ = the isotopes of Pu indexed by q

ρ_i^{MFPV} = density of glass that would be made from the i^{th} MFPV batch from a given HLW waste type (g_{glass}/m^3_{glass}), assumed to be 2.65×10^6 g/m^3

and f_q, m_{iq}^{MFPV}, and m_{ij}^{MFPV} are as previously defined following Eq. (A.1.2). Equation (A.7.1) provides two options for calculating $c_{i,Pu}^{MFPV}$. In the first option, g_{iq}^{MFPV} can be calculated using Eq. (A.1.3) with "q" in place of "j". In the second option, the quantities m_{ij}^{MFPV} and m_{iq}^{MFPV} (where q is treated as j) can be calculated by Eq. (A.1.2).

A.7.3 An Equation for the Concentration of Pu in Each MFPV Batch Based on Averages of Multiple Samples, Analyses, and Volume Determinations

During WTP IHLW production operations, several of the variables in Eq. (A.7.1) will be subject to various random uncertainties. If values for such variables can be determined more than once (i.e., by multiple samples, analyses per sample, or measurements), then it is possible to effectively reduce the random uncertainties by averaging over multiple determinations to estimate the values of the variables for a given MFPV batch. The "analyte-to-oxide conversion factor" f_q in Eq. (A.7.1) is assumed to be "known," and thus is not subject to random uncertainty.

In Eq. (A.7.1), the variables m_{iq}^{MFPV} and m_{ij}^{MFPV} (and hence g_{iq}^{MFPV}) will be subject to random uncertainties from (1) random inhomogeneity of MFPV contents, (2) sampling from the MFPV, (3) chemical analyses of the MFPV samples, and (4) MFPV volume determinations. Hence, the random uncertainties in these variables can be effectively reduced by taking more than one sample per MFPV batch and/or analyzing each sample more than once.

The variable ρ_i^{MFPV} will be subject to random measurement uncertainty if it is measured during production. If it can be measured more than once (e.g., for each of the multiple samples per MFPV batch), then its uncertainty can be effectively reduced by averaging the multiple determinations. However, if a pre-determined value of ρ_i^{MFPV} is used during production operations, it will be subject to an "uncertainty of estimation." That is, this predetermined value will not exactly represent the density of glass produced during production operations. Such an uncertainty cannot be effectively reduced because it is not possible to make multiple determinations of ρ_i^{MFPV} and average them.

The re-expression of Eq. (A.7.1) to include averages of multiple samples, analyses per sample, volume determinations, and density determinations (if possible) is given by

$$\bar{c}_{i,Pu}^{MFPV} = \left(\sum_{q \in Pu} \frac{\bar{g}_{iq}^{MFPV}}{f_q} \right) \bar{\rho}_i^{MFPV} = \left(\frac{\sum_{q \in Pu} \sum_{i=1}^{I} \left(\bar{m}_{iq}^{MFPV} \Big/ f_q \right)}{\sum_{i=1}^{I} \sum_{j=1}^{J} \bar{m}_{ij}^{MFPV}} \right) \left(\frac{\sum_{k=1}^{n_\rho} \rho_{ik}^{MFPV}}{n_\rho} \right) \qquad \text{(A.7.2)}$$

where

$\bar{c}_{i,Pu}^{MFPV}$ = mass-per-volume concentration of Pu isotopes in glass that would be made from the i^{th} MFPV batch from a given HLW waste type, based on averages over multiple samples, analyses per sample, volume determinations, and density determinations per MFPV batch (g/m^3)

$\bar{g}_{iq}^{MFPV}$ = oxide mass fraction of the q^{th} isotope of Pu in glass that would be made from the i^{th} MFPV batch from a given HLW waste type, based on averages of multiple

samples, analyses per sample, and volume determinations per MFPV batch (g_{oxide}/g_{oxides})

$\overline{\rho}_i^{MFPV}$ = density of glass that would be made from the i^{th} MFPV batch from a given HLW waste type, based on an average of n_ρ determinations for glass that would be made from each MFPV batch (g_{glass}/m^3_{glass})

ρ_{ik}^{MFPV} = the k^{th} determination of density of glass that would be made from the i^{th} MFPV batch from a given HLW waste type (g_{glass}/m^3_{glass})

n_ρ = number of determinations of density that would be associated with the i^{th} MFPV batch from a given HLW waste type

and f_q, $\overline{m}_{iq}^{MFPV}$, and $\overline{m}_{ij}^{MFPV}$ are as previously defined following Eq. (A.5.1). Equation (A.7.2) provides two options for calculating $\overline{c}_{i,Pu}^{MFPV}$. In the first option, $\overline{g}_{iq}^{MFPV}$ can be calculated using Eq. (A.1.5) with "q" in place of "j". In the second option, the quantities $\overline{m}_{ij}^{MFPV}$ and $\overline{m}_{iq}^{MFPV}$ (where q is treated as a j) can be calculated by Eq. (A.1.4). The averaging over multiple volume determinations of the i^{th} MFPV batch can be seen in Eq. (A.1.4).

A.8 Compliance Equations for IHLW Contract Specification 1.2.2.1.6: Product Loading

A statistically-based approach to demonstrating compliance with this specification was planned at one time, but the WTP compliance strategy was subsequently changed. Before the change in strategy, mass-balance-based equations for calculating waste loading had been developed and documented in a 29-page informal document. The informal document is available in case it is needed for adaptation in the future by the WTP Project.

Appendix B

Compliance Equations for ILAW Specifications

Appendix B: Compliance Equations for ILAW Specifications

This appendix contains derivations and descriptions of equations for calculating immobilized low-activity waste (ILAW) compliance quantities during ILAW production. The compliance equations are functions of process samples, analyses per sample, and measurements that will be available for demonstrating compliance with ILAW specifications during production, according to the Waste Treatment and Immobilization Plant (WTP) ILAW compliance strategy. The compliance strategy in the ILAW Product Compliance Plan (PCP) Rev. 0 (Nelson et al. 2003) was the primary guidance for the work in this report, along with scope revisions to reflect planned changes in compliance strategy. Shortly before this report was completed, the ILAW PCP Rev. 1 (Westsik et al. 2004) was issued. Any revisions to results in this appendix necessitated by revisions to the compliance strategies in the Rev. 1 ILAW PCP (Westsik et al. 2004) will be made in a future revision of this report.

Compliance equations are provided in this Appendix for ILAW specifications where the ILAW PCP Rev. 0 (Nelson et al. 2003) compliance strategy has statistical aspects. Compliance equations are also provided for ILAW specifications where the WTP compliance strategy previously had statistical aspects but was changed, and the equations had been developed before the strategy change. Such equations may still play roles in process control and revised WTP compliance strategies, and these are presented in this appendix.

Many aspects of the WTP ILAW compliance strategy are associated with reporting or demonstrating compliance for glass from a series of ILAW Melter Feed Preparation Vessel (MFPV) batches corresponding to a *low-activity waste (LAW) waste type* or an *ILAW production lot*. An LAW waste type is expected to correspond to an LAW waste tank, whereas an ILAW production lot is expected to correspond to the ILAW produced from a portion of an LAW waste type. The number of ILAW MFPV batches in an ILAW production lot (or corresponding to an LAW waste type) is denoted I, and the number of ILAW containers associated with that ILAW production lot (or LAW waste type) is denoted D. The D ILAW containers produced from the I ILAW MFPV batches will be those produced starting after the mean melter residence time plus the time of transfer from the ILAW MFPV to the melter. The total mass of glass oxides per ILAW MFPV batch will be summed for the I batches and divided by the mass of glass per container to determine the number of ILAW containers D represented by the I ILAW MFPV batches. For consistency in the discussion in this appendix, the term "LAW waste type" will always be used, but with the understanding that "ILAW production lot" or any other defined collection of MFPV batches could be used in its place.

B.1 Compliance Equations for ILAW Contract Specification 2.2.2.6.2: Chemical Composition During Production

ILAW Contract Specification 2.2.2.6.2 is listed verbatim to provide the context for the ILAW chemical compliance equations presented in this section.

Contract Specification 2.2.2.6.2: Chemical Composition During Production

The production documentation (Table C.5-1.1, Deliverable 6.7) shall provide the chemical composition of each waste form, optional filler, and package. The reported composition shall include

elements (excluding oxygen) present in concentrations greater than 0.5 percent by weight and elements and compounds required to meet regulatory or Contract requirements.

This section documents the equations for calculating the chemical composition of ILAW based on the results of process samples, analyses per sample, and measurements to be taken during production operations of the WTP ILAW facility. The sampling locations and other measurements to be taken are based on the WTP compliance strategy discussed in the ILAW Product Compliance Plan (PCP) (Nelson et al. 2003) for complying with ILAW specifications in the WTP contract (DOE-ORP 2003).

The ILAW chemical-composition equations presented in this section are based on work by (1) John Vienna representing the Waste Form Qualification (WFQ) area of the Research and Technology (R&T) organization within the WTP Project, and (2) Greg Piepel and Scott Cooley of Battelle—Pacific Northwest Division (PNWD).

The ILAW compliance strategy for ILAW chemical composition described in the ILAW PCP involves (1) sampling and analyzing waste in the Concentrate Receipt Vessel (CRV), (2) transferring a portion of the CRV contents to the MFPV, (3) calculating required amounts and then weighing those amounts of glass-forming chemicals (GFCs) to add to the MFPV to yield the desired ILAW glass composition, and (4) transferring the GFCs to the MFPV and mixing the contents. Additional details are described in the ILAW PCP (Nelson et al. 2003). For compliance purposes during ILAW production operations, the chemical composition of ILAW based on MFPV contents will be calculated based on chemical analyses of CRV samples and weights of individual GFCs. The composition and volume of the MFPV heel from the previous MFPV batch are also involved in the calculation of ILAW chemical composition for the current MFPV batch.

An important topic involves the list of glass components that will be used to represent the chemical composition of ILAW. The ILAW chemical-composition equations in this section treat this topic in a general way, with the total number of glass components denoted J and individual components indexed by j. However, to obtain accurate mass-fraction estimates of glass composition, the components used must comprise almost all of the mass that will end up in glass. This includes chemical composition components (oxides or halogens) and radionuclide composition components (oxides). Otherwise, mass fractions of glass components will be biased high. For example, suppose that the number of components chosen to represent ILAW composition corresponds to 98 wt% of the true composition for a given ILAW glass. Then, the mass-balance-based equations in this section would yield, on average, mass fractions that are biased high by the factor 1.0/0.98 = 1.0204 (i.e., slightly over a 2% positive bias). Hence, it is important that a sufficient number of components be included (e.g., in chemical and radiochemical analyses) to avoid obtaining biased estimates of the mass fractions of those glass components.

The ILAW chemical-composition equations do not at this time (per WTP Project R&T direction) account for possible volatility of components in the melter. If needed based on further consideration by the WTP Project, melter volatility aspects could be accounted for in future updates of the ILAW chemical-composition equations and related statistical compliance activities.

The ILAW chemical-composition equations presented in this appendix assume there are no biases in sampling, chemical analysis, and measurements that yield inputs for the equations. It is assumed that any significant long-term systematic biases in sampling, chemical analysis, or measurement processes will be

detected and corrected before operation of the WTP ILAW facility. If intermittent biases were to occur during WTP ILAW production, it is assumed the WTP will have methods for detecting and correcting such biases or rejecting the biased results. For example, Piepel and Weier (2003) present accept/reject, bias detection/correction, and weighted normalization methods for analyzed slurry and glass compositions. These methods could be included in the ILAW chemical-composition compliance equations in the future if desired by the WTP Project.

In summary, the ILAW chemical-composition equations presented in this section are intended for use during WTP ILAW production operations to calculate the chemical composition of ILAW that would result from vitrifying the contents of a given ILAW MFPV batch. The contents of an ILAW MFPV batch are formed by adding a portion of a CRV batch and weighed amounts of GFCs to the MFPV heel from the previous batch. The current equations do not (1) account for any biases in sampling, chemical analyses, or measurements yielding inputs for the equations, (2) account for volatility in the melter, and (3) implement the adjustment methods for analyzed compositions discussed by Weier and Piepel (2003).

Section B.1.1 presents general equations for calculating masses and mass fractions of ILAW components given a single determination of each input variable. Section B.1.2 extends these equations for calculating masses and mass fractions to accommodate averages over multiple ILAW MFPV samples, analyses per sample, and volume determinations.

B.1.1 Development of Compliance Equations for ILAW Chemical Composition

Composition of waste glass is typically expressed as mass fractions (summing to one) or mass percents (summing to 100) of the components in the glass. In this report, mass fractions are used. The general equation for the chemical composition (mass fractions) of ILAW formed from the i^{th} MFPV batch is

$$g_{ij}^{MFPV} = \frac{m_{ij}^{MFPV}}{M_i^{MFPV}} = \frac{m_{ij}^{CRV\ to\ MFPV} + m_{ij}^{GFCs} + m_{ij}^{MFPV\ Heel}}{M_i^{CRV\ to\ MFPV} + M_i^{GFCs} + M_i^{MFPV\ Heel}} \qquad \text{(B.1.1)}$$

where

g_{ij}^{MFPV} = mass fraction of the j^{th} glass oxide component in the i^{th} MFPV batch (g_{oxide}/g_{oxides})

m_{ij}^{MFPV} = mass of the j^{th} glass oxide component in the i^{th} MFPV batch (g)

I = total number of MFPV batches per reporting or compliance period

J = total number of glass oxide components

M_i^{MFPV} = $\sum_{j=1}^{J} m_{ij}^{MFPV}$ = total mass of glass oxide components $j = 1, 2, \ldots, J$ in the i^{th} MFPV batch (g)

$m_{ij}^{CRV\ to\ MFPV}$ = mass of the j^{th} glass oxide component in the portion of a CRV batch

transferred to the i^{th} MFPV batch (g)

m_{ij}^{GFCs} = mass of the j^{th} glass oxide component in GFCs for the i^{th} MFPV batch (g)

$m_{ij}^{MFPV\ Heel}$ = mass of the j^{th} glass oxide component in the MFPV Heel included in the i^{th} MFPV batch (g)

$M_i^{CRV\ to\ MFPV}$ = $\sum_{j=1}^{J} m_{ij}^{CRV\ to\ MFPV}$ = total mass of all glass oxide components in the portion of the CRV batch transferred to the i^{th} MFPV batch (g)

M_i^{GFCs} = $\sum_{j=1}^{J} m_{ij}^{GFCs}$ = total mass of all glass oxide components in GFCs for the i^{th} MFPV batch (g)

$M_i^{MFPV\ Heel}$ = $\sum_{j=1}^{J} m_{ij}^{MFPV\ Heel}$ = total mass of all glass oxide components in the MFPV Heel included in the i^{th} MFPV batch (g)

The masses of LAW glass oxide components in the (1) portion of the CRV transferred to the MFPV, (2) GFCs, and (3) MFPV Heel are respectively given by the following equations for the ILAW compliance strategy

$$m_{ij}^{CRV\ to\ MFPV} = c_{ij}^{CRV} f_j u V_i^{CRV to MFPV} \tag{B.1.2}$$

$$m_{ij}^{GFCs} = \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} \tag{B.1.3}$$

$$m_{ij}^{MFPV\ Heel} = m_{i-1,j}^{MFPV} \left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}} \right) \tag{B.1.4}$$

where

c_{ij}^{CRV} = concentration of the j^{th} element in the CRV batch, a portion of which is transferred to the i^{th} MFPV batch (μg/mL = mg/L). See the discussion regarding this notation after the following terminology definitions.

f_j = $\frac{MW_j^{oxide}}{MW_j^{analyte}} R_j$ where MW_j^{oxide} and $MW_j^{analyte}$ are the molecular weights of

oxide j and analyte j, respectively, and R_j is the ratio of moles of oxide j per mole of analyte j. Hence, f_j is the factor for converting the concentration of analyte j (μg analyte j/mL) to the concentration of oxide j (μg oxide j/mL). The quantity f_i is called the oxide factor for oxide j.

$V_i^{CRV\ to\ MFPV}$ = volume transfer from the CRV to the i^{th} MFPV batch (L)

u = $\frac{1\,(\mathrm{g})}{1000\,(\mathrm{mg})}$, a units conversion factor for converting mg to g

K = number of GFCs

a_{ik}^{GFC} = mass of the k^{th} GFC added to the i^{th} MFPV batch (g)

G_{ijk}^{GFC} = mass of the j^{th} glass oxide component per mass of the k^{th} GFC for the i^{th} MFPV batch ($g_{oxide\ j}/g_{GFC\ k}$). The mass fractions G_{ijk}^{GFC} $j = 1, 2, \ldots, J$ for the k^{th} GFC can sum to less than 1.0 to the extent the GFC contains interstitial water or other components that will not survive in the glass. The nominal G_{ijk}^{GFC} mass fractions of glass oxide components in the GFCs should not change frequently over MFPV batches. However, the i subscript was retained in case these mass fractions change (1) from one vendor to another for the same GFC or (2) for different lots of a given GFC from the same vendor.

$m_{i-1,j}^{MFPV}$ = mass of the j^{th} glass oxide component in the $(i-1)^{st}$ MFPV batch (g)

$V_i^{MFPV\ Heel}$ = volume of the MFPV Heel included in the i^{th} MFPV batch (L)

V_{i-1}^{MFPV} = volume of the $(i-1)^{st}$ MFPV batch (L). This is the total volume of the $(i-1)^{st}$ MFPV batch, including the MFPV Heel, waste transferred from the CRV, GFCs added, and any water that may be added. Water will typically be added to Envelope B LAW in the MFPV to lower the sodium molarity. It is not anticipated that LAW from Envelopes A and C will require adding water in the MFPV.

Note that Eq. (B.1.2) uses c_{ij}^{CRV} (the concentration of the j^{th} element in the CRV batch, a portion of which is transferred to the i^{th} MFPV batch) to calculate the mass of the j^{th} glass oxide component in the portion of the CRV batch transferred to the i^{th} MFPV batch. This wording is somewhat awkward, but is necessary because in the ILAW facility, one CRV batch will provide input to four MFPV batches (or more for Envelope B LAW when water must be added to the MFPV). The ILAW compliance strategy does not have a hold point at the CRV to wait for the chemical-analysis results for samples of a given CRV batch. In cases where the chemical-analysis results for a new CRV batch are ready in time to

determine the appropriate additions of GFCs for the first MFPV batch from the new CRV batch, then the concentrations c_{ij}^{CRV} can be used. Otherwise, the concentrations $c_{ij}^{CRV\ Previous}$ from the previous CRV batch will be used. It is expected that the chemical-analysis results for a given CRV batch (c_{ij}^{CRV}, j = 1, 2, … , J) will be available in time for the second, third, and fourth transfers from that CRV batch to the MFPV. If not, then $c_{ij}^{CRV\ Previous}$ would be used for as many remaining transfers from the current CRV batch as necessary until the current results c_{ij}^{CRV} become available. To simplify the notation, c_{ij}^{CRV} is used in Eq. (B.1.2) and subsequent equations with the understanding that it represents concentrations from the current CRV batch if available, and the previous CRV batch if not. Also note that Eq. (B.1.4) assumes uniform mixing of the ILAW MFPV.

Using elemental concentrations from the previous CRV batch as an estimate of the elemental concentrations in the current CRV batch is the simplest one-step-ahead forecast that can be made. If there is sufficient variation across CRV batches, a better one-step-ahead forecasting approach based on statistical time series models could be used. Because it is not clear whether such an approach would be worthwhile (i.e., sufficiently reducing the bias in the estimated concentrations), the time series approach is not included in the ILAW chemical-composition equations presented in this document.

Volume transfers will not be measured directly in the WTP, but calculated by differences in "before" and "after" volumes of a given vessel. Because volume transfers can be calculated for both the sending and receiving vessels, a more precise (less uncertain) estimate is obtained by using a weighted average of the volume transfer estimates from the sending and receiving vessels. In Eq. (B.1.2), the CRV is the sending vessel and the MFPV is the receiving vessel.

A volume transfer from vessel A to vessel B for the i^{th} batch is calculated as

$$\begin{aligned} V_i^{A\ to\ B} &= w_A V_i^{A\ transfer} + w_B V_i^{B\ transfer} \\ &= w_A \left(V_i^{A\ before} - V_i^{A\ after} \right) + w_B \left(V_i^{B\ after} - V_i^{B\ before} \right) \end{aligned} \tag{B.1.5}$$

where w_A and w_B are weights that reflect the relative magnitudes of the uncertainties associated with $\left(V_i^{A\ before} - V_i^{A\ after} \right)$ and $\left(V_i^{B\ after} - V_i^{B\ before} \right)$, respectively. It is reasonable to assume that $\left(V_i^{A\ before} - V_i^{A\ after} \right)$ and $\left(V_i^{B\ after} - V_i^{B\ before} \right)$ are statistically independent. If the additional assumptions are made that $V_i^{A\ before}$ and $V_i^{A\ after}$ are statistically independent, and that $V_i^{B\ after}$ and $V_i^{B\ before}$ are statistically independent, then the weights w_A and w_B can be written as:

$$w_A = \frac{\hat{\sigma}^2_{V_i^{B\ after}} + \hat{\sigma}^2_{V_i^{B\ before}}}{\hat{\sigma}^2_{V_i^{A\ before}} + \hat{\sigma}^2_{V_i^{A\ after}} + \hat{\sigma}^2_{V_i^{B\ after}} + \hat{\sigma}^2_{V_i^{B\ before}}} \tag{B.1.6}$$

and

$$w_B = \frac{\hat{\sigma}^2_{V_i^{A\,before}} + \hat{\sigma}^2_{V_i^{A\,after}}}{\hat{\sigma}^2_{V_i^{A\,before}} + \hat{\sigma}^2_{V_i^{A\,after}} + \hat{\sigma}^2_{V_i^{B\,after}} + \hat{\sigma}^2_{V_i^{B\,before}}} \tag{B.1.7}$$

where $\hat{\sigma}^2_{V_i^{A\,before}}$ denotes a previously determined estimate of the variance (squared standard deviation [SD]) of a volume measurement in Vessel A before a transfer. The other similar notations in Eqs. (B.1.6) and (B.1.7) denote previous estimates of the variance of a volume measurement in Vessel A after a transfer to Vessel B, and Vessel B before and after a transfer from Vessel A. Thus,

$$\begin{aligned} V_i^{CRV\,to\,MFPV} = & \frac{\hat{\sigma}^2_{V_i^{MFPV\,after}} + \hat{\sigma}^2_{V_i^{MFPV\,before}}}{\hat{\sigma}^2_{V_i^{CRV\,before}} + \hat{\sigma}^2_{V_i^{CRV\,after}} + \hat{\sigma}^2_{V_i^{MFPV\,after}} + \hat{\sigma}^2_{V_i^{MFPV\,before}}} \left(V_i^{CRV\,before} - V_i^{CRV\,after}\right) \\ & + \frac{\hat{\sigma}^2_{V_i^{CRV\,before}} + \hat{\sigma}^2_{V_i^{CRV\,after}}}{\hat{\sigma}^2_{V_i^{CRV\,before}} + \hat{\sigma}^2_{V_i^{CRV\,after}} + \hat{\sigma}^2_{V_i^{MFPV\,after}} + \hat{\sigma}^2_{V_i^{MFPV\,before}}} \left(V_i^{MFPV\,after} - V_i^{MFPV\,before}\right) \end{aligned} \tag{B.1.8}$$

where

$V_i^{CRV\,before}$ = volume of the CRV before the transfer of material to the i^{th} MFPV batch (L)

$V_i^{CRV\,after}$ = volume of the CRV after the transfer of material to the i^{th} MFPV batch (L)

$V_i^{MFPV\,before}$ = volume of the MFPV before receipt of CRV material for the i^{th} MFPV batch

= $V_i^{MFPV\,Heel}$ = volume of the MFPV Heel included in the i^{th} MFPV batch (L)

$V_i^{MFPV\,after}$ = volume of the MFPV after receipt of CRV material for the i^{th} MFPV batch but before receipt of GFCs or any added water (L).

It is important to note that $V_i^{MFPV\,after} \neq V_i^{MFPV}$ because V_i^{MFPV} is determined after the CRV material, GFCs, and any water are added to the MFPV. On the other hand, $V_i^{MFPV\,after}$ is determined after the CRV material is added but before the GFCs and any water are added to the MFPV. Thus, the equations in this document assume that both of these MFPV volumes will be determined during operation of the ILAW facility.

Note that vessel content volumes will not be directly measured in the WTP ILAW facility. Rather, the level of contents in a vessel will be measured and then the corresponding volume calculated using a

level-to-volume calibration equation. Because these calibration equations for the WTP ILAW CRV and MFPV will not be developed for some time, they cannot be included in the current equations for calculating ILAW chemical composition. The level-to-volume calibration equations for the ILAW CRV and MFPV will be included in a future update of the compliance equations and work for ILAW chemical composition.

The assumption of statistical independence between volume measurements (actually level measurements) in the CRV and MFPV is quite reasonable because there is no reason to expect the random errors in measuring volume (level) in one vessel will influence the random errors in measuring volume (level) in another vessel. The assumption of statistical independence between before and after volume (level) measurements in one vessel may not be quite as reasonable because ultimately the same level-to-volume calibration equation will be used to calculate before and after vessel volumes from before and after vessel levels. However, there is no reason to expect that random errors in measuring the "before level" in a vessel will influence the random errors in measuring the "after level" in a vessel. This second assumption of statistical independence of before and after volume (level) measurements within a given vessel will be revisited in the future when the work to develop level-to-volume calibration equations for the WTP ILAW CRV and MFPV is conducted.

Combining Eqs. (B.1.2), (B.1.3), and (B.1.4) with Eq. (B.1.1) yields

$$g_{ij}^{MFPV} = \frac{c_{ij}^{CRV} f_j V_i^{CRV\ to\ MFPV} u + \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + m_{i-1,j}^{MFPV} \left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}} \right)}{\sum_{j=1}^{J} \left(c_{ij}^{CRV} f_j V_i^{CRV\ to\ MFPV} u \right) + \sum_{j=1}^{J} \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \sum_{j=1}^{J} m_{i-1,j}^{MFPV} \left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}} \right)} \quad \text{(B.1.9)}$$

where all notation is as previously defined in this section. The quantities m_{ij}^{MFPV} and $m_{i-1,j}^{MFPV}$ are given by

$$m_{ij}^{MFPV} = c_{ij}^{CRV} f_j V_i^{CRV\ to\ MFPV} u + \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + m_{i-1,j}^{MFPV} \left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}} \right) \quad \text{(B.1.10a)}$$

and

$$m_{i-1,j}^{MFPV} = c_{i-1,j}^{CRV} f_j V_{i-1}^{CRV\ to\ MFPV} u + \sum_{k=1}^{K} a_{i-1,k}^{GFC} G_{i-1,jk}^{GFC} + m_{i-2,j}^{MFPV} \left(\frac{V_{i-1}^{MFPV\ Heel}}{V_{i-2}^{MFPV}} \right) \quad \text{(B.1.10b)}$$

Note that (B.1.10a) is just the numerator of Eq. (B.1.9), and Eq. (B.1.10b) is a version of Eq. (B.1.10a) for the previous MFPV batch. The expression for CRV to MFPV volume transfers in Eq. (B.1.8) and the expression for $m_{i-1,j}^{MFPV}$ in Eq. (B.1.10) could be substituted into Eq. (B.1.9) to yield a combined final equation for ILAW chemical composition, but that yields a very long equation. Hence, the final compliance equation for ILAW chemical composition is given by Eq. (B.1.9), where the volume

transfer $V^{CRV\ to\ MFPV}$ is given by Eq. (B.1.8) and $m_{i-1,j}^{MFPV}$ is given by Eq. (B.1.10). Note that each of these equations assumes uniform mixing of the ILAW MFPV.

B.1.2 Equations for Calculating ILAW Chemical Composition Corresponding to an MFPV Batch Based on Averages over Multiple Samples, Analyses, and Volume Determinations

All of the variables in Eq. (B.1.9), except the "units conversion factor" u and the "analyte-to-oxide conversion factor" f_i, are subject to various uncertainties. For example, there are random uncertainties caused by random inhomogeneity of CRV contents, sampling from the CRV, chemical analyses of CRV samples, weighing of GFCs, variation in the GFC mass fraction oxide compositions, and measuring CRV and MFPV volumes/levels). When level-to-volume calibration equations are developed for the ILAW CRV and MFPV, there will be uncertainties in the calibration equations (e.g., estimated coefficients). When the calibration equations are applied, there will be uncertainties in measuring vessel levels. Hence, calculated volumes will be uncertain because of level measurement uncertainties and uncertainties in the calibration equations.

The random uncertainties described in the preceding paragraph can be effectively reduced by (1) taking more than one CRV sample, (2) analyzing each CRV sample more than once, (3) using more determinations to quantify GFC compositions, (4) weighing GFCs more than once, and (5) measuring CRV and MFPV volumes/levels more than once. The uncertainties would be reduced by using averages over multiple determinations in Eq. (B.1.9), as well as in Eqs. (B.1.8) and (B.1.10), because averages over two or more determinations have smaller uncertainties than single determinations. The resulting re-expressions of these equations to include averages over multiple samples, analyses per sample, and volume determinations are now presented.

The re-expressions of Eqs. (B.1.9), (B.1.10), and (B.1.8) to include average determinations are given, respectively, by Eqs. (B.1.11), (B.1.12), and (B.1.13) following:

$$\bar{g}_{ij}^{MFPV} = \frac{\dfrac{1}{n_S^{CRV} n_A^{CRV}} \sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{ijlm}^{CRV} f_j \bar{V}_i^{CRV\,to\,MFPV} u + \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \bar{m}_{i-1,j}^{MFPV} \left(\dfrac{\dfrac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\ Heel}}{\dfrac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV}} \right)}{\sum_{j=1}^{J} \left(\dfrac{1}{n_S^{CRV} n_A^{CRV}} \sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{ijlm}^{CRV} f_j \bar{V}_i^{CRV\,to\,MFPV} u \right) + \sum_{j=1}^{J} \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \sum_{j=1}^{J} \bar{m}_{i-1,j}^{MFPV} \left(\dfrac{\dfrac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\ Heel}}{\dfrac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV}} \right)} \quad \text{(B.1.11)}$$

$$\bar{m}_{i-1,j}^{MFPV} = \frac{1}{n_S^{CRV} n_A^{CRV}} \sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{i-1,jlm}^{CRV} f_j \bar{V}_{i-1}^{CRV\,to\,MFPV} u + \sum_{k=1}^{K} a_{i-1,k}^{GFC} G_{i-1,jk}^{GFC} + \bar{m}_{i-2,j}^{MFPV} \left(\frac{\dfrac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV\ Heel}}{\dfrac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i-2,h}^{MFPV}} \right) \quad \text{(B.1.12)}$$

and

$$\overline{V}_i^{CRV\,to\,MFPV} = \frac{\hat{\sigma}^2_{\overline{V}_i^{MFPV\ after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\ before}}}{\hat{\sigma}^2_{\overline{V}_i^{CRV\ before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\ after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\ after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\ before}}} \left(\frac{\sum_{h=1}^{n_V^{CRV}} V_{ih}^{CRV\ before}}{n_V^{CRV}} - \frac{\sum_{h=1}^{n_V^{CRV}} V_{ih}^{CRV\ after}}{n_V^{CRV}} \right)$$

$$+ \frac{\hat{\sigma}^2_{\overline{V}_i^{CRV\ before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\ after}}}{\hat{\sigma}^2_{\overline{V}_i^{CRV\ before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\ after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\ after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\ before}}} \left(\frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV\ after}}{n_V^{MFPV}} - \frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV\ before}}{n_V^{MFPV}} \right) \qquad \text{(B.1.13)}$$

where the bars in certain notations (e.g., $\overline{V}_{i-1}^{CRV\,to\,MFPV}$) denote averages. The $\hat{\sigma}^2_{\overline{V}_i^{MFPV\ after}}$ notation in Eq. (B.1.13) represents the estimated variance of $\overline{V}_i^{MFPV\ after} = \frac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\ After}$.

The other variance notations in Eq. (B.1.13) have similar interpretations. Eq. (B.1.11) and Eq. (B.1.12) assume uniform mixing of the ILAW MFPV.

In Eqs. (B.1.11) to (B.1.13), the following notations for number of samples per CRV batch, number of analyses per CRV sample, and numbers of CRV and MFPV volume measurements are used:

n_S^{CRV} = number of samples per CRV batch

n_A^{CRV} = number of chemical analyses per CRV sample

n_V^{CRV} = number of volume determinations of the CRV batch before a transfer of material to the MFPV ($V_{ih}^{CRV\ before}$) and after a transfer of material to the MFPV ($V_{ih}^{CRV\ after}$). The numbers of these two CRV volume determinations are assumed to be the same and are given a single notation for simplicity in operation of the ILAW facility.

n_V^{MFPV} = number of volume determinations of the MFPV Heel ($V_{ih}^{MFPV\ before} = V_{ih}^{MFPV\ Heel}$), MFPV after transfer of CRV material ($V_{ih}^{MFPV\ after}$), and completed MFPV batch (V_{ih}^{MFPV}). The numbers of these three MFPV volume determinations are assumed to be the same and are given a single notation for simplicity in operation of the ILAW facility.

Note that n_A^{crv} is assumed to be the same for every CRV sample. An extension of this equation to the case of unequal numbers of analyses per sample can easily be made.

When level-to-volume calibration equations are eventually developed for ILAW vessels and factored into the ILAW chemical-composition compliance equations, notations such as n_V^{CRV} and n_V^{MFPV} will be replaced with n_L^{CRV} and n_L^{MFPV}. The notation n_L^{CRV} will denote the number of level measurements of the CRV (before and after transfer of material to the MFPV). The notation n_L^{MFPV} will denote the number of level measurements of the MFPV (before a CRV transfer, after a CRV transfer, and after a complete MFPV batch is prepared).

In Eqs. (B.1.11) to (B.1.13), it is assumed that the amount of the k^{th} GFC (a_{ik}^{GFC}) to be added to the i^{th} MFPV batch can only be weighed once. This assumption is required because there is no way to relieve the load cell on an individual GFC hopper in the GFC facility and obtain additional weight measurements. Hence, averages over multiple weight determinations of the GFCs (a_{ik}^{GFC} , $k = 1, 2, \ldots, K$) were not included in Eqs. (B.1.11) and (B.1.12). Further, it is assumed that the a_{ik}^{GFC} quantities will be well-determined average compositions of GFCs based on historical information from GFC vendors or WTP qualification and acceptance testing. Hence averages of the a_{ik}^{GFC} quantities were not included in Eqs. (B.1.11) and (B.1.12).

In summary, the calculating equations for mass-fraction composition of ILAW based on the WTP ILAW compliance strategy are given by Eqs. (B.1.11) to (B.1.13). These equations will serve as the basis for assessing the importance of multiple samples, multiple analyses per sample, and multiple volume determinations.

B.2 Compliance Equations for ILAW Contract Specification 2.2.2.7.2: Radionuclide Composition During Production

ILAW Contract Specification 2.2.2.7 and Sub-Specification 2.2.2.7.2 are listed verbatim to provide the context for the ILAW radionuclide compliance equations presented in this section.

Contract Specification 2.2.2.7: Radionuclide Composition During Production

Radiological Composition Documentation: The radionuclide composition of the waste form shall be documented. Radionuclides shall be identified that are significant as defined in NUREG/BR-0204 and 49CFR172.101 (Table 2). Technetium-99 (^{99}Tc) shall be considered to be significant at concentrations greater than 0.003 Ci/m3 in the ILAW form. The inventories shall be indexed to December 31, 2002. The documentation shall be consistent with the radiological description format described in NUREG/BR-0204.

2.2.2.7.2 Radionuclide Composition During Production: The ILAW production documentation (Table C.5-1.1, Deliverable 6.7) shall identify the radionuclide inventory in each ILAW package produced. The actual inventory indexed at the month of product transfer and the inventory indexed to December 31, 2002, shall be reported.

To address Contract Specification 2.2.2.7, the WTP project will determine which radionuclides satisfy the specification conditions or are reportable for other reasons. The WTP project's current list of

these ILAW radionuclides is given in Table 2.1 of Section 2. The equations to calculate required concentrations and inventories of the "reportable" radionuclides are discussed in the following subsections.

The following two subsections develop the equations for calculating the radionuclide inventories in each ILAW container. Section B.2.1 presents the equations for concentrations of radionuclides in CRV samples and discusses how mass fractions of radionuclide oxides in glass corresponding to a MFPV batch are calculated. The mass fractions of radionuclide oxides are needed in the equations for calculating radionuclide inventories. Section B.2.2 presents the equations for calculating the mean and SD of radionuclide inventory per container for each of the $q = 1, 2, \ldots, Q$ radionuclides where the mean and SD are over a collection of D ILAW containers corresponding to I MFPV batches.

B.2.1 Equations for Calculating Masses and Mass Fractions of Radionuclide Oxide Components in ILAW Corresponding to an MFPV Batch

During ILAW production, the concentrations of the reportable ILAW radionuclides listed in Table 2.1 of Section 2 will be measured in each LAW CRV batch. The measurements will be reported by the laboratory as activity-per-volume concentrations in units of μCi/mL. These radionuclide concentrations will be at the time of analysis. However, Contract Specification 2.2.2.7 requires reporting inventories indexed to the month of product transfer and the baseline of December 31, 2002. The activity-per-volume concentrations at the time of analysis will be indexed to December 31, 2002. These indexed concentrations (still in units of μCi/mL) will be used as inputs to all the following ILAW radionuclide compliance equations. Indexing these baseline results to the month of product transfer will be done at the time of transfer.

During ILAW production, radiochemical analyses of CRV samples will yield radionuclide concentrations in units of μCi/mL (= mCi/L). Such an activity-per-volume concentration of a radionuclide in the CRV can be converted to a mass-per-volume concentration by

$$c_{iq}^{CRV} = \frac{r_{iq}^{CRV}}{A_q} \tag{B.2.1}$$

where

c_{iq}^{CRV} = mass-per-volume concentration of the q^{th} radionuclide in the CRV batch contributing to the i^{th} MFPV batch (μg/mL = mg/L)

r_{iq}^{CRV} = activity-per-volume concentration of the q^{th} radionuclide in the CRV batch contributing to the i^{th} MFPV batch (μCi/mL = mCi/L)

A_q = specific activity of the q^{th} radionuclide (Ci/g = mCi/mg).

Values of A_q for a large number of radionuclides q are listed in Table A.2 of Appendix A. Table A.2 contains values for far more radionuclides than are reportable for ILAW (or immobilized high-level waste

[IHLW]), but the complete list is retained because the lists of reportable radionuclides are not yet finalized.

During operation of the WTP LAW vitrification facility, the measurements of activity-per-volume concentrations r_{iq}^{CRV} in Eq. (B.2.1) will be subject to uncertainties from (1) multiple waste samples taken from every CRV batch selected for analysis, and (2) possibly multiple laboratory analyses made on every sample. Averaging over multiple samples and multiple analyses per sample will reduce the uncertainty due to these sources. Rewriting Eq. (B.2.1) with means (averages) yields

$$\bar{c}_{iq}^{CRV} = \frac{\bar{r}_{iq}^{CRV}}{A_q} = \frac{1}{A_q}\left(\frac{1}{n_S^{CRV}\, n_A^{CRV}} \sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} r_{iqlm}^{CRV} \right) \tag{B.2.2}$$

where

$\bar{c}_{iq}^{CRV}$ = mass-per-volume concentration of the q^{th} radionuclide in the CRV batch contributing to the i^{th} MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations (μg/mL = mg/L)

$\bar{r}_{iq}^{CRV}$ = activity-per-volume concentration of the q^{th} radionuclide in the CRV batch contributing to the i^{th} MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations (μCi/mL = mCi/L)

n_S^{CRV} = number of samples per CRV batch, assuming all samples are analyzed for the q^{th} radionuclide[(a)]

n_A^{CRV} = number of radionuclide analyses per sample, assuming this number is the same for all radionuclides[(a)]

r_{iqlm}^{CRV} = activity-per-volume concentration of the q^{th} radionuclide in the CRV batch contributing to the i^{th} MFPV batch, based on the m^{th} radionuclide analysis of the l^{th} CRV sample (μCi/mL = mCi/L).

The average-based mass-per-volume concentrations $\bar{c}_{iq}^{CRV}$ from Eq. (B.2.2) can be used to calculate the average mass fractions of radionuclide oxides in the glass that would be made from the i^{th} MFPV batch ($\bar{g}_{iq}^{MFPV}$) using the compliance equations presented in Eqs. (B.1.11), (B.1.12), and (B.1.13). The ILAW radionuclides indexed by q in this section are treated as a subset of the components indexed by j in the ILAW chemical-composition compliance equations presented in Section B.1. Hence, the mass

(a) The number of samples (n_S^{CRV}) and number of radionuclide analyses per sample (n_A^{CRV}) need not be the same for each of the radionuclides. In such a case, these notations could be modified to include a q in the subscript to denote the dependence on the q^{th} radionuclide.

fraction compositions of ILAW are with respect to the total mass of "chemical composition" as well as "radionuclide composition" components. In the few cases where chemical analyses of selected radionuclides are performed in addition to radiochemical analyses, the masses must only be included once to avoid double-counting such radionuclides.

The ILAW compliance equations for mass and mass fraction of the q^{th} radionuclide oxide in the i^{th} ILAW MFPV batch in turn provide inputs for calculating the inventories of the q^{th} radionuclide in ILAW containers, as discussed in the following section.

B.2.2 Equations for Calculating Inventories of Radionuclides in ILAW Containers

To report the inventory of radionuclides in each ILAW container, the relationship between contents of individual ILAW MFPV batches and contents of individual containers would have to be estimated. Because of the time to process each ILAW MFPV batch through the melter, the volume of glass melt in the melter, and the mixing of MFPV batches that occurs, it is impossible to calculate and very difficult to estimate the composition of a specific ILAW container based on compositions of ILAW MFPV batches. Hence, the WTP ILAW compliance strategy (Nelson et al. 2003) is to report means and SDs of radionuclide inventories over containers of glass estimated to be produced from a series of ILAW MFPV batches.

B.2.2.1 Equation for a Mean Radionuclide Inventory per Container over D ILAW Containers

A general equation for the mean radionuclide inventory per container over D ILAW containers is first developed. Then this general equation is extended to include averages over multiple samples, analyses per sample, and volume determinations.

General Equation for the Mean Radionuclide Inventory per Container over *D* ILAW Containers

The mean inventory per container of radionuclide q in ILAW over an LAW waste type is calculated in three steps.

Step 1: The mean mass fraction of radionuclide oxide q in glass estimated to be produced from the I MFPV batches corresponding to an LAW waste type is calculated by

$$\bar{g}_q^{MFPV} = \frac{\sum_{i=1}^{I}\left(\sum_{j=1}^{J} m_{ij}^{MFPV}\right) g_{iq}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J} m_{ij}^{MFPV}} = \frac{\sum_{i=1}^{I} m_{iq}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J} m_{ij}^{MFPV}}$$

$$= \frac{\sum_{i=1}^{I}\left[c_{iq}^{CRV} f_q V_i^{CRV\ to\ MFPV} u + \sum_{k=1}^{K} a_{ik}^{GFC} G_{iqk}^{GFC} + m_{i-1,q}^{MFPV}\left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}}\right)\right]}{\sum_{i=1}^{I}\sum_{j=1}^{J}\left[c_{ij}^{CRV} f_j V_i^{CRV\ to\ MFPV} u + \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + m_{i-1,j}^{MFPV}\left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}}\right)\right]}$$

$$= \frac{\sum_{i=1}^{I}\left[\frac{r_{iq}^{CRV}}{A_q} f_q V_i^{CRV\ to\ MFPV} u + \sum_{k=1}^{K} a_{ik}^{GFC} G_{iqk}^{GFC} + m_{i-1,q}^{MFPV}\left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}}\right)\right]}{\sum_{i=1}^{I}\left[\sum_{j\in CHEM}^{J} c_{ij}^{CRV} f_j + \sum_{j\in RAD}^{J} \frac{r_{ij}^{CRV} f_j}{A_j} + \right] V_i^{CRV\ to\ MFPV} + \sum_{i=1}^{I}\sum_{j=1}^{J}\left[\sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + m_{i-1,j}^{MFPV}\left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}}\right)\right]} \quad \text{(B.2.3)}$$

where

$\bar{g}_q^{MFPV}$ = mean (mass-weighted-average) mass fraction of the q^{th} radionuclide oxide over I MFPV batches (g_{oxide}/g_{oxides})

m_{ij}^{MFPV} = mass of the j^{th} oxide (non-radionuclides as well as radionuclides) from the i^{th} MFPV batch (g_{oxide})

g_{iq}^{MFPV} = mass fraction of the q^{th} radionuclide oxide for glass that would be made from the i^{th} MFPV batch (g_{oxide}/g_{oxides})

I = number of MFPV batches corresponding to an LAW waste type

m_{iq}^{MFPV} = mass of the q^{th} radionuclide oxide from the i^{th} MFPV batch (g)

J = number of non-radionuclide oxides and radionuclide oxides estimated for the composition of each MFPV batch.

c_{iq}^{CRV} = mass-per-volume concentration of the q^{th} radionuclide in the CRV batch contributing to the i^{th} MFPV batch (µg/mL = mg/L)

c_{ij}^{CRV} = mass-per-volume concentration of the j^{th} analyte in the CRV batch contributing to the i^{th} MFPV batch (µg/mL = mg/L)

$V_i^{CRV\ to\ MFPV}$ = volume transfer from the CRV to the i^{th} MFPV batch (L)

r_{iq}^{CRV} = activity-per-volume concentration of the q^{th} radionuclide in the CRV contributing to the i^{th} MFPV batch (μCi/mL = mCi/L)

A_q = specific activity of the q^{th} radionuclide (Ci/g = mCi/mg)

$j \in CHEM$ = chemical composition components of ILAW

$j \in RAD$ = radionuclide composition components of ILAW

$CHEM$ = set of chemical composition components in ILAW

RAD = set of radionuclide components in ILAW

and the rest of the variables are as previously defined following Eq. (B.1.4). This equation assumes uniform mixing of the ILAW MFPV. The equation for g_{iq}^{MFPV} is given by Eq. (B.1.9) with "q" in place of "j". The equation for calculating m_{ij}^{MFPV} (where j denotes non-radionuclide oxides as well as radionuclide oxides) is given by Eq. (B.1.10a) in Section B.1. Substituting this equation in the first line yields the second line of Eq. (B.2.3). Substituting the expression in Eq. (B.2.1) for c_{iq}^{CRV} and c_{ij}^{CRV}, $j \in RAD$ yields the final form of Eq. (B.2.3). An expression for $m_{i-1,j}^{MFPV}$ (or $m_{i-1,q}^{MFPV}$) is given by Eq. (B.1.10b).

Step 2: The mean mass of the q^{th} radionuclide oxide over the D ILAW containers associated with an LAW waste type is calculated by multiplying the mean mass fraction of the q^{th} radionuclide oxide ($\overline{g}_q^{MFPV}$) from Eq. (B.2.3) times the mean mass of glass over the D ILAW containers estimated to correspond to the I MFPV batches:

$$\overline{m}_{Dq}^{Container} = \overline{g}_q^{MFPV}\,\overline{m}_D^{Container} \tag{B.2.4}$$

where

$\overline{m}_{Dq}^{Container}$ = mean mass of the q^{th} radionuclide oxide over the D ILAW containers associated with the I MFPV batches corresponding to an LAW waste type (g_{oxide})

$\overline{m}_D^{Container}$ = mean mass of glass in the D ILAW containers associated with an LAW waste type (g_{glass})

and $\overline{g}_q^{MFPV}$ is as previously defined and calculated by Eq. (B.2.3).

Step 3: The mean inventory per container of the q^{th} radionuclide over D ILAW containers associated with the I MFPV batches from an LAW waste type is given by the following general equation:

$$\overline{R}_{Dq}^{Container} = \frac{\overline{m}_{Dq}^{Container} A_q}{f_q} = \frac{\overline{g}_q^{MFPV} \overline{m}_D^{Container} A_q}{f_q}$$

$$= \frac{\sum_{i=1}^{I}\left[\frac{r_{iq}^{CRV}}{A_q} f_q V_i^{CRV\ to\ MFPV} u + \sum_{k=1}^{K} a_{ik}^{GFC} G_{iqk}^{GFC} + m_{i-1,q}^{MFPV}\left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}}\right)\right]\left(\frac{1}{D}\sum_{d=1}^{D} m_d^{Container}\right)\left(A_q / f_q\right)}{\sum_{i=1}^{I}\left[\sum_{j\in CHEM}^{J} c_{ij}^{CRV} f_j + \sum_{j\in RAD}^{J} \frac{r_{ij}^{CRV} f_j}{A_j} + \right] V_i^{CRV\ to\ MFPV} + \sum_{i=1}^{I}\sum_{j=1}^{J}\left[\sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + m_{i-1,j}^{MFPV}\left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}}\right)\right]} \quad \text{(B.2.5)}$$

where

$\overline{R}_{Dq}^{Container}$ = mean inventory per container of radionuclide q over the D ILAW containers associated with an LAW waste type (Ci)

f_q = $\frac{MW_q^{oxide}}{MW_q^{radionuclide}} K_q$ where MW_q^{oxide} and $MW_q^{radionuclide}$ are the molecular weights of radionuclide oxide q and radionuclide q, respectively, and K_q is the ratio of moles of radionuclide oxide q per mole of radionuclide q. Hence, f_j is the factor for converting the concentration of analyte j (µg analyte j/mL = mg analyte j/L) to the concentration of oxide j (µg oxide j/mL = mg oxide/L). The quantity f_q is called the oxide factor for oxide q ($g_{oxide}/g_{radionuclide}$),

and the remaining notation is as previously defined in this section. The expression for $\overline{m}_{Dq}^{Container}$ was substituted from Eq. (B.2.4) in the first line of Eq. (B.2.5). In the second line, $\overline{g}_q^{MFPV}$ was substituted from Eq. (B.2.3) and $\overline{m}_D^{Canister}$ is expanded using the usual formula for a mean. Eq. (B.2.5) assumes uniform mixing of the ILAW MFPV.

Equation for the Mean Radionuclide Inventory per Container over *D* ILAW Containers Based on Averages over Multiple Samples, Analyses, and Volume Determinations

Equation (B.2.5) provides the general formula for calculating the mean inventory per container of each reportable radionuclide q over the D ILAW containers associated with the I ILAW MFPV batches corresponding to a given LAW waste type. The variables in Eq. (B.2.5) are subject to several within-batch sources of uncertainty. These include CRV mixing and sampling uncertainty, CRV analytical uncertainty, glass forming chemical (GFC) composition uncertainty, uncertainty in masses of GFCs added to the MFPV, uncertainty in level/volume determinations of the CRV and MFPV before and after additions, and uncertainty in the mass of ILAW in containers. Some of these uncertainties can be effectively reduced by averaging results over multiple CRV samples per ILAW batch (n_A^{CRV}), multiple

chemical or radiochemical analyses per CRV sample (n_A^{CRV}), and multiple vessel level/volume measurements (n_V^{MFPV}). It is assumed that the mass of ILAW per container ($m_d^{Container}$) will be determined only once and thus that the uncertainty associated with it will not be eligible for reduction by averaging. This assumption was made because the uncertainty in determining this mass is expected to be fairly small, and thus not much would be gained by averaging multiple determinations.

The re-expression of Eq. (B.2.5) to include the average analyte concentrations over multiple CRV samples and analyses, as well as the average volume determinations for the CRV and MFPV, is given by:

$$\overline{\overline{R}}_{Dq}^{Container} = \frac{\overline{\overline{g}}_q^{MFPV}\,\overline{m}_D^{Container}\,A_q}{f_q} = \frac{\left(\dfrac{\sum_{i=1}^{I}\overline{m}_{iq}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J}\overline{m}_{ij}^{MFPV}}\right)\left(\dfrac{1}{D}\sum_{d=1}^{D}m_d^{Container}\right)A_q}{f_q}$$

$$= \frac{\sum_{i=1}^{I}\left[\begin{array}{l}\left(\dfrac{\sum_{l=1}^{n_S^{CRV}}\sum_{m=1}^{n_A^{CRV}}c_{iqlm}^{CRV}}{n_S^{CRV}\,n_A^{CRV}}\right)\overline{V}_i^{CRV\ to\ MFPV}\,f_q u \\ \quad + \sum_{k=1}^{K}a_{ik}^{GFC}G_{iqk}^{GFC} + \overline{m}_{i-1,q}^{MFPV}\left(\dfrac{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}}V_{i,h}^{MFPV\ Heel}}{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}}V_{i-1,h}^{MFPV}}\right)\end{array}\right]\left(\dfrac{1}{D}\sum_{d=1}^{D}m_d^{Container}\right)\left(\dfrac{A_q}{f_q}\right)}{\sum_{i=1}^{I}\sum_{j=1}^{J}\left[\left(\dfrac{\sum_{l=1}^{n_S^{CRV}}\sum_{m=1}^{n_A^{CRV}}c_{ijlm}^{CRV}}{n_S^{CRV}\,n_A^{CRV}}\right)\overline{V}_i^{CRV\ to\ MFPV}\,f_j u + \sum_{k=1}^{K}a_{ik}^{GFC}G_{ijk}^{GFC} + \overline{m}_{i-1,j}^{MFPV}\left(\dfrac{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}}V_{i,h}^{MFPV\ Heel}}{\frac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}}V_{i-1,h}^{MFPV}}\right)\right]}$$

$$= \sum_{i=1}^{I} \left[\left(\frac{\sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} r_{iqlm}^{CRV} / A_q}{n_S^{CRV} n_A^{CRV}} \right) \overline{V}_i^{CRV\ to\ MFPV} f_q u + \sum_{k=1}^{K} a_{ik}^{GFC} G_{iqk}^{GFC} + \overline{m}_{i-1,q}^{MFPV} \left(\frac{\frac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\ Heel}}{\frac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV}} \right) \right] \left[\left(\frac{1}{D} \sum_{d=1}^{D} m_d^{Container} \right) \frac{A_q}{f_q} \right]$$

(B.2.6)

$$\left[\sum_{i=1}^{I} \left[\left(\sum_{j \in CHEM}^{J} \frac{\sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{ijlm}^{CRV} f_j u}{n_S^{CRV} n_A^{CRV}} + \sum_{j \in RAD}^{J} \frac{\sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} r_{ijlm}^{CRV} f_j u / A_j}{n_S^{CRV} n_A^{CRV}} \right) \overline{V}_i^{CRV\ to\ MFPV} \right] + \sum_{i=1}^{I} \sum_{j=1}^{J} \left(\sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \overline{m}_{i-1,j}^{MFPV} \left(\frac{\frac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\ Heel}}{\frac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV}} \right) \right) \right]$$

where

$\overline{\overline{R}}_{Dq}^{Container}$ = mean inventory per container of the q^{th} radionuclide over the D ILAW containers associated with an LAW waste type, based on averages over multiple samples, analyses per sample, and volume determinations (Ci)

$$\overline{\overline{g}}_q^{MFPV} = \frac{\sum_{i=1}^{I} \overline{m}_{iq}^{MFPV}}{\sum_{i=1}^{I} \sum_{j=1}^{J} \overline{m}_{ij}^{MFPV}} = \text{mass weighted average of the mass fractions of the} \quad \text{(B.2.7)}$$

q^{th} radionuclide oxide over the I ILAW containers associated with an LAW waste type, based on averages over multiple samples per CRV batch, analyses per CRV sample, and volume determinations (g_{oxide}/g_{oxides})

$\overline{V}_i^{CRV\ to\ MFPV}$ is given by Eq. (B.1.13), and the remaining notation is as previously defined following Eq. (B.1.4). From the first to second lines of the derivation, $\overline{m}_{iq}^{MFPV}$ and $\overline{m}_{ij}^{MFPV}$ are substituted using

Eq. (B.1.10a). From the second to third lines, Eq. (B.2.2) is applied for the subset of ILAW components determined by radiochemical analysis (denoted *RAD*). This equation assumes uniform mixing of the ILAW MFPV.

Despite the reductions of some within-batch uncertainties, it should be recognized that values of $\overline{\overline{R}}_{Dq}^{Container}$ calculated via Eq. (B.2.6) will be subject to reduced within-MFPV-batch uncertainty as well as MFPV batch-to-batch variations.

B.2.2.2 Equation for the SD of a Radionuclide Inventory per Container over D ILAW Containers

The standard deviation of the inventory per container of radionuclide q over the D ILAW containers associated with the I ILAW MFPV batches corresponding to an ILAW production batch can be obtained by applying variance propagation methods to a conceptual equation for the inventory of radionuclide q in a single ILAW container. First, a general equation for the inventory of radionuclide q in a single ILAW container is presented. Then this general equation is extended to include averages over multiple samples, analyses per sample, and volume determinations.

General Equation for the SD of a Radionuclide Inventory per Container over *D* ILAW Containers

A general, conceptual equation for the inventory of radionuclide q in a single ILAW container is given by:

$$R_{dq}^{Container} = \frac{g_{iq}^{MFPV} m_d^{Container} A_q}{f_q} \tag{B.2.8}$$

where

$R_{dq}^{Container}$ = inventory of radionuclide q in the d^{th} ILAW container (Ci)

g_{iq}^{MFPV} = mass fraction of the q^{th} radionuclide oxide in the i^{th} MFPV batch (g_{oxide}/g_{oxides}), defined in Eq. (B.1.1) using the subscript "q" instead of "j"

$m_d^{Container}$ = measured mass of glass in the d^{th} ILAW container (g_{glass})

and A_q.and f_q are as previously defined. Values of f_q and A_q are listed in Tables A.1 and A.2 of Appendix A, respectively The quantity f_q is a known constant for each radionuclide q and hence is not subject to uncertainty. The A_q are subject to uncertainty corresponding to uncertainties in radionuclide half-lives. However, there is no compiled, complete table of such uncertainties. Hence, for now the A_q values will be treated as being known without uncertainty.

Equation (B.2.8) for $R_{dq}^{Container}$ provides a general, conceptual formula for calculating the inventory of each reportable radionuclide q for the d^{th} ILAW container associated with the i^{th} MFPV batch corresponding to a given LAW waste type. The formula is conceptual because it is not possible to directly calculate an ILAW radionuclide inventory for a given ILAW container as represented in the equation. The impossibility stems from the inability to easily relate the composition of the i^{th} ILAW MFPV batch to that of the d^{th} ILAW container. However, a subsequent variation of Eq. (B.2.8) is useful for calculating the SD of a radionuclide inventory per container over the D containers of ILAW and corresponding I MFPV batches corresponding to a given LAW waste type.

Equation for the SD of Radionuclide Inventory per Container over *D* ILAW Containers Based on Averages over Multiple Samples, Analyses, and Volume Determinations

The variables in Eq. (B.2.8) are subject to several within-batch sources of uncertainty. These include CRV mixing and sampling uncertainty, CRV analytical uncertainty, GFC composition uncertainty, uncertainty in masses of GFCs added to the MFPV, uncertainty in level/volume determinations of the CRV and MFPV before and after additions, and uncertainty in the mass of ILAW in containers. Some of these uncertainties can be effectively reduced by averaging results over multiple CRV samples per ILAW batch (n_A^{CRV}), multiple chemical or radiochemical analyses per CRV sample (n_A^{CRV}), and multiple vessel level/volume measurements (n_V^{MFPV}). It is assumed that the mass of ILAW per container ($m_d^{Container}$) will be determined only once, and thus that the uncertainty associated with it will not be eligible for reduction by averaging. This assumption was made because the uncertainty in determining this mass is expected to be fairly small, and thus not much would be gained by averaging multiple determinations.

The re-expression of Eq. (B.2.8) to include the average analyte concentrations over multiple CRV samples and analyses, and the average volume determinations for the CRV and MFPV is given by:

$$\overline{R}_{dq}^{Container} = \frac{\overline{g}_{iq}^{MFPV} m_d^{Container} A_q}{f_q} \qquad \text{(B.2.9)}$$

where

$\overline{R}_{dq}^{Container}$ = inventory of radionuclide q for the d^{th} ILAW container, based on averages over multiple samples, analyses per sample, and volume determinations (Ci),

$\overline{g}_{iq}^{MFPV}$ is given by Eq. (B.1.11) with "q" in place of "j", and the other notation is as previously defined. Note that $\overline{g}_{iq}^{MFPV}$ incorporates averages of analyte concentrations over multiple CRV samples and analyses per sample, and averages over multiple CRV and MFPV volume determinations.

The equation for the standard deviation of $\overline{R}_{dq}^{Container}$ over D containers associated with I ILAW MFPV batches was obtained by applying the variance propagation method of Goodman (1960) to Eq. (B.2.9) and assuming statistical independence among the radionuclide oxide mass fractions in an

ILAW MFPV batch and the measured mass of glass in an ILAW container.[a] The standard deviation equation is:

$$SD(\overline{R}_{dq}^{Container}) = \left(\frac{A_q}{f_q}\right)\left[\begin{array}{l}\left[\overline{\overline{g}}_q^{MFPV}\right]^2\left[SD(m_d^{Container})\right]^2 + \left[\overline{m}_D^{Container}\right]^2\left[SD(\overline{g}_{iq}^{MFPV})\right]^2 \\ -\left[SD(m_d^{Container})\right]^2\left[SD(\overline{g}_{iq}^{MFPV})\right]^2\end{array}\right]^{1/2} \quad \text{(B.2.10)}$$

where

$SD(\overline{R}_{dq}^{Container})$ = standard deviation of the average inventory per container of radionuclide q for the d^{th} ILAW container, where the average is based on multiple samples, analyses per sample, and volume determinations (Ci)

$SD(m_d^{Container})$ = standard deviation of the measured mass of glass in the d^{th} ILAW container (g_{glass})

$SD(\overline{g}_{iq}^{MFPV})$ = standard deviation of the average mass fraction of the q^{th} radionuclide oxide in the i^{th} MFPV batch, where the average is based on multiple samples, analyses per sample, and volume determinations (g_{oxide}/g_{oxides})

$\overline{\overline{g}}_q^{MFPV}$ is given by Eq. (B.2.7), $\overline{m}_D^{Container}$ is defined implicitly in Eq. (B.2.6), $\overline{g}_{iq}^{MFPV}$ is given by Eq. (B.1.11) with "q" in place of "j", and the remaining notation is as previously defined. Note that the minus sign in front of the third term in the square-bracketed portion of Eq. (B.2.10) is correct for estimating the standard deviation, as discussed by Goodman (1960).

The term $SD(\overline{g}_{iq}^{MFPV})$ includes variation in mass fractions of the q^{th} radionuclide oxide across all I MFPV batches associated with an LAW waste type as well as uncertainties in determining mass fractions of radionuclide oxides for each MFPV batch. These uncertainties include random inhomogeneities in mixing the CRV contents, random uncertainties associated with the MFPV sampling system, random irreproducibility of the chemical-analysis techniques employed, random uncertainties in volume measurements, and random uncertainties in the masses of GFCs added to the MFPV. The first four of these are effectively reduced by averaging when multiple samples, analyses per sample, and

(a) The assumption of statistical independence between radionuclide oxide mass fractions in the MFPV and mass of glass in an ILAW container is clearly reasonable as the process of filling containers is independent of the glass composition. It is not clear the extent to which the assumption of statistical independence among mass fractions of radionuclide oxides in the MFPV is appropriate. However, from a practical standpoint, it would be very difficult to estimate the many within-batch and batch-to-batch covariances between pairs of radionuclide oxide mass fractions. However, treating the radionuclide covariances as negligible is probably justified given the relatively tiny fractions of glass made up by radionuclides.

volume determinations per CRV and MFPV batch are made. A value of $SD(\overline{g}_{iq}^{MFPV})$ is calculated from the $\overline{g}_{iq}^{MFPV}$ (i = 1, 2, … , I) values using the usual standard deviation formula.

In a similar way, the term $SD(m_d^{Container})$ includes uncertainties associated with measuring the mass of glass in an ILAW container as well as the variation in the masses of glass that occur across containers associated with an LAW waste type. A value of $SD(m_d^{Container})$ is calculated from the $m_d^{Container}$ (d = 1, 2, … , D) values using the usual standard deviation formula.

B.3 Compliance Equations for ILAW Contract Specification 2.2.2.8: Radionuclide Concentration Limits

ILAW Contract Specification 2.2.2.8 is listed verbatim to provide the context for the ILAW radionuclide compliance equations presented in this section.

Contract Specification 2.2.2.8: Radionuclide Concentration Limits

> *The radionuclide concentration of the ILAW form shall be less than Class C limits as defined in 10 CFR 61.55. In addition, the average concentrations of ^{137}Cesium (^{137}Cs) and ^{90}Strontium (^{90}Sr) shall be limited as follows: $^{137}Cs < 3$ Ci/m^3 and $^{90}Sr < 20$ Ci/m^3. The method used to perform concentration averaging should be identified in the ILAW Product Compliance Plan.*

To comply with Specification 2.2.2.8, the radionuclides with Class C limits in 10CFR61.55, as well as radionuclides with limits from the specification, must be considered. Table B.1 summarizes the radionuclides and the corresponding limits.

According to 10 CFR 61.55(a)(8) for purposes of comparison to Class C limits, the concentration of a radionuclide may be averaged over the (1) volume of the ILAW when the radionuclide limit is expressed in units of Ci/m^3 or (2) weight of the ILAW when the radionuclide limit is expressed in units of nCi/g. The U.S. Nuclear Regulatory Commission's (NRC's) *Branch Technical Position on Concentration Averaging and Encapsulation* (NRC 1995) clarifies that radionuclide concentrations can be averaged over the contents of a waste container (i.e., an ILAW container in this instance). However, there is no indication that averaging over multiple containers is allowable. This is a difference from the second part of Contract Specification 2.2.2.8, which prescribes comparing average concentrations (over some group of containers) of ^{137}Cs and ^{90}Sr to their respective limits. Hence, the approaches to comply with the two parts of Specification 2.2.2.8 must be different.

Section B.3.1 develops the compliance equations for satisfying Class C limits. Section B.3.2 presents the compliance equations for satisfying the ^{137}Cs and ^{90}Sr limits given in Specification 2.2.2.8. In both sections, it is assumed that the radionuclide concentrations determined by the analytical laboratory will first be indexed to December 31, 2002 before use in the compliance equations, as discussed in Section B.2.1.

Table B.1. Class C and Contract Limits for Radionuclides in ILAW

Isotope[a]	10 CFR 61.55 Class C Limit		Contract Limit	Comments
	Table 1	Table 2		
^{14}C	8 Ci/m^3	N/A[b]	(c)	Not present in glass due to volatility
^{99}Tc	3 Ci/m^3	N/A	(c)	No comment.
^{129}I	0.08 Ci/m^3	N/A	(c)	Not present in glass due to volatility
TRU	100 nCi/g	N/A	(c)	TRU defined as alpha-emitting transuranics with half-lives > 5 yr[d]
^{241}Pu	3500 nCi/g	N/A	(c)	No comment.
^{242}Cm	20000 nCi/g	N/A	(c)	No comment.
^{63}Ni	N/A	700 Ci/m^3	(c)	Table 2 limits are applicable only if the concentrations of Table 1 radionuclides do not exceed 0.1 times their respective limits in Table 1
^{90}Sr	N/A	7000 Ci/m^3	20 Ci/m^3	
^{137}Cs	N/A	4600 Ci/m^3	3 Ci/m^3	

(a) WTP LAW does not contain radionuclides in activated metals, so those rows of 10 CFR 61.55 Tables 1 and 2 have been omitted.
(b) N/A = not applicable.
(c) No limit.
(d) TRU radionuclides include the alpha-emitting transuranic elements with half-lives > 5 y, namely ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Am, and ^{244}Cm.

B.3.1 Compliance Equations for Comparing Radionuclide Concentrations to Class C Limits

Section 5.3.3 presents the steps of the procedure for demonstrating compliance with Class C limits based on the requirements of 10 CFR 61.55(a)(5). Because WTP LAW may contain mixtures of both long-lived (10 CFR 61.55 Table 1) and short-lived (10 CFR 61.55 Table 2) radionuclides, a sum-of-fractions approach is used to assess compliance in both cases. This section presents the equations needed for the statistical implementations of the sum-of-fractions approach presented in Sections 5.3.3.1 and 5.3.3.2.

Section B.3.1.1 presents the equations for the mean and SD of radionuclide concentration sum-of-fractions, which are used in the statistical approach for demonstrating compliance over the *D* ILAW containers corresponding to an LAW waste type (as discussed in Section 5.3.3.1). Section B.3.1.2 presents the equations for calculating radionuclide sum-of-fractions needed to assess compliance with Class C limits for each ILAW MFPV batch (as discussed in Section 5.3.3.2).

B.3.1.1 Compliance Equations for Sum-of-Fractions of Class C Radionuclide Concentrations over *D* ILAW Containers

Equations to calculate the means and standard deviations of the sum-of-fractions of 10 CFR 61.55 Table 1 and Table 2 radionuclides for Class C limits over *D* ILAW containers corresponding to an LAW waste type are presented in this subsection.

Equations for the Means of Sum-of-Fractions of Class C Radionuclides over *D* ILAW Containers

Mean Sum-of-Fractions of Radionuclides in 10 CFR 61.55 Table 1

The equation to calculate the mean sum-of-fractions of 10 CFR 61.55 Table 1 radionuclides for Class C limits over *D* ILAW containers corresponding to an LAW waste type is of the general form:

$$\overline{SF1}_D^{Containers} = \sum_{k=TRU,\ ^{241}Pu,\ ^{242}Cm} \left(\frac{\sum_{q=1}^{N_k} \bar{\bar{s}}_{Dqk}^{Container}}{L_k^s} \right) + \left[\frac{\bar{\bar{r}}_{Dq}^{Container}}{L_q^r} \right]_{q=^{99}Tc} \qquad \text{(B.3.1)}$$

where

$\overline{SF1}_D^{Containers}$ = mean sum-of-fractions for Class C radionuclides from 10 CFR61.55 Table 1 over *D* ILAW containers associated with *I* ILAW MFPV batches corresponding to an LAW waste type, based on averages over multiple samples, analyses per sample, and volume determinations (unitless)

$\bar{\bar{s}}_{Dqk}^{Container}$ = mean activity-per-mass concentration of the q^{th} radionuclide in the k^{th} group of radionuclides in glass from *D* ILAW containers, based on averages over multiple samples, analyses per sample, and volume determinations (nCi/g)

N_k = number of radionuclides in the k^{th} group of radionuclides (one, except for TRU)

L_k^s = limiting activity-per-mass concentration for the k^{th} group of radionuclides (nCi/g)

$\bar{\bar{r}}_{Dq}^{Container}$ = mean activity-per-volume concentration of the q^{th} radionuclide ($q = {}^{99}$Tc) in glass from *D* ILAW containers, based on averages over multiple samples, analyses per sample, and volume determinations (Ci/m^3)

L_q^r = limiting activity-per-volume concentration for the q^{th} radionuclide ($q = {}^{99}$Tc) (Ci/m^3)

and TRU is as previously defined in Table B.1. The term before the plus sign in Eq. (B.3.1) corresponds to long-lived radionuclides expected in WTP LAW (TRU, ^{241}Pu, and ^{242}Cm) whose limits are specified in units of nCi/g. The term after the plus sign corresponds to long-lived radionuclides expected in WTP ILAW whose limits are specified in units of Ci/m^3 (only ^{99}Tc). Note that only radionuclides expected by the WTP Project to occur in LAW are included in the equations, as discussed in Section 5.3.3.

Expanding the mean concentrations $\overline{\overline{s}}_{Dqk}^{Container}$ and $\overline{\overline{r}}_{Dq}^{Container}$ in Eq. (B.3.1) yields

$$\overline{SF1}_D^{Containers} = \sum_{k=TRU,\ ^{241}Pu,\ ^{242}Cm} \left[\frac{1}{L_k^s} \left(\frac{\left(10^9\right) \sum_{q=1}^{N_k} \overline{\overline{R}}_{Dqk}^{Container}}{\overline{m}_D^{Container}} \right) \right] + \left[\frac{1}{L_q^r} \left(\frac{\overline{\overline{R}}_{Dq}^{Container}}{\overline{V}_D^{Container}} \right) \right]_{q=^{99}Tc} \quad \text{(B.3.2)}$$

where

$\overline{\overline{R}}_{Dqk}^{Container}$ = mean inventory per container of the q^{th} radionuclide in the k^{th} group of radionuclides in glass from D ILAW containers, based on averages over multiple samples, analyses per sample, and volume determinations and calculated similarly to Eq. (B.2.6) (Ci)

$\overline{m}_D^{Container}$ = mean mass of glass in D ILAW containers (g_{glass})

$\overline{\overline{R}}_{Dq}^{Container}$ = mean inventory per container of the q^{th} radionuclide ($q = {}^{99}$Tc) in glass from D ILAW containers, based on averages over multiple samples, analyses per sample, and volume determinations and calculated using Eq. (B.2.6) (Ci)

$\overline{V}_D^{Container}$ = mean volume of glass in D ILAW containers (m^3)

and $\overline{SF1}_D^{Containers}$, N_k, L_k^s, and L_q^r are as previously defined. The multiplier of 10^9 in the numerator of the first term in Eq. (B.3.2) converts inventory from Ci to nCi. This unit conversion is necessary for the remaining part of the first term to match the nCi/g units of the limit L_k^s.

Eq. (B.3.2) can be further expanded by substituting for $\overline{\overline{R}}_{Dqk}^{Container}$ and $\overline{\overline{R}}_{Dq}^{Container}$ using Eq. (B.2.6) and for $\overline{V}_D^{Container}$ using

$$\overline{V}_D^{Container} = \frac{\overline{m}_D^{Container}}{\overline{\rho}_D^{Container}} \quad \text{(B.3.3)}$$

where

$\overline{\rho}_D^{Container}$ = mean density of glass in D containers (g/m^3), assumed to be 2.65×10^6 g/m^3

and $\overline{V}_D^{Container}$ and $\overline{m}_D^{Container}$ are as previously defined. Equation (B.3.3) is used to calculate the average volume of ILAW over D containers because it is not impacted by voids in the ILAW within a container.

An equation that averaged ILAW volumes calculated from container fill heights would be impacted by voids.

The resulting expansion of Eq. (B.3.2) is

$$\overline{SF1}_D^{Containers} = \sum_{k=TRU,\ ^{241}Pu,\ ^{242}Cm} \left[\frac{1}{L_k^s} \left(\sum_{q=1}^{N_k} \frac{\left(10^9\right) \overline{\overline{g}}_q^{MFPV} A_q}{f_q} \right) \right] + \left[\frac{1}{L_q^r} \left(\frac{\overline{\overline{g}}_q^{MFPV} \overline{\rho}_D^{Container} A_q}{f_q} \right) \right]_{q=^{99}Tc} \quad \text{(B.3.4)}$$

where $\overline{\overline{g}}_q^{MFPV}$ is calculated according to Eq. (B.2.7), and all other quantities in the equation are as previously defined.

Mean Sum-of-Fractions of Radionuclides in 10 CFR 61.55 Table 2

The equation to calculate the mean sum-of-fractions of 10 CFR 61.55 Table 2 radionuclides for Class C limits over *D* ILAW containers corresponding to an LAW waste type is

$$\overline{SF2}_D^{Containers} = \sum_{q=^{63}Ni,\ ^{90}Sr,\ ^{137}Cs} \left[\frac{1}{L_q^r} \left(\frac{\overline{\overline{g}}_q^{MFPV} \overline{\rho}_D^{Container} A_q}{f_q} \right) \right] \quad \text{(B.3.5)}$$

where

$\overline{SF2}_D^{Containers}$ = mean sum-of-fractions for Class C radionuclides from 10 CFR61.55 Table 2 over *D* ILAW containers associated with *I* ILAW MFPV batches corresponding to an LAW waste type, based on averages over multiple samples, analyses per sample, and volume determinations (unitless)

and all remaining notation is as previously defined in this subsection. Equation (B.3.5) is a simplification of Eq. (B.3.4) because (1) there are no radionuclides in 10 CFR 61.55 Table 2 with a group limit (e.g., TRU), and (2) all three radionuclide concentrations have their corresponding limits expressed in units of Ci/m^3.

Equations for the SDs of the Sum-of-Fractions for Class C Radionuclides Over *D* ILAW Containers

Standard Deviation of Sum-of-Fractions of Radionuclides in 10 CFR 61.55 Table 1

The standard deviation of the sum-of-fractions of 10 CFR 61.55 Table 1 radionuclides for Class C limits over the *D* ILAW containers associated with the *I* ILAW MFPV batches corresponding to an LAW waste type can be obtained by applying variance propagation methods to the following conceptual equation for a single container:

$$\overline{SF1}_d^{Container} = \sum_{k=TRU,\ ^{241}Pu,\ ^{242}Cm} \left[\frac{1}{L_k^s} \left(\sum_{q=1}^{N_k} \frac{\left(10^9\right) \overline{g}_{iq}^{MFPV} A_q}{f_q} \right) \right] + \left[\frac{1}{L_q^r} \left(\frac{\overline{g}_{iq}^{MFPV} \rho_d^{Container} A_q}{f_q} \right) \right]_{q=^{99}Tc} \quad \text{(B.3.6)}$$

where

$\overline{SF1}_d^{Container}$ = sum-of-fractions for Class C radionuclides from 10 CFR 61.55 for the d^{th} ILAW container, based on averages over multiple samples, analyses per sample, and volume determinations (unitless)

$\overline{g}_{iq}^{MFPV}$ = mass fraction of the q^{th} radionuclide oxide in the i^{th} MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations (g_{oxide}/g_{oxides})

$\rho_d^{Container}$ = density of glass for the d^{th} ILAW container (g_{glass}/m^3_{glass})

$\overline{g}_{iq}^{MFPV}$ is given by Eq. (B.1.11) with "q" in place of "j", and A_q and f_q are as previously defined. The f_q are known constants for each radionuclide q and hence are not subject to uncertainty. The A_q are subject to uncertainty corresponding to uncertainties in radionuclide half-lives. However, there is no compiled, complete table of such uncertainties, and so for now the A_q values will be treated as known without uncertainty. For purposes of calculating the standard deviation of $\overline{SF}_d^{Container}$, $\rho_d^{Container}$ is assumed to have a mean value of 2.65×10^6 g/m^3 with some variation over ILAW containers corresponding to an LAW waste type.

Note that Eq. (B.3.6) for $\overline{SF1}_d^{Container}$ is conceptual and is used only to calculate the standard deviation of $\overline{SF1}_d^{Container}$ over the D ILAW containers associated with the I ILAW MFPV batches corresponding to an LAW waste type. Eq. (B.3.6) is conceptual because it is not possible to directly calculate an ILAW sum-of-fractions for a given ILAW container as represented in the equation. The impossibility stems from the inability to easily relate the composition of the i^{th} ILAW MFPV batch to that of the d^{th} ILAW container. However, the equation is useful for calculating the standard deviation of $\overline{SF1}_d^{Container}$, as described following.

The equation for the standard deviation of $\overline{SF1}_d^{Container}$ was obtained by applying the variance propagation methods described by Hines et al. (2003) and Goodman (1960) to Eq. (B.3.6) and assuming statistical independence among the radionuclide oxide mass fractions in an ILAW MFPV batch and the measured density of glass in an ILAW container.[(a)] The standard deviation equation is:

(a) The assumption of statistical independence between radionuclide oxide mass fractions in the MFPV and glass density in an ILAW container is reasonable because density will depend primarily on major glass components, not minor radionuclide components. It is not clear the extent to which the assumptions of statistical independence among mass fractions of radionuclide oxides in the MFPV are appropriate, but from a practical

$$SD(\overline{SF1}_d^{Container}) = \left\{ \sum_{k=TRU,\ ^{241}Pu,\ ^{242}Cm} \left(\frac{10^9}{L_k^s} \right)^2 \sum_{q=1}^{N_k} \left(\frac{A_q}{f_q} \right)^2 \left(SD(\overline{g}_{iq}^{MFPV}) \right)^2 \right.$$

$$\left. + \left[\left[\frac{A_q}{L_q^r f_q} \right]^2 \left(\begin{array}{l} (\overline{\overline{g}}_q^{MFPV})^2 \left(SD(\rho_d^{Container}) \right)^2 \\ + (\overline{\rho}_D^{Container})^2 \left(SD(\overline{g}_{iq}^{MFPV}) \right)^2 - \left(SD(\rho_d^{Container}) \right)^2 \left(SD(\overline{g}_{iq}^{MFPV}) \right)^2 \end{array} \right) \right]_{q=^{99}Tc} \right\}^{1/2} \quad \text{(B.3.7)}$$

where

$SD(\overline{SF1}_d^{Container})$ = standard deviation of the sum-of-fractions for Class C radionuclides from 10 CFR 61.55 Table 1 over the $d = 1, 2, \ldots, D$ ILAW containers (unitless)

$SD(\overline{g}_{iq}^{MFPV})$ = standard deviation of the mass fraction of the q^{th} radionuclide oxide over the $i = 1, 2, \ldots, I$ batches associated with the D ILAW containers, where $\overline{g}_{iq}^{MFPV}$ for the i^{th} MFPV batch is based on averages over multiple samples, analyses per sample, and volume determinations (g_{oxide}/g_{oxides})

$SD(\rho_d^{Container})$ = standard deviation of the density of glass over the $d = 1, 2, \ldots, D$ ILAW containers (g_{glass}/m^3_{glass})

$\overline{\overline{g}}_{iq}^{MFPV}$ is given by Eq (B.1.11) with "q" in place of "j", $\overline{\overline{g}}_q^{MFPV}$ is given by Eq. (B.2.7), and the rest of the variables are as previously defined. Note that the minus sign in front of the third term in the square-bracketed portion of Eq. (B.3.7) is correct for estimating the standard deviation, as discussed by Goodman (1960).

The term $SD(\overline{g}_{iq}^{MFPV})$ includes variation in mass fractions of the q^{th} radionuclide oxide across all I MFPV batches associated with an LAW waste type, as well as uncertainties in determining mass fractions of radionuclide oxides for each MFPV batch. These uncertainties include random inhomogeneities in mixing the CRV, uncertainties in sampling and analyzing the CRV, uncertainties in volume measurements, and uncertainties in the masses of GFCs added to the MFPV. A value of $SD(\overline{g}_{iq}^{MFPV})$ is calculated from the $\overline{g}_{iq}^{MFPV}$ ($i = 1, 2, \ldots, I$) values using the usual standard deviation formula.

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standpoint, it would be very difficult to estimate the many within-batch and batch-to-batch covariances. However, treating the radionuclide covariances as negligible is probably justified given the relatively tiny fractions of glass made up by radionuclides.

In a similar way, the term $SD(\rho_d^{Container})$ includes uncertainties associated with measuring or estimating the density of glass in a single container, as well as the variation in the density of glass in containers corresponding to an LAW waste type. A value of $SD(\rho_d^{Container})$ is calculated from the $\rho_d^{Container}$ ($d = 1, 2, \ldots, D$) values using the usual standard deviation formula.

Standard Deviation of Sum-of-Fractions of Radionuclides in 10 CFR 61.55 Table 2

The standard deviation of the sum-of-fractions of 10 CFR 61.55 Table 2 radionuclides for Class C limits over the D ILAW containers associated with the I ILAW MFPV batches corresponding to an LAW waste type can be obtained by applying variance propagation methods to the following conceptual equation for a single container:

$$\overline{SF2}_d^{Container} = \sum_{q={}^{63}Ni,\ {}^{90}Sr,\ {}^{137}Cs} \left[\frac{1}{L_q^r} \left(\frac{\bar{g}_{iq}^{MFPV} \rho_d^{Container} A_q}{f_q} \right) \right] \tag{B.3.8}$$

where all notation is as previously defined. Note that Eq. (B.3.8) is a simplified form of Eq. (B.3.6). Hence, the equation for the standard deviation of $\overline{SF2}_d^{Container}$ is a simplified form of Eq. (B.3.7) given by:

$$SD(\overline{SF2}_d^{Container}) = \left[\sum_{q={}^{63}Ni+{}^{90}Sr+{}^{137}Cs} \left[\frac{A_q}{L_q^r f_q} \right]^2 \left(\begin{array}{l} (\bar{\bar{g}}_q^{MFPV})^2 \left(SD(\rho_d^{Container}) \right)^2 \\ + (\bar{\rho}_D^{Container})^2 \left(SD(\bar{g}_{iq}^{MFPV}) \right)^2 \\ - \left(SD(\rho_d^{Container}) \right)^2 \left(SD(\bar{g}_{iq}^{MFPV}) \right)^2 \end{array} \right) \right]^{1/2} \tag{B.3.9}$$

where

$SD(\overline{SF2}_d^{Container})$ = standard deviation of the sum-of-fractions for Class C radionuclides from 10 CFR 61.55 Table 2 over the $d = 1, 2, \ldots, D$ ILAW container (unitless)

and all remaining notation is as previously defined.

B.3.1.2 Compliance Equations for Sum-of-Fractions of Class C Radionuclide Concentrations in Glass that Would Be Made from an ILAW MFPV Batch

The equation to calculate the sum-of-fractions of radionuclides from 10 CFR 61.55 Table 1 for Class C limits for ILAW that would be made from the i^{th} MFPV batch is of the general form:

$$\overline{SF1}_i^{MFPV} = \sum_{k=TRU,\ {}^{241}Pu,\ {}^{242}Cm} \left[\frac{1}{L_k^s} \left(\sum_{q=1}^{N_k} \frac{\left(10^9\right) \bar{g}_{iq}^{MFPV} A_q}{f_q} \right) \right] + \left[\frac{1}{L_q^r} \left(\frac{\bar{g}_{iq}^{MFPV} \rho_i^{MFPV} A_q}{f_q} \right) \right]_{q={}^{99}Tc} \tag{B.3.10}$$

where

$\overline{SF1}_i^{MFPV}$ = sum-of-fractions for Class C radionuclides from 10 CFR 61.55 Table 1 in ILAW that would be made from the i^{th} ILAW MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations (unitless)

$\overline{g}_{iq}^{MFPV}$ = mass fraction of the q^{th} radionuclide oxide in glass that would be made from the i^{th} ILAW MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations (g_{oxide}/g_{oxides})

ρ_i^{MFPV} = density of glass that would be made from the i^{th} ILAW MFPV batch (g_{glaaa}/m^3_{glass}), assumed to be 2.65×10^6 g/m^3

$\overline{g}_{iq}^{MFPV}$ is given by Eq. (B.1.11) with "q" in place of "j", and L_k^s, L_q^r, A_q,f_q, and the 10^9 unit conversion factor are as previously defined.

The equation to calculate the sum-of-fractions of radionuclides from 10 CFR 61.55 Table 2 for Class C limits for ILAW that would be made from the i^{th} MFPV batch is of the general form:

$$\overline{SF2}_i^{MFPV} = \sum_{q={}^{63}Ni,\ {}^{90}Sr,\ {}^{137}Cs} \left[\frac{1}{L_q^r} \left(\frac{\overline{g}_{iq}^{MFPV}\ \rho_i^{MFPV}\ A_q}{f_q} \right) \right] \qquad \text{(B.3.11)}$$

where

$\overline{SF2}_i^{MFPV}$ = sum-of-fractions for Class C radionuclides from 10 CFR 61.55 Table 2 in ILAW that would be made from the i^{th} ILAW MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations (unitless)

and all remaining notation is as previously defined.

In Eq. (B.3.10) for calculating $\overline{SF1}_i^{MFPV}$ and Eq. (B.3.11) for calculating $\overline{SF2}_i^{MFPV}$, the quantity $\overline{g}_{iq}^{MFPV}$ is subject to several within-batch sources of uncertainty, including CRV sampling, CRV analytical, GFC composition, GFC addition in the MFPV, and level/volume measurements of the CRV and MFPV before and after additions. In Eq. (B.3.10), the assumed value for ρ_i^{MFPV} will also be subject to uncertainty. Some of these uncertainties are effectively reduced by averaging results over the number of CRV samples per ILAW batch (n_A^{CRV}), the number of chemical or radiochemical analyses per CRV sample (n_A^{CRV}), and the number of vessel level/volume measurements (n_V^{MFPV}). This averaging is denoted by the "bar" notation on $\overline{g}_{iq}^{MFPV}$.

B.3.2 Compliance Equation for ILAW Radionuclide Running-Average Concentrations

Two equations for calculating running averages of ^{137}Cs and ^{90}Sr concentrations in ILAW are presented. The first equation, discussed in Section B.3.2.1, is for demonstrating compliance over the *D* ILAW containers produced at any point in time. The second equation, discussed in Section B.3.2.2, is for assessing compliance for each ILAW MFPV batch.

B.3.2.1 Compliance Equation for Running Averages of ILAW Radionuclide Concentrations over D ILAW Containers

The equation for comparing the running average of activity-per-volume concentrations of the q^{th} radionuclide (q = ^{137}Cs and ^{90}Sr) over *D* ILAW containers ($\overline{\overline{r}}_{Dq}^{Container}$) to the Contract limits (L_q^r) shown in Table B.1 is

$$\overline{\overline{r}}_{Dq}^{Container} \le L_q^r \quad . \tag{B.3.12}$$

In the notation $\overline{\overline{r}}_{Dq}^{Container}$, the first "bar" denotes averaging over multiple samples, analyses per sample, and volume determinations corresponding to each MFPV batch. The second "bar" and subscript *D* denotes averaging $\overline{r}_{dq}^{Container}$ values over *D* containers. The equation for calculating $\overline{\overline{r}}_{Dq}^{Container}$ follows from the derivations in Section B.3.1, and is given by

$$\overline{\overline{r}}_{Dq}^{Container} = \frac{\overline{\overline{g}}_q^{MFPV}\,\overline{\rho}_D^{Container}\,A_q}{f_q} = \left(\frac{\sum_{i=1}^{I} \overline{m}_{iq}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J} \overline{m}_{ij}^{MFPV}} \right) \left(\frac{\overline{\rho}_D^{Container}\,A_q}{f_q} \right) \tag{B.3.13}$$

where

$\overline{\overline{r}}_{Dq}^{Container}$ = running average of activity-per-volume concentrations of the q^{th} radionuclide (q = ^{137}Cs and ^{90}Sr) over the *D* ILAW containers produced through a given point in time, based on averages over multiple samples, analyses per sample, and volume determinations (Ci/m^3)

$\overline{m}_{iq}^{MFPV}$ = mass of the q^{th} radionuclide oxide from the i^{th} MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations (g)

I = number of MFPV batches produced to date

$\overline{m}_{ij}^{MFPV}$ = mass of the j^{th} oxide (non-radionuclides as well as radionuclides) from the i^{th} MFPV batch, based on averages over multiple samples, analyses per sample, and volume determinations (g_{oxide})

J = number of non-radionuclide oxides and radionuclide oxides estimated for the composition of each MFPV batch

and all remaining variables are as previously defined in Section B.3.1.

B.3.2.2 Compliance Equation for Running Averages of ILAW Radionuclide Concentrations in Glass that Would Be Made from ILAW MFPV Batches

The equation for comparing the running average of activity-per-volume concentrations of the q^{th} radionuclide (q = ^{137}Cs and ^{90}Sr) over I ILAW MFPV batches ($\overline{\overline{r}}_{Iq}^{MFPV}$) to the Contract limits (L_q^r) shown in Table B.1 is

$$\overline{\overline{r}}_{Iq}^{MFPV} \le L_q^r \ . \tag{B.3.14}$$

In the notation $\overline{\overline{r}}_{Iq}^{MFPV}$, the first "bar" denotes averaging over multiple samples, analyses per sample, and volume determinations corresponding to each MFPV batch. The second "bar" and subscript I denotes averaging $\overline{r}_{iq}^{MFPV}$ values over I MFPV batches. The equation for calculating $\overline{\overline{r}}_{Iq}^{MFPV}$ is given by

$$\overline{\overline{r}}_{Iq}^{MFPV} = \frac{\overline{\overline{g}}_q^{MFPV}\ \overline{\rho}_I^{MFPV}\ A_q}{f_q} = \left(\frac{\sum_{i=1}^{I} \overline{m}_{iq}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J} \overline{m}_{ij}^{MFPV}} \right) \left(\frac{\overline{\rho}_I^{MFPV}\ A_q}{f_q} \right) \tag{B.3.15}$$

where

$\overline{\overline{r}}_{Iq}^{MFPV}$ = running average of activity-per-volume concentrations of the q^{th} radionuclide (q = ^{137}Cs and ^{90}Sr) over the I ILAW MFPV batches produced through a given point in time, based on averages over multiple samples, analyses per sample, and volume determinations (Ci/m^3)

$\overline{\rho}_I^{MFPV}$ = mean density of glass that would be made from I ILAW MFPV batches (g/m^3), assumed to be 2.65×10^6 g/m^3

$\overline{\overline{g}}_q^{MFPV}$ is given by Eq. (B.2.7), and all remaining variables in Eq. (B.3.15) are as previously defined in Section B.3.1. Note that there is no difference between Eqs. (B.3.13) and (B.3.15), except for notation, if the same assumed mean density is used for $\overline{\rho}_D^{Container}$ in Eq. (B.313) and for $\overline{\rho}_I^{MFPV}$ in Eq. (B.3.15).

For each MFPV batch, the running average concentrations for ^{137}Cs and ^{90}Sr can be calculated according to Eq. (B.3.15) and the averages compared to the limits as in Eq. (B.3.14). Variations (over MFPV batches) and uncertainties (for each MFPV batch) are not accounted for in comparing calculated concentrations to limits, per the WTP compliance strategy.

B.4 Compliance Equations for ILAW Contract Specifications 2.2.2.17.2: Product Consistency Test (PCT) and 2.2.2.17.3: Vapor Hydration Test (VHT)

This section documents the general form of equations for calculating predicted property values for ILAW as well as the uncertainties associated with the predicted property values.

For a particular glass property *P* of interest (e.g., PCT or VHT response), predicted property values $\hat{y} = \hat{f}(P)$ are nominally calculated using a model of the general form

$$\hat{y} = \hat{f}(P) = \boldsymbol{x}^T \boldsymbol{b} \tag{B.4.1}$$

where $\hat{y} = \hat{f}(P)$ denotes the predicted value of a possibly mathematically transformed property (such as a logarithmic transformation), $\boldsymbol{x}^T$ is a row-vector containing the composition for a particular glass formulation for which a predicted property value is to be calculated, and $\boldsymbol{b}$ is a $p \times 1$ column-vector of model coefficients. The model coefficients in the $\boldsymbol{b}$ vector are uncertain because the model is an approximation to the real property-composition relationship and because the model form is fitted to experimental property-composition data subject to uncertainty. During operation of the WTP ILAW facility, estimated glass compositions $\boldsymbol{x}$ will be subject to several sources of uncertainty. Because the model uncertainty and glass composition uncertainty are statistically independent, the variance of $\hat{y}$ is given by

$$\text{var}(\hat{y}) = \text{var}(\boldsymbol{b}^T \boldsymbol{x}) = \boldsymbol{b}^T \boldsymbol{\Sigma}_x \boldsymbol{b} + \boldsymbol{x}^T \boldsymbol{\Sigma}_b \boldsymbol{x} \tag{B.4.2}$$

where $\boldsymbol{b}^T$ and $\boldsymbol{x}^T$ are transposes of $\boldsymbol{b}$ and $\boldsymbol{x}$, respectively, $\boldsymbol{\Sigma}_x$ is the composition variance-covariance matrix, and $\boldsymbol{\Sigma}_b$ is the variance-covariance matrix for the model coefficients. The first term of Eq. (B.4.2) represents compositional uncertainty, while the second term represents model uncertainty.

When a model is fitted to property-composition data using unweighted least squares (ULS) regression, an algebraic expression to estimate $\boldsymbol{\Sigma}_b$ is given by

$$\hat{\boldsymbol{\Sigma}}_b = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \hat{\sigma}_U^2 \tag{B.4.3}$$

where $\boldsymbol{X}$ is the design matrix used to generate the property-composition model, $\boldsymbol{X}^T$ is the matrix transpose of $\boldsymbol{X}$, and $\hat{\sigma}_U^2$ is the estimated mean square for error associated with the ULS fit of the model. In the ULS case, the second term in Eq. (B.4.2) representing model uncertainty can be written as

$$\boldsymbol{x}^T (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{x}\, \hat{\sigma}_U^2 \,. \tag{B.4.4}$$

When a model is fitted to property-composition data using weighted least squares (WLS) regression, an algebraic expression to estimate $\boldsymbol{\Sigma_b}$ is given by

$$\hat{\boldsymbol{\Sigma}}_b = (\boldsymbol{X}^T \boldsymbol{W} \boldsymbol{X})^{-1} \hat{\sigma}_W^2 \tag{B.4.5}$$

where $\boldsymbol{W}$ is a diagonal matrix of weights associated with the data points used to fit the property-composition model, $\hat{\sigma}_W^2$ is estimated mean square for error associated with the WLS fit of the model, and the remaining notation is as previously defined. In the WLS case, the second term in Eq. (B.4.2) representing model uncertainty can be written as

$$\boldsymbol{x}^T (\boldsymbol{X}^T \boldsymbol{W} \boldsymbol{X})^{-1} \boldsymbol{x}\, \hat{\sigma}_W^2 \,. \tag{B.4.6}$$

In Eq. (B.4.2), the variance-covariance matrix $\boldsymbol{\Sigma_x}$ associated with a glass composition $\boldsymbol{x}$ must be estimated from replicate experimental data rather than via a formula as in the case of model uncertainty. Because the number of glass components appearing in ILAW property-composition models is expected to be at least 8 to 12, an extremely large number of replicate compositions would be needed to adequately estimate $\boldsymbol{\Sigma_x}$. Further, variance-covariance matrices can have several sources of uncertainty (e.g., sampling, chemical analysis) associated with an estimate of glass composition associated with an ILAW MFPV batch. Batch-to-batch variation in ILAW composition can also be written as a variance-covariance matrix. Hence, because ILAW composition is multivariate, coupled with the presence of batch-to-batch variation and within-batch uncertainty (with several contributing sources of uncertainty), it is essentially impossible to collect sufficient replicate data to estimate composition variance-covariance matrices. However, there are practical alternatives that allow for quantifying the second term in Eq. (B.4.2).

As described in Section 3.4.2, Monte Carlo simulation can be used to simulate multiple sources of uncertainty and the total uncertainty in ILAW composition corresponding to a single MFPV batch. Then, every simulated ILAW composition for a given MFPV batch can be plugged into a property-composition model, resulting in a set of predicted property values for the simulated compositions. These property values are now univariate rather than multivariate, and standard formulas for SDs (or variances) can be used to quantify composition uncertainty in property units. Similarly, during WTP ILAW facility operations, estimated compositions for multiple MFPV batches can be substituted into a property-composition model, yielding multiple property values. Again, the usual standard deviation (or variance) formulas can be used to calculate batch-to-batch variation of ILAW composition in property units.

B.5 Compliance Equations for ILAW Contract Specification 2.2.2.20: Dangerous Waste Limitations

The WTP Project's compliance strategy and relevant equations for ILAW compliance quantities are discussed in the *Data Quality Objectives Process in Support of LDR/Delisting at the RPP-WTP* (Cook and Blumenkranz 2003).

B.6 Compliance Equations for ILAW Contract Specification 2.2.2.2: Waste Loading

ILAW Contract Specification 2.2.2.2 is listed verbatim to provide the context for the ILAW waste-loading compliance equations presented in this section.

Contract Specification 2.2.2.2: Waste Loading

> *The loading of waste sodium from Envelope A in the ILAW glass shall be greater than 14 weight percent based on Na_2O. The loading of waste sodium from Envelope B in the ILAW glass shall be greater than 3.0 weight percent based on Na_2O. The loading of waste sodium from Envelope C in the ILAW glass shall be greater than 10 weight percent based on Na_2O.*

The scope to develop compliance equations and the statistical methodology for demonstrating compliance with ILAW Contract Specification 2.2.2.2 on waste loading was originally included in the work covered by this report. However, this scope was deleted by the WTP Project before the report was completed. The scope reduction was based on a decision that waste-loading requirements would be easily met during ILAW production and hence that a statistical approach for demonstrating compliance was not needed. However, because compliance equations for waste loading were already completed before deleting the scope to develop statistical methods for demonstrating compliance, the equations are included here for documentation purposes. However, the equations are included in the form in which they were developed before the work scope was cut, and they do not reflect all of the revisions to previous sections. In particular, revisions to account for averaging over multiple samples, analyses per sample, and volume determinations per MFPV batch have not been made to the equations in this section.

This section documents the equations for calculating the waste loading of ILAW based on the results of process samples, analyses per sample, and measurements to be taken during production operations of the Waste Treatment Plant (WTP) ILAW facility. The section closely follows the format and uses the same notation as Section B.1[(a)]. The sampling locations and other measurements to be taken are based on the WTP compliance strategy discussed in the ILAW PCP (Nelson et al. 2003) for complying with ILAW specifications in the WTP Contract (DOE-RPP 2003). The equations are based on work by (1) John Vienna representing the Waste Form Qualification (WFQ) area of the Research and Technology (R&T) organization within the WTP Project and (2) Greg Piepel, Dennis Weier, and Scott Cooley of Battelle–Pacific Northwest Division (PNWD).

The ILAW compliance strategy for ILAW waste loading described in the ILAW PCP involves: (1) establishing the proportion of Na_2O in Concentrate Receipt Vessel (CRV) batches that comes from waste, (2) sampling and analyzing waste in the CRV, (3) transferring a portion of the CRV contents to the Melter Feed Preparation Vessel (MFPV), (4) calculating required amounts and then weighing those amounts of GFCs to add to the MFPV to yield the desired ILAW glass composition, and (5) transferring the GFCs to the MFPV and mixing the contents. Additional details are described in the ILAW PCP

(a) There is considerable duplication of formulas in this section that are in Section B.1, which could have been avoided by re-writing this section to refer to the earlier formulas. However, because the PNWD waste loading scope was cut, it was only possible to insert here the material as it existed before the scope was cut.

(Nelson et al. 2003). For compliance purposes, the chemical composition of ILAW based on MFPV contents and the subsequent waste loading of Na_2O is calculated based on chemical analyses of CRV samples and weights of individual GFCs. The composition and volume of the MFPV heel from the previous MFPV batch are also involved in the calculation of ILAW chemical composition and waste loading for the current MFPV batch.

Based on a decision by staff from the WTP Project R&T WFQ organization, the ILAW waste-loading equation does not at this time account for possible volatility of components in the melter. If needed based on further consideration by the WTP Project, melter volatility aspects could be accounted for in future updates of the ILAW waste-loading equation and related statistical compliance activities.

The ILAW waste-loading equation also does not account for possible biases in sampling, chemical analysis, and measurements that yield inputs for the equations. It is assumed that any significant long-term systematic biases in sampling, chemical analysis, or measurement processes will be detected and corrected before operation of the WTP ILAW facility. If intermittent biases were to occur during WTP ILAW production, it is assumed the WTP will have methods for detecting and correcting such biases or rejecting the biased results. For example, Weier and Piepel (2003) present accept/reject, bias detection/correction, and weighted normalization methods for analyzed slurry and glass compositions. These methods could be included in the ILAW waste-loading compliance equations in the future if desired by the WTP Project.

In summary, the ILAW waste-loading equations presented in this section are intended for use during WTP ILAW production operations to determine if ILAW waste-loading requirements are met in vitrifying the contents of a given MFPV batch. The contents of an MFPV batch are formed by adding a portion of a CRV batch and weighed amounts of GFCs to the MFPV heel from the previous batch. The current equations do not (1) account for any biases in sampling, chemical analyses, or measurements yielding inputs for the equations, (2) account for volatility in the melter, and (3) implement the adjustment methods for analyzed compositions discussed by Weier and Piepel (2003).

B.6.1 Development of Compliance Equations for ILAW Waste Loading

Consider the following quantities:

g_{ij}^{MFPV} = mass fraction of the j^{th} glass oxide component in the i^{th} MFPV batch (g_{oxide}/g_{oxides})

m_{ij}^{MFPV} = mass of the j^{th} glass oxide component in the i^{th} MFPV batch (g)

I = total number of MFPV batches per reporting or compliance period

J = total number of glass oxide components

M_i^{MFPV} = $\sum_{j=1}^{J} m_{ij}^{MFPV}$ = total mass of glass oxide components $j = 1, 2, \ldots, J$ in the i^{th} MFPV batch (g)

$m_{ij}^{CRV\ to\ MFPV}$ = mass of the j^{th} glass oxide component in the portion of a CRV batch transferred to the i^{th} MFPV batch (g)

m_{ij}^{GFCs} = mass of the j^{th} glass oxide component in GFCs for the i^{th} MFPV batch (g)

$m_{ij}^{MFPV\ Heel}$ = mass of the j^{th} glass oxide component in the MFPV Heel included in the i^{th} MFPV batch (g)

$M_i^{CRV\ to\ MFPV}$ = $\sum_{j=1}^{J} m_{ij}^{CRV\ to\ MFPV}$ = total mass of all glass oxide components in the portion of the CRV batch transferred to the i^{th} MFPV batch (g)

M_i^{GFCs} = $\sum_{j=1}^{J} m_{ij}^{GFCs}$ = total mass of all glass oxide components in GFCs for the i^{th} MFPV batch (g)

$M_i^{MFPV\ Heel}$ = $\sum_{j=1}^{J} m_{ij}^{MFPV\ Heel}$ = total mass of all glass oxide components in the MFPV Heel included in the i^{th} MFPV batch (g)

$p_{ij}^{CRV\ to\ MFPV}$ = proportion that is from waste of the mass of the j^{th} glass oxide component in a CRV transfer to the i^{th} MFPV batch

p_{ij}^{MFPV} = proportion that is from waste of the mass of the j^{th} glass oxide component in the i^{th} MFPV batch

WL_{ij}^{MFPV} = waste loading of the j^{th} glass oxide component in the i^{th} MFPV batch.

For ILAW loading requirements, interest is specifically in the j^{th} glass oxide in the above expressions being Na_2O. Note also that the composition of the i^{th} MFPV Heel is taken to be the same as the composition of the $(i\text{-}1)^{st}$ MFPV batch.

B.6.2 Compliance Equations for ILAW Waste Loading in a Single MFPV Batch

As stated earlier, the ILAW waste-loading requirement for a single MFPV batch is that

$$L_{Na_2O} \le 100\, WL_{i,Na_2O}^{MFPV} \tag{B.6.1}$$

where L_{Na_2O} is 14, 5, or 10 wt%, depending on the LAW envelope.

Consider the i^{th} MFPV batch that includes the i^{th} transfer from the CRV to the MFPV, the MFPV heel included as part of the i^{th} MFPV batch (which has the composition of the $(i\text{-}1)^{st}$ MFPV batch), and the i^{th} addition of GFCs. Then the proportion from waste of Na_2O in the MFPV batch (or equivalently, in glass made from the MFPV batch) is

$$p_{i,Na_2O}^{MFPV} = \frac{m_{i,Na_2O}^{CRV\ to\ MFPV}\ p_{i,Na_2O}^{CRV\ to\ MFPV} + m_{i,Na_2O}^{MFPV\ Heel}\ p_{i-1,Na_2O}^{MFPV}}{m_{i,Na_2O}^{CRV\ to\ MFPV} + m_{i,Na_2O}^{GFCs} + m_{i,Na_2O}^{MFPV\ Heel}} \tag{B.6.2}$$

Note that $p_{0,Na_2O}^{MFPV} = 0.0$ and that $p_{i,Na_2O}^{CRV\ to\ MFPV}$ (with associated uncertainty) is provided for each CRV batch as information from pretreatment activities. The proportion of Na_2O from waste in the MFPV batch is thus dependent on the proportion of Na_2O from waste in the CRV transfer and in the proportion of Na_2O from waste in the previous MFPV batch, which generated the currently included MFPV Heel. Note that one strategy is to take $p_{i,Na_2O}^{CRV\ to\ MFPV}$ to be constant as long as the waste is from the same LAW batch transfer or LAW type. Then the associated uncertainty of this constant quantity within a particular CRV batch would likely be larger to reflect the actual variability in the addition of Na_2O in the pretreatment of the current CRV batch material. If, instead, separate $p_{i,Na_2O}^{CRV\ to\ MFPV}$ estimates are provided for each CRV batch, then their uncertainties would likely be reduced by not including this pretreatment Na_2O addition variability source. In the assumed constant case, the first time the CRV is filled from a new waste envelope, a CRV heel remains from the previous waste envelope with a potentially different value for $p_{i,Na_2O}^{CRV\ to\ MFPV}$. This special case is expected to have minimal impact and is not included in the waste-loading equation.

Given Eq. (B.6.2), ILAW waste loading for a single MFPV batch is calculated as

$$WL_{i,Na_2O}^{MFPV} = \frac{m_{i,Na_2O}^{CRV\ to\ MFPV}\ p_{i,Na_2O}^{CRV\ to\ MFPV} + m_{i,Na_2O}^{MFPV\ Heel}\ p_{i-1,Na_2O}^{MFPV}}{M_i^{CRV\ to\ MFPV} + M_i^{GFCs} + M_i^{MFPV\ Heel}} \tag{B.6.3}$$

The masses of glass oxide components in the (1) portion of the CRV transferred to the MFPV, (2) GFCs, and (3) MFPV Heel are respectively given by the following equations for the ILAW compliance strategy

$$m_{ij}^{CRV\ to\ MFPV} = c_{ij}^{CRV}\ f_j V_i^{CRV to MFPV}\ u \tag{B.6.4}$$

$$m_{ij}^{GFCs} = \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} \tag{B.6.5}$$

$$m_{ij}^{MFPV\ Heel} = m_{i-1,j}^{MFPV} \left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}} \right) \tag{B.6.6}$$

where

c_{ij}^{CRV} = concentration of the j^{th} element in the CRV batch, a portion of which is transferred to the i^{th} MFPV batch (μg/mL). See the discussion regarding this notation after the following terminology definitions.

f_j = $\frac{MW_j^{oxide}}{MW_j^{analyte}} R_j$ where MW_j^{oxide} and $MW_j^{analyte}$ are the molecular weights of oxide j and analyte j, respectively, and R_j is the ratio of moles of oxide j per mole of analyte j. Hence, f_j is the factor for converting the concentration of analyte j (μg analyte j/mL) to the concentration of oxide j (μg oxide j/mL). The quantity f_i is called the oxide factor for oxide j.

$V_i^{CRV\ to\ MFPV}$ = volume transfer from the CRV to the i^{th} MFPV batch (L)

u = $\frac{1000\ (\text{mL} / \text{L})}{1000000\ (\mu\text{g} / \text{g})}$, a units conversion factor for converting mL to L and μg to g

K = number of GFCs

a_{ik}^{GFC} = mass of the k^{th} GFC added to the i^{th} MFPV batch (g)

G_{ijk}^{GFC} = mass of the j^{th} glass oxide component per mass of the k^{th} GFC for the i^{th} MFPV batch ($g_{oxide\ j}/g_{GFC\ k}$). The mass fractions G_{ijk}^{GFC} $j = 1, 2, \ldots, J$ for the k^{th} GFC can sum to less than 1.0 to the extent the GFC contains interstitial water or other components that will not survive in the glass. The nominal G_{ijk}^{GFC} mass fractions of glass oxide components in the GFCs should not change frequently over MFPV batches. However, the i subscript was retained in case these mass fractions change (1) from one vendor to another for the same GFC or (2) for different lots of a given GFC from the same vendor.

$m_{i-1,j}^{MFPV}$ = mass of the j^{th} glass oxide component in the $(i-1)^{st}$ MFPV batch (g)

$V_i^{MFPV\ Heel}$ = volume of the MFPV Heel included in the i^{th} MFPV batch (L)

V_{i-1}^{MFPV} = volume of the $(i-1)^{st}$ MFPV batch (L). This is the total volume of the $(i-1)^{st}$ MFPV batch, including the MFPV Heel, waste transferred from the CRV, GFCs added, and any water that may be added. Water will typically be added to Envelope B LAW in the MFPV to lower the sodium molarity. It is not anticipated that LAW from Envelopes A and C will require addition of water in the MFPV.

Note that Eq. (B.6.4) uses c_{ij}^{CRV} (the concentration of the j^{th} element in the CRV batch, a portion of which is transferred to the i^{th} MFPV batch) to calculate the mass of the j^{th} glass oxide component in the portion of the CRV batch transferred to the i^{th} MFPV batch. This wording is somewhat awkward, but is necessary because in the ILAW facility, one CRV batch will provide input to four MFPV batches (or more for Envelope B LAW when water must be added to the MFPV). The ILAW compliance strategy does not have a hold point at the CRV to wait for the chemical-analysis results for samples of a given CRV batch. In cases where the chemical-analysis results for a new CRV batch are ready in time to determine the appropriate additions of GFCs for the first MFPV batch from the new CRV batch, then the concentrations c_{ij}^{CRV} can be used. Otherwise, the concentrations $c_{ij}^{CRV\ Previous}$ from the previous CRV batch will be used. It is expected that the chemical-analysis results for a given CRV batch (c_{ij}^{CRV}, j = 1, 2, … , J) will be available in time for the second, third, and fourth transfers from that CRV batch to the MFPV. If not, then $c_{ij}^{CRV\ Previous}$ would be used for as many remaining transfers from the current CRV batch as necessary until the current results c_{ij}^{CRV} become available. To simplify the notation, c_{ij}^{CRV} is used in Eq. (B.6.4) and subsequent equations, with the understanding it represents concentrations from the current CRV batch if available, and the previous CRV batch if not. Also note that Eq. (B.6.6) assumes uniform mixing of the ILAW MFPV.

Using elemental concentrations from the previous CRV batch as an estimate of the elemental concentrations in the current CRV batch is the simplest one-step-ahead forecast that can be made. If there is sufficient variation across CRV batches, a better one-step-ahead forecasting approach based on time series models could be used. Because it is not clear whether such an approach would be worthwhile (i.e., sufficiently reducing the bias in the estimated concentrations), the time series approach is not included in the ILAW chemical-composition equations presented in this document.

Volume transfers will not be measured directly in the WTP, but calculated by differences in "before" and "after" volumes of a given vessel. Because volume transfers can be calculated for both the sending and receiving vessels, a more precise (less uncertain) estimate is obtained by using a weighted average of the volume transfer estimates from the sending and receiving vessels. In Eq. (B.6.4), the CRV is the sending vessel and the MFPV is the receiving vessel. Because the Melter Feed Vessel (MFV) will continually feed the melter, a weighted average of the volume transfer estimates from the MFPV (sending vessel) and MFV (receiving vessel) cannot be used in Eq. (B.6.6) for calculating the MFPV to MFV volume transfer.

A volume transfer from vessel A to vessel B for the i^{th} batch is calculated as

$$\begin{aligned} V_i^{A\ to\ B} &= w_A V_i^{A\ transfer} + w_B V_i^{B\ transfer} \\ &= w_A \left(V_i^{A\ before} - V_i^{A\ after} \right) + w_B \left(V_i^{B\ after} - V_i^{B\ before} \right) \end{aligned} \tag{B.6.7}$$

where w_A and w_B are weights that reflect the relative magnitudes of the uncertainties associated with $\left(V_i^{A\ before} - V_i^{A\ after} \right)$ and $\left(V_i^{B\ after} - V_i^{B\ before} \right)$, respectively. It is reasonable to assume that

$\left(V_i^{A\,before} - V_i^{A\,after}\right)$ and $\left(V_i^{B\,after} - V_i^{B\,before}\right)$ are statistically independent. If the additional assumptions are made that $V_i^{A\,before}$ and $V_i^{A\,after}$ are statistically independent, and that $V_i^{B\,after}$ and $V_i^{B\,before}$ are statistically independent, then the weights w_A and w_B can be written as:

$$w_A = \frac{\hat{\sigma}^2_{V_i^{B\,after}} + \hat{\sigma}^2_{V_i^{B\,before}}}{\hat{\sigma}^2_{V_i^{A\,before}} + \hat{\sigma}^2_{V_i^{A\,after}} + \hat{\sigma}^2_{V_i^{B\,after}} + \hat{\sigma}^2_{V_i^{B\,before}}} \tag{B.6.8}$$

and

$$w_B = \frac{\hat{\sigma}^2_{V_i^{A\,before}} + \hat{\sigma}^2_{V_i^{A\,after}}}{\hat{\sigma}^2_{V_i^{A\,before}} + \hat{\sigma}^2_{V_i^{A\,after}} + \hat{\sigma}^2_{V_i^{B\,after}} + \hat{\sigma}^2_{V_i^{B\,before}}} \tag{B.6.9}$$

where $\hat{\sigma}^2_{V_i^{A\,before}}$ denotes a previously determined estimate of the variance (squared standard deviation) of a volume measurement in Vessel A before a transfer. The other similar notations in Eqs. (B.6.8) and (B.6.9) denote previous estimates of the variance of a volume measurement in Vessel A after a transfer, and Vessel B before and after a transfer. Thus,

$$V_i^{CRV\,to\,MFPV} = \frac{\hat{\sigma}^2_{V_i^{MFPV\,after}} + \hat{\sigma}^2_{V_i^{MFPV\,before}}}{\hat{\sigma}^2_{V_i^{CRV\,before}} + \hat{\sigma}^2_{V_i^{CRV\,after}} + \hat{\sigma}^2_{V_i^{MFPV\,after}} + \hat{\sigma}^2_{V_i^{MFPV\,before}}} \left(V_i^{CRV\,before} - V_i^{CRV\,after}\right)$$

$$+ \frac{\hat{\sigma}^2_{V_i^{CRV\,before}} + \hat{\sigma}^2_{V_i^{CRV\,after}}}{\hat{\sigma}^2_{V_i^{CRV\,before}} + \hat{\sigma}^2_{V_i^{CRV\,after}} + \hat{\sigma}^2_{V_i^{MFPV\,after}} + \hat{\sigma}^2_{V_i^{MFPV\,before}}} \left(V_i^{MFPV\,after} - V_i^{MFPV\,before}\right) \tag{B.6.10}$$

where

$V_i^{CRV\,before}$ = volume of the CRV before the transfer of material to the i^{th} MFPV batch (L)

$V_i^{CRV\,after}$ = volume of the CRV after the transfer of material to the i^{th} MFPV batch (L)

$V_i^{MFPV\,before}$ = volume of the MFPV before receipt of CRV material for the i^{th} MFPV batch
= $V_i^{MFPV\,Heel}$ = volume of the MFPV Heel included in the i^{th} MFPV batch (L)

$V_i^{MFPV\,after}$ = volume of the MFPV after receipt of CRV material for the i^{th} MFPV batch but before receipt of GFCs or any added water (L).

It is important to note that $V_i^{MFPV\ after} \neq V_i^{MFPV}$ because V_i^{MFPV} is determined after the CRV material, GFCs, and any water are added to the MFPV. On the other hand, $V_i^{MFPV\ after}$ is determined after the CRV material is added but before the GFCs and any water are added to the MFPV. Thus, the equations in this document assume that both of these MFPV volumes will be determined during operation of the ILAW facility.

Note that vessel volumes will not be directly measured in the WTP ILAW facility. Rather, the level of contents in a vessel will be measured and then the corresponding volume calculated using a level-to-volume calibration equation. Because these calibration equations for the WTP ILAW CRV and MFPV will not be developed for some time, they cannot be included in the current equations for calculating ILAW chemical composition. The level-to-volume calibration equations for the ILAW CRV and MFPV will be included in a future update of the compliance equations and work for ILAW chemical composition.

The assumption of statistical independence between volume measurements (actually level measurements) in the CRV and MFPV is quite reasonable because there is no reason to expect the random errors in measuring volume (level) in one vessel will influence the random errors in measuring volume (level) in another vessel. The assumption of statistical independence between before and after volume (level) measurements in one vessel may not be quite as reasonable because ultimately, the same level-to-volume calibration equation will be used to calculate before and after vessel volumes from before and after vessel levels. However, there is no reason to expect that random errors in measuring the "before level" in a vessel will influence the random errors in measuring the "after level" in a vessel. This second assumption of statistical independence of before and after volume (level) measurements within a given vessel will be revisited in the future when the work to develop level-to-volume calibration equations for the WTP ILAW CRV and MFPV is conducted.

Combining Eqs. (B.6.4), (B.6.5), and (B.6.6) with Eq. (B.6.2) yields

$$p_{i,Na_2O}^{MFPV} = \frac{c_{i,Na_2O}^{CRV} f_{Na_2O} V_i^{CRV\,to\,MFPV} u\, p_{i,Na_2O}^{CRV\ to\ MFPV} + m_{i-1,Na_2O}^{MFPV} \left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}} \right) p_{i-1,Na_2O}^{MFPV}}{\left(c_{i,Na_2O}^{CRV} f_{Na_2O} V_i^{CRV\,to\,MFPV} u \right) + \sum_{k=1}^{K} a_{ik}^{GFC} G_{i,Na_2Ok}^{GFC} + m_{i-1,Na_2O}^{MFPV} \left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}} \right)} \tag{B.6.11}$$

where p_{i,Na_2O}^{MFPV} is the proportion of Na_2O from waste in the i^{th} MFPV batch (or equivalently, in glass made from the i^{th} MFPV batch). Combining Eqs. (B.6.4), (B.6.5), and (B.6.6) with Eq. (B.6.3) yields

$$WL_{i,Na_2O}^{MFPV} = \frac{c_{i,Na_2O}^{CRV} f_{Na_2O} V_i^{CRV\,to\,MFPV} u\, p_{i,Na_2O}^{CRV\ to\ MFPV} + m_{i-1,Na_2O}^{MFPV} \left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}} \right) p_{i-1,Na_2O}^{MFPV}}{\sum_{j=1}^{J} \left(c_{ij}^{CRV} f_j V_i^{CRV\,to\,MFPV} u \right) + \sum_{j=1}^{J} \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \sum_{j=1}^{J} m_{i-1,j}^{MFPV} \left(\frac{V_i^{MFPV\ Heel}}{V_{i-1}^{MFPV}} \right)} \tag{B.6.12}$$

where WL_{i,Na_2O}^{MFPV} is the waste loading of Na_2O in the i^{th} MFPV batch (or equivalently, in glass made from the i^{th} MFPV batch).

Note that $m_{i-1,j}^{MFPV}$ is given by

$$m_{i-1,j}^{MFPV} = c_{i-1,j}^{CRV} f_j V_{i-1}^{CRV\,to\,MFPV} u + \sum_{k=1}^{K} a_{i-1,k}^{GFC} G_{i-1,jk}^{GFC} + m_{i-2,j}^{MFPV} \left(\frac{V_{i-1}^{MFPV\ heel}}{V_{i-2}^{MFPV}} \right) \qquad \text{(B.6.13)}$$

The expression for $V_i^{CRV\,to\,MFPV}$ in Eq. (B.6.10), and the expression for $m_{i-1,j}^{MFPV}$ in Eq. (B.6.13) could be substituted into Eq. (B.6.11). Equation (B.6.11) could similarly be substituted into Eq. (B.6.12) to yield a combined final equation for ILAW waste loading, but that yields a very long equation. Hence, the final compliance equation for ILAW waste loading is given by Eq. (B.6.12), where p_{i,Na_2O}^{MFPV} is given by Eq. (B.6.11), $V_i^{CRV\,to\,MFPV}$ is given by Eq. (B.6.10), and $m_{i-1,j}^{MFPV}$ is given by Eq. (B.6.13). Note that each of these equations assumes uniform mixing of the ILAW MFPV.

B.6.3 Compliance Equations for ILAW Waste Loading with Averages over Multiple Samples, Analyses, and Volume Determinations for a Single Batch

All of the variables in Eqs. (B.6.12), (B.6.11), (B.6.10), and (B.6.13), except the "units conversion factor" u and the "analyte-to-oxide conversion factor" f_i, are subject to various random uncertainties (e.g., from: random inhomogeneity of CRV contents, the proportion of CRV Na_2O from waste, sampling from the CRV, chemical analyses of CRV samples, weighing of GFCs, variation in the GFC mass fraction oxide compositions, and measuring CRV and MFPV volumes/levels). When level-to-volume calibration equations are developed for the ILAW CRV and MFPV, there will be uncertainties in the calibration equations (e.g., estimated coefficients). When the calibration equations are applied, there will be uncertainties in measuring vessel levels. Hence, calculated volumes will be uncertain because of level measurement uncertainties and uncertainties in the calibration equations.

The random uncertainties described in the preceding paragraph can be effectively reduced by (1) taking more than one CRV sample, (2) analyzing each CRV sample more than once, (3) using more determinations to quantify GFC compositions, (4) weighing GFCs more than once, and (5) measuring CRV and MFPV volumes/levels more than once. The uncertainties would be reduced by using averages over multiple determinations in Eq. (B.6.12), as well as Eqs. (B.6.11), (B.6.10), and (B.6.13), because averages over two or more determinations have smaller uncertainties than single determinations. The resulting re-expressions of these equations to include averages over multiple samples, analyses per sample, and volume determinations are now presented.

The re-expressions of Eqs. (B.6.12), (B.6.11), (B.6.10), and (B.6.13) to include average determinations are given, respectively, by Eqs. (B.6.14), (B.6.15), (B.6.16), and (B.6.17) following:

$$\overline{WL}_{i,Na_2O}^{MFPV} = \frac{\frac{1}{n_S^{CRV} n_A^{CRV}} \left(\sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{i,Na_2O,l,m}^{CRV} \right) f_{Na_2O} \overline{V}_i^{CRV to MFPV} \; u \; p_{i,Na_2O}^{CRV\ to\ MFPV} + \overline{m}_{i-1,Na_2O}^{MFPV} \left(\frac{\sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\ Heel}}{n_V^{MFPV}} - \frac{\sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV}}{n_V^{MFPV}} \right) \overline{p}_{i-1,Na_2O}^{MFPV}}{\frac{1}{n_S^{CRV} n_A^{CRV}} \sum_{j=1}^{J} \left[\left(\sum_{l=1}^{n_S} \sum_{m=1}^{n_A} c_{ijlm}^{CRV} \right) f_j \overline{V}_i^{CRV to MFPV} \; u \right] + \sum_{j=1}^{J} \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC} + \sum_{j=1}^{J} \overline{m}_{i-1,j}^{MFPV} \left(\frac{\sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\ Heel}}{n_V^{MFPV}} - \frac{\sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV}}{n_V^{MFPV}} \right)} \tag{B.6.14}$$

$$\overline{p}_{i,Na_2O}^{MFPV} = \frac{\frac{1}{n_S^{CRV} n_A^{CRV}} \left(\sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{i,Na_2O,l,m}^{CRV} \right) f_{Na_2O} \overline{V}_i^{CRV to MFPV} \; u \; p_{i,Na_2O}^{CRV\ to\ MFPV} + \overline{m}_{i-1,Na_2O}^{MFPV} \left(\frac{\sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPVHeel}}{n_V^{MFPV}} - \frac{\sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV}}{n_V^{MFPV}} \right) p_{i-1,Na_2O}^{MFPV}}{\frac{1}{n_S^{CRV} n_A^{CRV}} \left(\sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{i,Na_2O,l,m}^{CRV} \right) f_{Na_2O} \overline{V}_i^{CRV to MFPV} u + \sum_{k=1}^{K} a_{ik}^{GFC} G_{i,Na_2O,k}^{GFC} + \overline{m}_{i-1,Na_2O}^{MFPV} \left(\frac{\sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\ Heel}}{n_V^{MFPV}} - \frac{\sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV}}{n_V^{MFPV}} \right)} \tag{B.6.15}$$

$$\overline{V}_i^{CRV to MFPV} = \frac{\hat{\sigma}^2_{\overline{V}_i^{MFPV\ after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\ before}}}{\hat{\sigma}^2_{\overline{V}_i^{CRV\ before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\ after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\ after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\ before}}} \left(\frac{\sum_{h=1}^{n_V^{CRV}} V_{ih}^{CRV\ before}}{n_V^{CRV}} - \frac{\sum_{h=1}^{n_V^{CRV}} V_{ih}^{CRV\ after}}{n_V^{CRV}} \right)$$

$$+ \frac{\hat{\sigma}^2_{\overline{V}_i^{CRV\ before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\ after}}}{\hat{\sigma}^2_{\overline{V}_i^{CRV\ before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\ after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\ after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\ before}}} \left(\frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV\ after}}{n_V^{MFPV}} - \frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV\ before}}{n_V^{MFPV}} \right) \tag{B.6.16}$$

$$\overline{m}_{i-1,j}^{MFPV} = \frac{1}{n_S^{CRV} n_A^{CRV}} \left(\sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{i-1,jlm}^{CRV} \right) f_j \, \overline{V}_{i-1}^{CRV\,to\,MFPV} u + \sum_{k=1}^{K} a_{i-1,k}^{GFC} G_{i-1,jk}^{GFC} + \overline{m}_{i-2,j}^{MFPV} \left(\frac{\dfrac{\sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV\,Heel}}{n_V^{MFPV}}}{\dfrac{\sum_{h=1}^{n_V^{MFPV}} V_{i-2,h}^{MFPV}}{n_V^{MFPV}}} \right) \quad \text{(B.6.17)}$$

where the bars in certain notations (e.g., $\overline{V}_{i-1}^{CRV\,to\,MFPV}$) denote averages. The $\hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}}$ notation in Eq. (B.6.16) represents the estimated variance of $\overline{V}_i^{MFPV\,after} = \frac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\,After}$. The other variance notations in Eq. (B.6.16) have similar interpretations. Note that Eqs. (B.6.14) to (B.6.17) assume uniform mixing of the ILAW MFPV.

In Eqs. (B.6.14) to (B.6.17), the following notations for number of samples per CRV batch, number of analyses per CRV sample, and numbers of CRV and MFPV volume measurements are used:

n_S^{CRV} = number of samples per CRV batch

n_A^{CRV} = number of chemical analyses per CRV sample

n_V^{CRV} = number of volume determinations of the CRV batch before a transfer of material to the MFPV ($V_{ih}^{CRV\,before}$) and after a transfer of material to the MFPV ($V_{ih}^{CRV\,after}$). The numbers of these two CRV volume determinations are assumed to be the same and given a single notation for simplicity in operation of the ILAW facility.

n_V^{MFPV} = number of volume determinations of the MFPV Heel ($V_{ih}^{MFPV\,before} = V_{ih}^{MFPV\,Heel}$), MFPV after transfer of CRV material ($V_{ih}^{MFPV\,after}$), and completed MFPV batch (V_{ih}^{MFPV}). The numbers of these three MFPV volume determinations are assumed to be the same and given a single notation for simplicity in operation of the ILAW facility.

When level-to-volume calibration equations are eventually developed for ILAW vessels and factored into the ILAW chemical-composition compliance equations, notations such as n_V^{CRV} and n_V^{MFPV} will be replaced with n_L^{CRV} and n_L^{MFPV} . The notation n_L^{CRV} will denote the number of level measurements of the CRV (before and after transfer of material to the MFPV). The notation n_L^{MFPV} will denote the number of level measurements of the MFPV (before a CRV transfer, after a CRV transfer, and after a complete MFPV batch is prepared).

In Eqs. (B.6.14) to (B.6.17), it is assumed that the amount of the k^{th} GFC (a_{ik}^{GFC}) to be added to the i^{th} MFPV batch can only be weighed once. This assumption is required because there is no way to relieve the load cell on an individual GFC hopper in the GFC facility and obtain additional weight measurements. Hence, averages over multiple weight determinations of the GFCs (a_{ik}^{GFC} , $k = 1, 2, \ldots, K$) were not included in Eqs. (B.6.14), (B.6.15), and (B.6.17). Further, it is assumed that the G_{ijk}^{GFC} quantities will be well-determined average compositions of GFCs based on historical information from GFC vendors or WTP qualification and acceptance testing. Hence averages of the G_{ijk}^{GFC} quantities were not included in Eqs. (B.6.14), (B.6.15), and (B.6.17).

In summary, the calculating equation for ILAW waste loading based on the WTP ILAW compliance strategy is given by Eq. (B.6.14) with substitution of Eqs. (B.6.15), (B.6.16) and (B.6.17). These equations will serve as the basis for assessing the importance of multiple samples, multiple analyses per sample, and multiple volume determinations in calculated ILAW waste loadings and their uncertainties.

B.6.4 Compliance Equations for ILAW Waste Loading over Multiple Batches

Equation (B.6.14), with substitution of Eqs. (B.6.15), (B.6.16), and (B.6.17), is appropriate for demonstrating that single MFPV batches comply with ILAW waste-loading requirements. However, the WTP compliance strategy also calls for demonstrating compliance with ILAW waste-loading requirements over an LAW waste type. However, the ILAW waste-loading compliance equations that follow do not directly depend on how an LAW waste type is defined. Ultimately, the period of production corresponding to a waste type or any other specified quantity of waste corresponds to some number of CRV and MFPV batches. Hence, the equations for demonstrating compliance over multiple batches depend only on the number of MFPV batches I over which ILAW waste-loading compliance is to be demonstrated.

To demonstrate compliance with ILAW waste-loading requirements over I MFPV batches, the dominant contributors are (1) transfers from the CRV to MFPV and (2) additions of GFCs. For all ILAW produced from a waste type, the inclusion of an MFPV Heel from a previous waste type and the exclusion of a final MFPV Heel from the current waste type would have a minimal impact on waste loading relative to the multiple MFPV batches expected from a single LAW waste type. Hence, cases of transitioning between two waste types are not covered in the compliance equations at this time.

Consider a waste type that includes a total of I CRV-to-MFPV transfers and the resulting I MFPV batches. When the initial CRV heel and the final MFPV heel are ignored as having insignificant impact, the waste loading over all I batches is

$$WL_{I,Na_2O}^{MFPV} = \frac{\sum_{i=1}^{I}\left(m_{i,Na_2O}^{CRV\,to\,MFPV}\; p_{i,Na_2O}^{CRV\,to\,MFPV}\right)}{\sum_{i=1}^{I}\left(M_i^{CRV\,to\,MFPV} + M_i^{GFCs}\right)} = \frac{\sum_{i=1}^{I}\left(c_{i,Na_2O}^{CRV} f_{Na_2O}\, V_i^{CRV\,to\,MFPV}\, u\; p_{i,Na_2O}^{CRV\,to\,MFPV}\right)}{\sum_{i=1}^{I}\sum_{j=1}^{J}\left(c_{ij}^{CRV} f_j\, V_i^{CRV\,to\,MFPV}\, u\right) + \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K} a_{ik}^{GFC}\, G_{ijk}^{GFC}} \qquad \text{(B.6.21)}$$

where all variables are as previously defined, and $V_i^{CRV\,to\,MFPV}$ is given by Eq. (B.6.10).

Suppose the estimate of $p_{i,Na_2O}^{CRV\,to\,MFPV}$ over a waste type is constant (that is, over the *I* CRV transfers resulting from a waste type), say with value $p_{I,Na_2O}^{CRV\,to\,MFPV}$.[(a)] Then Eq. (B.6.21) reduces to

$$WL_{I,Na_2O}^{MFPV} = \frac{\left(\sum_{i=1}^{I} m_{i,Na_2O}^{CRV\,to\,MFPV}\right) p_{I,Na_2O}^{CRV\,to\,MFPV}}{\sum_{i=1}^{I}\left(M_i^{CRV\,to\,MFPV} + M_i^{GFCs}\right)} = \frac{\left(\sum_{i=1}^{I} c_{i,Na_2O}^{CRV} f_{Na_2O} V_i^{CRV\,to\,MFPV} u\right) p_{I,Na_2O}^{CRV\,to\,MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J}\left(c_{ij}^{CRV} f_j V_i^{CRV\,to\,MFPV} u\right) + \sum_{i=1}^{I}\sum_{j=1}^{J}\sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC}} \quad \text{(B.6.22)}$$

where again all variables are as previously defined, and $V_i^{CRV\,to\,MFPV}$ is given by Eq. (B.6.10).

B.6.5 Compliance Equations for ILAW Waste Loading over Multiple Batches with Averages over Multiple Samples, Analyses, and Volume Determinations for Each Batch

All of the variables in Eqs. (B.6.21) or (B.6.22), except the "units conversion factor" *u* and the "analyte-to-oxide conversion factor" f_i, are subject to various random uncertainties (e.g., from: random inhomogeneity of CRV contents, the proportion of CRV Na_2O from waste, sampling from the CRV, chemical analyses of CRV samples, weighing of GFCs, variation in the GFC mass fraction oxide compositions, and measuring CRV and MFPV volumes/levels). When level-to-volume calibration equations are developed for the ILAW CRV and MFPV, there will be uncertainties in the calibration equations (e.g., estimated coefficients). When the calibration equations are applied, there will be uncertainties in measuring vessel levels. Hence, calculated volumes will be uncertain because of level measurement uncertainties and uncertainties in the calibration equations.

The random uncertainties described in the preceding paragraph can be effectively reduced by (1) taking more than one CRV sample, (2) analyzing each CRV sample more than once, (3) using more determinations to quantify GFC compositions, (4) weighing GFCs more than once, and (5) measuring CRV and MFPV volumes/levels more than once. The uncertainties would be reduced by using averages over multiple determinations in Eq. (B.6.21) or (B.6.22), as well as Eq. (B.6.10), because averages over two or more determinations have smaller uncertainties than single determinations.

The uncertainties discussed in the preceding paragraphs are within-batch uncertainties. To demonstrate compliance with the ILAW waste-loading requirements over a waste type (i.e., a specified number of batches *I*), batch-to-batch variations must also be addressed. However, "total" waste loading over *I* batches is of interest [per Eq. (B.6.21) or (B.6.22)] and not the average waste loading over *I* batches. Hence, the number of batches *I* does not reduce batch-to-batch uncertainty via averaging.

The re-expressions of Eqs. (B.6.21), (B.6.22), and (B.6.10) to include averages over multiple samples, analyses per sample, and volume determinations for each of the *I* batches are given, respectively, by Eqs. (B.6.23), (B.6.24), and (B.6.25) following:

(a) This is not to say the estimate does not have uncertainty, just that the estimate does not change over the course of a waste type.

$$\overline{WL}_{I,Na_2O}^{MFPV} = \frac{\dfrac{1}{n_S^{CRV} n_A^{CRV}} \sum_{i=1}^{I} \left[\left(\sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{i,Na_2O,l,m}^{CRV} \right) f_{Na_2O} \overline{V}_i^{CRV\,to\,MFPV} u\, p_{i,Na_2O}^{CRV\,to\,MFPV} \right]}{\dfrac{1}{n_S^{CRV} n_A^{CRV}} \sum_{i=1}^{I} \sum_{j=1}^{J} \left[\left(\sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{ijlm}^{CRV} \right) f_j\, \overline{V}_i^{CRV\,to\,MFPV} u \right] + \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC}} \tag{B.6.23}$$

$$\overline{WL}_{I,Na_2O}^{MFPV} = \frac{\dfrac{1}{n_S^{CRV} n_A^{CRV}} \sum_{i=1}^{I} \left[\left(\sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{i,Na_2O,l,m}^{CRV} \right) f_{Na_2O} \overline{V}_i^{CRV\,to\,MFPV} u \right] p_{I,Na_2O}^{CRV\,to\,MFPV}}{\dfrac{1}{n_S^{CRV} n_A^{CRV}} \sum_{i=1}^{I} \sum_{j=1}^{J} \left[\left(\sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{ijlm}^{CRV} \right) f_j\, \overline{V}_i^{CRV\,to\,MFPV} u \right] + \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} a_{ik}^{GFC} G_{ijk}^{GFC}} \tag{B.6.24}$$

$$\overline{V}_i^{CRV\,to\,MFPV} = \frac{\hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,before}}}{\hat{\sigma}^2_{\overline{V}_i^{CRV\,before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,before}}} \left(\frac{\sum_{h=1}^{n_V^{CRV}} V_{ih}^{CRV\,before}}{n_V^{CRV}} - \frac{\sum_{h=1}^{n_V^{CRV}} V_{ih}^{CRV\,after}}{n_V^{CRV}} \right)$$

$$+ \frac{\hat{\sigma}^2_{\overline{V}_i^{CRV\,before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\,after}}}{\hat{\sigma}^2_{\overline{V}_i^{CRV\,before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,before}}} \left(\frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV\,after}}{n_V^{MFPV}} - \frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV\,before}}{n_V^{MFPV}} \right) \tag{B.6.25}$$

The variables in Eqs. (B.6.23), (B.6.24), and (B.6.25) are all as previously defined. Note that Eq. (B.6.25) is the same as Eq. (B.6.16) given previously. Also, note that the uncertainties of $p_{i,Na_2O}^{CRV\,to\,MFPV}$ in Eq. (B.6.23) and $p_{I,Na_2O}^{CRV\,to\,MFPV}$ in Eq. (B.6.24) are not reduced by averaging multiple determinations. It is assumed that only one determination of $p_{i,Na_2O}^{CRV\,to\,MFPV}$ will be available for each batch, and only one determination of $p_{I,Na_2O}^{CRV\,to\,MFPV}$ will be available for each waste type.

Using Eq. (B.6.23) or (B.6.24) as appropriate with substitution of Eq. (B.6.25), the ILAW waste-loading compliance requirement over multiple batches is

$$L_{Na_2O} \le 100\, WL_{I,Na_2O}^{MFPV} \tag{B.6.26}$$

where again L_{Na_2O} is 14, 5, or 10 wt% for LAW Envelopes A, B, and C, respectively.

Appendix C

Nominal Concentrations and Estimates of Uncertainties Associated with the IHLW Compliance Strategy for Three HLW Waste Tanks

Appendix C: Nominal Concentrations and Estimates of Uncertainties Associated with the IHLW Compliance Strategy for Three HLW Waste Tanks

This appendix summarizes the immobilized high-level waste (IHLW) process composition and uncertainty inputs provided by the Waste Treatment and Immobilization Plant (WTP) Project that are relevant to IHLW compliance (i.e., reporting chemical or radionuclide composition, and demonstrating that compliance quantities satisfy specified limits). Because the WTP compliance strategy for IHLW is focused on estimating glass composition corresponding to each MFPV batch, the composition and uncertainty estimates provided by the WTP Project are associated with the MFPV. The IHLW MFPV composition and uncertainty information was provided for three HLW tanks to represent different possible realistic situations. Actual waste composition data from HLW tanks AY-102, AZ-102, and C-104 were used by the WTP Project to generate the inputs summarized in this appendix.

The estimates of mixing/sampling uncertainty [$\%RSD_S(c_j^{MFPV})$], and analytical uncertainty [$\%RSD_A(c_j^{MFPV})$] of MFPV chemical-composition elemental concentration in each of the three HLW waste tanks are listed in Table C.1. The estimates of MFPV chemical-composition concentrations represent the completed state of an MFPV (i.e., after GFC addition) before transfer to an MFV. However, the WTP Project had to combine different sources of information to construct the inputs in Table C.1. They began with measured sludge concentrations and augmented them using target concentrations of the various GFCs. Hence, the estimates provided by the WTP Project in Table C.1 are not based on direct measurements of the MFPV after GFC addition because there was no representative testing to obtain such information.

Mixing/sampling denotes combined random uncertainty caused by (1) random inhomogeneity in mixing an MFPV and (2) random uncertainty in taking samples from the MFPV by the designated sampling method. Mixing and sampling uncertainties cannot be separately estimated during WTP IHLW production operations, so combined estimates of these uncertainties were used. The MFPV mixing/sampling uncertainty [$\%RSD_S(c_j^{MFPV})$] values for the low and high cases of each of the low (L) and high (H) uncertainty categories of nonradionuclide analytes are listed in Table C.1. Low and high cases represent the lower and upper expected values of the uncertainty for a given analyte, while each analyte is classified into a low or high category for $\%RSD_S(c_j^{MFPV})$.

Table C.2 lists the nominal concentrations of HLW radionuclides in the MFPV (after adding glass-forming chemicals [GFCs]) for each of three HLW tanks. Table C.2 lists the low and high case mixing/sampling[(a)] uncertainties [$\%RSD_S(c_j^{MFPV})$] for HLW radionuclides in the MFPV (after GFC addition) for each of the three HLW tanks. Table C.3 provides HLW radionuclide analytical uncertainties

(a) Mixing/sampling denotes combined random uncertainty caused by (1) random inhomogeneity in mixing an IHLW MFPV and (2) random uncertainty in taking samples from the IHLW MFPV by the designated sampling method. Mixing and sampling uncertainties cannot be separately estimated during WTP IHLW production operations, so combined estimates of these uncertainties were used.

[$\%RSD_A(c_j^{MFPV})$] dependent on the concentration of HLW radionuclides in the MFPV (after GFC addition). Table C.4 lists the $\%RSD_S(c_j^{MFPV})$ for HLW radionuclides in the MFPV (after GFC addition) for each of three HLW tanks. These uncertainties were determined from Table C.3 based on the nominal concentrations in Table C.2.

Data on the GFC compositions (mass fractions of oxides) and corresponding low and high case uncertainties are summarized in Tables D.7 and D.8 of Appendix D. The 12 GFCs listed in those tables are the ones that will be used by the WTP to produce both IHLW and ILAW. However, it is currently expected that only five of the GFCs (silica, zincite, borax, sodium carbonate, and lithium carbonate) will be used to produce IHLW.

Table C.5 lists the nominal volumes as well as the low and high case uncertainty estimates (standard deviations [SDs]) of the HLW MFPV contents (1) before waste transfer from the HBV, (2) after the waste transfer from the HBV, and (3) after transfer of GFCs to the MFPV. Table C.6 lists the nominal compositions (in mass fractions) for glass made from the IHLW MFPV for each of three HLW tanks.

It is important to note that Tables C.1 to C.4 use slightly modified notation in order to better fit within the tables. The MFPV concentration mixing/sampling %RSD, usually denoted as $\%RSD_S(c_j^{MFPV})$, is referred to as $\%RSD_S$. The MFPV concentration analytical relative standard deviation, usually denoted as $\%RSD_A(c_j^{MFPV})$, is referred to as $\%RSD_A$.

Finally, note that the MFPV nominal concentration data in Tables C.1 and C.2 were based on samples and analyses of actual waste tank samples. However, those analyses were not adjusted or normalized as described by Weier and Piepel (2003). Normalizing and adjusting compositions can be used to eliminate possible biases and reduce uncertainties in analyzed slurry and glass compositions. Applying the adjustment and normalization procedures discussed by Weier and Piepel (2003) to the WTP data provided by the WTP Project was beyond the scope of the present work. However, it remains an option to determine the extent to which the adjustments and normalization would affect the composition variations and uncertainties.

Table C.1. Nominal Chemical Composition Analyte Concentrations, Mixing/Sampling Uncertainties (%RSD$_S$), and Analytical Uncertainties (%RSD$_A$) in the IHLW MFPV (After GFC Addition) for Three HLW Tanks

Analyte	AY-102			AZ-102			C-104		
	MFPV Conc. (mg/L)	Mixing/ Sampling %RSD$_S$[(a)]	Analytical %RSD$_A$[(b)]	MFPV Conc. (mg/L)	Mixing/ Sampling %RSD$_S$[(a)]	Analytical %RSD$_A$[(b)]	MFPV Conc. (mg/L)	Mixing/ Sampling %RSD$_S$[(a)]	Analytical %RSD$_A$[(b)]
Ag	744.48	5 (15)	5 (10)	87.56	5 (15)	ND[(c)]	306.22	5 (15)	10 (20)
Al	11257.92	5 (15)	5 (10)	21009.76	5 (15)	5 (10)	6451.15	5 (15)	5 (10)
B	14516.64	5 (15)	5 (10)	6348.56	5 (15)	5 (10)	14107.44	5 (15)	5 (10)
Ba	290.88	5 (15)	10 (20)	171.55	5 (15)	15 (30)	85.06	5 (15)	15 (30)
Be	-[(d)]	-	-	5.55	1 (5)	ND	9.16	1 (5)	ND
Bi	-	-	-	-	-	-	11.40	5 (15)	ND
Ca	1548.00	5 (15)	10 (20)	1765.22	5 (15)	10 (20)	1658.53	5 (15)	10 (20)
Cd	47.52	5 (15)	ND	6257.73	5 (15)	5 (10)	268.21	5 (15)	ND
Ce	383.04	5 (15)	ND	245.03	5 (15)	ND	348.81	5 (15)	ND
Cl	-	-	-	274.48	1 (5)	10 (20)	7.38	1 (5)	ND
Co	-	-	-	24.21	5 (15)	ND	8.99	5 (15)	ND
Cr	656.64	5 (15)	10 (20)	328.48	5 (15)	10 (20)	480.51	5 (15)	10 (20)
Cs	2.88	1 (5)	ND	48.39	1 (5)	15 (30)	61.53	1 (5)	15 (30)
Cu	118.08	5 (15)	20 (40)	117.49	5 (15)	20 (40)	102.94	5 (15)	20 (40)
Dy	-	-	-	-	-	-	12.18	5 (15)	ND
Eu	-	-	-	-	-	-	5.49	5 (15)	ND
F	-	-	-	63.28	1 (5)	10 (20)	-	-	-
Fe	42037.92	5 (15)	5 (10)	43533.74	5 (15)	5 (10)	16628.44	5 (15)	5 (10)
K	37.44	1 (5)	ND	112.15	1 (5)	ND	250.64	1 (5)	15 (30)
La	279.36	5 (15)	15 (30)	1310.92	5 (15)	10 (20)	81.28	5 (15)	ND
Li	5237.28	1 (5)	10 (20)	11929.60	1 (5)	10 (20)	11721.60	1 (5)	5 (10)
Mg	411.84	5 (15)	ND	387.77	5 (15)	ND	196.88	5 (15)	ND
Mn	9370.08	5 (15)	5 (10)	3658.08	5 (15)	5 (10)	9927.65	5 (15)	5 (10)
Mo	92.16	5 (15)	15 (30)	-	-	-	7.55	5 (15)	ND
Na	40629.60	1 (5)	5 (10)	50564.26	1 (5)	5 (10)	32040.49	1 (5)	5 (10)
Nd	-	-	-	919.30	5 (15)	10 (20)	190.80	5 (15)	ND
Ni	1393.92	5 (15)	10 (20)	3084.07	5 (15)	5 (10)	933.82	5 (15)	10 (20)
P	1051.20	5 (15)	10 (20)	1038.16	5 (15)	10 (20)	725.13	5 (15)	10 (20)
Pb	2149.92	5 (15)	10 (20)	447.69	5 (15)	ND	716.97	5 (15)	15 (30)
Pd	-	-	-	-	-	-	48.24	5 (15)	25 (50)
Pr	-	-	-	-	-	-	19.98	5 (15)	25 (50)
Rh	-	-	-	-	-	-	131.86	5 (15)	25 (50)
Ru	-	-	-	-	-	-	62.72	5 (15)	ND
Sb	136.80	5 (15)	25 (50)	-	-	-	-	-	-
Se	-	-	-	-	-	-	12.66	5 (15)	ND
Si	95495.04	5 (15)	5 (10)	115275.34	5 (15)	5 (10)	112859.25	5 (15)	5 (10)
S	360.00	1 (5)	15 (30)	54.51	1 (5)	ND	7.72	1 (5)	ND
Sn	217.44	5 (15)	15 (30)	666.78	5 (15)	10 (20)	272.19	5 (15)	15 (30)
Sr	614.88	5 (15)	5 (10)	6458.22	5 (15)	5 (10)	14422.12	5 (15)	5 (10)

(a) MFPV mixing/sampling %RSD values are represented by %RSD$_S$ instead of $\%RSD_S(c_j^{MFPV})$ for space reasons. Low case value listed first, followed by the high case value in parentheses.

(b) MFPV analytical %RSD values are represented by %RSD$_A$ instead of $\%RSD_A(c_j^{MFPV})$ for space reasons. Low case value listed first, followed by the high case value in parentheses.

(c) %RSD$_A$ = 50 was used for non-detectable (ND) analytes for both low and high cases. Detection limits were used in place of concentration amounts for non-detects.

(d) A "-" means that no data were recorded for that analyte for that HLW tank, and hence mixing/sampling and analytical uncertainties were not estimated.

Table C.1. Nominal Chemical Composition Analyte Concentrations, Mixing/Sampling Uncertainties (%RSD$_S$), and Analytical Uncertainties (%RSD$_A$) in the IHLW MFPV (After GFC Addition) for Three HLW Tanks (cont.)

Analyte	AY-102			AZ-102			C-104		
	MFPV Conc. (mg/L)	Mixing/ Sampling %RSD$_S$[(a)]	Analytical %RSD$_A$[(b)]	MFPV Conc. (mg/L)	Mixing/ Sampling %RSD$_S$[(a)]	Analytical %RSD$_A$[(b)]	MFPV Conc. (mg/L)	Mixing/ Sampling %RSD$_S$[(a)]	Analytical %RSD$_A$[(b)]
Th	-	-	-	-	-	-	18124.08	5 (15)	5 (10)
Ti	83.52	5 (15)	ND	43.33	5 (15)	ND	64.23	5 (15)	ND
U	1893.60	5 (15)	20 (40)	7333.91	5 (15)	10 (20)	16113.77	5 (15)	5 (10)
V	38.88	5 (15)	50 (50)	-	-	-	10.67	5 (15)	ND
Y	-	-	-	61.95	5 (15)	ND	12.00	5 (15)	ND
Zn	2473.92	5 (15)	5 (10)	170.37	5 (15)	10 (20)	8096.31	5 (15)	5 (10)
Zr	1467.36	5 (15)	5 (10)	5570.60	5 (15)	5 (10)	18033.49	5 (15)	5 (10)

(a) MFPV mixing/sampling %RSD values are represented by %RSD$_S$ instead of $\%RSD_S(c_j^{MFPV})$ for space reasons. Low case value listed first, followed by the high case value in parentheses.

(b) MFPV analytical %RSD values are represented by %RSD$_A$ instead of $\%RSD_A(c_j^{MFPV})$ for space reasons. Low case value listed first, followed by the high case value in parentheses.

(c) %RSD$_A$ = 50 was used for non-detectable (ND) analytes for both low and high cases. Detection limits were used in place of concentration amounts for non-detects.

(d) A "-" means that no data were recorded for that analyte for that HLW tank, and hence mixing/sampling and analytical uncertainties were not estimated.

Table C.2. Nominal Concentrations and Mixing/Sampling Uncertainties (%RSD$_S$) for HLW Radionuclides in the MFPV (After GFC Addition) for Each of Three HLW Tanks

Isotope	AY-102		AZ-102		C-104	
	MFPV Conc. (µCi/mL)[a]	Mixing/ Sampling %RSD$_S$[b]	MFPV Conc. (µCi/mL)[a]	Mixing/ Sampling %RSD$_S$[b]	MFPV Conc. (µCi/mL)[a]	Mixing/ Sampling %RSD$_S$[b]
Am-241	2.016	1 (5)	35.18031	1 (5)	1.975684	1 (5)
Ce-144[d]	-[c]	1 (5)	-	1 (5)	-	1 (5)
Cm-242	-	1 (5)	-	1 (5)	0.002744	1 (5)
Cm-243+Cm-244	-	1 (5)	0.051736	1 (5)	0.029129	1 (5)
Co-60	0.144	1 (5)	1.323573	1 (5)	0.129602	1 (5)
Cs-134	-	1 (5)	0.042251	1 (5)	0.067545	1 (5)
Cs-137	242.064	1 (5)	365.1682	1 (5)	540.3581	1 (5)
Eu-152	-	1 (5)	-	1 (5)	-	1 (5)
Eu-154	1.44	1 (5)	12.54592	1 (5)	0.527694	1 (5)
Eu-155	0.72	1 (5)	23.10864	1 (5)	0.308173	1 (5)
Ni-63	-	1 (5)	-	1 (5)	-	1 (5)
Np-237	-	1 (5)	0.014917	1 (5)	0.001689	1 (5)
Pu-238	0.144	1 (5)	0.275924	1 (5)	0.187015	1 (5)
Pu-239	1.296	1 (5)	1.70728	1 (5)	1.709727	1 (5)
Pu-240	-	1 (5)	-	1 (5)	-	1 (5)
Pu-241	-	1 (5)	6.941214	1 (5)	4.896996	1 (5)
Rh-106[e]	-	1 (5)	-	1 (5)	-	1 (5)
Ru-103[d]	-	1 (5)	-	1 (5)	-	1 (5)
Ru-106	-	1 (5)	-	1 (5)	-	1 (5)
Sb-125	-	1 (5)	6.941214	1 (5)	0.05488	1 (5)
Se-79	-	1 (5)	-	1 (5)	-	1 (5)
Sm-151	-	1 (5)	-	1 (5)	-	1 (5)
Sn-113	-	1 (5)	-	1 (5)	-	1 (5)
Sn-126	-	1 (5)	-	1 (5)	-	1 (5)
Sr-90	2334.528	1 (5)	5087.349	1 (5)	218.6762	1 (5)
Tc-99	0.000181	1 (5)	0.004048	1 (5)	0.00591	1 (5)
Th-232	-	1 (5)	-	1 (5)	-	1 (5)
U-233	-	1 (5)	0.002673	1 (5)	0.138467	1 (5)
U-234	-	1 (5)	0.002966	1 (5)	0.005784	1 (5)
U-235	-	1 (5)	0.00012	1 (5)	0.000198	1 (5)
U-236	-	1 (5)	0.000215	1 (5)	0.000265	1 (5)
U-238	1.32E-09	1 (5)	0.002182	1 (5)	0.004129	1 (5)
Y-88[d]	-	1 (5)	-	1 (5)	-	1 (5)

(a) The estimated concentrations are based on measurements of actual pretreated sludge samples and then scaled to account for GFC additions. The references for the sludge work are Hansen and Crawford (2005) for AY-102 and Smith et al. (2001) for AZ-102 and C-104.

(b) MFPV mixing/sampling %RSD values are represented by %RSD$_S$ instead of $\%RSD_S(r_q^{MFPV})$ for space reasons.

Low case value listed first, followed by the high case value in parentheses. Low and high case values were chosen by the WTP Project to span the range of expected mixing/sampling uncertainties (%RSD$_S$) for radionuclides. The WTP Project has no basis at this time to estimate different %RSD$_S$ for different radionuclides or different HLW tanks, so the range of 1 to 5 %RSD$_S$ was selected for all radionuclides and each of the three HLW tanks.

(c) A "-" means no recorded data for that analyte.

(d) These short-lived radionuclides will be deleted in future work.

(e) This radionuclide will be combined with Ru-106 in future work.

Table C.3. HLW Radionuclide Analytical Uncertainties (%RSD_A) Dependent on the Concentration Range of the Radionuclide in the MFPV (After GFC Addition)[a]

Isotope	Concentration Range (µCi/g)[b]	%RSD_A[c]	Concentration Range (µCi/g) [b]	%RSD_A[c]	Comments
Am-241	1E-5 – 1E-3	25	1E-3 - 3E+3	5	
Am-243	5E-3 – 1E-1	40	1E-1 - 1E+2	25	
Ce-144[f]	No data	Assume 25			284 day half-life
Cm-242	3E-6 – 1E-4	60	1E-4 - 1E+0	20	
Cm-243+244	1E-4 – 1E-1	30	1E-1 - 1E+1	10	
Co-60	1E-4 – 1E-2	25	1E-2 - 1E+2	5	
Cs-134	1E-2 – 1E+0	30	1E+0 - 1E+3	20	High radiation from Cs-137
Cs-135	1E-3 – 1E+0	20	>1E+0	10	
Cs-137	1E-2 – 1E+2	5	1E+2 - 1E+5	10	(d)
Eu-152	2E-2 – 1E+0	10	1E+0 - 1E+3	5	
Eu-154	1E-4 – 1E-1	15	1E-1 - 1E+1	10	
Eu-155	1E-4 – 1E-2	10	1E-2 - 1E+0	5	
Nb-94	1E-1 - 1E+1	15	>1E+1	10	
Ni-59	1E-3 - 1E-1	20	1E-1 - 1E+1	10	
Ni-63	5E-3 - 1E+0	15	1E+0 - 1E+2	10	
Np-237	1E-4 - 1E-2	25	1E-2 - 1E+1	10	
Pu-238	1E-6 - 1E-2	25	1E-2 - 1E+0	10	
Pu-239	1E-4 - 1E-2	15	1E-2 - 1E+0	10	
Pu-240	1E-3 - 1E-1	50	1E-1 - 1E+1	20	
Pu-239/240	1E-6 - 1E-2	20	1E-2 - 1E+0	10	
Pu-241	5E-2 - 1E+0	25	1E+0 - 1E+3	15	
Ru-106	1E-5 - 1E-2	15	1E-2 - 1E+2	10	368 day half-life
Sm-151	No Data	Assume 50	No data		
Sn-113	No data	Assume 50	No data		
Sn-126	1E-4 - 1E-2	20	1E-2 - 1E+0	10	
Sr-90	1E-6 - 1E-2	20	1E-2 - 1E+4	10	
Tc-99	1E-5 - 1E-2	10	1E-2 - 1E+2	20	(e)
U-233	1E-4 - 1E+0	10	1E+0 - 1E+2	5	
U-234	1E-4 - 1E-2	50	1E-2 - 1E+1	30	
U-235	1E-2 - 1E+0	20	1E+0 - 1E+2	10	
U-236	3E-3 - 1E+0	50	1E+0 - 1E+3	15	
U-238	1E-2 - 1E+0	15	1E+0 - 1E+4	5	
Zr-93	No data	Assume 100	No data	No data	

(a) The data in this table were gathered by the WTP analytical laboratory group from the following documents: Brooks et al. (2000), Hay et al. (2003a,b), and Martin et al. (2003).

(b) Concentrations within this range have the corresponding %RSD_A (next column) for analytical uncertainty.

(c) MFPV analytical %RSD values are represented by %RSD_A instead of $\%RSD_A(c_q^{MFPV})$ for space reasons.

(d) The %RSD_A is estimated to be larger for higher concentrations because of additional requirements for dilution and handling in the hot cell.

(e) The %RSD_A is estimated to be larger for higher concentrations because of more probability of complexed species.

(f) These short-lived radionuclides will be deleted in future work.

Table C.4. Analytical Uncertainties (%RSD$_A$)[(a)] of HLW Radionuclides in the MFPV (After GFC Addition) for Each of Three HLW Tanks

Isotope	AY-102		AZ-102		C-104	
	Low[(b)] %RSD$_A$	High[(b)] %RSD$_A$	Low %RSD$_A$	High %RSD$_A$	Low %RSD$_A$	High %RSD$_A$
Am-241	25	50	5	10	25	50
Cm-242	-[(c)]	-	-	-	60	120
Cm-243+Cm-244	-	-	30	60	30	60
Co-60	25	50	25	50	25	50
Cs-134	-	-	30	60	30	60
Cs-137	5	10	5	10	5	10
Eu-154	15	30	15	30	15	30
Eu-155	10	20	10	20	10	20
Np-237	-	-	10	20	25	50
Pu-238	25	50	25	50	25	50
Pu-239	10	20	10	20	10	20
Pu-241	-	-	25	50	25	50
Sb-125	-	-	25	50	25	50
Sr-90	10	20	10	20	20	40
Tc-99	10	20	10	20	10	20
U-233	-	-	10	20	10	20
U-234	-	-	50	100	50	100
U-235	-	-	20	40	20	40
U-236	-	-	50	100	50	100
U-238	15	30	5	10	5	10

(a) MFPV analytical %RSD values are represented by %RSD$_A$ instead of $\%RSD_A(c_q^{MFPV})$ for space reasons. %RSD$_A$ values were determined from Table C.3 based on the nominal values in Table C.2 after applying a conversion factor of 1.48 to change the units from µCi/g to µCi/mL.

(b) Low and high case %RSD$_A$ values were chosen by the WTP Project to span the range of expected analytical uncertainties for radionuclides.

(c) A dash (–) indicates that the nominal value is zero, and hence there can be no %RSD$_A$ value.

Table C.5. Nominal HLW MFPV Volumes and Estimated SDs (in liters)

IHLW Process Stage	Nominal Volume (L)	Volume SDs (L)[(a)]	
		Low Case	High Case
MFPV Before Waste Addition from HBV	6113.06	112.05	224.1
MFPV After Waste Addition from HBV	23,147.8	112.05	224.1
MFPV After HBV and GFC Additions	26,932.83	112.05	224.1

(a) Low-case SDs are based on values from Table 5.12 in Heredia-Langner et al. (2003). High-case SDs are twice the low-case SDs.

Table C.6. Nominal Compositions for Glass Made from the HLW MFPV (in mass fractions) for Each of Three HLW Tanks[a]

Component	Mass Fractions			Component	Mass Fractions		
	AY-102	AZ-102	C-104		AY-102	AZ-102	C-104
Ag_2O	0.00185	0.00018	0.00065	V_2O_5	0.00016	0	3.77E-05
Al_2O_3	0.04915	0.07718	0.02412	Y_2O_3	0	0.00015	3.02E-05
B_2O_3	0.10800	0.03974	0.08987	ZnO	0.00711	0.00041	0.01994
BaO	0.00075	0.00037	0.00019	ZrO_2	0.00458	0.01463	0.04819
BeO	0	2.99E-05	5.03E-05	**Radionuclide Oxide**	**Mass Fractions**		
Bi_2O_3	0	0	2.51E-05		**AY-102[b]**	**AY-102[b]**	**AY-102[b]**
CaO	0.00500	0.00480	0.00459	$^{241}Am_2O_3$	1.51E-06	2.21E-05	1.26E-06
CdO	0.00013	0.01390	0.00061	$^{144}Ce_2O_3$[e]	0	0	0
Ce_2O_3	0.00104	0.00056	0.00081	$^{242}Cm_2O_3$	0	0	1.81E-12
Cl	0	0.00053	1.46E-05	$^{243+244}Cm_2O_3$	0	2.12E-09	1.22E-09
CoO	0	5.98E-05	2.26E-05	^{60}CoO	3.83E-10	2.96E-09	2.95E-10
Cr_2O_3	0.00222	0.00093	0.00139	$^{134}Cs_2O$	0	6.70E-11	1.09E-10
Cs_2O	7.06E-06	9.97E-05	0.00013	$^{137}Cs_2O$	6.80E-06	8.64E-06	1.30E-05
CuO	0.00034	0.00029	0.00025	$^{152}Eu_2O_3$	0	0	0
Dy_2O_3	0	0	2.76E-05	$^{154}Eu_2O_3$	1.48E-08	1.08E-07	4.64E-09
Eu_2O_3	0	0	1.26E-05	$^{155}Eu_2O_3$	3.92E-09	1.06E-07	1.44E-09
F	0	0.00012	0	$^{95}Nb_2O_5$	0	0	0
Fe_2O_3	0.13888	0.12101	0.04704	^{63}NiO	0	0	0
K_2O	0.00010	0.00026	0.00060	$^{237}NpO_2$	0	4.64E-05	5.34E-06
La_2O_3	0.00076	0.00299	0.00019	$^{238}PuO_2$	2.22E-08	3.58E-08	2.47E-08
Li_2O	0.02605	0.04992	0.04992	$^{239}PuO_2$	5.48E-05	6.07E-05	6.19E-05
MgO	0.00158	0.00125	0.00065	$^{240}PuO_2$	0	0	0
MnO	0.02796	0.00918	0.02536	$^{241}PuO_2$	0	1.53E-07	1.10E-07
MoO_3	0.00032	0	2.24E-05	$^{106}Rh_2O_3$[e]	0	0	0
Na_2O	0.12655	0.13251	0.08545	$^{103}RuO_2$[d]	0	0	0
Nd_2O_3	0	0.00208	0.00044	$^{106}RuO_2$	0	0	0
NiO	0.00410	0.00763	0.00235	$^{125}Sb_2O_3$	0	1.61E-08	1.29E-10
P_2O_5	0.00557	0.00462	0.00329	$^{79}SeO_2$	0	0	0
PbO	0.00535	0.00094	0.00153	$^{151}Sm_2O_3$	0	0	0
PdO	0	0	0.00011	$^{113}SnO_2$	0	0	0
Pr_2O_3	o	0	4.63E-05	$^{126}SnO_2$	0	0	0
Rh_2O_3	0	0	0.00032	^{90}SrO	4.54E-05	8.32E-05	3.64E-06
RuO_2	0	0	0.00016	$^{99}Tc_2O_7$	3.85E-08	7.25E-07	1.08E-06
Sb_2O_3	0.00038	0	0	$^{232}ThO_2$	0	0	0
SeO_2	0	0	3.52E-05	$^{233}U_3O_8$	0	6.46E-07	3.41E-05
SiO_2	0.47205	0.47945	0.47768	$^{234}U_3O_8$	0	1.12E-06	2.22E-06
SO_3	0.00208	0.00026	3.81E-05	$^{235}U_3O_8$	0	0.00013	0.00021
SnO_2	0.00064	0.00165	0.00068	$^{236}U_3O_8$	0	7.73E-06	9.70E-06
SrO	0.00168	0.01485	0.03374	$^{238}U_3O_8$	1.08E-08	0.01499	0.02887
ThO_2	0	0	0.04080	$^{88}Y_2O_3$[d]	0	0	0
TiO_2	0.00032	0.00014	0.00021	**Total[c]**	1.000	1.000	1.000
UO_3	0.00526	0.01713	0.03831				

(a) These nominal compositions were provided by the WTP Project. They are based on Kot et al. (2004a) for AY-102 and on Smith et al. (2001) for AZ-102 and C-104.

(b) Shaded cells denote radionuclide oxides that were considered to be already included in the chemical-composition oxides (e.g., the isotopes of U were considered to be already included in U_3O_8). The mass fractions of these radionuclide oxides were not counted as part of the total. If the chemical composition was greater than zero, the associated radionuclides were not included. If the chemical composition was zero or not reported, the associated radionuclides were included.

(c) Total does not include the gray-shaded entries to avoid double counting some radioactive components. The table values may not sum to one exactly because of rounding, but the electronic data values to more decimal places sum to one.

(d) These short-lived radionuclide oxides will be deleted in future work.

(e) This radionuclide oxide will be combined with that of Ru-106 in future work.

Appendix D

Nominal Concentrations and Estimates of Uncertainties Associated with the ILAW Compliance Strategy for Three LAW Waste Tanks

Appendix D: Nominal Concentrations and Estimates of Uncertainties Associated with the ILAW Compliance Strategy for Three LAW Waste Tanks

This appendix summarizes the ILAW process composition and uncertainty inputs provided by the WTP Project that are relevant to ILAW compliance (i.e., reporting chemical or radionuclide composition, and demonstrating that compliance quantities satisfy specified limits). The WTP compliance strategy for ILAW is focused on analyses of CRV samples, quantifying transfer volumes, weighing GFCs added to the MFPV, and ultimately on estimating glass composition corresponding to each MFPV batch and other compliance quantities. Hence, the composition and uncertainty estimates provided by the WTP Project are associated with the ILAW CRV, GFCs, and MFPV. The ILAW process composition and uncertainty information was provided for three LAW tanks representing Envelopes A (AP-101), B (AZ-101), and C (AN-107). Actual waste composition data from these tanks were used by the WTP Project to generate the inputs summarized in this appendix.

Table D.1 lists the nominal elemental concentrations of chemical-composition components (mg/L) for pre-treated LAW in the CRV corresponding to one tank each of Envelopes A, B, and C (as discussed in the preceding paragraph). Table D.1 also lists the CRV mixing/sampling[(a)] uncertainties [$\%RSD_S(c_j^{CRV})$] and the CRV analytical uncertainties [$\%RSD_A(c_j^{CRV})$] for the elemental concentrations, again corresponding to one tank each of Envelopes A, B, and C.

Table D.2 lists the nominal concentrations and corresponding mixing/sampling uncertainties [$\%RSD_S(c_j^{CRV})$] of LAW radionuclides (μCi/mL) for pre-treated LAW in the CRV corresponding to one tank each of Envelopes A, B, and C. Table D.3 provides LAW radionuclide analytical uncertainties [$\%RSD_A(c_j^{CRV})$] dependent on the concentrations of LAW radionuclides in the CRV. Table D.4 lists the CRV analytical uncertainties [$\%RSD_A(c_j^{CRV})$], again corresponding to one tank each of Envelopes A, B, and C. These uncertainties were determined from Table D.3 based on the nominal concentrations in Table D.2.

Table D.5 lists the nominal masses of GFCs added per liter of LAW for one tank each of Envelopes A, B, and C. Table D.6 lists the uncertainties for masses of GFCs [$\%RSD(a_k^{GFC})$] added to the ILAW MFPV. These uncertainties include all uncertainties associated with batching, weighing, and transferring GFCs until they are added to the MFPV. Data on the GFC compositions (mass fractions of oxides) and corresponding low- and high-case uncertainties are summarized in Tables D.7 and D.8. Table D.7 provides nominal values and low- and high-uncertainty-case ranges for each GFC component (oxide or halide). Table D.8 provides nominal values as well as low- and high-case standard deviations

(a) Mixing/sampling denotes combined random uncertainty caused by (1) random inhomogeneity in mixing an LAW CRV and (2) random uncertainty in taking samples from the LAW CRV by the designated sampling method. Mixing and sampling uncertainties cannot be separately estimated during WTP ILAW production operations, so combined estimates of these uncertainties were used.

[$SD(G_{jk}^{GFC})$] for each GFC component. The standard deviations were obtained using a formula assuming that the nominal values and ranges in Table D.7 specify triangular distributions for the GFC composition uncertainties. This formula is given by

$$SD(G_{jk}^{GFC}) = \sqrt{\frac{\Delta_l^2 + \Delta_u^2 + \Delta_n^2 - \Delta_l * \Delta_u - \Delta_l * \Delta_n - \Delta_u * \Delta_n}{18}} \quad \text{(D.1)}$$

where

Δ_l = lower limit value specified for the triangular distribution

Δ_u = upper limit value specified for the triangular distribution

Δ_n = nominal value specified for the triangular distribution.

The 12 GFCs listed in Tables D.7 and D.8 will be used by the WTP to produce ILAW and/or IHLW.

Table D.9 lists the nominal volumes as well as low- and high-case-uncertainty estimates (SDs) of (1) the LAW CRV contents before a transfer to the MFPV, (2) the LAW contents after a transfer to the MFPV, (3) the MFPV contents before a transfer from the CRV, and (4) the MFPV contents after a transfer from the CRV but before the GFCs are added.

Table D.10 lists the nominal volume (in liters) of water added to an ILAW MFPV to lower sodium molarity. The water is added before the last volume measurement in the ILAW MFPV, so the information is relevant for the illustrations and investigations using realistic data in this report. Currently, the WTP Project expects to add water to Envelope B wastes only.

Table D.11 lists the nominal compositions (in mass fractions) for glass made from the ILAW MFPV for each of three LAW tanks. These nominal compositions are based on the nominal CRV compositions, transfers, and GFC additions as discussed previously.

It is important to note that Tables D.1 to D.4 use slightly modified notation in order to better fit within the tables. The CRV concentration mixing/sampling %RSD, usually denoted as $\%RSD_S(c_j^{CRV})$, is referred to as $\%RSD_S$. The CRV concentration analytical percent relative standard deviation, usually denoted as $\%RSD_A(c_j^{CRV})$, is referred to as $\%RSD_A$.

Finally, note that the CRV nominal concentration data in Tables D.1 and D.2 were based on samples and analyses of actual waste tank samples. However, those analyses were not adjusted or normalized as described by Weier and Piepel (2003). Normalizing and adjusting compositions can be used to eliminate possible biases and reduce uncertainties in analyzed slurry and glass compositions. Applying the adjustment and normalization procedures discussed by Weier and Piepel (2003) to the WTP data provided by the WTP Project was beyond the scope of the present work. However, it remains an interesting option to determine the extent to which the adjustments and normalization would affect the composition variations and uncertainties.

Table D.1. Nominal Chemical Composition Analyte Concentrations of Pre-Treated LAW, Mixing/Sampling Uncertainties (%RSD_S), and Analytical Uncertainties (%RSD_A) in the CRV Corresponding to One Tank Each of Envelopes A, B, and C

Analyte	AP-101 (Envelope A)			AZ-101 (Envelope B)			AN-107 (Envelope C)		
	CRV Conc. (mg/L)[a]	Mixing/ Sampling %RSD_S[b]	Analytical %RSD_A[c]	CRV Conc. (mg/L)[a]	Mixing/ Sampling %RSD_S[b]	Analytical %RSD_A[c]	CRV Conc. (mg/L)[a]	Mixing/ Sampling %RSD_S[b]	Analytical %RSD_A[c]
Ag	< 0.9005[d]	1 (5)	10 (20)	< 0.3168	1 (5)	20 (40)	-[e]	-	-
Al	9919.5196	5 (15)	5 (10)	3345.6221	5 (15)	5 (10)	3845	5 (15)	5 (10)
As	1.7990	1 (5)	15 (30)	8.5541	1 (5)	10 (20)	-	-	-
B	21.4069	1 (5)	5 (10)	4.9107	1 (5)	15 (30)	-	-	-
Ba	0.4714	5 (15)	5 (10)	< 0.1267	5 (15)	15 (30)	-	-	-
Be	1.8894	1 (5)	5 (10)	< 0.1267	1 (5)	15 (30)	-	-	-
Bi	< 3.5779	1 (5)	5 (10)	< 1.2673	1 (5)	10 (20)	-	-	-
Ca	11.0552	5 (15)	10 (20)	< 3.1682	5 (15)	15 (30)	317	5 (15)	5 (10)
Ce	< 0.1106	1 (5)	20 (40)	< 2.5346	1 (5)	15 (30)	-	-	-
Cd	2.8542	5 (15)	5 (10)	< 0.1901	5 (15)	15 (30)	-	-	-
Cl	2834.1484	1 (5)	8 (16)	< 82.3733	1 (5)	10 (20)	1036	1 (5)	10 (20)
Cr	204.0185	5 (15)	5 (10)	360.8583	5 (15)	5 (10)	168	5 (15)	5 (10)
Cs	7.2763	1 (5)	5 (10)	-	-	-	2000	1 (5)	5 (10)
Cu	2.2914	1 (5)	5 (10)	< 0.3168	1 (5)	10 (20)	-	-	-
F	4140.6708	1 (5)	6 (12)	1203.9171	1 (5)	10 (20)	1869	1 (5)	20 (40)
Fe	3.5779	5 (15)	8 (16)	< 0.3168	5 (15)	10 (20)	1556	5 (15)	5 (10)
K	44622.7628	1 (5)	20 (40)	2407.8341	1 (5)	20 (40)	910	1 (5)	10 (20)
La	< 1.8593	1 (5)	10 (20)	< 0.6336	1 (5)	10 (20)	19	1 (5)	10 (20)
Li	0.4864	5 (15)	20 (40)	< 0.3802	5 (15)	10 (20)	-	-	-
Mg	< 3.5779	5 (15)	10 (20)	< 1.2673	5 (15)	15 (30)	-	-	-
Mo	20.7034	1 (5)	5 (10)	54.0495	1 (5)	5 (10)	-	-	-
Mn	< 1.8593	5 (15)	20 (40)	< 0.6336	5 (15)	10 (20)	-	-	-
Na	183918.1440	1 (5)	8 (16)	62730.4148	1 (5)	5 (10)	137940	1 (5)	5 (10)
Nd	< 3.5779	5 (15)	10 (20)	< 1.2673	5 (15)	10 (20)	-	-	-
Ni	11.2562	5 (15)	8 (16)	< 0.3802	5 (15)	10 (20)	273	5 (15)	5 (10)
Pb	21.4069	1 (5)	10 (20)	4.2137	1 (5)	10 (20)	220	1 (5)	5 (10)
Pd	< 27.1355	1 (5)	10 (20)	< 9.5046	1 (5)	15 (30)	-	-	-
Rh	< 10.8542	1 (5)	10 (20)	< 3.8018	1 (5)	15 (30)	-	-	-
Ru	< 39.9997	1 (5)	10 (20)	< 13.9401	1 (5)	10 (20)	-	-	-
Sb	0.0600	1 (5)	10 (20)	< 6.3364	1 (5)	20 (40)	-	-	-
Se	< 3.2864	1 (5)	10 (20)	< 3.1682	1 (5)	20 (40)	-	-	-
Si	195.9784	5 (15)	20 (40)	33.2661	5 (15)	5 (10)	-	-	-
Sn	-	-	-	27.8802	1 (5)	15 (30)	-	-	-
Sr	< 0.5437	1 (5)	15 (30)	< 0.1901	1 (5)	15 (30)	-	-	-
Th	< 0.0157	1 (5)	15 (30)	< 12.6728	1 (5)	20 (40)	-	-	-
Tl	0.0257	1 (5)	15 (30)	< 6.3364	1 (5)	10 (20)	-	-	-
Ti	< 0.9005	5 (15)	15 (30)	1.6158	5 (15)	15 (30)	-	-	-
U	73.0647	5 (15)	5 (10)	< 25.3456	5 (15)	20 (40)	-	-	-
V	< 1.1055	1 (5)	10 (20)	0.8554	1 (5)	20 (40)	-	-	-
W	40.9042	1 (5)	5 (10)	32.3157	1 (5)	20 (40)	-	-	-
Zn	8.0100	1 (5)	10 (20)	1.0455	1 (5)	15 (30)	-	-	-
Zr	2.0000	5 (15)	12 (24)	1.2356	5 (15)	10 (20)	-	-	-
PO_4	1457.2749	1 (5)	5 (10)	1013.8249	1 (5)	5 (10)	2030	1 (5)	5 (10)
SO_4	5758.7484	1 (5)	5 (10)	10455.0691	1 (5)	5 (10)	4723	1 (5)	5 (10)

(a) The AP-101 data are based on waste tank sample analyses in Goheen et al. (2002) at 4.85 molar Na, but were scaled to 8.0 molar for this table. The AZ-101 data are waste tank sample analyses from Smith et al. (2004). The AN-107 data are based on a pilot melter test (Matlack et al. 2002).

(b) MFPV mixing/sampling %RSD_S low case value listed first, followed by the high case value in parentheses.

(c) MFPV analytical %RSD_A low case values listed first, followed by the high case value in parentheses.

(d) A "<" denotes a measured value less than the detection limit (DL), in which case the value shown is one-half the DL.

(e) A "-" means no recorded data for that analyte.

Table D.2. Nominal Radionuclide Concentrations and Mixing/Sampling Uncertainties (%RSD_S) of Pre-Treated LAW in the CRV Corresponding to One Tank Each of Envelopes A, B, and C

Isotope	AP-101 (Envelope A)		AZ-101 (Envelope B)		AN-107 (Envelope C)	
	CRV Conc. (µCi/mL)[a]	Mixing/ Sampling %RSD_S[b]	CRV Conc. (µCi/mL)[a]	Mixing/ Sampling %RSD_S[b]	CRV Conc. (µCi/mL)[a]	Mixing/ Sampling %RSD_S[b]
Am-241	0.000167	1 (5)	4.31E-07	1 (5)	0.001967	1 (5)
Ce-144[e]	< 9.90E-05[c]	1 (5)	< 1.90E-04	1 (5)	-[d]	-
Cm-242	1.29E-07	1 (5)	< 3.17E-08	1 (5)	-	-
Cm-243+Cm-244	1.37E-06	1 (5)	< 6.34E-08	1 (5)	-	-
Co-60	0.003381	1 (5)	1.08E-05	1 (5)	0.057697	1 (5)
Cs-134	< 1.48E-05	1 (5)	< 1.27E-05	1 (5)	-	-
Cs-137	0.000132	1 (5)	2.28E-02	1 (5)	0.106797	1 (5)
Eu-152	< 3.30E-05	1 (5)	< 1.27E-05	1 (5)	-	-
Eu-154	8.61E-05	1 (5)	< 1.27E-05	1 (5)	0.004517	1 (5)
Eu-155	4.24E-05	1 (5)	< 1.27E-04	1 (5)	0.003162	1 (5)
Fe-59[e]	< 3.30E-05	1 (5)	< 1.27E-05	1 (5)	-	-
Nb-95	< 1.32E-05	1 (5)	-	-	0.001588	1 (5)
Ni-63	0.003414	1 (5)	-	-	-	-
Np-237	-	-	6.97E-06	1 (5)	1.78E-05	1 (5)
Pu-238	3.96E-06	1 (5)	6.97E-07	1 (5)	-	-
Pu-239	2.87E-05	1 (5)	5.83E-06	1 (5)	0.000565	1 (5)
Pu-241	0.000188	1 (5)	3.29E-05	1 (5)	-	-
Rh-106[f]	0.00099	1 (5)	-	-	-	-
Ru-103[e]	< 1.32E-05	1 (5)	< 3.17E-05	1 (5)	-	-
Ru-106	0.00099	1 (5)	-	-	-	-
Sb-125	0.002078	1 (5)	6.34E-03	1 (5)	< 1.22E-04	1 (5)
Se-79	1.48E-05	1 (5)	8.87E-05	1 (5)	< 2.91E-06	1 (5)
Sm-151	0.001285	1 (5)	3.80E-05	1 (5)	-	-
Sn-113	< 1.65E-05	1 (5)	< 4.44E-05	1 (5)	8.14E-05	1 (5)
Sn-126	0.000363	1 (5)	1.39E-03	1 (5)	< 5.25E-05	1 (5)
Sr-90	0.088742	1 (5)	1.01E-01	1 (5)	0.00354	1 (5)
Tc-99	0.000564	1 (5)	-	-	0.071392	1 (5)
Th-232	< 3.30E-05	1 (5)	-	-	-	-
Y-88[e]	< 1.65E-05	1 (5)	< 6.34E-06	1 (5)	< 3.50E-04	1 (5)

(a) The AP-101 data are based on waste tank sample analyses in Goheen et al. (2002) at 4.85 molar Na, but were scaled to 8.0 molar Na for this table. The AZ-101 data are waste tank sample analyses from Smith et al. (2004). The AN-107 data are based on waste tank sample analyses in Smith et al. (2000) at 4.12 molar Na, but were scaled to 6.0 molar Na based on work by Matlack et al. (2002).

(b) MFPV mixing/sampling %RSD_S low case value listed first, followed by the high case value in parentheses. Low case and high case values were chosen by the WTP Project to span the range of expected mixing/sampling uncertainties (%RSD_S) for radionuclides. The WTP Project has no basis at this time to estimate different %RSD_S for different radionuclides or different HLW tanks, so the range of 1 to 5 %RSD_S was selected for all radionuclides and each of the three HLW tanks.

(c) A "<" denotes a measured value less than the detection limit (DL), in which case the value used in the simulation is one-half the DL (the value listed is the DL).

(d) A "-" means no recorded data for that analyte.

(e) These short-lived radionuclides will be deleted in future work.

(f) This radionuclide will be combined with Ru-106 in future work.

Table D.3. LAW Radionuclide Concentration Boundaries for Determining CRV Radionuclide Analytical Uncertainties (%RSD_A)[a]

Isotope	Analytical %RSD_A[b]		Isotope Concentration Lower Limit to Determine Analytical %RSD_A (µCi/mL)	Analytical %RSD_A[c]		Isotope Concentration Upper Limit to Determine Analytical %RSD_A (µCi/mL)	Analytical %RSD_A[d]	
	Low[e]	High[e]		Low[e]	High[e]		Low[e]	High[e]
Am-241	5	10	1.01E-03	15	30	5.05E-06	25	50
Ce-144[f]	5	10	5.05E-01	15	30	5.05E-03	25	50
Cm-242	5	10	5.50E-03	15	30	5.05E-04	25	50
Cm-243+244	5	10	5.05E-02	15	30	5.50E-04	25	50
Co-60	5	10	5.50E-04	15	30	5.05E-05	25	50
Cs-134	5	10	5.01E-01	15	30	5.05E-04	25	50
Cs-137	5	10	5.50E-03	15	30	5.01E-04	25	50
Eu-152	5	10	5.01E-01	15	30	5.50E-04	25	50
Eu-154	5	10	5.05E-03	15	30	1.00E-04	25	50
Eu-155	5	10	5.05E-03	15	30	5.50E-05	25	50
Fe-59[f]	5	10	5.05E-03	15	30	5.50E-05	25	50
Nb-95	5	10	5.01E+00	15	30	5.05E-03	25	50
Ni-63	5	10	5.05E+00	15	30	5.50E-02	25	50
Np-237	5	10	5.01E-05	15	30	5.05E-08	25	50
Pu-238	5	10	5.05E-03	15	30	5.05E-05	25	50
Pu-239	5	10	5.50E-04	15	30	5.05E-05	25	50
Pu-241	5	10	5.05E-01	15	30	5.50E-03	25	50
Rh-106[g]	5	10	5.00E+01	15	30	5.05E-04	25	50
Ru-103[f]	5	10	5.00E+02	15	30	5.50E-02	25	50
Ru-106	5	10	5.00E+01	15	30	5.05E-04	25	50
Sb-125	5	10	5.01E-02	15	30	5.50E-05	25	50
Se-79	5	10	5.01E-01	15	30	5.05E-04	25	50
Sm-151	5	10	5.50E+00	15	30	5.01E-01	25	50
Sn-113	5	10	5.05E+01	15	30	5.50E-01	25	50
SnSb-126	5	10	5.05E-02	15	30	5.50E-04	25	50
Sr-90	5	10	5.50E-02	15	30	5.01E-03	25	50
Tc-99	5	10	5.05E-02	15	30	5.05E-04	25	50
Th-232	5	10	5.50E-03	15	30	5.50E-04	25	50
Y-88[f]	5	10	5.50E+00	15	30	5.05E-01	25	50

(a) The contents of this table were supplied by the WTP analytical laboratory group.
(b) These %RSD_A values apply for concentrations greater than those in the column to the right.
(c) These %RSD_A values applied for concentrations between those to the left and the right.
(d) These %RSD_A values apply for concentrations less than those in the column to the left.
(e) %RSD_A values for the low and high cases correspond to the lower and upper limits of estimated ranges on %RSD_A. High-case values are assumed to be two times the low-case values.
(f) These short-lived radionuclides will be deleted in future work.
(g) This radionuclide will be combined with Ru-106 in future work.

Table D.4. CRV Radionuclide Analytical Uncertainties (%RSD_A)[(a)] for One Tank Each of LAW Waste Envelopes A, B, and C

Isotope	AP-101 Envelope A		AZ-101 Envelope B		AN-107 Envelope C	
	Low %RSD_A	High %RSD_A	Low %RSD_A	High %RSD_A	Low %RSD_A	High %RSD_A
Am-241	15	30	25	50	5	10
Ce-144[(c)]	25	50	25	50	-(b)	-
Cm-242	25	50	25	50	-	-
Cm-243+244	25	50	25	50	-	-
Co-60	5	10	25	50	5	10
Cs-134	25	50	25	50	-	-
Cs-137	25	50	5	10	5	10
Eu-152	25	50	25	50	-	-
Eu-154	25	50	25	50	15	30
Eu-155	25	50	15	30	15	30
Fe-59[(c)]	25	50	25	50	-	-
Nb-95	25	50	-	-	25	50
Ni-63	25	50	-	-	-	-
Np-237	-	-	15	30	15	30
Pu-238	25	50	25	50	-	-
Pu-239	25	50	25	50	5	10
Pu-241	25	50	25	50	-	-
Rh-106[(d)]	15	30	-	-	-	-
Ru-103[(c)]	25	50	25	50	-	-
Ru-106	15	30	-	-	-	-
Sb-125	15	30	15	30	15	30
Se-79	25	50	25	50	25	50
Sm-151	25	50	25	50	-	-
Sn-113	25	50	25	50	25	50
SnSb-126	25	50	15	30	25	50
Sr-90	5	10	5	10	25	50
Tc-99	15	30	-	-	5	10
Th-232	25	50	-	-	-	-
Y-88[(c)]	25	50	25	50	25	50

(a) %RSD_A values were determined from Table D.7 based on the concentrations in Table D.6. The high case values are two times the low case values.

(b) A dash "-" means that the analyte was not measured for that envelope, generally because of its small amount. Hence, the WTP Project did not estimate the radionuclide analytical uncertainty for such isotopes.

(c) These short-lived radionuclides will be deleted in future work.

(d) This radionuclide will be combined with Ru-106 in future work.

Table D.5. Masses of GFCs (a_{ik}^{GFC}) per Liter of LAW for One Tank Each of Envelopes A, B, and C[(a)]

GFC	Formula [(b)]	AP-101 Envelope A (g/L)	AZ-101 Envelope B (g/L)	AN-107 Envelope C (g/L)
Kyanite	Al_2SiO_5	108.12	155.08	133.48
Boric Acid	H_3BO_3	238.45	280.85	233.71
Wollastonite	$CaSiO_3$	56.87	234.79	138.68
Hematite	Fe_2O_3	69.96	75.36	65.19
Olivine	Mg_2SiO_4	41.94	94.9	40.95
Silica	SiO_2	481.65	514.03	437.27
Rutile	TiO_2	28.19	23.45	15.41
Zincite	ZnO	39.97	76.41	39.58
Zircon	$ZrSiO_4$	60.61	75.36	58.46
Borax	$Na_2B_4O_7$-$10H_2O$	0	0	0
Sodium Carbonate	Na_2CO_3	0	0	0
Lithium Carbonate	Li_2CO_3	0	169.4	0

(a) These quantities were calculated and provided by the WTP Project.
(b) The nominal chemical formulas of the corresponding minerals are listed, although GFCs will contain other elements/oxides in minor amounts.

Table D.6. Uncertainties for Masses of Individual GFCs [$\%RSD(a_k^{GFC})$] Added to the ILAW MFPV

Uncertainty Category	$\%RSD(a_k^{GFC})$ Low Case[(a)]	$\%RSD(a_k^{GFC})$ High Case[(b)]
Low (>100 g/L)	0.67	1.34
High (<100 g/L)	2.0	4.0

(a) The low-case $\%RSD(a_k^{GFC})$ for the low uncertainty category is based on a WTP estimate of 2% total precision, which was assumed to represent three times $\%RSD(a_k^{GFC})$, thus yielding 2/3 = 0.67 %RSD. The low-case $\%RSD(a_k^{GFC})$ for the high-uncertainty category was based on the assumption that GFCs added in smaller quantities will be subject to a higher relative standard deviation. All GFCs with greater than 100 g added per liter of LAW were considered to be in the low-uncertainty category. All others were considered to be in the high-uncertainty category.
(b) The high-case values are two times the low-case values.

Table D.7. GFC Compositions (G_{ijk}^{GFC}) and Uncertainty Ranges Expressed as Mass Fractions.[a] These GFCs are the total set used in ILAW and IHLW.

Oxide	Kyanite		Boric Acid		Wollastonite		Hematite	
	Nominal	Case Ranges[b]	Nominal	Case Ranges	Nominal	Case Ranges	Nominal	Case Ranges
Al_2O_3	0.5703	0.5400 – 0.6000 0.5097 – 0.6297	0	(e)	0.0020	0.0013 – 0.0027 0.0006 – 0.0034	0.0150	0.0099 – 0.0201 0.0048 – 0.0252
B_2O_3	0	(e)	0.5652	0.5625 – 0.5680 0.5598 – 0.5708	0	(e)	0	(e)
CaO	0.0003	0 – 0.0004 0 – 0.0005	0	(e)	0.4750	0.4477 – 0.5023 0.4204 – 0.5296	0.0004	0 – 0.0008 0 – 0.0011
CdO	0	(e)	0	(e)	0	(e)	0	(e)
Cl	0	(e)	0	(e)	0	(e)	0	(e)
Cr_2O_3	0	(e)	0	(e)	0	(e)	0	(e)
Fe_2O_3	0.0078	0.0042 – 0.0100 0.0006 – 0.0122	0	(e)	0.0040	0.0029 – 0.0051 0.0018 – 0.0062	0.9700	0.9615 – 0.9785 0.9530 – 0.9870
K_2O	0	0 – 0.0007 0 – 0.0014	0	(e)	0	(e)	0	(e)
Li_2O	0	(e)	0	(e)	0	(e)	0	(e)
MgO	0.0001	0 – 0.0004 0 – 0.0007	0	(e)	0.0010	0 – 0.0010 0 – 0.0010	0.0010	0.0001 – 0.0037 0 – 0.0054
MnO	0	(e)	0	(e)	0.0010	0.0009 – 0.0011 0.0008 – 0.0012	0.0012	0.0003 – 0.0039 0 – 0.0066
Na_2O	0.0042	0 – 0.0042 0 – 0.0042	0	(e)	0	(e)	0	(e)
NiO	0	(e)	0	(e)	0	(e)	0	(e)
P_2O_5	0	(e)	0	(e)	0	(e)	0.0027	0.0018 – 0.0054 0.0009 – 0.0081
PbO	0	(e)	0	(e)	0	(e)	0	
SiO_2	0.4067	0.3900 – 0.4200 0.3733 – 0.4333	0	(e)	0.5100	0.4800 – 0.5300 0.4500 – 0.5500	0.0135	0.0084 – 0.0186 0.0033 – 0.0237
SO_3	0	(e)	0	0 – 0.0003 0 – 0.0006	0	(e)	0.0007	0.0006 – 0.0009 0.0005 – 0.0011
TiO_2	0.0079	0.0050 – 0.0160 0.0021 – 0.0241	0	(e)	0.0002	0.0001 – 0.0003 0 – 0.0004	0	(e)
UO_2	0	(e)	0	(e)	0	(e)	0	(e)
V_2O_5	0	(e)	0	(e)	0	(e)	0	(e)
ZnO	0	(e)	0	(e)	0	(e)	0	(e)
ZrO_2	0	(e)	0	(e)	0	(e)	0	(e)
Total[c]	0.9973	0.9392 – 1.0517 0.8857 – 1.1061	0.5652	0.5625 – 0.5683 0.5598 – 0.5714	0.9932	0.9329 – 1.0918 0.8736 – 1.0425	1.0045[d]	0.9826 – 1.0319 0.9625 – 1.0582

(a) The information in this table is based on Table 5.14 of Heredia-Langner et al. (2003) with the high-case ranges added.

(b) The top range is the low case, and the bottom range is the high case. The high case generally doubles the range about the nominal value compared to the low case.

(c) Total mass fractions less than one indicate GFCs containing water or other volatile components that will not be present in the glass. Ranges shown for the total were obtained by summing the lower values and summing the upper values of the ranges for the individual oxide components. Obviously, a total mass fraction value greater than 1 is not possible and must be dealt with appropriately in the use of the information in this table.

(d) This was the result of converting minor components from element to oxide bases. The mass fractions of Hematite will need to be corrected based on updated/corrected vendor information.

(e) Case range cells are left blank for oxides with zero nominal value.

Table D.7. GFC Compositions (G_{ijk}^{GFC}) and Uncertainty Ranges Expressed as Mass Fractions of Oxides. These GFCs are the total set used in ILAW and IHLW (cont.)

Oxide	Olivine		Silica		Rutile		Zincite	
	Nominal	Case Ranges	Nominal	Case Ranges[(a)]	Nominal	Case Ranges	Nominal	Case Ranges
Al_2O_3	0.0019	0.0003 – 0.0078 0 – 0.0137	0.0014	0.0004 – 0.0040 0 – 0.0067	0.0050	0 – 0.0075 0 – 0.0100	0	(e)
B_2O_3	0	(e)	0	(e)	0	(e)	0	(e)
CaO	0.0002	0 – 0.0003 0 – 0.0004	0.0001	0 – 0.0002 0 – 0.0003	0	(e)	0	(e)
CdO	0	(e)	0	(e)	0	(e)	0.0001	0 – 0.0002 0 – 0.0003
Cl	0	(e)	0	(e)	0	(e)	0	(e)
Cr_2O_3	0.0013	0 – 0.0078 0 – 0.0143	0	(e)	0.0016	0 – 0.0075 0 – 0.0134	0	(e)
Fe_2O_3	0.0768	0.0468 – 0.1068 0.0168 – 0.1368	0.0002	0.0001 – 0.0004 0 – 0.0005	0.0070	0 – 0.0250 0 – 0.0430	0	0 – 0.0001 0 – 0.0001
K_2O	0	(e)	0	0 – 0.0002 0 – 0.0004	0	(e)	0	(e)
Li_2O	0	(e)	0	(e)	0	(e)	0	(e)
MgO	0.4801	0.4634 – 0.4934 0.4467 – 0.5067	0.0001	0 – 0.0001 0 – 0.0001	0	(e)	0	(e)
MnO	0	(e)	0	(e)	0	(e)	0	0 – 0.0001 0 – 0.0001
Na_2O	0.0003	0 – 0.0004 0 – 0.0005	0.0002	0 – 0.0002 0 – 0.0002	0	(e)	0	(e)
NiO	0.0037	0.0022 – 0.0052 0.0007 – 0.0067	0	(e)	0	(e)	0	(e)
P_2O_5	0	(e)	0	(e)	0	0 – 0.0007 0 – 0.0014	0	(e)
PbO	0	(e)	0	(e)	0	(e)	0	0 – 0.0001 0 – 0.0001
SiO_2	0.4252	0.4085 – 0.4385 0.3918 – 0.4518	0.9970	0.9920 – 0.9990 0.9870 – 1.0000	0.0220	0 – 0.0250 0 – 0.0280	0	(e)
SO_3	0	(e)	0	(e)	0	0 – 0.0007 0 – 0.0014	0	(e)
TiO_2	0	(e)	0.0001	0 – 0.0005 0 – 0.0009	0.9320	0.9280 – 0.9360 0.9240 – 0.9400	0	(e)
UO_2	0	(e)	0	(e)	0	(e)	0	(e)
V_2O_5	0	(e)	0	(e)	0.0045	0 – 0.0075 0 – 0.0105	0	(e)
ZnO	0	(e)	0	(e)	0	(e)	0.9990	0.9930 – 0.9999 0.9870 – 1.0000
ZrO_2	0	(e)	0	(e)	0.0190	0 – 0.0250 0 – 0.0310	0	(e)
Total[(b)]	0.9895	0.9217 – 1.0602 0.8560 – 1.1309	0.9987	0.9925 – 1.0046 0.9870 – 1.0091	0.9911	0.9320 – 1.0349 0.9240 – 1.0787	0.9991	0.9931 – 1.0004 0.9870 – 1.0006

(a) The top range is the low case, and the bottom range is the high case. The high case generally doubles the range about the nominal value compared to the low case.

(b) Total mass fractions less than one indicate GFCs containing water or other volatile components that will not be present in the glass. Ranges shown for the total were obtained by summing the lower values and summing the upper values of the ranges for the individual oxide components. Obviously, a total mass fraction value greater than 1 is not possible and must be dealt with appropriately in the use of the information in this table.

(e) Case range cells are left blank for oxides with zero nominal value.

Table D.7. GFC Compositions (G_{ijk}^{GFC}) and Uncertainty Ranges Expressed as Mass Fractions of Oxides. These GFCs are the total set used in ILAW and IHLW (cont.)

Oxide	Zircon		Borax		Sodium Carbonate		Lithium Carbonate	
	Nominal	Case Ranges	Nominal	Case Ranges[a]	Nominal	Case Ranges	Nominal	Case Ranges
Al_2O_3	0.0025	0.0010 – 0.0040 0 – 0.0055	0	(e)	0	(e)	0	(e)
B_2O_3	0	(e)	0.3750	0.3690 – 0.3820 0.3630 – 0.3890	0	(e)	0	(e)
CaO	0	(e)	0	(e)	0	0 – 0.0001 0 – 0.0002	0	0 – 0.0220 0 – 0.0439
CdO	0	(e)	0	(e)	0	(e)	0	(e)
Cl	0	(e)	0	0 – 0.0007 0 – 0.0014	0.0002	(e)	0.0001	(e)
Cr_2O_3	0	(e)	0	(e)	0	0 – 0.0006 0 – 0.0010	0.0001	0 – 0.0002 0 – 0.0002
Fe_2O_3	0.0008	0.0006 – 0.0009 0.0004 – 0.0010	0	0 – 0.0001 0 – 0.0001	0	0 – 0.0001 0 – 0.0001	0	0 – 0.0001 0 – 0.0001
K_2O	0	(e)	0	(e)	0	(e)	0	0 – 0.0001 0 – 0.0001
Li_2O	0	(e)	0	(e)	0	(e)	0.4020	0.4000 – 0.4044 0.3980 – 0.4068
MgO	0	(e)	0	(e)	0	0 – 0.0001 0 – 0.0002	0.0001	0 – 0.0002 0 – 0.0002
MnO	0	(e)	0	(e)	0	(e)	0	(e)
Na_2O	0	(e)	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	(e)	0	(e)	0	(e)	0	(e)
P_2O_5	0	(e)	0	(e)	0	(e)	0	(e)
PbO	0	(e)	0	(e)	0	(e)	0	(e)
SiO_2	0.3225	0.3200 – 0.3250 0.3175 – 0.3275	0	(e)	0	(e)	0	(e)
SO_3	0	(e)	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	0.0010	0.0007 – 0.0014 0.0004 – 0.0018	0	(e)	0	(e)	0	(e)
UO_2	0.0004	0.0003 – 0.0008 0.0002 – 0.0012	0	(e)	0	(e)	0	(e)
V_2O_5	0	(e)	0	(e)	0	(e)	0	(e)
ZnO	0	(e)	0	(e)	0	(e)	0	(e)
ZrO_2	0.6600	0.6500 – 0.6700 0.6400 – 0.6800	0	(e)	0	(e)	0	(e)
Total[b]	0.9908	0.9753 – 1.0021 0.9583 – 1.0170	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) The top range is the low case, and the bottom range is the high case. The high case generally doubles the range about the nominal value compared to the low case.

(b) Total mass fractions less than one indicate GFCs containing water or other volatile components that will not be present in the glass. Ranges shown for the total were obtained by summing the lower values and summing the upper values of the ranges for the individual oxide components. Obviously, a total mass fraction value greater than 1 is not possible and must be dealt with appropriately in the use of the information in this table.

(e) Case range cells are left blank for oxides with zero nominal value.

Table D.8. GFC Nominal Compositions (G_{ijk}^{GFC}) and SDs Expressed as Mass Fractions of Oxides

Oxide	Value Type	Kyanite	Boric Acid	Wollastonite	Hematite	Olivine	Silica
Al_2O_3	Nominal	0.5703	(b)	0.0020	0.0150	0.0019	0.0014
	Low SD[(a)]	0.0122	(b)	0.0003	0.0021	0.0016	0.0008
	High SD[(a)]	0.0245	(b)	0.0006	0.0042	0.0030	0.0014
B_2O_3	Nominal	(b)	0.5652	(b)	(b)	(b)	(b)
	Low SD	(b)	0.0011	(b)	(b)	(b)	(b)
	High SD	(b)	0.0022	(b)	(b)	(b)	(b)
CaO	Nominal	0.0003	(b)	0.4750	0.0004	0.0002	0.0001
	Low SD	0.00008	(b)	0.0111	0.0002	0.00006	0.00004
	High SD	0.00010	(b)	0.0223	0.0002	0.00008	0.00006
Cr_2O_3	Nominal	(b)	(b)	(b)	(b)	0.0013	(b)
	Low SD	(b)	(b)	(b)	(b)	0.0016	(b)
	High SD	(b)	(b)	(b)	(b)	0.0032	(b)
Fe_2O_3	Nominal	0.0078	(b)	0.0040	0.9700	0.0768	0.0002
	Low SD	0.0012	(b)	0.0004	0.0035	0.0122	0.00006
	High SD	0.0024	(b)	0.0009	0.0069	0.0250	0.00010
K_2O	Nominal	0	(b)	(b)	(b)	(b)	0
	Low SD	0.0002	(b)	(b)	(b)	(b)	0.00005
	High SD	0.0003	(b)	(b)	(b)	(b)	0.00009
MgO	Nominal	0.0001	(b)	0.0010	0.0010	0.4801	0.0001
	Low SD	0.00008	(b)	0.0002	0.0008	0.0061	0.00002
	High SD	0.00015	(b)	0.0002	0.0012	0.0123	0.00002
MnO	Nominal	(b)	(b)	0.0010	0.0012	(b)	(b)
	Low SD	(b)	(b)	0.00004	0.0008	(b)	(b)
	High SD	(b)	(b)	0.00008	0.0014	(b)	(b)
Na_2O	Nominal	0.0042	(b)	(b)	(b)	0.0003	0.0002
	Low SD	0.0011	(b)	(b)	(b)	0.00008	0.00005
	High SD	0.0012	(b)	(b)	(b)	0.00010	0.00005
NiO	Nominal	(b)	(b)	(b)	(b)	0.0037	(b)
	Low SD	(b)	(b)	(b)	(b)	0.0006	(b)
	High SD	(b)	(b)	(b)	(b)	0.0012	(b)
P_2O_5	Nominal	(b)	(b)	(b)	0.0027	(b)	(b)
	Low SD	(b)	(b)	(b)	0.0008	(b)	(b)
	High SD	(b)	(b)	(b)	0.0015	(b)	(b)
SO_3	Nominal	(b)	0	(b)	0.0007	(b)	(b)
	Low SD	(b)	0.00007	(b)	0.00006	(b)	(b)
	High SD	(b)	0.00014	(b)	0.00012	(b)	(b)
SiO_2	Nominal	0.4067	(b)	0.5100	0.0135	0.4252	0.9970
	Low SD	0.0061	(b)	0.0103	0.0021	0.0061	0.0015
	High SD	0.0123	(b)	0.0205	0.0042	0.0123	0.0028
TiO_2	Nominal	0.0079	(b)	0.0002	(b)	(b)	0.0001
	Low SD	0.0023	(b)	0.00004	(b)	(b)	0.0001
	High SD	0.0047	(b)	0.00008	(b)	(b)	0.0002

(a) The low- and high-case SDs were obtained using Eq. (D.1) with inputs to the equation given by the nominal values and the low- and high-case range values in Table D.10.

(b) An empty cell means that the GFC does not contain the given oxide in measurable quantities.

Table D.8. GFC Nominal Compositions (G_{ijk}^{GFC}) and SDs Expressed as Mass Fractions of Oxides (cont.)

Oxide	Value Type	Rutile	Zincite	Zircon	Borax	Sodium Carbonate	Lithium Carbonate
Al_2O_3	Nominal	0.0050(a)	(b)	0.0025	(b)	(b)	(b)
	Low SD[(a)]	0.0016	(b)	0.0006	(b)	(b)	(b)
	High SD[(a)]	0.0020	(b)	0.0011	(b)	(b)	(b)
B_2O_3	Nominal	(b)	(b)	(b)	0.3750	(b)	(b)
	Low SD	(b)	(b)	(b)	0.0027	(b)	(b)
	High SD	(b)	(b)	(b)	0.0053	(b)	(b)
CaO	Nominal	(b)	(b)	(b)	(b)	0	0
	Low SD	(b)	(b)	(b)	(b)	0.00002	0.0052
	High SD	(b)	(b)	(b)	(b)	0.00005	0.0103
CdO	Nominal	(b)	0.0001	(b)	(b)	(b)	(b)
	Low SD	(b)	0.00002	(b)	(b)	(b)	(b)
	High SD	(b)	0.00006	(b)	(b)	(b)	(b)
Cl	Nominal	(b)	(b)	(b)	0	0.0002	0.0001
	Low SD	(b)	(b)	(b)	0.0002	0.00004	0.00002
	High SD	(b)	(b)	(b)	0.0003	0.00005	0.00002
Cr_2O_3	Nominal	0.0016	(b)	(b)	(b)	0	0.0001
	Low SD	0.0015	(b)	(b)	(b)	0.0001	0.00004
	High SD	0.0030	(b)	(b)	(b)	0.0002	0.00004
Fe_2O_3	Nominal	0.0070	0	0.0008	0	0	0
	Low SD	0.0053	0.00002	0.00006	0.00002	0.00002	0.00002
	High SD	0.0094	0.00002	0.00012	0.00002	0.00002	0.00002
K_2O	Nominal	(b)	(b)	(b)	(b)	(b)	0
	Low SD	(b)	(b)	(b)	(b)	(b)	0.00002
	High SD	(b)	(b)	(b)	(b)	(b)	0.00002
Li_2O	Nominal	(b)	(b)	(b)	(b)	(b)	0.4020
	Low SD	(b)	(b)	(b)	(b)	(b)	0.0009
	High SD	(b)	(b)	(b)	(b)	(b)	0.0018
MgO	Nominal	(b)	(b)	(b)	(b)	0	0.0001
	Low SD	(b)	(b)	(b)	(b)	0.00002	0.00004
	High SD	(b)	(b)	(b)	(b)	0.00005	0.00004
MnO	Nominal	(b)	0	(b)	(b)	(b)	(b)
	Low SD	(b)	0.00002	(b)	(b)	(b)	(b)
	High SD	(b)	0.00002	(b)	(b)	(b)	(b)
Na_2O	Nominal	(b)	(b)	(b)	0.1670	0.5837	0.0008
	Low SD	(b)	(b)	(b)	0.0012	0.0004	0.0002
	High SD	(b)	(b)	(b)	0.0024	0.0007	0.0003
P_2O_5	Nominal	0	(b)	(b)	(b)	(b)	(b)
	Low SD	0.0002	(b)	(b)	(b)	(b)	(b)
	High SD	0.0003	(b)	(b)	(b)	(b)	(b)
PbO	Nominal	(b)	0	(b)	(b)	(b)	(b)
	Low SD	(b)	0.00002	(b)	(b)	(b)	(b)
	High SD	(b)	0.00002	(b)	(b)	(b)	(b)
SO_3	Nominal	0	(b)	(b)	0	0.0001	0.0003
	Low SD	0.0002	(b)	(b)	0.0001	0.00004	0.00008
	High SD	0.0003	(b)	(b)	0.0002	0.00006	0.00010
SiO_2	Nominal	0.0220	(b)	0.3225	(b)	(b)	(b)
	Low SD	0.0053	(b)	0.0010	(b)	(b)	(b)
	High SD	0.0060	(b)	0.0020	(b)	(b)	(b)
TiO_2	Nominal	0.9320	(b)	0.0010	(b)	(b)	(b)
	Low SD	0.0016	(b)	0.0001	(b)	(b)	(b)
	High SD	0.0033	(b)	0.0003	(b)	(b)	(b)
UO_3	Nominal	(b)	(b)	0.0004	(b)	(b)	(b)
	Low SD	(b)	(b)	0.00006	(b)	(b)	(b)
	High SD	(b)	(b)	0.00022	(b)	(b)	(b)

Table D.8. GFC Nominal Compositions (G_{ijk}^{GFC}) and SDs Expressed as Mass Fractions of Oxides (cont.)

Oxide	Value Type	Rutile	Zincite	Zircon	Borax	Sodium Carbonate	Lithium Carbonate
V2O5	Nominal	0.0045	(b)	(b)	(b)	(b)	(b)
	Low SD	0.0009	(b)	(b)	(b)	(b)	(b)
	High SD	0.0022	(b)	(b)	(b)	(b)	(b)
ZnO	Nominal	(b)	0.9990	(b)	(b)	(b)	(b)
	Low SD	(b)	0.0015	(b)	(b)	(b)	(b)
	High SD	(b)	0.0030	(b)	(b)	(b)	(b)
ZrO2	Nominal	0.0190	(b)	0.6600	(b)	(b)	(b)
	Low SD	0.0053	(b)	0.0041	(b)	(b)	(b)
	High SD	0.0064	(b)	0.0082	(b)	(b)	(b)

(a) The low-case and high-case SDs were obtained via a formula for the SD of a triangular distribution whereas the low-case and high-case distributions are specified by the nominal and range values in Table D.10.

(b) An empty cell means that the GFC does not contain the given oxide in measurable quantities.

Table D.9. Nominal ILAW Vessel Volumes and Estimated SDs (in liters)

Volume[(a)]	Nominal Value (L)	SDs (L)[(b)]	
		Low SD (L)	High SD (L)
CRV Before	50,084.783	181.62	363.24
CRV After	41,458.776	181.62	363.24
MFPV Before (Heel)	9,577.092	112.12	224.24
MFPV After	18,203.099	112.12	224.24

(a) "CRV Before" refers to the full CRV before a transfer to the MFPV. "CRV After" refers to the CRV after the first transfer to the MFPV. "MFPV Before" refers to the MFPV before a transfer from the CRV (i.e., the MFPV heel). "MFPV After" refers to the MFPV after a CRV transfer, but before GFCs are added.

(b) Low-case SDs are based on values from Table 5.13 in Heredia-Langner et al. (2003). High-case SDs are twice the low-case SDs.

Table D.10. Nominal ILAW Volume (in liters) of Water Added to MFPV to Lower Sodium Molarity

AP-101 Envelope A (L)	AZ-101 Envelope B (L)	AN-107 Envelope C (L)
0	4980.6[(a)]	0

(a) Based on a calculation by the WTP Project to lower sodium molarity from 4.31 to 2.75.

Table D.11. Nominal Compositions for Glass Made from the LAW MFPV (in mass fractions) for One Tank Each of LAW Waste Envelopes A, B, and C[a]

Component	AP-101 Envelope A	AZ-101 Envelope B	AN-107 Envelope C	Component	AP-101 Envelope A	AZ-101 Envelope B	AN-107 Envelope C
Ag_2O	3.58E-07	1.08E-07	0	ZnO	0.029488	0.048417	0.031067
Al_2O_3	0.060875	0.061757	0.06708	ZrO_2	0.029928	0.031829	0.030545
As_2O_5	2.04E-06	8.33E-06	0	Cl	0.002096	2.61E-05	0.000814
B_2O_3	0.099512	0.100654	0.103749	F	0.003062	0.000764	0.001468
BaO	3.89E-07	4.49E-08	0	SO_3	0.003601	0.005579	0.003144
BeO	3.88E-06	1.12E-07	0	**Radionuclide Oxide**	**AP-101 Envelope A**	**AZ-101 Envelope B**	**AN-107 Envelope C**
Bi_2O_3	0	0	0				
CaO	0.019954	0.070738	0.052105	$^{241}Am_2O_3$	3.98E-11	8.84E-11	5.00E-07
Ce_2O_3	0	0	0	$^{144}Ce_2O_3$[c]	2.67E-14	4.40E-11	0
CdO	2.41E-06	6.89E-08	0	$^{242}Cm_2O_3$	3.17E-17	6.70E-15	0
Cr_2O_3	0.000293	0.000425	0.000249	$^{243+244}Cm_2O_3$	2.14E-14	8.50E-13	0
Cs_2O	5.71E-06	0	0.001666	^{60}CoO	2.88E-12	7.87E-12	5.22E-08
CuO	2.12E-06	1.26E-07	0	$^{51}Cr_2O_3$	1.36E-15	2.57E-12	0
Fe_2O_3	0.053485	0.052536	0.055314	$^{134}Cs_2O$	8.95E-15	6.56E-12	0
K_2O	0.039755	0.001841	0.000861	$^{137}Cs_2O$	1.19E-12	1.76E-07	1.02E-06
La_2O_3	8.06E-07	2.36E-07	1.75E-05	$^{152}Eu_2O_3$	1.57E-13	5.17E-11	0
Li_2O	7.74E-07	0.043086	0	$^{154}Eu_2O_3$	2.83E-13	3.58E-11	1.58E-08
MgO	0.014958	0.029197	0.015604	$^{155}Eu_2O_3$	7.39E-14	1.90E-10	5.85E-09
MnO	9.45E-05	0.000197	0.00016	$^{59}Fe_2O_3$[c]	6.86E-16	2.26E-13	0
MoO_3	0.000023	5.15E-05	0	$^{95}Nb_2O_5$	3.56E-16	0	4.55E-11
Na_2O	0.183674	0.054066	0.146512	^{63}NiO	5.56E-11	0	0
Nd_2O_3	0	0	0	$^{237}NpO_2$	0	0	0
NiO	0.000134	0.000241	0.000402	$^{236}PuO_2$	1.05E-16	5.17E-14	0
P_2O_5	0.00096	0.000624	0.001346	$^{238}PuO_2$	1.95E-13	2.95E-11	0
PbO	1.71E-05	2.88E-06	0.000186	$^{239}PuO_2$	3.88E-10	6.77E-08	8.12E-06
PdO	0	0	0	$^{241}PuO_2$	1.58E-12	2.37E-10	0
Rh_2O_3	0	0	0	$^{106}Rh_2O_3$[d]	2.53E-19	0	0
RuO_2	0	0	0	$^{103}RuO_2$[c]	4E-16	8.24E-13	0
Sb_2O_3	5.31E-08	2.41E-06	0	$^{106}RuO_2$	2.89E-13	0	0
SeO_2	1.71E-06	1.41E-06	0	$^{125}Sb_2O_3$	0	0	0
SiO_2	0.437526	0.483091	0.470281	$^{79}SeO_2$	2.2E-10	1.13E-06	4.60E-08
SnO_2	0	0	0	$^{151}Sm_2O_3$	4.24E-11	1.08E-09	0
SrO	2.38E-07	7.13E-08	0	$^{113}SnO_2$	1.57E-15	3.61E-12	8.21E-12
ThO_2	6.6E-09	4.58E-06	0	$^{126}SnO_2$	1.2E-08	3.96E-05	1.85E-06
TiO_2	0.020082	0.014698	0.012169	^{90}SrO	5.52E-10	5.41E-07	2.34E-08
Tl_2O	1.98E-08	2.09E-06	0	$^{99}Tc_2O_7$	0	0	0
UO_3	6.49E-05	9.67E-06	0	$^{232}ThO_2$	0.000252	0	0
V_2O_5	0.000105	7.53E-05	6.05E-05	$^{88}Y_2O_3$[c]	1.11E-15	3.66E-13	2.50E-11
WO_3	3.82E-05	2.59E-05	0	**Total**[b]	1.000	1.000	1.000

(a) The compositions in this table were provided by the WTP Project.
(b) The table values may not sum to one exactly due to rounding, but the electronic data values to more decimal places do sum to one.
(c) These short-lived radionuclide oxides will be deleted in future work.
(d) This radionuclide oxide will be combined with that of Ru-106 in future work.

Appendix E

Derivations and Details of Compliance Methods for IHLW Specifications

Appendix E: Derivations and Details of Compliance Methods for IHLW Specifications

This appendix presents the derivations or additional details of immobilized high-level waste (IHLW) compliance methods presented in Section 4. Only those methods needing derivation or additional detail are addressed here.

E.1 Equation for Calculating the Means of IHLW Chemical Composition Components over an HLW Waste Type

This section presents the derivation of the equation for calculating the means of IHLW chemical composition components over a high-level waste (HLW) waste type. This equation is required to implement the Waste Treatment and Immobilization Plant (WTP) IHLW compliance strategy for the Waste Acceptance Product Specifications (WAPS) 1.1.2, Chemical Composition During Production. The methods for implementing the strategy are presented in Section 4.1.4.

The derivation of Eq. (4.1.2) in Section 4.1.4 for the mean (mass-weighted-average) mass fraction of the j^{th} IHLW component (oxide or halogen) over the I Melter Feed Preparation Vessel (MFPV) batches corresponding to an HLW waste type is given by:

$$\bar{\bar{g}}_j^{MFPV} = \frac{\sum_{i=1}^{I}\left(\sum_{j=1}^{J}\bar{m}_{ij}^{MFPV}\right)\bar{g}_{ij}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J}\bar{m}_{ij}^{MFPV}} = \frac{\sum_{i=1}^{I}\left(\sum_{j=1}^{J}\bar{m}_{ij}^{MFPV}\right)\dfrac{\bar{m}_{ij}^{MFPV}}{\sum_{j=1}^{J}\bar{m}_{ij}^{MFPV}}}{\sum_{i=1}^{I}\sum_{j=1}^{J}\bar{m}_{ij}^{MFPV}}$$

$$= \frac{\sum_{i=1}^{I}\bar{m}_{ij}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J}\bar{m}_{ij}^{MFPV}} = \frac{\sum_{i=1}^{I}\bar{c}_{ij}^{MFPV} f_j u\bar{V}_i^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J}\bar{c}_{ij}^{MFPV} f_j u\bar{V}_i^{MFPV}}$$

$$= \frac{\sum_{i=1}^{I}\left(\dfrac{1}{n_S^{MFPV} n_A^{MFPV}}\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}} c_{ijlm}^{MFPV}\right)\left(\dfrac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV}\right) f_j}{\sum_{i=1}^{I}\sum_{j=1}^{J}\left(\dfrac{1}{n_S^{MFPV} n_A^{MFPV}}\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}} c_{ijlm}^{MFPV}\right)\left(\dfrac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV}\right) f_j} \quad \text{for } j = 1,\cdots,J \tag{E.1.1}$$

where:

$\bar{\bar{g}}_j^{MFPV}$ = mean (mass-weighted-average) mass fraction of the j^{th} IHLW component over I MFPV batches, based on averages over n_S^{MFPV} samples per MFPV batch, n_A^{MFPV}

analyses per sample, and n_V^{MFPV} volume determinations per MFPV batch (g_{oxide}/g_{oxides})

I = number of MFPV batches corresponding to an HLW waste type

J = number of IHLW components (non-radionuclide and radionuclide oxides and halogens) estimated for the IHLW composition corresponding to each MFPV batch

$\overline{m}_{ij}^{MFPV}$ = mass of the j^{th} IHLW component for the i^{th} MFPV batch averaged over n_S^{MFPV} samples per MFPV batch, n_A^{MFPV} analyses per sample, and n_V^{MFPV} volume determinations per MFPV batch (g_{oxide})

$\overline{g}_{ij}^{MFPV}$ = mass fraction of the j^{th} IHLW component in glass that would be made from the i^{th} MFPV batch averaged over n_S^{MFPV} samples per MFPV batch and n_A^{MFPV} analyses per sample (g_{oxide}/g_{oxides})

$\overline{c}_{ij}^{MFPV}$ = concentration of the j^{th} analyte (element or radionuclide) averaged over n_S^{MFPV} samples per MFPV batch and n_A^{MFPV} analyses per sample (μg/mL = mg/L)

f_j = $\frac{MW_j^{oxide}}{MW_j^{analyte}} R_j$ where MW_j^{oxide} and $MW_j^{analyte}$ are the molecular weights of oxide j and analyte j, respectively, and R_j is the ratio of moles of oxide per mole of analyte for oxide j. Hence, f_j is the factor for converting the concentration of analyte j (μg analyte j/mL = mg analyte j/L) to the concentration of oxide j (μg oxide j/mL = mg oxide/L). The quantity f_j is called the oxide factor for oxide j.

u = $\frac{1\,(g)}{1000\,(mg)}$, a units conversion factor for converting mg to g

$\overline{V}_i^{MFPV}$ = average volume over n_V^{MFPV} volume determinations of the i^{th} MFPV batch (L)

n_S^{MFPV} = number of samples per MFPV batch

n_A^{MFPV} = number of chemical analyses per MFPV sample

c_{ijlm}^{MFPV} = analyzed concentration of the j^{th} analyte from the m^{th} analysis of the l^{th} sample from the i^{th} MFPV batch (μg/mL = mg/L)

n_V^{MFPV} = number of volume measurements per MFPV batch

V_{ih}^{MFPV} = the h^{th} volume determination of the i^{th} MFPV batch (L).

Note that the "units correction factor" u, which is a constant, cancels out of the equation.

E.2 Equation for CL% Upper Combined Confidence Intervals on PCT Normalized Releases of B, Li, and Na for a Single IHLW MFPV Batch

This section presents the derivation of the equation for calculating CL% upper combined confidence interval (CL% UCCI) values for Product Consistency Test (PCT) normalized releases of B, Li, and Na corresponding to a single IHLW MFPV batch. The equation is derived for the case $n_S^{MFPV} > 1$ and $n_A^{MFPV} \geq 1$. This equation is required to implement one aspect of the WTP IHLW compliance strategy for WAPS 1.3, Product Consistency. The methods for implementing the strategy are presented in Section 4.3.3.2.

An appropriate statistical interval for demonstrating compliance with WAPS 1.3 for each IHLW MFPV batch is a CL% UCCI, the concept of which was introduced in Section 3.1. Section A.3 of Appendix A discusses the statistical method for combining model and composition uncertainties that is used in forming a CL% UCCI. The CL% UCCI formula is given in general by

$$CL\%\ UCCI\left(y_i^h\right) = \bar{\hat{y}}_i^h + CHW_{i,CL\%\ UCI}^h + MHW_{i,CL\%\ SUCI}^h \qquad \text{(E.2.1)}$$

where

$CL\%\ UCCI\left(y_i^h\right)$ = CL% UCCI for the true, unknown mean value of $y_i^h = ln\left(r_i^{PCT\ h}\right)$, that is, the natural logarithm of the PCT normalized release of element h (= B, Li, or Na) from IHLW corresponding to the i^{th} MFPV batch [ln(g/L)]

$\bar{\hat{y}}_i^h$ = mean of model-predicted $\hat{y}_{ilm}^h = \hat{ln}\left(r_{ilm}^{PCT\ h}\right)$ values over the n_S^{MFPV} samples and n_A^{MFPV} analyses per sample of the i^{th} MFPV batch [ln(g/L)]

$CHW_{i,CL\%\ UCI}^h$ = composition uncertainty half-width for a CL% upper confidence interval (CL% UCI) for the PCT normalized release of element h for IHLW corresponding to the i^{th} MFPV batch

$MHW^{h}_{i,CL\%\ SUCI}$ = model uncertainty half-width for a CL% simultaneous upper confidence interval (CL% SUCI) for the PCT normalized release of element *h* for IHLW corresponding to the i^{th} MFPV batch.

Equations for the terms on the right hand side of Eq. (E.2.1) are now given for the case of $n_S^{MFPV} > 1$ samples and $n_A^{MFPV} \geq 1$ analyses per sample of the i^{th} MFPV batch.

The quantity $\bar{\hat{y}}_i^h$ in Eq. (E.2.1) is given by

$$\bar{\hat{y}}_i^h = \frac{\sum_{l=1}^{n_S^{MFPV}} \sum_{m=1}^{n_A^{MFPV}} \left(\sum_{k=1}^{n_{mc}^h} b_k^h \, x_{iklm}^{MFPV} \right)}{n_S^{MFPV} \, n_A^{MFPV}} \tag{E.2.2}$$

where the notation is as defined in Sections 4.3.3.1 and 4.3.3.2.

The quantity $CHW^{h}_{i,CL\%\ UCI}$ in Eq. (E.2.1) is given by

$$CHW^{h}_{i,CL\%\ UCI} = t_{1-\alpha,df} \sqrt{\frac{\left[SD_S^{MFPV}(\hat{y}_{ilm}^h)\right]^2}{n_S^{MFPV}} + \frac{\left[SD_A^{MFPV}(\hat{y}_{ilm}^h)\right]^2}{n_S^{MFPV} \, n_A^{MFPV}}} \tag{E.2.3}$$

where

$t_{1-\alpha,df}$ = CL% = 100(1 – α) percentile of Student's t-distribution with *df* degrees of freedom

$SD_S^{MFPV}(\hat{y}_{ilm}^h)$ = standard deviation of $\hat{y}_{ilm}^h$ values due to composition uncertainty resulting from mixing/sampling uncertainty for the i^{th} MFPV batch [ln(g/L)]

$SD_A^{MFPV}(\hat{y}_{ilm}^h)$ = standard deviation of $\hat{y}_{ilm}^h$ values due to composition uncertainty resulting from analytical uncertainty for the i^{th} MFPV batch [ln(g/L)]

and the remaining notation is as previously defined following Eq. (E.1.1). When $n_A^{MFPV} > 1$, statistical variance component estimation methods must be applied to the $\hat{y}_{ilm}^h$ ($l = 1, 2, \ldots, n_S^{MFPV}$; $m = 1, 2, \ldots, n_A^{MFPV}$) values to calculate $SD_S^{MFPV}(\hat{y}_{ilm}^h)$ and $SD_A^{MFPV}(\hat{y}_{ilm}^h)$. For balanced data (i.e., n_A^{MFPV} the same for every MFPV sample), the analysis of variance (ANOVA) method can be used to estimate the variance components. First, the ANOVA mean squares for mixing/sampling and analytical are given respectively by

$$MS_S^{MFPV} = n_A^{MFPV} \sum_{l=1}^{n_S^{MFPV}} \left(\bar{\hat{y}}_{il}^h - \bar{\hat{y}}_i^h\right)^2 \Big/ \left(n_S^{MFPV} - 1\right) \tag{E.2.4}$$

and

$$MS_A^{MFPV} = \sum_{l=1}^{n_S^{MFPV}} \sum_{m=1}^{n_A^{MFPV}} \left(\hat{y}_{ilm}^h - \bar{\hat{y}}_{il}^h\right)^2 \Big/ \left(n_A^{MFPV} - 1\right) \tag{E.2.5}$$

Equating these mean squares to the quantities they estimate gives

$$\begin{aligned} MS_S^{MFPV} &= n_A^{MFPV} \left[SD_S^{MFPV}(\hat{y}_{ilm}^h)\right]^2 + \left[SD_A^{MFPV}(\hat{y}_{ilm}^h)\right]^2 \\ MS_A^{MFPV} &= \left[SD_A^{MFPV}(\hat{y}_{ilm}^h)\right]^2 \end{aligned} \tag{E.2.6}$$

Solving these equations for the two variance components gives

$$\begin{aligned} \left[SD_S^{MFPV}(\hat{y}_{ilm}^h)\right]^2 &= \frac{MS_S^{MFPV} - MS_A^{MFPV}}{n_A^{MFPV}} \\ \left[SD_A^{MFPV}(\hat{y}_{ilm}^h)\right]^2 &= MS_A^{MFPV} \end{aligned} \tag{E.2.7}$$

Finally, the quantity inside the square root symbol in Eq. (E.2.3) can be obtained from Eqs. (E.2.7) and (E.2.4) as

$$\begin{aligned} &\frac{\left[SD_S^{MFPV}(\hat{y}_{ilm}^h)\right]^2}{n_S^{MFPV}} + \frac{\left[SD_A^{MFPV}(\hat{y}_{ilm}^h)\right]^2}{n_S^{MFPV} n_A^{MFPV}} = \frac{MS_S^{MFPV} - MS_A^{MFPV}}{n_S^{MFPV} n_A^{MFPV}} + \frac{MS_A^{MFPV}}{n_S^{MFPV} n_A^{MFPV}} \\ &= \frac{MS_S^{MFPV}}{n_S^{MFPV} n_A^{MFPV}} = \frac{n_A^{MFPV} \sum_{l=1}^{n_S^{MFPV}} \left(\bar{\hat{y}}_{il}^h - \bar{\hat{y}}_i^h\right)^2 \Big/ \left(n_S^{MFPV} - 1\right)}{n_S^{MFPV} n_A^{MFPV}} = \frac{\sum_{l=1}^{n_S^{MFPV}} \left(\bar{\hat{y}}_{il}^h - \bar{\hat{y}}_i^h\right)^2 \Big/ \left(n_S^{MFPV} - 1\right)}{n_S^{MFPV}} \end{aligned} \tag{E.2.8}$$

Substituting Eq. (E.2.8.) into Eq. (E.2.3) yields

$$\begin{aligned} CHW_{i,CL\%\ UCI}^h &= t_{1-\alpha,df} \sqrt{\frac{\left[SD_S^{MFPV}(\hat{y}_{ilm}^h)\right]^2}{n_S^{MFPV}} + \frac{\left[SD_A^{MFPV}(\hat{y}_{ilm}^h)\right]^2}{n_S^{MFPV} n_A^{MFPV}}} \\ &= t_{1-\alpha,n_S^{MFPV}-1} \sqrt{\frac{\sum_{l=1}^{n_S^{MFPV}} \left(\bar{\hat{y}}_{il}^h - \bar{\hat{y}}_i^h\right)^2 \Big/ \left(n_S^{MFPV} - 1\right)}{n_S^{MFPV}}} \end{aligned} \tag{E.2.9}$$

Note that the degrees of freedom in Eq. (E.2.19) is $df = n_S^{MFPV} - 1$, so n_S^{MFPV} must be > 1.

The quantity $MHW_{i,CL\%\ SUCI}^{h}$ in Eq. (E.2.1) is given by

$$MHW_{i,CL\%\ SUCI}^{h} = \sqrt{p\, F_{1-\alpha}(p, n-p)}\left(\sqrt{(\bar{\boldsymbol{x}}_i^{MFPV})^{\mathrm{T}}\, \hat{\boldsymbol{\Sigma}}_{\boldsymbol{b}}^{h}\, \bar{\boldsymbol{x}}_i^{MFPV}}\right) \tag{E.2.10}$$

where

p = number of coefficients in the property-composition model for the PCT normalized release of element h = B, Li, or Na. For a model of the form in Eq. (4.3.2a), $p = n_{mc}^{h}$.

$F_{1-\alpha}(p, n-p)$ = CL% = 100(1 – α) percentile of an F-distribution with p numerator degrees of freedom and $n - p$ denominator degrees of freedom, where n is the number of data points used to fit the model for $ln\left(r^{PCT\ h}\right)$, and p is the number of model coefficients estimated from the data

$\bar{\boldsymbol{x}}_i^{MFPV}$ = $p \times 1$ column vector whose entries $\bar{x}_{ik}^{MFPV}$, $k = 1, 2, \cdots, p$ are means of the x_{iklm}^{MFPV} [as given by Eq. (4.3.3)] values where l = 1, 2, … , n_S^{MFPV}, and m = 1, 2, … , n_A^{MFPV}

$\hat{\boldsymbol{\Sigma}}_b^h$ = estimate of the $p \times p$ variance-covariance matrix of the model coefficient vector $\boldsymbol{b}^h$ for the PCT normalized release of h = B, Li, or Na. The variances of the coefficients are located on the diagonal of the matrix, and the covariances between pairs of coefficients are located on the off-diagonal positions of the matrix

and the remaining notation is as previously defined following Eq. (4.3.2a). General equations for calculating model variance-covariance matrices such as $\hat{\boldsymbol{\Sigma}}_b^h$ are given in Section A.3 of Appendix A.

In summary, the formula for calculating a CL% UCCI in the case of $n_S^{MFPV} > 1$ and $n_A^{MFPV} \geq 1$ is given by Eq. (E.2.1) with substitutions of its parts from Eqs. (E.2.2), E.2.9), and (E.2.10).

E.3 Equation for X%/Y% Upper Tolerance Intervals on PCT Normalized Releases of B, Li, and Na over an HLW Waste Type

This section presents the derivation of the equation for calculating X%/Y% upper tolerance interval (X%/Y% UTI) values for IHLW PCT normalized releases of B, Li, and Na over an HLW waste type.

This equation is required to implement the WTP IHLW compliance strategy for WAPS 1.3, Product Consistency. The methods for implementing the strategy are presented in Section 4.3.5.

An appropriate statistical interval for demonstrating with high (X%) confidence that a high percentage (Y%) of IHLW produced from an HLW waste type satisfies the PCT limits in Eq. (4.3.1) is a X%/Y% UTI, the concept of which was introduced in Section 3.2. Section A.3 of Appendix A discusses the statistical method for combining model and composition uncertainties that is used in forming a X%/Y% UTI. Piepel and Cooley (2002) derived the equations necessary to calculate an X%/Y% UTI for a compliance strategy that matches the current WTP Project's IHLW compliance strategy (see Section 2.2).

The general formula for a one-sided X%/Y% UTI applicable to IHLW PCT property-composition models is

$$\text{X\%/Y\% UTI} = \tilde{\mu} + k(X,Y)\,\tilde{\sigma} \qquad \text{(E.3.1)}$$

where

X%/Y% UTI = a value that with X% confidence captures Y% of the distribution (population) of true mean ln(PCT releases) over the MFPV batches corresponding to an HLW waste type [ln(g/L)]

$\tilde{\mu}$ = estimate of the population mean that is calculated by forming the average model-predicted ln(PCT release) for each MFPV batch and averaging them across all MFPV batches corresponding to an HLW waste type [ln(g/L)]

$k(X, Y)$ = tolerance interval multiplier that is implicitly a function of X, Y, degrees of freedom associated with $\tilde{\sigma}$ and other parameters

$\tilde{\sigma}$ = estimate of the population standard deviation that properly accounts for (1) variation in ln(PCT release) across MFPV batches corresponding to an HLW waste type, (2) mixing/sampling and analytical uncertainties for each MFPV batch, and (3) model uncertainty [ln(g/L)].

The parameters X and Y generally should have values between 90% (or 95%) and 100% to provide high confidence that a high percentage of IHLW produced from an HLW waste type satisfies the WAPS 1.3 requirements. However, X and Y can never take values of 100% because it is impossible to be 100% confident about 100% of the true distribution of ln(PCT releases) given estimated IHLW composition variation as well as IHLW composition and model uncertainties.

Equations for the terms on the right hand side of Eq. (E.3.1) are given in Section 4.3.5 for the case of $n_S^{MFPV} > 1$ samples and $n_A^{MFPV} = 1$ analyses per sample of the i^{th} MFPV batch. In this section, the equations for the terms on the right hand side of Eq. (E.3.1) are given for the more general case of $n_S^{MFPV} > 1$ samples and $n_A^{MFPV} \geq 1$ analyses per sample of the i^{th} MFPV batch.

The equation for $\tilde{\mu}$ in Eq. (E.3.1) is given by

$$\tilde{\mu} = \bar{\bar{\hat{y}}}^{h}_{I} = \frac{\sum_{i=1}^{I} \bar{\hat{y}}^{h}_{i}}{I} = \frac{1}{I}\sum_{i=1}^{I}\left[\frac{\sum_{l=1}^{n_S^{MFPV}}\sum_{m=1}^{n_A^{MFPV}}\left(\sum_{k=1}^{n^{h}_{mc}} b^{h}_{k}\, x^{MFPV}_{iklm}\right)}{n_S^{MFPV}\, n_A^{MFPV}}\right] \tag{E.3.2}$$

where

$\bar{\bar{\hat{y}}}^{h}_{I}$ = average of the $\bar{\hat{y}}^{h}_{i}$, $i = 1, 2, \ldots, I$ values for the I MFPV batches corresponding to an HLW waste type

and the remaining notation is as previously defined in Section E.2 and in Section 4.3. Note that Eq. (E.3.2) calculates the ordinary mean (average) of the model-predicted property values over the IHLW compositions resulting from the n_S^{MFPV} samples per MFPV batch, the n_A^{MFPV} analyses per MFPV sample, and the I IHLW MFPV batches corresponding to an HLW waste type. An alternative approach would be to use $\hat{y}(\bar{\bar{\boldsymbol{x}}}^{MFPV})$, the model-predicted value for the normalized version of the mass-weighted-averaged composition over the I MFPV batches ($\bar{\bar{x}}^{MFPV}_{k}$, $k = 1, \ldots, n^{h}_{mc}$) that would result from supplying ($\bar{\bar{g}}^{MFPV}_{j}$, $j = 1, \ldots, J$) [calculated per Eq. (4.1.2) for balanced data and Eq. (4.1.5) for unbalanced data] to the normalizing transformation given in Eq. (4.3.3). Although this alternative approach would be consistent with some of the other compliance methods and calculations adopted in this report, it is contrary to the typical method for developing tolerance intervals.

In general, $k(X, Y)$ in Eq. (E.3.1) is calculated using the following equation

$$k(X,Y) = \frac{t(X,Y,df_{\tilde{\sigma}},\delta)}{\sqrt{I}} \tag{E.3.3}$$

where $t(X,Y,df_{\tilde{\sigma}},\delta)$ represents a non-centralized t-distribution with degrees of freedom $df_{\tilde{\sigma}}$ and non-centrality parameter δ, and I is the number of MFPV batches associated with an HLW waste type. This is Eq. (3.18d) in Piepel and Cooley (2002) adapted to the notation in this report. It is important to note that $k(X, Y)$ is determined so as to compensate for the effects of MFPV mixing/sampling uncertainty and analytical uncertainty, which are "nuisance uncertainties" with respect to the population for which an X%/Y% UTI is desired.

The expression for $df_{\tilde{\sigma}}$ in Eq. (E.3.3) is given by

$$df_{\tilde{\sigma}} \approx \frac{\left[\left(SD_M\left[\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})\right]\right)^2 + \frac{MS_I}{n_S^{MFPV} n_A^{MFPV}}\right]^2}{\frac{\left[\left(SD_M\left[\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})\right]\right)^2\right]^2}{df_m} + \frac{\left[\frac{MS_I}{n_S^{MFPV} n_A^{MFPV}}\right]^2}{df_I}}$$

$$= \frac{\left[\left[(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^T \hat{\boldsymbol{\Sigma}}_b^h \bar{\bar{\boldsymbol{x}}}_I^{MFPV}\right] + \frac{n_S^{MFPV} n_A^{MFPV}\left[\sum_{i=1}^{I}(\bar{\hat{y}}_i^h - \bar{\bar{\hat{y}}}_I^h)^2 \Big/ (I-1)\right]}{n_S^{MFPV} n_A^{MFPV}}\right]^2}{\frac{\left[(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^T \hat{\boldsymbol{\Sigma}}_b^h \bar{\bar{\boldsymbol{x}}}_I^{MFPV}\right]^2}{df_m} + \frac{\frac{n_S^{MFPV} n_A^{MFPV}\left[\sum_{i=1}^{I}(\bar{\hat{y}}_i^h - \bar{\bar{\hat{y}}}_I^h)^2 \Big/ (I-1)\right]^2}{n_S^{MFPV} n_A^{MFPV}}}{I-1}}$$

$$= \frac{\left[\left[(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^T \hat{\boldsymbol{\Sigma}}_b^h \bar{\bar{\boldsymbol{x}}}_I^{MFPV}\right] + \sum_{i=1}^{I}(\bar{\hat{y}}_i^h - \bar{\bar{\hat{y}}}_I^h)^2 \Big/ (I-1)\right]^2}{\frac{\left[(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^T \hat{\boldsymbol{\Sigma}}_b^h \bar{\bar{\boldsymbol{x}}}_I^{MFPV}\right]^2}{df_m} + \frac{\left[\sum_{i=1}^{I}(\bar{\hat{y}}_i^h - \bar{\bar{\hat{y}}}_I^h)^2 \Big/ (I-1)\right]^2}{I-1}} \qquad \text{(E.3.4)}$$

where

$df_{\tilde{\sigma}}$ = approximate degrees of freedom associated with $\tilde{\sigma}$

$\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ = $p \times 1$ column vector whose entries $\bar{\bar{x}}_k^{MFPV}, k = 1, 2, \cdots, p$ are model-component-normalized versions of the $\bar{\bar{g}}_k^{MFPV}, k = 1, 2, \cdots, p$, which are mass-weighted-average compositions over the i = 1, 2, … , I MFPV batches, with ordinary averaging over the l = 1, 2, … , n_S^{MFPV} samples per MPFV batch and m = 1, 2, … , n_A^{MFPV} analyses per sample. Note that $p = n_{mc}^h$ because of the model form in Eq. (4.3.2a).

$\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})$ = model prediction of the PCT normalized release of h = B, Li, or Na for the mass-weighted-average IHLW composition $\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ [ln(g/L)]

$SD_M[\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})]$ = standard deviation of the model prediction for the mass-weighted-average IHLW composition $\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ [ln(g/L)]

MS_I = mean square for IHLW MFPV batches over the $I \times n_S^{MFPV} \times n_A^{MFPV}$ values of $\hat{y}_{ilm}^h$

I = number of IHLW MFPV batches corresponding to an HLW waste type

n_S^{MFPV} = number of samples per IHLW MFPV batch

n_A^{MFPV} = number of analyses per IHLW MFPV sample

$\hat{\boldsymbol{\Sigma}}_b^h$ = estimated $p \times p$ variance-covariance matrix of the model coefficient vector $\boldsymbol{b}^h$ for the PCT normalized release of h = B, Li, or Na

df_m = degrees of freedom for the model relating PCT normalized releases of h = B, Li, or Na to IHLW composition. This quantity is given by $n - p$ where n is the number of data points used to fit the model, and p is the number of model coefficients estimated using the data.

df_I = degrees of freedom for the I MFPV batches associated with an HLW waste type. This quantity is given by $I - 1$.

Note that $\bar{\hat{y}}_i^h$ is given by Eq. (E.2.2) and $\bar{\bar{\hat{y}}}_I^h$ is given by Eq. (E.3.2). The preceding derivation is based on the results in Appendix D of Piepel and Cooley (2002).

The expression for δ in Eq. (E.3.3) is given by

$$\delta = z_{1-\beta}\sqrt{I}\,\frac{\sigma_g}{\sigma} \tag{E.3.5}$$

where

$z_{1-\beta}$ = $100(1-\beta)$ percentile of the standard normal distribution

I = number of IHLW MFPV batches corresponding to an HLW waste type

σ_g = standard deviation of the distribution of true ln(PCT normalized release) values for IHLW produced from a given HLW waste type [ln(g/L)]

σ = $\left[\sigma_g^2 + \bar{\sigma}_m^2 + \frac{(\sigma_S^{MFPV})^2}{n_S^{MFPV}} + \frac{(\sigma_A^{MFPV})^2}{n_S^{MFPV} n_A^{MFPV}} \right]^{0.5}$ = standard deviation of the distribution of possible $\bar{\hat{y}}_i^h$ values over the *I* IHLW MFPV batches corresponding to an HLW waste type. Here $\bar{\sigma}_m$ denotes the model prediction standard deviation for the true average IHLW composition over an HLW waste type, σ_S^{MFPV} denotes the true sampling standard deviation expressed in model units, and σ_A^{MFPV} represents the true analytical standard deviation expressed in model units. [ln(g/L)]

Equations (E.3.4) and (E.3.5) for *f* and δ are based on Eqs. (3.18f) and (3.18e) in Section 3.7 and development work in Appendix H of Piepel and Cooley (2002).

The estimate of the population standard deviation $\tilde{\sigma}$ is discussed in Sections 3.4 and 3.5 of Piepel and Cooley (2002). Applying the notation used in this report to Eq. (3.18c) of Piepel and Cooley (2002) yields the following general equation for $\tilde{\sigma}$

$$\tilde{\sigma} = \sqrt{\left(SD_I(\hat{y}_{ilm}^h)\right)^2 + \left[SD_M\left(\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})\right)\right]^2 + \frac{\left(SD_S(\hat{y}_{ilm}^h)\right)^2}{n_S^{MFPV}} + \frac{\left(SD_A(\hat{y}_{ilm}^h)\right)^2}{n_S^{MFPV} n_A^{MFPV}}} \qquad \text{(E.3.6)}$$

where

$SD_I(\hat{y}_{ilm}^h)$ = standard deviation of $\hat{y}_{ilm}^h = \hat{l}n(r_{ilm}^{PCT\,h})$, $i = 1, 2, \ldots, I$; $l = 1, 2, \ldots, n_S^{MFPV}$; $m = 1, 2, \ldots, n_A^{MFPV}$ values corresponding to variation in IHLW composition over a waste type. The result is expressed in PCT model units [ln(g/L)]

$SD_M[\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})]$ = standard deviation of the model prediction for the mass-weighted-average IHLW composition $\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ [ln(g/L)]

$SD_S(\hat{y}_{ilm}^h)$ = standard deviation of $\hat{y}_{ilm}^h = \hat{l}n(r_{ilm}^{PCT\,h})$ values corresponding to MFPV mixing/sampling uncertainty in estimating IHLW compositions for MFPV samples. The result is expressed in PCT model units [ln(g/L)]

$SD_A(\hat{y}_{ilm}^h)$ = standard deviation in $\hat{y}_{ilm}^h = \hat{l}n(r_{ilm}^{PCT\,h})$ values corresponding to analytical uncertainty in estimating IHLW compositions for MFPV samples. The result is expressed in PCT model units [ln(g/L)]

n_S^{MFPV} = number of samples per MFPV batch

n_A^{MFPV} = number of analyses per MFPV sample.

The first term in Eq. (E.3.6) represents variation in PCT normalized release of B, Li, or Na for IHLW produced from a given HLW waste type. The second term represents model uncertainty. The third and fourth terms represent reduced (by averaging over multiple samples per MFPV batch) mixing/sampling uncertainty and reduced (by averaging over multiple analyses per MFPV sample) analytical uncertainty, where these uncertainties are expressed in model units.

The equation for $SD_M[\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})]$ in Eq. (E.3.6) is given by

$$SD_M[\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})] = \sqrt{(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^{\mathrm{T}}\,\hat{\boldsymbol{\Sigma}}_{\boldsymbol{b}}^h\,\bar{\bar{\boldsymbol{x}}}_I^{MFPV}} \tag{E.3.7}$$

where all notation is as defined in this section or Section 4.3.

The quantities $SD_I(\hat{y}_{ilm}^h)$, $SD_S(\hat{y}_{ilm}^h)$, and $SD_A(\hat{y}_{ilm}^h)$ in Eq. (E.3.6) can be estimated from the $\hat{y}^h(\boldsymbol{x}_{ilm}^{MFPV})$ values where $i = 1, 2, \ldots, I$; $l = 1, 2, \ldots, n_S^{MFPV}$; and $m = 1, 2, \ldots, n_A^{MFPV}$ using statistical variance component estimation methods. However, that is unnecessary because the sum of the first, third, and fourth terms on the right hand side of Eq. (E.3.6) can be jointly estimated as follows

$$\sqrt{\left(SD_I(\hat{y}_{ilm}^h)\right)^2 + \frac{\left(SD_S(\hat{y}_{ilm}^h)\right)^2}{n_S^{MFPV}} + \frac{\left(SD_A(\hat{y}_{ilm}^h)\right)^2}{n_S^{MFPV}\,n_A^{MFPV}}} = SD(\bar{\bar{\hat{y}}}_i^h) = \sqrt{\frac{\sum_{i=1}^{I}(\bar{\hat{y}}_i^h - \bar{\bar{\hat{y}}}_I^h)^2}{I-1}} \tag{E.3.8}$$

where the notation has been previously defined following Eq. (E.1.1) and Eq. (E.3.6).

Hence, the formula for calculating $\tilde{\sigma}$ in Eq. (E.3.1) is given by

$$\tilde{\sigma} = \sqrt{(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^{\mathrm{T}}\,\hat{\boldsymbol{\Sigma}}_{\boldsymbol{b}}^h\,\bar{\bar{\boldsymbol{x}}}_I^{MFPV} + \sum_{i=1}^{I}(\bar{\hat{y}}_i^h - \bar{\bar{\hat{y}}}_I^h)^2 \Big/ (I-1)} \tag{E.3.9}$$

after substituting Eqs. (E.3.7) and (E.3.8) into Eq. (E.3.6).

In summary, Eq. (E.3.1) is the basic equation for calculating an X%/Y% UTI, along with Eqs. (E.3.2), (E.3.3), (E.3.4), (E.3.5), and (E.3.9).

Appendix F

Derivations and Details of Compliance Methods for ILAW Specifications

Appendix F: Derivations and Details of Compliance Methods for ILAW Specifications

This appendix presents the derivations or additional details of immobilized low-activity waste (ILAW) compliance methods presented in Section 5. Only those methods needing derivation or additional detail are addressed here.

F.1 Equation for Calculating the Means of ILAW Chemical Composition Components over an LAW Waste Type

This section presents the derivation of the equation for calculating the means of ILAW chemical composition components over a low-activity waste (LAW) waste type. This equation is required to implement the Waste Treatment and Immobilization Plant (WTP) ILAW compliance strategy for Contract Specification 2.2.2.6.2, Chemical Composition During Production. The methods for implementing the strategy are presented in Section 5.1.4.

The derivation of Eq. (5.1.2) in Section 5.1.4 for the mean (mass-weighted-average) mass fraction of the j^{th} ILAW component (oxide or halogen) over the I Melter Feed Preparation Vessel (MFPV) batches corresponding to an LAW waste type is given by:

$$\overline{\overline{g}}_j^{MFPV} = \frac{\sum_{i=1}^{I}\left(\sum_{j=1}^{J}\overline{m}_{ij}^{MFPV}\right)\overline{g}_{ij}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J}\overline{m}_{ij}^{MFPV}} = \frac{\sum_{i=1}^{I}\left(\sum_{j=1}^{J}\overline{m}_{ij}^{MFPV}\right)\dfrac{\overline{m}_{ij}^{MFPV}}{\sum_{j=1}^{J}\overline{m}_{ij}^{MFPV}}}{\sum_{i=1}^{I}\sum_{j=1}^{J}\overline{m}_{ij}^{MFPV}} = \frac{\sum_{i=1}^{I}\overline{m}_{ij}^{MFPV}}{\sum_{i=1}^{I}\sum_{j=1}^{J}\overline{m}_{ij}^{MFPV}}$$

$$= \frac{\sum_{i=1}^{I}\left[\dfrac{1}{n_S^{CRV}n_A^{CRV}}\sum_{l=1}^{n_S^{CRV}}\sum_{m=1}^{n_A^{CRV}}c_{ijlm}^{CRV}f_j\overline{V}_i^{CRV\,to\,MFPV}u + \sum_{k=1}^{K}a_{ik}^{GFC}G_{ijk}^{GFC} + \overline{m}_{i-1,j}^{MFPV}\left(\dfrac{\dfrac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}}V_{i,h}^{MFPV\,Heel}}{\dfrac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}}V_{i-1,h}^{MFPV}}\right)\right]}{\sum_{i=1}^{I}\left[\sum_{j=1}^{J}\left(\dfrac{1}{n_S^{CRV}n_A^{CRV}}\sum_{l=1}^{n_S^{CRV}}\sum_{m=1}^{n_A^{CRV}}c_{ijlm}^{CRV}f_j\overline{V}_i^{CRV\,to\,MFPV}u\right) + \sum_{j=1}^{J}\sum_{k=1}^{K}a_{ik}^{GFC}G_{ijk}^{GFC} + \sum_{j=1}^{J}\overline{m}_{i-1,j}^{MFPV}\left(\dfrac{\dfrac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}}V_{i,h}^{MFPV\,Heel}}{\dfrac{1}{n_V^{MFPV}}\sum_{h=1}^{n_V^{MFPV}}V_{i-1,h}^{MFPV}}\right)\right]} \quad \text{(F.1.1)}$$

for $j = 1, \cdots, J$

with

$$\overline{m}_{i-1,j}^{MFPV} = \frac{1}{n_S^{CRV} n_A^{CRV}} \sum_{l=1}^{n_S^{CRV}} \sum_{m=1}^{n_A^{CRV}} c_{i-1,jlm}^{CRV} f_j \overline{V}_{i-1}^{CRV\,to\,MFPV} u + \sum_{k=1}^{K} a_{i-1,k}^{GFC} G_{i-1,jk}^{GFC} + \overline{m}_{i-2,j}^{MFPV} \left(\frac{\frac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i-1,h}^{MFPV\,Heel}}{\frac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i-2,h}^{MFPV}} \right) \qquad \text{(F.1.2)}$$

and

$$\overline{V}_i^{CRV\,to\,MFPV} = \frac{\hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,before}}}{\hat{\sigma}^2_{\overline{V}_i^{CRV\,before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,before}}} \left(\frac{\sum_{h=1}^{n_V^{CRV}} V_{ih}^{CRV\,before}}{n_V^{CRV}} - \frac{\sum_{h=1}^{n_V^{CRV}} V_{ih}^{CRV\,after}}{n_V^{CRV}} \right)$$

$$+ \frac{\hat{\sigma}^2_{\overline{V}_i^{CRV\,before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\,after}}}{\hat{\sigma}^2_{\overline{V}_i^{CRV\,before}} + \hat{\sigma}^2_{\overline{V}_i^{CRV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}} + \hat{\sigma}^2_{\overline{V}_i^{MFPV\,before}}} \left(\frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV\,after}}{n_V^{MFPV}} - \frac{\sum_{h=1}^{n_V^{MFPV}} V_{ih}^{MFPV\,before}}{n_V^{MFPV}} \right) \qquad \text{(F.1.3)}$$

where the bars in certain notations (e.g., $\overline{V}_{i-1}^{CRV\,to\,MFPV}$) denote averages. The $\hat{\sigma}^2_{\overline{V}_i^{MFPV\,after}}$ notation in Eq. (F.1.3) represents the variance of $\overline{V}_i^{MFPV\,after} = \frac{1}{n_V^{MFPV}} \sum_{h=1}^{n_V^{MFPV}} V_{i,h}^{MFPV\,After}$. The other variance notations in Eq. (F.1.3) have similar interpretations.

In Eqs. (F.1.1) to (F.1.3), the following notation is used:

$\overline{\overline{g}}_j^{MFPV}$ = mean (mass-weighted-average) mass fraction of the j^{th} ILAW component over I MFPV batches, based on averages over n_S^{CRV} samples per CRV batch, n_A^{CRV} analyses per sample, and n_V^{CRV} and n_V^{MFPV} volume determinations for CRV and MFPV volumes (g_{oxide}/g_{oxides})

I = number of MFPV batches per reporting or compliance period

n_S^{CRV} = number of samples per CRV batch

n_A^{CRV} = number of chemical analyses per CRV sample

c_{ijlm}^{CRV} = analyzed concentration of the j^{th} analyte from the m^{th} analysis of the l^{th} sample from the i^{th} CRV batch (μg/mL = mg/L)

J = number of glass oxide components

f_j = $\frac{MW_j^{oxide}}{MW_j^{analyte}} R_j$ where MW_j^{oxide} and $MW_j^{analyte}$ are the molecular weights of oxide j and analyte j, respectively, and R_j is the ratio of moles of oxide per mole of analyte for oxide j. Hence, f_j is the factor for converting the concentration of analyte j (µg analyte j/mL = mg analyte j/L) to the concentration of oxide j (µg oxide j/mL = mg oxide/L). The quantity f_j is called the oxide factor for oxide j.

u = $\frac{1(\text{g})}{1000(\text{mg})}$, a units conversion factor for converting mg to g

K = number of glass-forming chemicals (GFCs)

a_{ik}^{GFC} = mass of the k^{th} GFC added to the i^{th} MFPV batch (g)

G_{ijk}^{GFC} = mass of the j^{th} glass oxide component per mass of the k^{th} GFC for the i^{th} MFPV batch ($g_{\text{oxide } j}/g_{\text{GFC } k}$). The mass fractions G_{ijk}^{GFC} $j = 1, 2, \ldots, J$ for the k^{th} GFC can sum to less than 1.0 to the extent the GFC contains interstitial water or other components that will not survive in the glass. The nominal G_{ijk}^{GFC} mass fractions of glass oxide components in the GFCs should not change frequently over MFPV batches. However, the i subscript was retained in case these mass fractions change (1) from one vendor to another for the same GFC or (2) for different lots of a given GFC from the same vendor.

$\overline{m}_{i-1,j}^{MFPV}$ = mass of the j^{th} glass oxide component in the $(i-1)^{\text{st}}$ MFPV batch based on averages over multiple samples, analyses per sample, and volume determinations (g)

n_V^{MFPV} = number of volume determinations per MFPV batch

$V_i^{MFPV\ Heel}$ = volume of the MFPV Heel included in the i^{th} MFPV batch (L)

V_{i-1}^{MFPV} = volume of the $(i-1)^{\text{st}}$ MFPV batch (L). This is the total volume of the $(i\text{-}1)^{\text{st}}$ MFPV batch, including the MFPV Heel, waste transferred from the CRV, GFCs added, and any water that may be added. Water will typically be added to Envelope B LAW in the MFPV to lower the sodium molarity. It is not anticipated that LAW from Envelopes A and C will require adding water in the MFPV.

n_V^{CRV} = number of volume determinations per CRV batch

$V_i^{CRV\ before}$ = volume of the CRV before the transfer of material to the i^{th} MFPV batch (L)

$V_i^{CRV\ after}$ = volume of the CRV after the transfer of material to the i^{th} MFPV batch (L)

$V_i^{MFPV\ before}$ = volume of the MFPV before receipt of CRV material for the i^{th} MFPV batch

$V_i^{MFPV\ after}$ = volume of the MFPV after receipt of CRV material for the i^{th} MFPV batch but before receipt of GFCs or any added water (L).

The notations similar to V_{ih}^{MFPV}, but with different superscripts and subscripts, have similar meanings where the (1) superscripts indicate the different vessel conditions for which volume determinations are made and (2) subscripts denote the MFPV batch (i.e., "*i*-1" or "*i*-2").

F.2 Formula for the Tolerance Interval Multiplier Used in Demonstrating that ILAW Radionuclide Concentrations over an LAW Waste Type Meet Class C Limits

This section presents the derivation of the equation for the multiplier of an X%/Y% upper tolerance interval (X%/Y% UTI) for demonstrating that ILAW radionuclide concentrations over an LAW waste type meet Class C limits. X%/Y% UTIs on the sum-of-fractions of Class C ILAW radionuclide concentrations (see Section B.3.1.1 of Appendix B) are required to implement the WTP ILAW compliance strategy for one aspect of Contract Specification 2.2.2.8, Radionuclide Concentration Limits. The method for implementing this strategy is presented in Section 5.3.3.1.

The formula for an X%/Y% UTI on the sum-of-fractions of Class C ILAW radionuclide concentrations is given by

$$X\%/Y\%\ UTI = \overline{SF}_D^{Containers} + k(X,Y)\ SD(\overline{SF}_d^{Container}) \qquad \text{(F.2.1)}$$

where $\overline{SF}_D^{Containers}$ and $SD(\overline{SF}_d^{Container})$ are generic notations, with the specific notation and equations determined by whether the sum-of-fractions is for radionuclides in Table 1 or Table 2 of 10 CFR 61.55:

- Table 1: $\overline{SF1}_D^{Containers}$ and $SD(\overline{SF1}_d^{Container})$ are given respectively by Eq. (B.3.4) and (B.3.7) in Section B.3.1.1 of Appendix B
- Table 2: $\overline{SF2}_D^{Containers}$ and $SD(\overline{SF2}_d^{Container})$ are given respectively by Eqs. (B.3.5) and (B.3.9) in Section B.3.1.1 of Appendix B.

The remainder of this section discusses how to obtain the $k(X, Y)$ multiplier.

As discussed in Section B.3.1.1, $SD(\overline{SF1}_d^{Container})$ and $SD(\overline{SF2}_d^{Container})$ include (1) variation in sum-of-fractions values across the I MFPV batches and D ILAW containers associated with an ILAW waste type, (2) all uncertainties associated with estimating ILAW composition for each ILAW MFPV batch, and (3) the uncertainty associated with the estimate or measurement of the density of LAW glass in an ILAW container. Ideally, the desired X%/Y% UTI should be a statement about a distribution of sum-of-fractions subject to the variation in (1), but not the nuisance uncertainties in (2) and (3). An approach similar to that of Piepel and Cooley (2002) would ideally be used to obtain a multiplier $k(X, Y)$ that is adjusted for the inflation of $SD(\overline{SF1}_d^{Container})$ or $SD(\overline{SF2}_d^{Container})$ by nuisance uncertainties. The Piepel and Cooley (2002) approach was adapted in this report to obtain X%/Y% UTIs for IHLW Product Consistency Test (PCT) (Section 4.3.5), ILAW PCT, and Vapor Hydration Test (VHT) (Section 5.4.5). However, the situation for a sum-of-fractions of Class C radionuclides is quite different than for property-composition models for PCT and VHT, so that the Piepel and Cooley (2002) results could not be easily adapted. It was beyond the scope of the work documented in this report to develop the formula for a multiplier $k(X, Y)$ that is adjusted for the inflation of $SD(\overline{SF1}_d^{Container})$ or $SD(\overline{SF2}_d^{Container})$ by nuisance uncertainties. For now, the multiplier $k(X, Y)$ for a standard, textbook X%/Y% UTI is used. Such multipliers can be looked up in tables (e.g., Table A-7 in Natrella 1966) as a function of X (percent confidence), Y (percent of the distribution), and number of data points (i.e., number of ILAW MFPV batches). Such standard multipliers do not adjust for nuisance uncertainties so that the X%/Y% UTI is an X% confidence statement about at least Y% of the distribution of sum-of-fractions values that includes variation over the I ILAW MFPV batches and D ILAW containers corresponding to an LAW waste type. However, it also includes (or is inflated by) the nuisance uncertainties mentioned previously.

F.3 Equation for a CL% Upper Confidence Interval on the Running Average of ^{137}Cs or ^{90}Sr Concentrations over *D* ILAW Containers

This section presents the derivation of the equation for a CL% upper confidence interval (CL% UCI) on the running average of ^{137}Cs or ^{90}Sr concentrations in ILAW over an LAW waste type or other specified period of ILAW production. CL% UCIs are required to implement the WTP ILAW compliance strategy for demonstrating that running averages of ^{137}Cs and ^{90}Sr concentrations in ILAW are below the limits in Contract Specification 2.2.2.8. The methods for implementing the strategy are presented in Section 5.3.5.

The formula for a CL% UCI on the running average of ^{137}Cs or ^{90}Sr concentrations in ILAW, given by Eq. (5.3.3) in Section 5.3.5, is

$$CL\%\ UCI = \bar{\bar{r}}_{Dq}^{Container} + t_{1-\alpha,df}\ SD(\bar{\bar{r}}_{Dq}^{Container}) \qquad \text{(F.3.1)}$$

where the notation is as defined in Section 5.3.5. The running average $\bar{\bar{r}}_{Dq}^{Container}$ can be calculated using Eq. (B.3.13) in Section B.3.2.1 of Appendix B. The balance of this section derives the formula for $SD(\bar{\bar{r}}_{Dq}^{Container})$ and discusses the determination of df in $t_{1-\alpha,df}$.

The development of $SD(\bar{\bar{r}}_{Dq}^{Container})$ is now presented. To begin, the formula for $\bar{\bar{r}}_{Dq}^{Container}$ given in Eq. (B.3.13) is repeated here for clarity of the development

$$\bar{\bar{r}}_{Dq}^{Container} = \frac{\bar{\bar{g}}_q^{MFPV}\,\bar{\rho}_D^{Container}\,A_q}{f_q} \tag{F.3.2}$$

where

$\bar{\bar{r}}_{Dq}^{Container}$ = running average of activity-per-volume concentrations of the q^{th} radionuclide (q = ^{137}Cs and ^{90}Sr) over the D ILAW containers produced through a given point in time, based on averages over multiple samples, analyses per sample, and volume determinations (Ci/m^3)

and the remaining notation is as defined in Section B.3.2.1. The development of the formula for $SD(\bar{\bar{r}}_{Dq}^{Container})$ follows the procedure described in Goodman (1960), which was used to develop formulas for other standard deviations in Appendices A and B. The resulting formula is

$$\begin{aligned} SD(\bar{\bar{r}}_{Dq}^{Container}) &= \left(\frac{A_q}{f_q}\right)\left[\begin{array}{l}\left[\bar{\bar{g}}_q^{MFPV}\right]^2\left[SD(\bar{\rho}_D^{Container})\right]^2 + \left[\bar{\rho}_D^{Container}\right]^2\left[SD(\bar{\bar{g}}_q^{MFPV})\right]^2 \\ -\left[SD(\bar{\rho}_D^{Container})\right]^2\left[SD(\bar{\bar{g}}_q^{MFPV})\right]^2\end{array}\right]^{1/2} \\ &= \left(\frac{A_q}{f_q}\right)\left[\begin{array}{l}\left[\bar{\bar{g}}_q^{MFPV}\right]^2\left[SD(\bar{\rho}_D^{Container})\right]^2 + \left[\bar{\rho}_D^{Container}\right]^2\left[SD(\bar{g}_{iq}^{MFPV})/\sqrt{I}\right]^2 \\ -\left[SD(\bar{\rho}_D^{Container})\right]^2\left[SD(\bar{g}_{iq}^{MFPV})/\sqrt{I}\right]^2\end{array}\right]^{1/2}\end{aligned} \tag{F.3.3}$$

where

$SD(\bar{\bar{r}}_{Dq}^{Container})$ = standard deviation of $\bar{\bar{r}}_{Dq}^{Container}$, which is sometimes referred to as a *standard error* because it is the standard deviation of an average (Ci/m^3)

$\bar{\bar{g}}_q^{MFPV}$ = mean (mass-weighted-average) mass fraction of the q^{th} radionuclide oxide in glass over I ILAW MFPV batches, based on averages over multiple samples per CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations (g_{oxide}/g_{oxides})

$SD(\bar{\bar{g}}_q^{MFPV})$ = standard deviation of $\bar{\bar{g}}_q^{MFPV}$ (g_{oxide}/g_{oxides})

$\bar{g}_{iq}^{MFPV}$ = mass fraction of the q^{th} radionuclide oxide in glass that would be made from the i^{th} ILAW MFPV batch, based on averages over multiple samples per CRV batch, analyses per CRV sample, and CRV and MFPV volume determinations (g_{oxide}/g_{oxides})

$SD(\bar{g}_{iq}^{MFPV})$ = standard deviation of $\bar{g}_{iq}^{MFPV}$ (g_{oxide}/g_{oxides})

$\bar{\rho}_{D}^{Container}$ = mean density of glass in D ILAW containers (g/m^3)

$SD(\bar{\rho}_{d}^{Container})$ = standard deviation of $\bar{\rho}_{D}^{Container}$ (g_{glass}/m^3_{glass})

In this report, the value of $\bar{\rho}_{D}^{Container}$ is assumed to be 2.65×10^6 g/m^3.

To determine the numerical value of the term $t_{1-\alpha,df}$ in Eq. (F.3.1), which is also Eq. (5.3.3), the degrees of freedom (*df*) associated with $SD(\bar{\bar{r}}_{Dq}^{Container})$ must be determined. Ordinarily, the number of degrees of freedom can be easily calculated as the number of observations of the variable for which the confidence interval is being constructed minus one. In the case of Equation (5.3.3), however, this may not be such a simple task. Data to calculate $\bar{\bar{r}}_{Dq}^{Container}$ may consist of $\bar{g}_{iq}^{MFPV}, i = 1, 2, \ldots, I$ observations and possibly $\rho_{d}^{Container}, d = 1,2 \ldots D$ density measurements, where D and I are not necessarily equal. Or, it may be that prior estimates of the average density $\bar{\rho}_{d}^{Container}$ and its uncertainty $SD(\rho_{d}^{Container})$ will be used rather than measuring or otherwise estimating the density of glass in each of the D ILAW containers. Under these circumstances, several possibilities for calculating *df* arise. Because it is not clear what the final structure of the data for calculating $\bar{\bar{r}}_{Dq}^{Container}$ will be, the exact procedure for determining *df* is not explored in any more detail at this time. Until such time that more information is available

$$df = I - 1 \tag{F.3.4}$$

will be used as a placeholder formula, where I denotes the number of ILAW MFPV batches corresponding to the D ILAW containers for which a concentration running average is being calculated.

F.4 Equation for X%/Y% Upper Tolerance Intervals on PCT Normalized Releases of B and Na and VHT Alteration Depth over an LAW Waste Type

This section presents the derivation of the equation for calculating X%/Y% UTI values for ILAW PCT normalized B and Na releases and VHT alteration depth over an LAW waste type. This equation is required to implement the WTP ILAW compliance strategy for Contract Specification 2.2.2.17.2, Product Consistency Test and Contract Specification 2.2.2.17.3, Vapor Hydration Test. The methods for implementing the strategy are presented in Section 5.4.5.

An appropriate statistical interval for demonstrating with high (X%) confidence that a high percentage (Y%) of ILAW produced from an LAW waste type satisfies the PCT or VHT limits in Eq. (5.4.1) is an X%/Y% UTI, the concept of which was introduced in Section 3.2. Section B.4 of Appendix B discusses the statistical method for combining model and composition uncertainties that is used in forming an X%/Y% UTI. Piepel and Cooley (2002) derived the equations necessary to calculate an X%/Y% UTI for IHLW and ILAW compliance strategies that involved estimating glass composition based on analyses of samples from a single process location (i.e., the MFPV for IHLW and shards from the top of containers for ILAW). The WTP IHLW compliance strategy remains unchanged, and so the results of Piepel and Cooley (2002) are applicable. However, the current WTP ILAW compliance strategy (see Section 2.3) is substantially different than (1) the previous WTP ILAW shard-sample-based compliance strategy and (2) the current WTP IHLW compliance strategy (see Section 2.2). However, it is possible to adapt the methodology and formulas developed by Piepel and Cooley (2002) for the current WTP ILAW compliance strategy. The adaptation is discussed in the remainder of this section.

The general formula for a one-sided X%/Y% UTI applicable to ILAW PCT and VHT property-composition models is

$$\text{X\%/Y\% UTI} = \tilde{\mu} + k(X, Y)\,\tilde{\sigma} \qquad \text{(F.4.1)}$$

where

X%/Y% UTI = a value that with X% confidence captures Y% of the distribution (population) of true mean ln(PCT release) or ln(VHT alteration depth) over the MFPV batches corresponding to an LAW waste type [ln(g/L) for PCT and ln(μm) for VHT]

$\tilde{\mu}$ = estimate of the population mean that is calculated by forming the model-predicted ln (PCT release) or ln(VHT alteration depth) for each MFPV batch and averaging them across all MFPV batches corresponding to an LAW waste type [ln(g/L) for PCT and ln(μm) for VHT]

$k(X, Y)$ = tolerance interval multiplier that is implicitly a function of X, Y, degrees of freedom associated with $\tilde{\sigma}$, and other parameters

$\tilde{\sigma}$ = estimate of the population standard deviation that properly accounts for (1) variation in ln(PCT release) or ln(VHT alteration depth) across MFPV batches corresponding to an LAW waste type, (2) all ILAW process uncertainties affecting each MFPV batch, and (3) model uncertainty [ln(g/L) for PCT and ln(μm) for VHT].

The parameters X and Y generally should have values between 90% (or 95%) and 100% to provide high confidence that a high percentage of ILAW produced from an LAW waste type satisfies the requirements of Contract Specifications 2.2.2.17.2 and 2.2.2.17.3. However, X and Y can never take values of 100% because it is impossible to be 100% confident about 100% of the true distribution of ln(PCT releases) or ln(VHT alteration depth) given estimated ILAW composition variation as well as ILAW composition and model uncertainties.

Equations for the terms on the right hand side of Eq. (F.4.1) are given in Section 5.4.5 for the case of $n_S^{CRV} > 1$ samples and $n_A^{CRV} = 1$ analyses per sample of the i^{th} CRV batch. In this section, the equations for the terms on the right hand side of Eq. (F.4.1) are given for the more general case of $n_S^{CRV} > 1$ samples and $n_A^{CRV} \geq 1$ analyses per sample of the i^{th} CRV batch.

The equation for $\tilde{\mu}$ in Eq. (F.4.1) is given by

$$\tilde{\mu} = \bar{\hat{\bar{y}}}_I^h = \frac{\sum_{i=1}^{I} \hat{\bar{y}}_i^h}{I} = \frac{1}{I} \sum_{i=1}^{I} \left[\sum_{k=1}^{n_{mc}^h} b_k^h \, \bar{x}_{ik}^{MFPV} + Selected \left\{ \sum_{k=1}^{n_{mc}^h} b_{kk} \left(\bar{x}_{ik}^{MFPV} \right)^2 + \sum_{k<}^{n_{mc}^h - 1} \sum_{l}^{n_{mc}^h} b_{kl} \bar{x}_{ik}^{MFPV} \bar{x}_{il}^{MFPV} \right\} \right] \quad \text{(F.4.2)}$$

where

$\bar{\hat{\bar{y}}}_I^h$ = average of the $\hat{\bar{y}}_i^h$, i = 1, 2, … , I values for the I MFPV batches corresponding to an LAW waste type

and the remaining notation is as defined in Section 5.4. Note that Eq. (F.4.2) calculates the ordinary mean (average) of the model-predicted property values over the ILAW compositions corresponding to the I ILAW MFPV batches. An alternative approach would be to use $\hat{y}(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})$, the model-predicted value for the normalized version of the mass-averaged composition over the I MFPV batches ($\bar{\bar{x}}_k^{MFPV}, k = 1, \ldots, n_{mc}^h$) that would result from supplying ($\bar{\bar{g}}_j^{MFPV}, j = 1, \ldots, J$) [calculated per Eq. (5.1.2) for balanced data and Eq. (5.1.7) for unbalanced data] to the normalizing transformation given in Eq. (5.4.4). Although this alternative approach would be consistent with some of the other compliance methods and calculations adopted in this report, it is contrary to the typical method for developing tolerance intervals.

In general, $k(X, Y)$ in Eq. (F.4.1) is calculated using the following equation

$$k(X,Y) = \frac{t(X, Y, df_{\tilde{\sigma}}, \delta)}{\sqrt{I}} \quad \text{(F.4.3)}$$

where $t(X, Y, df_{\tilde{\sigma}}, \delta)$ represents a non-centralized t-distribution with degrees of freedom $df_{\tilde{\sigma}}$ and non-centrality parameter δ, and I is the number of MFPV batches associated with an LAW waste type. This is Eq. (3.18d) in Piepel and Cooley (2002), adapted to the notation in this report. It is important to note that $k(X, Y)$ is determined so as to compensate for the effects of all ILAW process uncertainties (e.g., CRV mixing/sampling uncertainty, analytical uncertainty, GFC uncertainties, and volume uncertainties), which are "nuisance uncertainties" with respect to the population for which a X%/Y% UTI is desired.

The expression for $df_{\tilde{\sigma}}$ in Eq. (F.4.3) is given by

$$df_{\tilde{\sigma}} \approx \frac{\left[\left(SD_M\left[\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})\right]\right)^2 + \left(SD_I\left[\hat{y}_i^h(\bar{\boldsymbol{x}}_i^{MFPV})\right]\right)^2\right]^2}{\frac{\left[\left(SD_M\left[\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})\right]\right)^2\right]^2}{df_m} + \frac{\left[\left(SD_I\left[\hat{y}_i^h(\bar{\boldsymbol{x}}_i^{MFPV})\right]\right)^2\right]^2}{df_I}}$$

$$= \frac{\left[\left((\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^T\,\hat{\boldsymbol{\Sigma}}_b^h\,\bar{\bar{\boldsymbol{x}}}_I^{MFPV}\right) + \sum_{i=1}^{I}(\hat{\bar{y}}_i^h - \bar{\hat{\bar{y}}}_I^h)^2 \Big/ (I-1)\right]^2}{\frac{\left((\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^T\,\hat{\boldsymbol{\Sigma}}_b^h\,\bar{\bar{\boldsymbol{x}}}_I^{MFPV}\right)^2}{df_m} + \frac{\left[\sum_{i=1}^{I}(\hat{\bar{y}}_i^h - \bar{\hat{\bar{y}}}_I^h)^2 \Big/ (I-1)\right]^2}{I-1}} \qquad \text{(F.4.4)}$$

where

$df_{\tilde{\sigma}}$ = approximate degrees of freedom associated with $\tilde{\sigma}$

$\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ = $p \times 1$ column vector whose first n_{mc}^h entries $\bar{\bar{x}}_k^{MFPV}, k = 1, 2, \cdots, n_{mc}^h$ are mass-weighted-averages of the $\bar{x}_{ik}^{MFPV}$, i = 1, 2, …, I values, which in turn are ordinary averages over the n_S^{CRV} samples per CRV batch, n_A^{CRV} analyses per sample, n_V^{CRV} determinations per CRV volume, and n_V^{MFPV} determinations per MFPV volume. The remaining entries $\bar{\bar{x}}_k^{MFPV}, k = n_{mc}^h + 1, \cdots, p$ are squares and/or crossproducts of the first n_{mc}^h entries according to the form of the PCT or VHT partial quadratic mixture model.

$\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})$ = model prediction of the PCT normalized release of *h* = B or Na or the VHT alteration depth for the mass-weighted-average ILAW composition $\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ [ln(g/L) for PCT and ln(μm) for VHT]

$SD_M[\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})]$ = standard deviation of the model prediction for the mass-weighted-average composition $\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ [ln(g/L) for PCT and ln(μm) for VHT]

MS_I = mean square for the ILAW MFPV batches corresponding to an LAW waste type, which is calculated over the $I \times n_S^{CRV} \times n_A^{CRV}$ values of $\hat{y}_{ilm}^h$

I = number of ILAW MFPV batches corresponding to an LAW waste type

n_S^{CRV} = number of samples per ILAW CRV batch

n_A^{CRV} = number of analyses per ILAW CRV sample

n_V^{CRV} = number of determinations for any CRV volume

n_V^{MFPV} = number of determinations for any MFPV volume

$\hat{\boldsymbol{\Sigma}}_b^h$ = estimated $p \times p$ variance-covariance matrix of the model coefficient vector $\boldsymbol{b}^h$ for the PCT normalized release of h = B or Na or VHT alteration depth

df_m = degrees of freedom for the model relating PCT normalized releases of h = B or Na or VHT alteration depth to ILAW composition. This quantity is given by $n - p$ where n is the number of data points used to fit the model, and p is the number of model coefficients estimated using the data.

df_I = degrees of freedom for the I MFPV batches associated with an LAW waste type. This quantity is given by $I - 1$.

Note that $\hat{\bar{y}}_i^h$ is given by a sub-equation of Eq. (F.4.2) and $\hat{\bar{y}}_I^h$ is given by Eq. (F.4.2). The preceding derivation is based on the results in Appendix D of Piepel and Cooley (2002).

The expression for δ in Eq. (F.4.3) is given by

$$\delta = z_{1-\beta}\sqrt{I}\,\frac{\sigma_g}{\sigma} \tag{F.4.5}$$

where

$z_{1-\beta}$ = $100(1-\beta)$ percentile of the standard normal distribution

I = number of ILAW MFPV batches corresponding to an LAW waste type

σ_g = standard deviation of the distribution of true ln(PCT normalized release) [ln(g/L)] or ln(VHT alteration depth) [ln(μm)] values for ILAW produced from a given LAW waste type

σ = $\left[\sigma_{\mathrm{g}}^2 + \bar{\sigma}_m^2 + (\bar{\sigma}_{\mathrm{U}}^{\mathrm{MFPV}})^2\right]^{0.5}$ = standard deviation of the distribution of possible $\hat{\bar{y}}_i^h$ values over the I ILAW MFPV batches corresponding to an LAW waste type for h = PCT B or Na [ln(g/L)] or VHT alteration depth [ln(μm)]. For each property h, $\bar{\sigma}_m$

denotes the model prediction standard deviation for the true average ILAW composition over an LAW waste type and σ_U^{MFPV} denotes the standard deviation for the true total uncertainty in the ILAW composition for an MFPV batch. Both standard deviations are expressed in model units [ln(g/L) for PCT and ln(μm) for VHT alteration depth].

Equations (F.4.4) and (F.4.5) for f and δ are based on Eqs. (3.18f) and (3.18e) in Section 3.7 and development work in Appendix H of Piepel and Cooley (2002).

The estimate of the population standard deviation $\tilde{\sigma}$ is discussed in Sections 3.4 and 3.5 of Piepel and Cooley (2002). Applying the notation used in this report to Eq. (3.18c) of Piepel and Cooley (2002) yields the following general equation for $\tilde{\sigma}$:

$$\tilde{\sigma} = \sqrt{\left[SD_I\left(\hat{y}_i^h(\bar{\boldsymbol{x}}_i^{MFPV})\right)\right]^2 + \left[SD_M\left(\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})\right)\right]^2 + \left(SD_U\left(\hat{y}_i^h(\bar{\boldsymbol{x}}_i^{MFPV})\right)\right)^2} \qquad \text{(F.4.6)}$$

where

$SD_I\left(\hat{y}_i^h(\bar{\boldsymbol{x}}_i^{MFPV})\right)$ = standard deviation of $\hat{\bar{y}}_i^h = \hat{ln}(r_i^{PCT\,h})$ or $\hat{\bar{y}}_i^h = \hat{ln}(D^{VHT})$, $i = 1, 2, \ldots, I$ values corresponding to variation in ILAW composition over a waste type [ln(g/L) for PCT or ln(μm) for VHT]

$SD_M[\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})]$ = standard deviation of the model prediction for the mass-weighted-average ILAW composition $\bar{\bar{\boldsymbol{x}}}_I^{MFPV}$ [ln(g/L) for PCT or ln(μm) for VHT]

$SD_U\left(\hat{y}_i^h(\bar{\boldsymbol{x}}_i^{MFPV})\right)$ = standard deviation in $\hat{\bar{y}}_i^h = ln(r_i^{PCT\,h})$ or $\hat{\bar{y}}_i^h = ln(D^{VHT})$ values representing all ILAW process uncertainties (e.g., CRV mixing/sampling, CRV analytical, CRV and MFPV volumes, GFC compositions and additions), where the process uncertainties in $\bar{\boldsymbol{x}}_i^{MFPV}$ are reduced by averaging over multiple determinations [ln(g/L) for PCT or ln(μm) for VHT].

The first term in Eq. (F.4.6) represents variation in PCT normalized release of B or Na or VHT alteration depth for ILAW produced from a given LAW waste type. The second term represents model uncertainty. The third term represents the total uncertainty in model-predicted values corresponding to all sources of uncertainty affecting the estimate of ILAW composition for a single MFPV batch. Note that this total uncertainty is reduced by averaging over multiple (1) samples per CRV batch, (2) analyses per CRV sample, and (3) determinations per CRV or MFPV volumes.

The equation for $SD_M[\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})]$ in Eq. (F.4.6) is given by

$$SD_M[\hat{y}^h(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})] = \sqrt{(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^{\mathrm{T}}\,\hat{\boldsymbol{\Sigma}}_{\boldsymbol{b}}^h\,\bar{\bar{\boldsymbol{x}}}_I^{MFPV}} \tag{F.4.7}$$

where all notation is as defined in this section or Section 5.4.

The quantity $SD_U\left(\hat{y}_i^h(\bar{\boldsymbol{x}}_i^{MFPV})\right)$ in Eq. (F.4.6) can be estimated using the Monte Carlo simulation method discussed in Section 3.4.2.1. The quantity $SD_I\left(\hat{y}_i^h(\bar{\boldsymbol{x}}_i^{MFPV})\right)$ can be estimated from the $\hat{\bar{y}}_i^h = \hat{y}_i^h(\bar{\boldsymbol{x}}_i^{MFPV})$ values and subtracting out the $SD_U\left(\hat{y}_i^h(\bar{\boldsymbol{x}}_i^{MFPV})\right)$ estimate. However, that is unnecessary because the sum of these two terms on the right hand side of Eq. (F.4.6) can be jointly estimated as follows:

$$\sqrt{\left[SD_I\left(\hat{y}_i^h(\bar{\boldsymbol{x}}_i^{MFPV})\right)\right]^2 + \left[SD_U\left(\hat{y}_i^h(\bar{\boldsymbol{x}}_i^{MFPV})\right)\right]^2} = SD(\hat{\bar{y}}_i^h) = \sqrt{\frac{\sum_{i=1}^{I}(\hat{\bar{y}}_i^h - \bar{\hat{\bar{y}}}_I^h)^2}{I-1}} \tag{F.4.8}$$

where the notation has been previously defined in this section.

Hence, the formula for calculating $\tilde{\sigma}$ in Eq. (F.4.1) is given by

$$\tilde{\sigma} = \sqrt{(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^{\mathrm{T}}\,\hat{\boldsymbol{\Sigma}}_{\boldsymbol{b}}^h\,\bar{\bar{\boldsymbol{x}}}_I^{MFPV} + \sum_{i=1}^{I}(\hat{\bar{y}}_i^h - \bar{\hat{\bar{y}}}_I^h)^2 \Big/ (I-1)} \tag{F.4.9}$$

after substituting Eqs. (F.4.7) and (F.4.8) into Eq. (F.4.6).

In summary, Eq. (F.4.1) is the basic equation for calculating an X%/Y% UTI, along with Eqs. (F.4.2), (F.4.3), (F.4.4), (F.4.5), and (F.4.9).

Appendix G

Detailed IHLW Waste Form Qualification Results Associated with Section 6

Appendix G: Detailed IHLW Waste Form Qualification Results Associated with Section 6

This appendix presents the additional details of IHLW waste form qualification results presented in Section 6. Sections 6.4 to 6.8 did not have any scope for this iteration, and therefore no results associated with those sections are included in this appendix.

G.1 Compliance Results for IHLW WAPS Specification 1.1.2: Chemical Composition During Production

Additional details of results from Section 6.1 are presented following. Detailed results from Sections 6.1.1 and 6.1.2 are, respectively, presented in Sections G.1.1 and G.1.2.

G.1.1 Detailed Results of Investigations to Assess the Effects of Process Uncertainties, Number of Samples per MFPV Batch, and Number of Analyses per MFPV Sample on Uncertainties in the Chemical Composition of IHLW from a MFPV Batch

Detailed results associated with Section 6.1.1 are presented in this section. Tables G.1 to G.14 contain the numbers of samples per immobilized high-level waste (IHLW) Melter Feed Process Vessel (MFPV) batch and analyses per MFPV sample necessary to achieve certain ranges of percent relative half-width (%RHW) for each of the IHLW reportable chemical composition components (oxides). Results for oxides that have the same MFPV mixing/sampling and analytical %RSDs are included on the same table. For example, Table G.1 contains the numbers of samples per MFPV batch and analyses per MFPV sample for Al_2O_3, B_2O_3, Fe_2O_3, MnO, SiO_2, SrO, and ZrO_2 because they were each expected to have $\%RSD_S(g_j^{MFPV})$ values of 5% for the low case and 15% for the high case, and $\%RSD_A(g_j^{MFPV})$ values of 5% for the low case and 10% for the high case. Any calculation that required more than 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) was reported as a dash in the tables.

As discussed in Section 4.1.3, values of $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ were not yet available at the time of this work. However, based on a preliminary investigation, values of $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ were used as substitutes in the calculations.

Table G.1. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of Al_2O_3, B_2O_3, Fe_2O_3, MnO, SiO_2, SrO, and ZrO_2 for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	Percent Relative Half-width (%RHW) on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
	15	5	90	29	1	9	1	6	1	4	1
			95	-[b]	-	13	1	7	1	5	1
		10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1
AZ-102	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
	15	5	90	29	1	9	1	6	1	4	1
			95	-	-	13	1	7	1	5	1
		10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1
C-104	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
	15	5	90	29	1	9	1	6	1	4	1
			95	-	-	13	1	7	1	5	1
		10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component *j* (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.2. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of CaO, Cr_2O_3, and P_2O_5 for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-[b]	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
	15	10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1
		20	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
AZ-102	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
	15	10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1
		20	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
C-104	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
	15	10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1
		20	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component j (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.3. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of CdO for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	5	50[b]	90	-[c]	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	15	50[b]	90	-	-	-	-	-	-	21	1
			95	-	-	-	-	-	-	29	1
AZ-102	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
	15	5	90	29	1	9	1	6	1	4	1
			95	-	-	13	1	7	1	5	1
		10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1
C-104	5	50[b]	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	15	50[b]	90	-	-	-	-	-	-	21	1
			95	-	-	-	-	-	-	29	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component *j* (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) MFPV concentration is less than detect so $\%RSD_A(g_j^{MFPV}) = 50$ was used for both the nominal and high levels.

(c) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.4. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of Li_2O for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	1	10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
		20	90	-[b]	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
	5	10	90	16	1	6	1	4	1	3	1
			95	-	-	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
AZ-102	1	10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
		20	90	-	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
C-104	1	5	90	5	1	3	1	3	1	3	1
			95	7	1	4	1	3	1	3	1
		10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component *j* (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.5. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of MgO for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	5	50[b]	90	-[c]	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	15	50[b]	90	-	-	-	-	-	-	21	1
			95	-	-	-	-	-	-	29	1
AZ-102	5	50[b]	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	15	50[b]	90	-	-	-	-	-	-	21	1
			95	-	-	-	-	-	-	29	1
C-104	5	50[b]	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	15	50[b]	90	-	-	-	-	-	-	21	1
			95	-	-	-	-	-	-	29	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component *j* (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) MFPV concentration is less than detect so $\%RSD_A(g_j^{MFPV}) = 50$ was used for both the nominal and high levels.

(c) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.6. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of Na_2O for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	1	5	90	5	1	3	1	3	1	3	1
			95	7	1	4	1	3	1	3	1
		10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
AZ-102	1	5	90	5	1	3	1	3	1	3	1
			95	7	1	4	1	3	1	3	1
		10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
C-104	1	5	90	5	1	3	1	3	1	3	1
			95	7	1	4	1	3	1	3	1
		10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component *j* (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

Table G.7. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of NiO for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-[b]	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
	15	10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1
		20	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
AZ-102	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
	15	5	90	29	1	9	1	6	1	4	1
			95	-	-	13	1	7	1	5	1
		10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1
C-104	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
	15	10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1
		20	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component *j* (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.8. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of PdO and Rh_2O_3 for One HLW Tank

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
C-104	5	25	90	-[b]	-	20	1	10	1	7	1
			95	-	-	28	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	15	25	90	-	-	25	1	13	1	8	1
			95	-	-	-	-	17	1	11	1
		50	90	-	-	-	-	-	-	21	1
			95	-	-	-	-	-	-	29	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component *j* (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.9. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of RuO_2 and SeO_2 for One HLW Tank

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
C-104	5	50[b]	90	-[c]	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	15	50[b]	90	-	-	-	-	-	-	21	1
			95	-	-	-	-	-	-	29	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component j (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) MFPV concentration is less than detect so $\%RSD_A(g_j^{MFPV}) = 50$ was used for both the nominal and high levels.

(c) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.10. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of Sb_2O_3 for One HLW Tank

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	5	25	90	-[b]	-	20	1	10	1	7	1
			95	-	-	28	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	15	25	90	-	-	25	1	13	1	8	1
			95	-	-	-	-	17	1	11	1
		50	90	-	-	-	-	-	-	21	1
			95	-	-	-	-	-	-	29	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component *j* (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.11. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of ThO_2 for One HLW Tank

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
C-104	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
	15	5	90	29	1	9	1	6	1	4	1
			95	-[b]	-	13	1	7	1	5	1
		10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component *j* (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.12. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of SO_3 for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	1	15	90	27	1	9	1	5	1	4	1
			95	-[b]	-	12	1	7	1	5	1
		30	90	-	-	27	1	13	1	9	1
			95	-	-	-	-	18	1	12	1
	5	15	90	29	1	9	1	6	1	4	1
			95	-	-	13	1	7	1	5	1
		30	90	-	-	27	1	14	1	9	1
			95	-	-	-	-	19	1	12	1
AZ-102	1	50[c]	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	5	50[c]	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
C-104	1	50[c]	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	5	50[c]	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component *j* (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

(c) MFPV concentration is less than detect so $\%RSD_A(g_j^{MFPV}) = 50$ was used for both the nominal and high levels.

Table G.13. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of U_3O_8 for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	5	20	90	-[b]	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
		40	90	-	-	-	-	22	1	13	1
			95	-	-	-	-	-	-	19	1
	15	20	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
		40	90	-	-	-	-	24	1	15	1
			95	-	-	-	-	-	-	20	1
AZ-102	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
	15	10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1
		20	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
C-104	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
	15	5	90	29	1	9	1	6	1	4	1
			95	-	-	13	1	7	1	5	1
		10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component *j* (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.14. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Component Mass Fractions of ZnO for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
	15	5	90	29	1	9	1	6	1	4	1
			95	-[b]	-	13	1	7	1	5	1
		10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1
AZ-102	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
	15	10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1
		20	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
C-104	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
	15	5	90	29	1	9	1	6	1	4	1
			95	-	-	13	1	7	1	5	1
		10	90	-	-	11	1	6	1	5	1
			95	-	-	15	1	9	1	6	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW component *j* (oxide or halogen) in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

G.1.2 Details of the Illustration for Calculating Means and Standard Deviations of IHLW Chemical Composition over an HLW Waste Type

There are no detailed results associated with Section 6.1.2 at this time.

G.2 Compliance Results for IHLW WAPS Specification 1.1.2: Radionuclide Inventory During Production

Additional details of results from Section 6.2 are presented following. Detailed results from Sections 6.2.1 and 6.2.2 are, respectively, presented in Sections G.2.1 and G.2.2.

G.2.1 Detailed Results of Investigations to Assess the Effects of Process Uncertainties, Number of Samples per MFPV Batch, and Number of Analyses per MFPV Sample on Uncertainties in the Radionuclide Composition of IHLW from a MFPV Batch

Detailed results associated with Section 6.2.1 are presented in this section. Tables G.15 to G.28 contain the numbers of samples per IHLW MFPV batch and analyses per MFPV sample necessary to achieve certain ranges of %RHW for each of the IHLW reportable radionuclide composition components (oxides). Results for radionuclide oxides that have the same MFPV mixing/sampling and analytical %RSDs are included on the same table. For example, Table G.18 contains the numbers of samples per MFPV batch and analyses per MFPV sample for Co^{60} and Pu^{238} because they were each expected to have $\%RSD_S(g_j^{MFPV})$ values of 1% for the low case and 5% for the high case, and $\%RSD_A(g_j^{MFPV})$ values of 25% for the low case and 50% for the high case. Any calculation that required more than 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) was reported as a dash in the tables.

As discussed in Section 4.1.3, values of $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ were not yet available at the time of this work. However, based on a preliminary investigation, values of $\%RSD_S(c_j^{MFPV})$ and $\%RSD_A(c_j^{MFPV})$ were used as substitutes in the calculations.

Table G.15. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of $^{241}Am_2O_3$ for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	1	25	90	-[b]	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	5	25	90	-	-	20	1	10	1	7	1
			95	-	-	28	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
AZ-102	1	5	90	5	1	3	1	3	1	3	1
			95	7	1	4	1	3	1	3	1
		10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
C-104	1	25	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	5	25	90	-	-	20	1	10	1	7	1
			95	-	-	28	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.16. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of $^{242}Cm_2O_3$ for One HLW Tank

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
C-104	1	60	90	-[a]	-	-	-	-	-	27	1
			95	-	-	-	-	-	-	-	-
		120	90	-	-	-	-	-	-	-	-
			95	-	-	-	-	-	-	-	-
	5	60	90	-	-	-	-	-	-	27	1
			95	-	-	-	-	-	-	-	-
		120	90	-	-	-	-	-	-	-	-
			95	-	-	-	-	-	-	-	-

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.17. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of $^{243+244}Cm_2O_3$ and $^{134}Cs_2O$ for Each of Two HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AZ-102	1	30	90	-[b]	-	27	1	13	1	9	1
			95	-	-	-	-	18	1	12	1
		60	90	-	-	-	-	-	-	27	1
			95	-	-	-	-	-	-	-	-
	5	30	90	-	-	27	1	14	1	9	1
			95	-	-	-	-	19	1	12	1
		60	90	-	-	-	-	-	-	27	1
			95	-	-	-	-	-	-	-	-
C-104	1	30	90	-	-	27	1	13	1	9	1
			95	-	-	-	-	18	1	12	1
		60	90	-	-	-	-	-	-	27	1
			95	-	-	-	-	-	-	-	-
	5	30	90	-	-	27	1	14	1	9	1
			95	-	-	-	-	19	1	12	1
		60	90	-	-	-	-	-	-	27	1
			95	-	-	-	-	-	-	-	-

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.18. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of ^{60}CoO and $^{238}PuO_2$ for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	1	25	90	-[b]	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	5	25	90	-	-	20	1	10	1	7	1
			95	-	-	28	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
AZ-102	1	25	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	5	25	90	-	-	20	1	10	1	7	1
			95	-	-	28	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
C-104	1	25	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	5	25	90	-	-	20	1	10	1	7	1
			95	-	-	28	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.19. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of $^{137}Cs_2O$ for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	1	5	90	5	1	3	1	3	1	3	1
			95	7	1	4	1	3	1	3	1
		10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
AZ-102	1	5	90	5	1	3	1	3	1	3	1
			95	7	1	4	1	3	1	3	1
		10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
C-104	1	5	90	5	1	3	1	3	1	3	1
			95	7	1	4	1	3	1	3	1
		10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

Table G.20. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of $^{154}Eu_2O_3$ for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	1	15	90	27	1	9	1	5	1	4	1
			95	-[b]	-	12	1	7	1	5	1
		30	90	-	-	27	1	13	1	9	1
			95	-	-	-	-	18	1	12	1
	5	15	90	29	1	9	1	6	1	4	1
			95	-	-	13	1	7	1	5	1
		30	90	-	-	27	1	14	1	9	1
			95	-	-	-	-	19	1	12	1
AZ-102	1	15	90	27	1	9	1	5	1	4	1
			95	-	-	12	1	7	1	5	1
		30	90	-	-	27	1	13	1	9	1
			95	-	-	-	-	18	1	12	1
	5	15	90	29	1	9	1	6	1	4	1
			95	-	-	13	1	7	1	5	1
		30	90	-	-	27	1	14	1	9	1
			95	-	-	-	-	19	1	12	1
C-104	1	15	90	27	1	9	1	5	1	4	1
			95	-	-	12	1	7	1	5	1
		30	90	-	-	27	1	13	1	9	1
			95	-	-	-	-	18	1	12	1
	5	15	90	29	1	9	1	6	1	4	1
			95	-	-	13	1	7	1	5	1
		30	90	-	-	27	1	14	1	9	1
			95	-	-	-	-	19	1	12	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.21. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of $^{155}Eu_2O_3$, $^{239}PuO_2$, and $^{99}Tc_2O_7$ for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	1	10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
		20	90	-[b]	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
AZ-102	1	10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
		20	90	-	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
C-104	1	10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
		20	90	-	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.22. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of $^{237}NpO_2$ for Each of Two HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AZ-102	1	10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
		20	90	-[a]	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
C-104	1	25	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	5	25	90	-	-	20	1	10	1	7	1
			95	-	-	28	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.23. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of $^{241}PuO_2$ and $^{125}Sb_2O_3$ for Each of Two HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AZ-102	1	25	90	-[b]	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	5	25	90	-	-	20	1	10	1	7	1
			95	-	-	28	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
C-104	1	25	90	-	-	19	1	10	1	7	1
			95	-	-	27	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
	5	25	90	-	-	20	1	10	1	7	1
			95	-	-	28	1	14	1	9	1
		50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.24. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of ^{90}SrO for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	1	10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
		20	90	-[b]	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
AZ-102	1	10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
		20	90	-	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
C-104	1	20	90	-	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
		40	90	-	-	-	-	22	1	13	1
			95	-	-	-	-	30	1	18	1
	5	20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
		40	90	-	-	-	-	22	1	13	1
			95	-	-	-	-	-	-	19	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.25. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of $^{233}U_3O_8$ for Each of Two HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AZ-102	1	10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
		20	90	-[b]	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
C-104	1	10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
		20	90	-	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
	5	10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
		20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.26. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of $^{234}U_3O_8$ and $^{236}U_3O_8$ for Each of Two HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AZ-102	1	50	90	-[b]	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
		100	90	-	-	-	-	-	-	-	-
			95	-	-	-	-	-	-	-	-
	5	50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
		100	90	-	-	-	-	-	-	-	-
			95	-	-	-	-	-	-	-	-
C-104	1	50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
		100	90	-	-	-	-	-	-	-	-
			95	-	-	-	-	-	-	-	-
	5	50	90	-	-	-	-	-	-	19	1
			95	-	-	-	-	-	-	27	1
		100	90	-	-	-	-	-	-	-	-
			95	-	-	-	-	-	-	-	-

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.27. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of $^{235}U_3O_8$ for Each of Two HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AZ-102	1	20	90	-[b]	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
		40	90	-	-	-	-	22	1	13	1
			95	-	-	-	-	30	1	18	1
	5	20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
		40	90	-	-	-	-	22	1	13	1
			95	-	-	-	-	-	-	19	1
C-104	1	20	90	-	-	13	1	7	1	5	1
			95	-	-	18	1	10	1	7	1
		40	90	-	-	-	-	22	1	13	1
			95	-	-	-	-	30	1	18	1
	5	20	90	-	-	14	1	8	1	5	1
			95	-	-	19	1	10	1	7	1
		40	90	-	-	-	-	22	1	13	1
			95	-	-	-	-	-	-	19	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

Table G.28. Required Number of IHLW MFPV Samples (n_S^{MFPV}) and Analyses per Sample (n_A^{MFPV}) to Satisfy Certain %RHWs on IHLW Radionuclide Component Mass Fractions of $^{238}U_3O_8$ for Each of Three HLW Tanks

HLW Tank	$\%RSD_S(g_j^{MFPV})$[a]	$\%RSD_A(g_j^{MFPV})$[a]	% Confidence	%RHW on the Mass Fraction of an IHLW Radionuclide Component							
				< 5%		< 10%		< 15%		< 20%	
				n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}	n_S^{MFPV}	n_A^{MFPV}
AY-102	1	15	90	27	1	9	1	5	1	4	1
			95	-[b]	-	12	1	7	1	5	1
		30	90	-	-	27	1	13	1	9	1
			95	-	-	-	-	18	1	12	1
	5	15	90	29	1	9	1	6	1	4	1
			95	-	-	13	1	7	1	5	1
		30	90	-	-	27	1	14	1	9	1
			95	-	-	-	-	19	1	12	1
AZ-102	1	5	90	5	1	3	1	3	1	3	1
			95	7	1	4	1	3	1	3	1
		10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1
C-104	1	5	90	5	1	3	1	3	1	3	1
			95	7	1	4	1	3	1	3	1
		10	90	13	1	5	1	4	1	3	1
			95	18	1	7	1	5	1	4	1
	5	5	90	8	1	4	1	3	1	3	1
			95	11	1	5	1	4	1	3	1
		10	90	16	1	6	1	4	1	3	1
			95	22	1	8	1	5	1	4	1

(a) The notation $\%RSD_S(g_j^{MFPV})$ and $\%RSD_A(g_j^{MFPV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the mass fraction of IHLW radionuclide oxide *j* in the MFPV. See Section 4.1.3 for discussion related to this notation and the values used.

(b) A dash (–) indicates that over 30 total analyses ($n_S^{MFPV} \times n_A^{MFPV}$) would be necessary to satisfy that %RHW category.

G.2.2 Details of the Illustration for Calculating Means and Standard Deviations of IHLW Radionuclide Inventory per Canister over an HLW Waste Type

There are no details of the illustration associated with Section 6.2.2 at this time.

G.3 Compliance Results for IHLW WAPS Specification 1.3: Product Consistency

The ratio σ_g / σ was estimated for the product consistency test (PCT) normalized B release example calculations in Section 6.3.3 as follows. First, re-expressing the equation found below Eq. (4.3.13) yields

$$\sigma = \left(\sigma_g^2 + \bar{\sigma}_m^2 + \frac{\sigma_S^2 + \sigma_A^2}{n_S^{MFPV}} \right)^{0.5} \quad \Rightarrow \quad \sigma_g = \left(\sigma^2 - \bar{\sigma}_m^2 - \frac{\sigma_S^2 + \sigma_A^2}{n_S^{MFPV}} \right)^{0.5} \tag{G.3.1}$$

Then, an estimate of σ using Eq. (4.3.14) is $\tilde{\sigma} = 0.47$, the details of which are included in the example calculation for PCT normalized B release in Section 6.3.3. An estimate of $\bar{\sigma}_m^2$ is given by $(\bar{\bar{\boldsymbol{x}}}_I^{MFPV})^{\mathrm{T}} \hat{\boldsymbol{\Sigma}}_b^h \bar{\bar{\boldsymbol{x}}}_I^{MFPV} = 0.021$, which is obtained from the simulated data discussed in Section 6.3.3. Finally, the simulated data yields a combined estimate of $\sigma_S^2 + \sigma_A^2 = 0.04$. Substituting these values into Eq. (G.3.1) gives

$$\sigma_g = \left(\sigma^2 - \bar{\sigma}_m^2 - \frac{\sigma_S^2 + \sigma_A^2}{n_S^{MFPV}} \right)^{0.5} = \left((0.47)^2 - 0.021 - \frac{0.04}{8} \right)^{0.5} = 0.44 .$$

as an estimate of σ_g. This results in an estimate for the ratio $\sigma_g / \sigma = 0.44/0.47 = 0.94$.

Appendix H

Detailed ILAW Waste Form Qualification Results Associated with Section 7

Appendix H: Detailed ILAW Waste Form Qualification Results Associated with Section 7

This appendix presents the additional details of immobilized low-activity waste (ILAW) waste form qualification results presented in Section 7. Sections 7.6 and 7.7 did not have any scope for this iteration, and therefore no results associated with those sections are included in this appendix.

H.1 Compliance Results for ILAW Contract Specification 2.2.2.6.2: Chemical Composition During Production

Additional details of results from Section 7.1 are presented following. Detailed results from Sections 7.1.1 and 7.1.2 are, respectively, presented in Sections H.1.1 and H.1.2.

H.1.1 Detailed Results of Simulations to Assess the Effects of Process Uncertainties and Numbers of Samples, Analyses, and Measurements on Uncertainties in the Chemical Composition of ILAW from a MFPV Batch

Detailed results associated with Section 7.1.1 are presented in this section. Tables H.1 to H.16 contain numbers of samples per LAW CRV batch and analyses per CRV sample necessary to achieve certain ranges of percent relative half-width (%RHW) for each of the ILAW reportable chemical composition components (oxides and halogens). Any calculation that required more than the number of samples (n_S^{CRV}) and number of analyses per sample (n_A^{CRV}) that were simulated as listed in Table 3.3 was reported as a dash in the tables.

The values in this section are a result of the ILAW simulations discussed in Section 3.4.2 and Section 5.1.3.

Table H.1. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Component Mass Fractions for Al_2O_3 for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(b)]	$\%RSD_A(c_j^{CRV})$[(b)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(c)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(c)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	5	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
AZ-101 (Envelope B)	5	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
AN-107 (Envelope C)	5	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the Concentrate Receipt Vessel (CRV).

(c) Other uncertainties include glass-forming chemicals (GFC) uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

Table H.2. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of B_2O_3 for a Waste Tank in Each of Two LAW Waste Envelopes[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	5	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
AZ-101 (Envelope B)	1	15	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		30	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	5	15	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		30	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) B_2O_3 is not reported for AN-107.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

Table H.3. Required Number of ILAW CRV Samples (n_S^{CRV})[a] and Analyses per Sample (n_A^{CRV})[a] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of CaO for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[b]	$\%RSD_A(c_j^{CRV})$[b]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[c] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[c] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	5	10	90	1	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	-[d]	-	1	1	1	1	1	1
		20	90	1	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	-	-	1	1	1	1	1	1
	15	10	90	1	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	-	-	1	1	1	1	1	1
		20	90	1	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	-	-	1	1	1	1	1	1
AZ-101 (Envelope B)	5	15	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		30	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	15	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		30	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
AN-107 (Envelope C)	5	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.4. Required Number of ILAW CRV Samples (n_S^{CRV})[a] and Analyses per Sample (n_A^{CRV})[a] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of Cl for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[b]	$\%RSD_A(c_j^{CRV})$[b]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[c] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[c] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	8	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
		16	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	3	2	1	2	2	1	1	1	3	2	1	2	2	1	1	1
	5	8	90	3	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
			95	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
		16	90	3	2	2	1	2	1	1	1	3	2	2	1	1	1	1	1
			95	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
AZ-101 (Envelope B)	1	10	90	2	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	-[d]	-	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		20	90	-	-	2	1	1	1	1	1	1	2	2	1	1	1	1	1
			95	-	-	1	2	1	1	1	1	2	2	2	1	1	1	1	1
	5	10	90	2	2	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	-	-	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		20	90	7	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	-	-	1	2	1	1	1	1	2	2	2	1	1	1	1	1
AN-107 (Envelope C)	1	10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	3	1	1	1	1	1	1	1	3	1	1	1	1	1	1
		20	90	3	2	1	2	2	1	1	1	3	2	1	2	2	1	1	1
			95	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
	5	10	90	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
		20	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	5	2	4	1	2	1	1	1	5	2	1	3	2	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.5. Required Number of ILAW CRV Samples (n_S^{CRV})[a] and Analyses per Sample (n_A^{CRV})[a] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of F for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[b]	$\%RSD_A(c_j^{CRV})$[b]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[c] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[c] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	6	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		12	90	1	2	2	1	1	1	1	1	1	3	1	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
	5	6	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	3	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
		12	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	3	2	2	1	1	1	1	1	3	2	2	1	1	1	1	1
AZ-101 (Envelope B)	1	10	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
		20	90	-[d]	-	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	5	2	1	2	2	1	1	1	10	1	1	2	2	1	1	1
	5	10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
		20	90	3	2	2	1	1	1	1	1	3	2	2	1	1	1	1	1
			95	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
AN-107 (Envelope C)	1	20	90	3	2	1	2	2	1	1	1	3	2	1	2	2	1	1	1
			95	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
		40	90	-	-	3	2	1	3	1	2	-	-	5	2	1	3	1	2
			95	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	2
	5	20	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	5	2	1	2	2	1	2	1	5	2	4	1	2	1	1	1
		40	90	-	-	3	2	1	3	1	2	-	-	5	2	2	2	1	2
			95	-	-	5	2	2	2	1	3	-	-	5	2	2	2	1	2

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.6. Required Number of ILAW CRV Samples (n_S^{CRV})[a] and Analyses per Sample (n_A^{CRV})[a] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of Fe_2O_3 for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[b]	$\%RSD_A(c_j^{CRV})$[b]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[c] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[c] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	5	8	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		16	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	8	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		16	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
AZ-101 (Envelope B)	5	10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		20	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		20	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
AN-107 (Envelope C)	5	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

Table H.7. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of K_2O for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(b)]	$\%RSD_A(c_j^{CRV})$[(b)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(c)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(c)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	5	20	90	3	2	1	2	2	1	1	1	-[(d)]	-	1	2	2	1	1	1
			95	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
		40	90	-	-	3	2	1	3	1	2	-	-	-	-	1	3	1	2
			95	-	-	5	2	2	2	1	2	-	-	3	2	2	2	1	2
	15	20	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	5	2	1	2	2	1	1	1	5	2	1	3	2	1	1	1
		40	90	-	-	3	2	2	2	1	2	-	-	3	2	2	2	1	2
			95	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	2
AZ-101 (Envelope B)	5	20	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	3	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
		40	90	-	-	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	3	2	2	2	1	2	-	-	3	2	1	3	1	2
	15	20	90	3	2	2	1	1	1	1	1	3	2	2	1	1	1	1	1
			95	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
		40	90	-	-	-	-	1	2	2	1	-	-	-	-	1	2	2	1
			95	-	-	3	2	1	3	1	2	-	-	3	2	2	2	1	2
AN-107 (Envelope C)	5	10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
		20	90	3	2	1	2	2	1	1	1	3	2	1	2	2	1	1	1
			95	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
	15	10	90	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
		20	90	5	2	1	2	2	1	1	1	10	1	1	2	2	1	1	1
			95	5	2	4	1	2	1	2	1	5	2	2	2	2	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.8. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of Li_2O for a Waste Tank in Each of Two LAW Waste Envelopes[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	5	20	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	5	2	1	3	2	1	1	1	7	2	2	2	1	2	2	1
		40	90	-[(e)]	-	3	2	2	2	1	2	-	-	3	2	2	2	1	2
			95	-	-	5	2	2	2	1	3	-	-	5	2	2	2	1	3
	15	20	90	-	-	4	1	1	2	1	1	-	-	5	1	2	1	2	1
			95	-	-	6	1	4	1	2	1	-	-	6	1	3	1	2	1
		40	90	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	2
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2
AZ-101 (Envelope B)	5	10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		20	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		20	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) Li_2O is not reported for AN-107.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(e) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.9. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of MgO for a Waste Tank in Each of Two LAW Waste Envelopes[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	5	10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		20	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
	15	10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		20	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1
AZ-101 (Envelope B)	5	15	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		30	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	15	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		30	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) MgO is not reported for AN-107.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

Table H.10. Required Number of ILAW CRV Samples (n_S^{CRV})[a] and Analyses per Sample (n_A^{CRV})[a] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of Na_2O for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[b]	$\%RSD_A(c_j^{CRV})$[b]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[c] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[c] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	8	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		16	90	2	2	2	1	1	1	1	1	4	1	2	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	-[d]	-	2	1	1	1	1	1
	5	8	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	3	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
		16	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	-	-	2	1	1	1	1	1	3	2	2	1	1	1	1	1
AZ-101 (Envelope B)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
	5	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	4	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
AN-107 (Envelope C)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
	5	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.11. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of P_2O_5 for a Waste Tank in Each of Two LAW Waste Envelopes[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
	5	5	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	3	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
		10	90	4	1	1	1	1	1	1	1	2	2	1	1	1	1	1	1
			95	6	1	2	1	1	1	1	1	3	2	2	1	1	1	1	1
AZ-101 (Envelope B)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	2	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	2	1	1	1	1	1	1	2	2	1	1	1	1	1	1
	5	5	90	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	4	1	1	1	1	1	1	1
			95	4	1	1	1	1	1	1	1	2	2	1	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) P_2O_5 is not reported for AN-107.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

Table H.12. Required Number of ILAW CRV Samples (n_S^{CRV})[a] and Analyses per Sample (n_A^{CRV})[a] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of SO_3 for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[b]	$\%RSD_A(c_j^{CRV})$[b]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[c] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[c] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	3	1	1	1	1	1	1	1	3	2	1	1	1	1	1
	5	5	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	3	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
		10	90	4	1	2	1	1	1	1	1	4	1	1	1	1	1	1	1
			95	6	1	2	1	1	1	1	1	2	2	2	1	1	1	1	1
AZ-101 (Envelope B)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
	5	5	90	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
AN-107 (Envelope C)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
	5	5	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
		10	90	3	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

Table H.13. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of SiO_2 for a Waste Tank in Each of Two LAW Waste Envelopes[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	5	20	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		40	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	20	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		40	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
AZ-101 (Envelope B)	5	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) SiO_2 is not reported for AN-107.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

Table H.14. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of TiO_2 for a Waste Tank in Each of Two LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(b)]	$\%RSD_A(c_j^{CRV})$[(b)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(c)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(c)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	5	15	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		30	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
	15	15	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		30	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
AZ-101 (Envelope B)	5	15	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		30	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	15	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		30	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

Table H.15. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of ZnO for a Waste Tank in Each of Two LAW Waste Envelopes[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		20	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	5	10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		20	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
AZ-101 (Envelope B)	1	15	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		30	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	5	15	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		30	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) ZnO is not reported for AN-107.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

Table H.16. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Component Mass Fractions of ZrO_2 for a Waste Tank in Each of Two LAW Waste Envelopes[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	5	12	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		24	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
	15	12	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		24	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
AZ-101 (Envelope B)	5	10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		20	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
	15	10	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		20	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) ZrO_2 is not reported for AN-107.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW analyte *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

H.1.2 Details of the Illustration for Reporting Means and Standard Deviations of ILAW Chemical Composition over an LAW Waste Type

There are no detailed results associated with Section 7.1.2 at this time.

H.2 Compliance Results for ILAW Contract Specification 2.2.2.7.2: Radionuclide Composition During Production

Additional details of results from Section 7.2 are presented following. Detailed results from Sections 7.2.1 and 7.2.2 are, respectively, presented in Sections H.2.1 and H.2.2.

H.2.1 Detailed Results of Simulations to Assess the Effects of Process Uncertainties and Numbers of Samples, Analyses, and Measurements on Uncertainties in ILAW Radionuclide Inventory

Detailed results associated with Section 7.2.1 are presented in this section. Tables H.17 to H.30 contain the numbers of samples per LAW CRV batch and analyses per CRV sample necessary to achieve certain ranges of %RHW for each of the ILAW reportable radionuclide composition components (oxides). Any calculation that required more than the number of samples (n_S^{CRV}) and number of analyses per sample (n_A^{CRV}) that were simulated as listed in Table 3.3 was not included in the tables.

The values in this section are a result of the ILAW simulations discussed in Section 3.4.2 and Section 5.2.3.

H.3 Boxplot Interpretation

Section 7 uses boxplots to help show a distribution of values for a given set of data. Boxplots can be found in Figures 7.2, 7.5, 7.6, and 7.7. To help in the discussion of interpreting boxplots, an example boxplot is given in Figure H.1. This boxplot was drawn from a data set consisting of the numbers 1 to 100, incremented by 1, for an easy illustration. Five parts of the boxplot are labeled A through E for the discussion. The bottom line ("A") is called a whisker, which shows the range of the first quartile (up to the 25th percentile). The lower part of the box ("B"), below the box midline, shows the range of the second quartile (25th to 50th percentile). The box midline ("C") shows the position of the median. The upper part of the box ("D"), above the box midline, shows the range of the third quartile (50th to 75th percentile). The top whisker ("E") shows the range of the last quartile (75th percentile to the maximum data point).

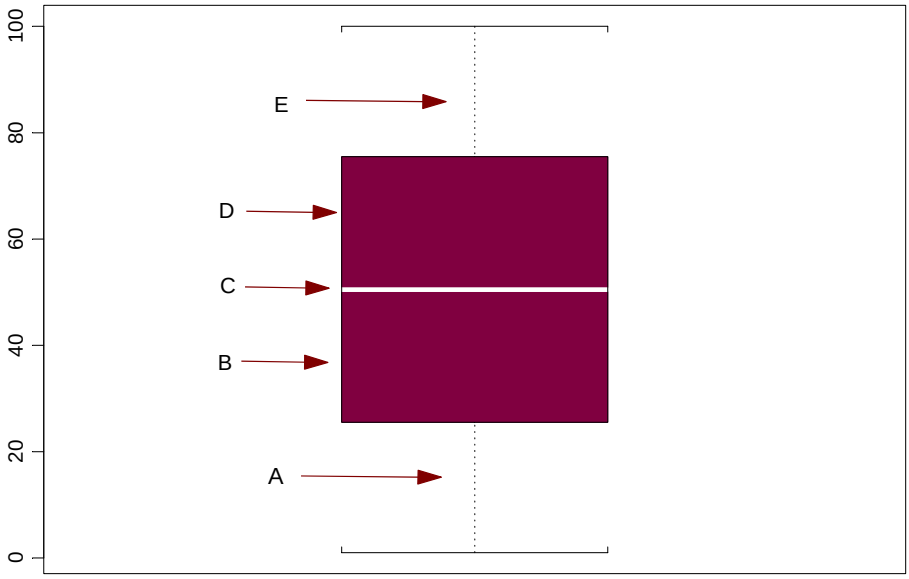

Figure H.1. An Example Boxplot

Table H.17. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of $^{241}Am_2O_3$ for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(b)]	$\%RSD_A(c_j^{CRV})$[(b)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	15	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	-[(d)]	-	1	2	1	1	1	1	3	2	1	2	1	1	1	1
		30	90	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	3	2	1	2	1	2	-	-	-	-	1	2	1	2
	5	15	90	3	2	2	1	1	1	1	1	-	-	2	1	1	1	1	1
			95	10	1	1	2	2	1	1	1	5	2	1	2	1	1	1	1
		30	90	-	-	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	-	-	1	2	1	2	-	-	3	2	1	3	1	2
AZ-101 (Envelope B)	1	25	90	3	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	5	2	1	2	1	2	1	1	5	2	4	1	2	1	2	1
		50	90	-	-	3	2	2	2	1	2	-	-	3	2	2	2	1	2
			95	-	-	5	2	2	2	1	2	-	-	5	2	2	2	4	1
	5	25	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	5	2	2	2	2	1	1	1	7	2	4	1	2	1	1	1
		50	90	-	-	3	2	2	2	1	2	-	-	3	2	2	2	1	2
			95	-	-	5	2	2	2	1	3	-	-	5	2	2	2	1	2
AN-107 (Envelope C)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	2	2	1	1	1	1	1	1	2	1	1	1	1	1	1
	5	5	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	3	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	5	1	2	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.18. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of $^{243+244}Cm_2O_3$ for a Waste Tank in Each of Two LAW Waste Envelopes[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	25	90	5	2	1	3	2	1	1	1	5	2	4	1	2	1	2	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-[(e)]	-	5	2	2	2	1	3	-	-	5	2	2	2	1	2
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2
	5	25	90	5	2	4	1	2	1	2	1	7	2	1	3	2	1	2	1
			95	7	2	2	2	1	2	2	1	-	-	2	2	1	2	2	1
		50	90	-	-	5	2	2	2	1	2	-	-	5	2	-	-	1	3
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2
AZ-101 (Envelope B)	1	25	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	5	2	1	3	2	1	1	1	5	2	1	2	1	2	2	1
		50	90	-	-	3	2	2	2	1	2	-	-	3	2	2	2	1	2
			95	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	2
	5	25	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	5	2	2	2	2	1	2	1	5	2	2	2	1	2	2	1
		50	90	-	-	3	2	2	2	1	2	-	-	5	2	2	2	1	2
			95	-	-	5	2	2	2	2	2	-	-	5	2	2	2	1	3

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) $^{243+244}Cm_2O_3$ is not reported for AN-107.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(e) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.19. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of ^{60}CoO for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(b)]	$\%RSD_A(c_j^{CRV})$[(b)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	3	2	1	1	1	1	1	1	3	2	1	1	1	1	1
	5	5	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	3	1	1	1	1	1	1	1	3	1	1	1	1	1	1	1
		10	90	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
			95	6	1	2	1	1	1	1	1	5	1	2	1	1	1	1	1
AZ-101 (Envelope B)	1	25	90	3	2	1	2	2	1	1	1	3	2	1	2	2	1	1	1
			95	5	2	1	2	2	1	1	1	5	2	1	3	1	2	1	1
		50	90	-[(d)]	-	3	2	2	2	1	2	-	-	3	2	2	2	1	2
			95	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	2
	5	25	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	7	2	2	2	1	2	2	1	5	2	2	2	1	2	2	1
		50	90	-	-	3	2	2	2	1	2	-	-	5	2	2	2	1	2
			95	-	-	5	2	2	2	1	3	-	-	5	2	2	2	1	2
AN-107 (Envelope C)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	3	1	1	1	1	1	1	1	3	1	1	1	1	1	1
	5	5	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
			95	6	1	2	1	1	1	1	1	5	1	2	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.20. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of $^{137}Cs_2O$ for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(b)]	$\%RSD_A(c_j^{CRV})$[(b)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	25	90	5	2	1	3	2	1	1	1	5	2	1	3	2	1	2	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-[(d)]	-	5	2	2	2	1	3	-	-	5	2	2	2	1	2
			95	-	-	7	2	3	2	2	2	-	-	5	2	3	2	2	2
	5	25	90	5	2	2	2	2	1	2	1	7	2	2	2	2	1	2	1
			95	7	2	2	2	1	2	2	1	-	-	2	2	1	2	2	1
		50	90	-	-	5	2	2	2	1	3	-	-	5	2	2	2	1	2
			95	-	-	5	2	3	2	2	2	-	-	7	2	3	2	2	2
AZ-101 (Envelope B)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	2	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
	5	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
AN-107 (Envelope C)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	3	2	1	1	1	1	1	1	3	2	1	1	1	1	1
	5	5	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	3	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	5	1	2	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.21. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses Per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of $^{154}Eu_2O_3$ for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(b)]	$\%RSD_A(c_j^{CRV})$[(b)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	25	90	5	2	1	3	2	1	2	1	5	2	1	3	2	1	2	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-[(d)]	-	5	2	2	2	1	2	-	-	5	2	2	2	1	2
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2
	5	5	90	5	2	1	3	2	1	2	1	7	2	1	3	1	2	2	1
			95	7	2	2	2	1	2	2	1	-	-	2	2	1	2	2	1
		10	90	-	-	5	2	2	2	1	2	-	-	5	2	-	-	1	3
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2
AZ-101 (Envelope B)	1	25	90	3	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	5	2	1	3	2	1	2	1	5	2	4	1	2	1	2	1
		50	90	-	-	3	2	1	3	1	2	-	-	3	2	2	2	1	2
			95	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	3
	5	25	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	7	2	1	3	1	2	2	1	5	2	2	2	2	1	1	1
		50	90	-	-	3	2	2	2	1	2	-	-	3	2	1	3	1	2
			95	-	-	5	2	2	2	2	2	-	-	5	2	2	2	1	3
AN-107 (Envelope C)	1	15	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	-	-	2	1	1	1	1	1	-	-	2	1	1	1	1	1
		30	90	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	2	2	1	2	2	1	-	-	-	-	1	2	1	2
	5	15	90	3	2	2	1	1	1	1	1	-	-	2	1	1	1	1	1
			95	3	2	1	2	2	1	1	1	10	1	1	2	2	1	1	1
		30	90	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	-	-	1	3	1	2	-	-	3	2	1	3	2	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.22. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of $^{155}Eu_2O_3$ for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(b)]	$\%RSD_A(c_j^{CRV})$[(b)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	25	90	5	2	1	2	2	1	2	1	5	2	1	3	2	1	1	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-[(d)]	-	7	2	2	2	1	3	-	-	5	2	2	2	1	3
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2
	5	25	90	5	2	2	2	2	1	2	1	7	2	2	2	2	1	2	1
			95	-	-	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-	-	5	2	2	2	1	3	-	-	5	2	2	2	1	2
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2
AZ-101 (Envelope B)	1	15	90	1	3	2	1	1	1	1	1	1	3	2	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
		30	90	5	2	1	3	2	1	2	1	5	2	1	2	1	2	2	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
	5	15	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	3	2	2	1	1	1	1	1	3	2	2	1	1	1	1	1
		30	90	5	2	2	2	2	1	2	1	5	2	2	2	2	1	2	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
AN-107 (Envelope C)	1	15	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	2	2	1	2	1	1	1	1	-	-	1	2	1	1	1	1
		30	90	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	-	-	1	2	2	1	-	-	2	2	1	2	1	2
	5	15	90	-	-	2	1	1	1	1	1	3	2	2	1	1	1	1	1
			95	10	1	1	2	2	1	1	1	10	1	1	2	2	1	1	1
		30	90	-	-	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	-	-	4	1	1	2	-	-	3	2	1	3	1	2

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.23. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of ^{63}NiO for a Waste Tank in One LAW Waste Envelope[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	25	90	5	2	1	3	2	1	2	1	5	2	1	2	2	1	2	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-[(e)]	-	5	2	2	2	1	2	-	-	5	2	2	2	1	2
			95	-	-	7	2	5	2	2	2	-	-	7	2	3	2	2	2
	5	25	90	7	2	1	3	1	2	1	1	7	2	2	2	2	1	2	1
			95	7	2	6	1	1	2	2	1	-	-	2	2	1	2	2	1
		50	90	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	3
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) ^{63}NiO is not reported for AZ-101 and AN-107.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(e) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.24. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of $^{237}NpO_2$ for a Waste Tank in Each of Two LAW Waste Envelopes[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AZ-101 (Envelope B)	1	15	90	1	3	1	1	1	1	1	1	1	3	2	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
		30	90	5	2	1	3	2	1	2	1	5	2	1	3	2	1	2	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
	5	15	90	2	2	2	1	1	1	1	1	2	2	1	1	1	1	1	1
			95	3	2	2	1	1	1	1	1	3	2	2	1	1	1	1	1
		30	90	7	2	2	2	2	1	1	1	5	2	2	2	2	1	1	1
			95	7	2	2	2	1	2	2	1	-[(e)]	-	2	2	1	2	2	1
AN-107 (Envelope C)	1	15	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	-	-	1	2	1	1	1	1	-	-	1	2	1	1	1	1
		30	90	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	-	-	1	2	1	2	-	-	-	-	1	3	2	1
	5	15	90	6	1	2	1	1	1	1	1	3	2	2	1	1	1	1	1
			95	3	2	1	2	2	1	1	1	3	2	1	2	1	1	1	1
		30	90	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	3	2	1	3	1	2	-	-	3	2	1	2	1	2

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) $^{237}NpO_2$ is not reported for AP-101.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(e) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.25. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of $^{238}PuO_2$ for a Waste Tank in Each of Two LAW Waste Envelopes[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	25	90	7	2	1	2	2	1	2	1	5	2	1	2	2	1	1	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-[(e)]	-	5	2	2	2	1	2	-	-	5	2	2	2	1	2
			95	-	-	7	2	-	-	2	2	-	-	7	2	3	2	2	2
	5	25	90	5	2	2	2	1	2	1	1	7	2	2	2	1	2	2	1
			95	-	-	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	2
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2
AZ-101 (Envelope B)	1	25	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	5	2	1	2	2	1	2	1	5	2	1	3	2	1	1	1
		50	90	-	-	3	2	2	2	1	2	-	-	3	2	2	2	1	2
			95	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	3
	5	25	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	5	2	2	2	2	1	2	1	5	2	2	2	1	2	2	1
		50	90	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	2
			95	-	-	5	2	2	2	1	3	-	-	5	2	2	2	1	3

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) $^{238}PuO_2$ is not reported for AN-107.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(e) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.26. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of $^{239}PuO_2$ for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(b)]	$\%RSD_A(c_j^{CRV})$[(b)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	25	90	5	2	1	3	2	1	1	1	5	2	1	3	2	1	1	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-[(d)]	-	5	2	2	2	1	3	-	-	5	2	2	2	1	2
			95	-	-	5	2	3	2	2	2	-	-	7	2	3	2	2	2
	5	25	90	5	2	2	2	2	1	2	1	5	2	2	2	1	2	2	1
			95	-	-	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-	-	5	2	2	2	1	3	-	-	5	2	2	2	1	3
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2
AZ-101 (Envelope B)	1	25	90	5	2	1	2	2	1	1	1	3	2	1	2	2	1	1	1
			95	5	2	1	3	2	1	2	1	5	2	1	3	2	1	1	1
		50	90	-	-	3	2	2	2	1	2	-	-	3	2	2	2	1	2
			95	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	3
	5	25	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	5	2	2	2	2	1	1	1	5	2	2	2	1	2	1	1
		50	90	-	-	3	2	2	2	1	2	-	-	5	2	2	2	1	2
			95	-	-	5	2	2	2	1	2	-	-	5	2	-	-	1	2
AN-107 (Envelope C)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	3	1	1	1	1	1	1	1	2	1	1	1	1	1	1
	5	5	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	3	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.27. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of $^{241}PuO_2$ for a Waste Tank in Each of Two LAW Waste Envelopes[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	25	90	5	2	1	3	2	1	2	1	5	2	1	3	2	1	2	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-[(e)]	-	5	2	2	2	1	2	-	-	5	2	-	-	1	2
			95	-	-	7	2	-	-	2	2	-	-	7	2	3	2	2	2
	5	25	90	5	2	4	1	2	1	2	1	7	2	2	2	2	1	1	1
			95	-	-	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	3
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2
AZ-101 (Envelope B)	1	25	90	5	2	1	2	2	1	1	1	3	2	1	2	2	1	1	1
			95	5	2	1	3	2	1	1	1	5	2	2	2	1	2	1	1
		50	90	-	-	3	2	2	2	1	2	-	-	3	2	2	2	1	2
			95	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	2
	5	25	90	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
			95	7	2	1	3	2	1	2	1	5	2	2	2	2	1	2	1
		50	90	-	-	3	2	2	2	1	2	-	-	3	2	2	2	1	2
			95	-	-	5	2	2	2	1	2	-	-	5	2	2	2	1	3

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) $^{241}PuO_2$ is not reported for AN-107.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(e) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.28. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of $^{125}Sb_2O_3$ for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(b)]	$\%RSD_A(c_j^{CRV})$[(b)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	15	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	-[(d)]	-	1	2	1	1	1	1	-	-	1	2	2	1	1	1
		30	90	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	-	-	1	3	1	2	-	-	-	-	1	2	1	2
	5	15	90	-	-	2	1	1	1	1	1	3	2	2	1	1	1	1	1
			95	5	2	1	2	2	1	1	1	5	2	1	2	2	1	1	1
		30	90	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	-	-	1	2	1	2	-	-	3	2	1	3	1	2
AZ-101 (Envelope B)	1	15	90	2	2	2	1	1	1	1	1	4	1	2	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
		30	90	5	2	1	3	2	1	1	1	5	2	1	3	2	1	2	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
	5	15	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	3	2	2	1	1	1	1	1	3	2	2	1	1	1	1	1
		30	90	5	2	1	2	2	1	2	1	7	2	2	2	2	1	2	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
AN-107 (Envelope C)	1	15	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	-	-	1	2	1	1	1	1	3	2	2	1	1	1	1	1
		30	90	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	-	-	1	2	1	2	-	-	-	-	1	2	1	2
	5	15	90	2	2	2	1	1	1	1	1	-	-	2	1	1	1	1	1
			95	10	1	1	2	1	1	1	1	3	2	1	2	2	1	1	1
		30	90	7	2	2	2	1	2	2	1	-	-	2	2	1	2	2	1
			95	-	-	-	-	1	2	2	1	-	-	3	2	4	1	1	2

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.29. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of ^{90}SrO for a Waste Tank in Each of Three LAW Waste Envelopes

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(b)]	$\%RSD_A(c_j^{CRV})$[(b)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(c)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	1	3	2	1	1	1	1	1
	5	5	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	1	2	1	1	1	1	1	1	3	1	1	1	1	1	1	1
		10	90	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
			95	2	2	2	1	1	1	1	1	5	1	2	1	1	1	1	1
AZ-101 (Envelope B)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
	5	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	3	1	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	4	1	1	1	1	1	1	1	4	1	1	1	1	1	1	1
AN-107 (Envelope C)	1	25	90	5	2	1	3	1	2	1	1	5	2	1	2	2	1	1	1
			95	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-[(d)]	-	5	2	2	2	1	3	-	-	5	2	2	2	1	2
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2
	5	25	90	5	2	2	2	2	1	2	1	7	2	2	2	2	1	2	1
			95	-	-	2	2	1	2	2	1	7	2	2	2	1	2	2	1
		50	90	-	-	5	2	2	2	1	3	-	-	5	2	2	2	1	3
			95	-	-	7	2	3	2	2	2	-	-	7	2	3	2	2	2

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(c) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(d) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

Table H.30. Required Number of ILAW CRV Samples (n_S^{CRV})[(a)] and Analyses per Sample (n_A^{CRV})[(a)] to Satisfy Certain %RHWs on ILAW Radionuclide Component Mass Fractions of $^{99}Tc_2O_7$ for a Waste Tank in Each of Two LAW Waste Envelopes[(b)]

Waste Tank (Envelope)	$\%RSD_S(c_j^{CRV})$[(c)]	$\%RSD_A(c_j^{CRV})$[(c)]	% Confidence	%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(d)] are at Low Values								%RHWs on the Mass Fraction of an ILAW Radionuclide Component when Other Uncertainties[(d)] are at High Values							
				< 5%		< 10%		< 15%		< 20%		< 5%		< 10%		< 15%		< 20%	
				n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A	n_S	n_A
AP-101 (Envelope A)	1	15	90	2	2	2	1	1	1	1	1	2	2	2	1	1	1	1	1
			95	3	2	1	2	2	1	1	1	2	2	1	2	1	1	1	1
		30	90	7	2	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-[(d)]	-	2	2	1	3	2	1	-	-	3	2	1	2	2	1
	5	15	90	-	-	2	1	1	1	1	1	-	-	2	1	1	1	1	1
			95	10	1	1	2	2	1	1	1	10	1	1	2	1	1	1	1
		30	90	-	-	2	2	1	2	2	1	7	2	2	2	1	2	2	1
			95	-	-	3	2	1	2	2	1	-	-	3	2	1	2	2	1
AN-107 (Envelope C)	1	5	90	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
			95	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
		10	90	1	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1
			95	1	3	1	1	1	1	1	1	1	2	1	1	1	1	1	1
	5	5	90	2	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
			95	3	1	1	1	1	1	1	1	2	1	1	1	1	1	1	1
		10	90	4	1	1	1	1	1	1	1	4	1	2	1	1	1	1	1
			95	5	1	2	1	1	1	1	1	2	2	2	1	1	1	1	1

(a) To conserve space within the table, n_S^{CRV} is labeled n_S, and n_A^{CRV} is labeled n_A.

(b) $^{99}Tc_2O_7$ is not reported for AZ-101.

(c) The notation $\%RSD_S(c_j^{CRV})$ and $\%RSD_A(c_j^{CRV})$ represent, respectively, the mixing/sampling and analytical uncertainties for the concentration of LAW radionuclide *j* in the CRV.

(d) Other uncertainties include GFC uncertainty, GFC weights uncertainty, and volume uncertainty. Their low and high values used for this work are listed in Tables D.6, D.7, and D.9.

(e) A dash (–) means that no number of samples and analyses tested as listed in Table 3.3 satisfied that %RHW category.

H.2.2 Details of the Illustration for Calculating Means and Standard Deviations of ILAW Radionuclide Inventory per Container over an LAW Waste Type

There are no details of the illustration associated with Section 7.2.2 at this time.

Appendix I

Simulated Data Used to Illustrate IHLW Compliance Methods

Appendix I: Simulated Data Used to Illustrate IHLW Compliance Methods

This appendix presents the simulated data used to illustrate in Section 6 the immobilized high-level waste (IHLW) compliance methods that were presented in Section 4. These simulated data are based on data from tank waste samples, glass formulation development work, melter testing, realistic estimates of variations and uncertainties, G2 software (Deng 2004; Vora 2004) simulations of the Waste Treatment Plant (WTP) high-level waste (HLW) vitrification process, and statistical simulations to include realistic uncertainties. Hence, the data included in this appendix have been "constructed" from various inputs and methods to provide, as much as is possible at this time, a realistic simulation of data that will be collected during operation of the WTP IHLW facility.

I.1 Simulated Data Used to Illustrate Calculating Means and Standard Deviations of IHLW Chemical Compositions

Simulated data were used in Section 6.1.2 to illustrate calculations of means, standard deviations, and percent relative standard deviations (%RSDs) with Eqs. (4.1.2), (4.1.3), and (4.1.4). The simulated data consist of elemental concentrations (g/L) [(a)] for 18 IHLW Melter Feed Process Vessel (MFPV) batches corresponding to an HLW waste type from Tank AY-102/C-106, with 8 samples per MFPV batch and one chemical analysis per sample. The simulated data were generated by starting with concentrations for 18 MFPV batches obtained from an Excel spreadsheet (Vienna 2004a) containing results from Run 3.1vv of the G2 dynamic simulation flowsheet (Deng 2004; Vora 2004). Note that G2 does not simulate multiple MFPV samples and/or analyses per sample and thus does not simulate MFPV mixing/sampling and analytical uncertainties. To address this issue, normally distributed random disturbances for mixing/sampling and analytical uncertainties (using the %RSD values given in Tables C.1 and C.2) were added to the elemental concentration data for the 18 MFPV batches from G2. This process created eight observations of elemental concentrations per MFPV batch that simulated mixing/sampling and analytical uncertainties in the AY-102/C-106 G2 run. The resulting simulated data were used "as is", with no attempt to apply realistic detection limits to small simulated concentration values.

Because the simulated data consist of 18 × 8 sets of elemental concentration data, they are not all displayed in this section. Table I.1 shows averages of the simulated concentrations for each of the 18 IHLW MFPV batches.

Table I.2 lists simulated volumes (in L) of the 18 MFPV batches corresponding to AY-102/C-106, as obtained directly from G2 Run 3.1vv (Vienna 2004a).

(a) Elsewhere in this report chemical composition elemental concentrations are assumed to be measured in units of mg/L. The simulated data here were generated in units of g/L and hence listed that way in tables. They could be converted to units of mg/L, but for calculating mass fractions of chemical composition components it is unnecessary as the units cancel.

Table I.3 contains averages of simulated IHLW chemical composition mass fractions for each of the 18 IHLW MFPV batches calculated from the simulated elemental concentrations using Eq. (A.1.5) in Section A.1 of Appendix A.

Table I.1. Averages of Simulated Elemental Concentrations ($\bar{c}_{ij}^{MFPV}$, g/L) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type for Tank AY-102/C-106. Values reported for each batch are averages of simulated concentrations for eight samples per batch with one chemical analysis per sample.

IHLW Element *j*	Average Elemental Concentrations (g/L) for MFPV Batch Numbers *i* = 1 to 9								
	1	2	3	4	5	6	7	8	9
Ag	4.56E-02	4.31E-02	4.30E-02	4.17E-02	4.18E-02	4.18E-02	4.16E-02	4.19E-02	4.15E-02
Al	3.43E+01	3.57E+01	3.43E+01	8.25E+00	3.37E+00	3.39E+01	8.60E+00	3.39E+00	3.27E+00
As	5.20E-02	5.08E-02	5.06E-02	5.17E-02	5.12E-02	4.91E-02	5.00E-02	4.85E-02	4.98E-02
B	6.74E+01	7.02E+01	6.96E+01	1.72E+02	2.04E+02	6.99E+01	6.96E+01	2.13E+02	1.73E+02
Ba	1.40E+00	1.37E+00	1.34E+00	1.34E+00	1.36E+00	1.33E+00	1.38E+00	1.31E+00	1.33E+00
Be	1.16E-02	1.16E-02	1.17E-02	1.12E-02	1.13E-02	1.16E-02	1.13E-02	1.14E-02	1.13E-02
Bi	2.58E-01	2.56E-01	2.62E-01	2.53E-01	2.49E-01	2.51E-01	2.61E-01	2.50E-01	2.48E-01
Ca	1.14E+01	1.14E+01	1.16E+01	1.15E+01	1.13E+01	1.15E+01	1.16E+01	1.15E+01	1.14E+01
Cd	1.81E-01	1.81E-01	1.78E-01	1.74E-01	1.79E-01	1.83E-01	1.78E-01	1.73E-01	1.76E-01
Ce	2.90E+00	2.88E+00	2.88E+00	2.85E+00	2.82E+00	2.87E+00	2.89E+00	2.85E+00	2.86E+00
Cl	2.55E-01	2.59E-01	2.58E-01	2.51E-01	2.54E-01	2.56E-01	2.59E-01	2.56E-01	2.55E-01
Cr	2.40E+00	2.44E+00	2.51E+00	2.34E+00	2.40E+00	2.43E+00	2.45E+00	2.40E+00	2.36E+00
Cs	7.95E-02	7.62E-02	7.51E-02	7.56E-02	7.30E-02	7.59E-02	7.45E-02	7.34E-02	7.46E-02
Cu	3.92E-01	3.93E-01	3.94E-01	3.85E-01	3.81E-01	3.88E-01	3.86E-01	3.76E-01	3.75E-01
F	4.91E-01	4.78E-01	4.87E-01	4.85E-01	4.71E-01	4.64E-01	4.91E-01	4.69E-01	4.61E-01
Fe	2.04E+02	2.12E+02	2.09E+02	2.01E+02	2.04E+02	2.08E+02	2.10E+02	2.06E+02	1.94E+02
K	5.51E+00	5.42E+00	5.48E+00	5.58E+00	5.52E+00	5.54E+00	5.75E+00	5.46E+00	5.47E+00
La	2.19E+00	2.21E+00	2.16E+00	2.19E+00	2.06E+00	2.16E+00	2.14E+00	2.20E+00	2.16E+00
Li	5.61E+01	5.73E+01	5.58E+01	5.25E+01	5.27E+01	5.42E+01	5.48E+01	5.42E+01	5.42E+01
Mg	4.51E+00	4.45E+00	4.47E+00	4.41E+00	4.31E+00	4.42E+00	4.46E+00	4.46E+00	4.42E+00
Mn	2.35E+01	2.32E+01	2.25E+01	2.24E+01	2.25E+01	2.30E+01	2.29E+01	2.27E+01	2.31E+01
Mo	2.36E-02	2.36E-02	2.32E-02	2.37E-02	2.33E-02	2.42E-02	2.39E-02	2.40E-02	2.39E-02
Na	1.38E+02	1.35E+02	1.39E+02	1.23E+02	7.86E+01	1.35E+02	1.60E+02	7.69E+01	1.21E+02
Nd	1.84E+00	1.82E+00	1.87E+00	1.83E+00	1.77E+00	1.86E+00	1.85E+00	1.84E+00	1.81E+00
Ni	5.49E+00	5.46E+00	5.43E+00	5.42E+00	5.30E+00	5.25E+00	5.37E+00	5.35E+00	5.46E+00

Table I.1. Averages of Simulated Elemental Concentrations ($\bar{c}_{ij}^{MFPV}$, g/L) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type for Tank AY-102/C-106. Values reported for each batch are averages of simulated concentrations for eight samples per batch with one chemical analysis per sample. (cont.)

IHLW Element *j*	Average Elemental Concentrations (g/L) for MFPV Batch Numbers *i* = 1 to 9								
	1	2	3	4	5	6	7	8	9
P	3.52E+00	3.68E+00	3.61E+00	3.63E+00	3.56E+00	3.60E+00	3.52E+00	3.40E+00	3.42E+00
Pb	1.57E+01	1.48E+01	1.54E+01	1.45E+01	1.48E+01	1.54E+01	1.53E+01	1.53E+01	1.51E+01
Pd	3.71E-05	3.71E-05	3.82E-05	3.51E-05	3.51E-05	3.64E-05	3.66E-05	3.51E-05	3.49E-05
Pr	5.43E-01	5.55E-01	5.52E-01	5.35E-01	5.36E-01	5.42E-01	5.43E-01	5.32E-01	5.20E-01
Rb	4.00E-03	4.10E-03	3.84E-03	3.97E-03	3.92E-03	3.91E-03	3.95E-03	3.85E-03	4.01E-03
Rh	3.77E-02	3.74E-02	3.70E-02	3.69E-02	3.58E-02	3.69E-02	3.66E-02	3.63E-02	3.62E-02
Ru	8.68E-01	8.62E-01	8.37E-01	8.35E-01	8.14E-01	8.65E-01	8.57E-01	8.15E-01	8.38E-01
Sb	5.96E-03	5.98E-03	6.00E-03	5.93E-03	5.95E-03	5.70E-03	5.94E-03	5.81E-03	5.83E-03
Se	5.63E-03	5.65E-03	5.64E-03	5.64E-03	5.52E-03	5.62E-03	5.68E-03	5.59E-03	5.50E-03
Si	5.85E+02	5.85E+02	5.77E+02	5.09E+02	5.09E+02	5.88E+02	5.84E+02	5.09E+02	5.24E+02
S	6.30E-01	6.35E-01	6.33E-01	6.26E-01	6.12E-01	6.40E-01	6.10E-01	6.22E-01	6.22E-01
Sr	5.09E-01	5.39E-01	5.29E-01	5.08E-01	4.92E-01	5.04E-01	5.24E-01	5.09E-01	5.10E-01
Ta	3.29E-03	3.18E-03	3.17E-03	3.26E-03	3.17E-03	3.30E-03	3.22E-03	3.23E-03	3.25E-03
Te	1.77E-01	1.76E-01	1.74E-01	1.74E-01	1.65E-01	1.70E-01	1.72E-01	1.68E-01	1.75E-01
Ti	2.70E-01	2.84E-01	2.71E-01	2.70E-01	2.76E-01	2.72E-01	2.80E-01	2.74E-01	2.76E-01
Tl	8.11E-03	7.69E-03	8.07E-03	7.68E-03	7.88E-03	7.84E-03	8.05E-03	7.97E-03	8.02E-03
V	7.77E-02	8.12E-02	7.93E-02	7.80E-02	7.98E-02	7.97E-02	7.88E-02	7.89E-02	8.07E-02
W	4.64E-01	4.79E-01	4.62E-01	4.41E-01	4.59E-01	4.62E-01	4.36E-01	4.54E-01	4.66E-01
Y	1.89E-01	1.85E-01	1.91E-01	1.80E-01	1.84E-01	1.94E-01	1.89E-01	1.84E-01	1.88E-01
Zn	2.88E-01	2.98E-01	2.90E-01	2.90E-01	2.81E-01	2.89E-01	2.99E-01	2.85E-01	2.93E-01
Zr	5.36E-02	5.56E-02	5.46E-02	5.37E-02	5.24E-02	5.39E-02	5.36E-02	5.24E-02	5.46E-02

Table I.1. Averages of Simulated Elemental Concentrations ($\bar{c}_{ij}^{MFPV}$, g/L) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type for Tank AY-102/C-106. Values reported for each batch are averages of simulated concentrations for eight samples per batch with one chemical analysis per sample. (cont.)

IHLW Element *j*	Average Elemental Concentrations (g/L) for MFPV Batch Numbers *i* = 10 to 18								
	10	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**
Ag	4.12E-02	4.17E-02	4.27E-02	4.27E-02	4.22E-02	4.28E-02	4.15E-02	4.29E-02	4.28E-02
Al	3.46E+01	8.60E+00	3.24E+00	3.32E+00	3.35E+00	3.26E+00	3.33E+00	3.29E+00	3.25E+00
As	5.08E-02	5.01E-02	5.07E-02	5.02E-02	5.09E-02	5.12E-02	5.29E-02	4.96E-02	4.94E-02
B	6.91E+01	7.13E+01	6.62E+01	6.96E+01	7.06E+01	6.87E+01	6.97E+01	6.85E+01	6.86E+01
Ba	1.37E+00	1.39E+00	1.32E+00	1.43E+00	1.36E+00	1.33E+00	1.35E+00	1.40E+00	1.35E+00
Be	1.13E-02	1.15E-02	1.16E-02	1.17E-02	1.12E-02	1.15E-02	1.13E-02	1.10E-02	1.16E-02
Bi	2.55E-01	2.55E-01	2.62E-01	2.68E-01	2.53E-01	2.59E-01	2.61E-01	2.52E-01	2.60E-01
Ca	1.14E+01	1.20E+01	1.17E+01	1.19E+01	1.15E+01	1.16E+01	1.14E+01	1.17E+01	1.19E+01
Cd	1.82E-01	1.81E-01	1.83E-01	1.79E-01	1.75E-01	1.82E-01	1.76E-01	1.75E-01	1.79E-01
Ce	2.99E+00	2.84E+00	2.89E+00	3.03E+00	2.79E+00	2.89E+00	2.91E+00	2.84E+00	2.94E+00
Cl	2.54E-01	2.46E-01	2.44E-01	2.45E-01	2.38E-01	2.48E-01	2.45E-01	2.39E-01	2.41E-01
Co	7.10E-10	6.87E-10	7.14E-10	6.78E-10	6.81E-10	6.79E-10	6.72E-10	6.78E-10	6.96E-10
Cr	2.43E+00	2.38E+00	2.45E+00	2.41E+00	2.37E+00	2.35E+00	2.45E+00	2.35E+00	2.44E+00
Cs	5.46E-02	4.30E-02	3.31E-02	2.93E-02	2.52E-02	2.46E-02	2.27E-02	2.22E-02	2.34E-02
Cu	3.95E-01	3.80E-01	3.78E-01	3.94E-01	3.89E-01	3.75E-01	3.84E-01	3.76E-01	3.96E-01
F	4.84E-01	4.74E-01	4.65E-01	4.57E-01	4.54E-01	4.65E-01	4.77E-01	4.52E-01	4.61E-01
Fe	2.09E+02	2.12E+02	2.02E+02	2.08E+02	2.05E+02	2.04E+02	2.08E+02	2.08E+02	2.08E+02
K	5.52E+00	5.55E+00	5.47E+00	5.37E+00	5.56E+00	5.50E+00	5.37E+00	5.38E+00	5.41E+00
La	2.16E+00	2.16E+00	2.20E+00	2.17E+00	2.13E+00	2.26E+00	2.16E+00	2.15E+00	2.23E+00
Li	5.60E+01	5.44E+01	5.65E+01	5.61E+01	5.33E+01	5.57E+01	5.38E+01	1.36E+01[(a)]	5.51E+01
Mg	4.39E+00	4.53E+00	4.52E+00	4.53E+00	4.47E+00	4.39E+00	4.51E+00	4.43E+00	4.79E+00
Mn	2.33E+01	2.28E+01	2.35E+01	2.33E+01	2.34E+01	2.34E+01	2.29E+01	2.30E+01	2.36E+01
Mo	2.37E-02	2.40E-02	2.37E-02	2.34E-02	2.34E-02	2.38E-02	2.41E-02	2.35E-02	2.38E-02
Na	1.31E+02	1.66E+02	1.63E+02	1.64E+02	1.09E+02	1.62E+02	1.11E+02	1.44E+02	1.62E+02
Nb	2.27E-08	2.29E-08	2.31E-08	2.30E-08	2.27E-08	2.20E-08	2.26E-08	2.26E-08	2.28E-08
Nd	1.87E+00	1.84E+00	1.82E+00	1.88E+00	1.86E+00	1.90E+00	1.83E+00	1.83E+00	1.90E+00
Ni	5.44E+00	5.60E+00	5.38E+00	5.56E+00	5.32E+00	5.37E+00	5.39E+00	5.36E+00	5.35E+00

(a) This outlying value was present in the data supplied by the WTP Project from the G2 results (Vienna 2004a). No attempt to remove or replace the apparent outlier was made for the example calculations in this report.

Table I.1. Averages of Simulated Elemental Concentrations ($\bar{c}_{ij}^{MFPV}$, g/L) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type for Tank AY-102/C-106. Values reported for each batch are averages of simulated concentrations for eight samples per batch with one chemical analysis per sample. (cont.)

IHLW Element *j*	Average Elemental Concentrations (g/L) for MFPV Batch Numbers *i* = 10 to 18								
	10	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**
Np	1.01E-02	9.99E-03	1.01E-02	1.02E-02	9.87E-03	1.03E-02	9.73E-03	9.98E-03	1.01E-02
P	3.54E+00	3.44E+00	3.55E+00	3.55E+00	3.59E+00	3.55E+00	3.47E+00	3.58E+00	3.55E+00
Pb	1.52E+01	1.52E+01	1.50E+01	1.53E+01	1.49E+01	1.50E+01	1.50E+01	1.51E+01	1.49E+01
Pd	3.51E-05	3.57E-05	3.60E-05	3.50E-05	3.51E-05	3.64E-05	3.56E-05	3.46E-05	3.52E-05
Pr	5.41E-01	5.49E-01	5.52E-01	5.39E-01	5.53E-01	5.39E-01	5.63E-01	5.27E-01	5.37E-01
Rb	3.90E-03	4.01E-03	4.03E-03	3.95E-03	3.99E-03	3.92E-03	3.86E-03	3.89E-03	4.01E-03
Rh	3.70E-02	3.79E-02	3.84E-02	3.74E-02	3.79E-02	3.75E-02	3.75E-02	3.71E-02	3.86E-02
Ru	8.36E-01	8.37E-01	8.43E-01	8.59E-01	8.48E-01	8.45E-01	8.44E-01	8.41E-01	8.28E-01
Sb	5.97E-03	5.92E-03	5.86E-03	5.78E-03	5.68E-03	5.91E-03	5.75E-03	5.73E-03	5.78E-03
Se	5.61E-03	5.47E-03	5.55E-03	5.66E-03	5.64E-03	5.70E-03	5.74E-03	5.47E-03	5.62E-03
Si	5.94E+02	5.81E+02	5.87E+02	6.07E+02	6.53E+02	5.99E+02	6.33E+02	6.37E+02	6.02E+02
S	6.22E-01	6.29E-01	6.10E-01	6.21E-01	6.11E-01	6.16E-01	6.00E-01	5.79E-01	5.91E-01
Sr	5.26E-01	5.20E-01	5.11E-01	5.06E-01	5.12E-01	5.32E-01	5.08E-01	5.09E-01	5.09E-01
Ta	3.21E-03	3.28E-03	3.22E-03	3.28E-03	3.22E-03	3.27E-03	3.27E-03	3.24E-03	3.28E-03
Tc	9.27E-04	9.04E-04	9.45E-04	9.23E-04	8.89E-04	9.21E-04	8.91E-04	8.60E-04	9.24E-04
Te	1.73E-01	1.72E-01	1.67E-01	1.77E-01	1.78E-01	1.74E-01	1.76E-01	1.75E-01	1.74E-01
Ti	2.76E-01	2.79E-01	2.78E-01	2.86E-01	2.90E-01	2.77E-01	2.76E-01	2.75E-01	2.90E-01
Tl	8.03E-03	8.23E-03	8.14E-03	8.10E-03	8.19E-03	7.97E-03	7.99E-03	8.10E-03	8.15E-03
V	7.83E-02	8.17E-02	8.00E-02	7.95E-02	7.91E-02	7.93E-02	8.00E-02	8.12E-02	8.12E-02
W	4.54E-01	4.66E-01	4.63E-01	4.59E-01	4.63E-01	4.71E-01	4.57E-01	4.51E-01	4.62E-01
Y	1.88E-01	1.90E-01	1.91E-01	1.94E-01	1.92E-01	1.91E-01	1.87E-01	1.89E-01	1.84E-01
Zn	2.94E-01	2.99E-01	2.93E-01	3.00E-01	2.98E-01	2.92E-01	2.90E-01	2.98E-01	2.91E-01
Zr	5.45E-02	5.44E-02	5.49E-02	5.55E-02	5.39E-02	5.43E-02	5.55E-02	5.32E-02	5.43E-02

Table I.2. Simulated MFPV Volumes (V_i^{MFPV}, L) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type of AY-102/C-106. Obtained from simulated data from G2 Run 3.1vv (Vienna 2004a).

Batch # *i*	Volume (L)
1	25718.3
2	24888.5
3	24864.1
4	25534.9
5	25650.5
6	24609.3
7	24851.1
8	25824.0
9	25270.0
10	24703.6
11	24873.9
12	24870.3
13	24876.0
14	24902.3
15	24861.8
16	24903.5
17	24920.1
18	24846.3

Table I.3. Averages of Simulated IHLW Chemical Composition Component Mass Fractions ($\bar{g}_{ij}^{MFPV}$) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type for Tank AY-102/C-106. Values reported for each batch are averages of simulated mass fractions for eight samples per batch with one chemical analysis per sample.

IHLW Comp. *j*	Average IHLW Component Mass Fractions for Batch Numbers *i* = 1 to 9								
	1	2	3	4	5	6	7	8	9
Ag_2O	1.84E-05	1.73E-05	1.75E-05	1.63E-05	1.62E-05	1.68E-05	1.69E-05	1.61E-05	1.62E-05
Al_2O_3	1.07E-01	1.06E-01	1.05E-01	8.43E-02	7.64E-02	1.05E-01	8.63E-02	7.70E-02	7.92E-02
As_2O_5	2.99E-05	2.90E-05	2.94E-05	2.89E-05	2.84E-05	2.81E-05	2.90E-05	2.66E-05	2.77E-05
B_2O_3	8.07E-02	8.35E-02	8.40E-02	1.99E-01	2.35E-01	8.33E-02	8.40E-02	2.42E-01	1.99E-01
BaO	5.84E-04	5.69E-04	5.65E-04	5.45E-04	5.48E-04	5.57E-04	5.82E-04	5.22E-04	5.39E-04
BeO	1.21E-05	1.20E-05	1.22E-05	1.13E-05	1.13E-05	1.20E-05	1.19E-05	1.13E-05	1.13E-05
Bi_2O_3	1.08E-04	1.06E-04	1.10E-04	1.03E-04	1.01E-04	1.05E-04	1.10E-04	9.95E-05	1.00E-04
CaO	5.97E-03	5.96E-03	6.13E-03	5.89E-03	5.72E-03	5.99E-03	6.13E-03	5.73E-03	5.80E-03
CdO	7.78E-05	7.73E-05	7.71E-05	7.26E-05	7.41E-05	7.80E-05	7.68E-05	7.08E-05	7.28E-05
Ce_2O_3	1.27E-03	1.26E-03	1.28E-03	1.22E-03	1.19E-03	1.26E-03	1.28E-03	1.19E-03	1.21E-03
Cl	9.58E-05	9.66E-05	9.75E-05	9.13E-05	9.18E-05	9.55E-05	9.82E-05	9.14E-05	9.24E-05
Cr_2O_3	1.31E-03	1.33E-03	1.39E-03	1.25E-03	1.27E-03	1.33E-03	1.35E-03	1.25E-03	1.25E-03
Cs_2O	3.16E-05	3.01E-05	3.01E-05	2.92E-05	2.80E-05	3.01E-05	2.99E-05	2.78E-05	2.87E-05
CuO	1.84E-04	1.83E-04	1.86E-04	1.75E-04	1.72E-04	1.81E-04	1.83E-04	1.68E-04	1.70E-04
F	1.84E-04	1.78E-04	1.84E-04	1.77E-04	1.70E-04	1.73E-04	1.86E-04	1.67E-04	1.67E-04
Fe_2O_3	1.09E-01	1.13E-01	1.13E-01	1.04E-01	1.05E-01	1.11E-01	1.13E-01	1.05E-01	1.00E-01
K_2O	4.98E-03	4.87E-03	4.99E-03	4.90E-03	4.81E-03	4.99E-03	5.25E-03	4.70E-03	4.78E-03
La_2O_3	9.62E-04	9.64E-04	9.59E-04	9.37E-04	8.72E-04	9.45E-04	9.48E-04	9.20E-04	9.17E-04
Li_2O	4.52E-02	4.59E-02	4.53E-02	4.11E-02	4.09E-02	4.35E-02	4.46E-02	4.16E-02	4.22E-02
MgO	2.82E-03	2.76E-03	2.82E-03	2.68E-03	2.60E-03	2.75E-03	2.81E-03	2.65E-03	2.67E-03
MnO	1.14E-02	1.12E-02	1.10E-02	1.05E-02	1.05E-02	1.11E-02	1.12E-02	1.04E-02	1.08E-02
MoO_3	1.33E-05	1.32E-05	1.32E-05	1.29E-05	1.26E-05	1.36E-05	1.35E-05	1.29E-05	1.30E-05
Na_2O	1.39E-01	1.37E-01	1.37E-01	1.28E-01	1.03E-01	1.38E-01	1.50E-01	1.00E-01	1.26E-01
Nd_2O_3	8.07E-04	7.91E-04	8.25E-04	7.77E-04	7.47E-04	8.10E-04	8.15E-04	7.65E-04	7.67E-04
NiO	2.62E-03	2.59E-03	2.61E-03	2.51E-03	2.44E-03	2.50E-03	2.58E-03	2.43E-03	2.52E-03
P_2O_5	3.03E-03	3.14E-03	3.13E-03	3.03E-03	2.95E-03	3.08E-03	3.05E-03	2.78E-03	2.84E-03
PbO	6.33E-03	5.94E-03	6.27E-03	5.69E-03	5.76E-03	6.20E-03	6.22E-03	5.87E-03	5.90E-03
PdO	1.60E-08	1.59E-08	1.66E-08	1.47E-08	1.46E-08	1.56E-08	1.60E-08	1.44E-08	1.46E-08
Pr_2O_3	2.38E-04	2.42E-04	2.44E-04	2.28E-04	2.27E-04	2.37E-04	2.41E-04	2.22E-04	2.21E-04
Rb_2O	1.64E-06	1.67E-06	1.59E-06	1.58E-06	1.55E-06	1.60E-06	1.64E-06	1.50E-06	1.59E-06
Rh_2O_3	1.74E-05	1.72E-05	1.73E-05	1.66E-05	1.60E-05	1.70E-05	1.71E-05	1.60E-05	1.62E-05
RuO_2	4.29E-04	4.23E-04	4.17E-04	4.01E-04	3.88E-04	4.26E-04	4.27E-04	3.83E-04	4.00E-04
Sb_2O_5	2.97E-06	2.96E-06	3.01E-06	2.87E-06	2.86E-06	2.83E-06	2.99E-06	2.75E-06	2.80E-06
SeO_2	2.97E-06	2.96E-06	3.00E-06	2.89E-06	2.80E-06	2.95E-06	3.02E-06	2.80E-06	2.80E-06
SiO_2	4.71E-01	4.67E-01	4.68E-01	3.97E-01	3.94E-01	4.71E-01	4.74E-01	3.89E-01	4.07E-01
SO_3	5.91E-04	5.92E-04	5.99E-04	5.70E-04	5.54E-04	5.98E-04	5.78E-04	5.55E-04	5.64E-04
SrO	2.26E-04	2.37E-04	2.36E-04	2.19E-04	2.10E-04	2.23E-04	2.34E-04	2.15E-04	2.18E-04

Table I.3. Averages of Simulated IHLW Chemical Composition Component Mass Fractions ($\bar{g}_{ij}^{MFPV}$) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type for Tank AY-102/C-106. Values reported for each batch are averages of simulated mass fractions for eight samples per batch with one chemical analysis per sample. (cont.)

IHLW Comp. *j*	Average IHLW Component Mass Fractions for Batch Numbers *i* = 1 to 9								
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
Ta_2O_5	1.51E-06	1.45E-06	1.46E-06	1.45E-06	1.40E-06	1.51E-06	1.49E-06	1.41E-06	1.44E-06
TeO_2	8.32E-05	8.20E-05	8.25E-05	7.94E-05	7.45E-05	7.95E-05	8.13E-05	7.48E-05	7.94E-05
TiO_2	1.69E-04	1.76E-04	1.71E-04	1.64E-04	1.67E-04	1.69E-04	1.77E-04	1.63E-04	1.67E-04
TlO	3.28E-06	3.09E-06	3.29E-06	3.02E-06	3.07E-06	3.16E-06	3.28E-06	3.07E-06	3.13E-06
V_2O_5	5.20E-05	5.40E-05	5.35E-05	5.07E-05	5.15E-05	5.31E-05	5.32E-05	5.03E-05	5.22E-05
WO_3	2.19E-04	2.25E-04	2.20E-04	2.03E-04	2.09E-04	2.18E-04	2.08E-04	2.04E-04	2.13E-04
Y_2O_3	9.02E-05	8.77E-05	9.19E-05	8.32E-05	8.43E-05	9.19E-05	9.06E-05	8.34E-05	8.64E-05
ZnO	1.35E-04	1.38E-04	1.37E-04	1.32E-04	1.27E-04	1.35E-04	1.41E-04	1.27E-04	1.32E-04
ZrO_2	2.71E-05	2.80E-05	2.79E-05	2.64E-05	2.56E-05	2.72E-05	2.74E-05	2.53E-05	2.67E-05
Rads[(a)]	2.63E-03	2.59E-03	2.61E-03	2.50E-03	2.46E-03	2.56E-03	2.58E-03	2.38E-03	2.50E-03
Total[(b)]	1.00E+00	1.00E-00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00

(a) The total mass fractions of all radionuclide oxides, as listed specifically in Table I.5.

(b) Mass fractions in the table are rounded to two three significant figures. Before rounding, the mass fractions for each batch sum to a total of 1.00 as shown. However, the rounded values may not sum exactly to 1.00.

Table I.3. Averages of Simulated IHLW Chemical Composition Component Mass Fractions ($\bar{g}_{ij}^{MFPV}$) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type for Tank AY-102/C-106. Values reported for each batch are averages of simulated mass fractions for eight samples per batch with one chemical analysis per sample. (cont.)

IHLW Comp. *j*	Average IHLW Component Mass Fractions for MFPV Batch Numbers *i* = 10 to 18								
	10	11	12	13	14	15	16	17	18
Ag_2O	1.65E-05	1.67E-05	1.74E-05	1.70E-05	1.67E-05	1.73E-05	1.67E-05	1.75E-05	1.71E-05
Al_2O_3	1.04E-01	8.95E-02	8.26E-02	8.62E-02	8.16E-02	8.21E-02	8.32E-02	8.25E-02	8.47E-02
As_2O_5	2.90E-05	2.87E-05	2.96E-05	2.85E-05	2.88E-05	2.96E-05	3.04E-05	2.90E-05	2.83E-05
B_2O_3	8.20E-02	8.51E-02	8.03E-02	8.21E-02	8.30E-02	8.24E-02	8.33E-02	8.32E-02	8.17E-02
BaO	5.70E-04	5.82E-04	5.59E-04	5.90E-04	5.62E-04	5.60E-04	5.67E-04	5.95E-04	5.64E-04
BeO	1.17E-05	1.19E-05	1.22E-05	1.20E-05	1.15E-05	1.20E-05	1.18E-05	1.16E-05	1.20E-05
Bi_2O_3	1.06E-04	1.06E-04	1.11E-04	1.10E-04	1.04E-04	1.09E-04	1.09E-04	1.07E-04	1.08E-04
CaO	5.95E-03	6.27E-03	6.25E-03	6.17E-03	5.94E-03	6.13E-03	5.98E-03	6.24E-03	6.22E-03
CdO	7.72E-05	7.72E-05	7.94E-05	7.58E-05	7.39E-05	7.83E-05	7.52E-05	7.60E-05	7.65E-05
Ce_2O_3	1.30E-03	1.24E-03	1.29E-03	1.31E-03	1.21E-03	1.27E-03	1.28E-03	1.27E-03	1.29E-03
Cl	9.46E-05	9.20E-05	9.27E-05	9.05E-05	8.78E-05	9.34E-05	9.17E-05	9.09E-05	9.00E-05
Cr_2O_3	1.32E-03	1.30E-03	1.36E-03	1.30E-03	1.28E-03	1.29E-03	1.34E-03	1.31E-03	1.33E-03
Cs_2O	2.15E-05	1.71E-05	1.34E-05	1.15E-05	9.86E-06	9.79E-06	9.01E-06	8.94E-06	9.27E-06
CuO	1.84E-04	1.78E-04	1.80E-04	1.82E-04	1.79E-04	1.76E-04	1.80E-04	1.79E-04	1.85E-04
F	1.80E-04	1.77E-04	1.77E-04	1.69E-04	1.67E-04	1.75E-04	1.79E-04	1.72E-04	1.72E-04
Fe_2O_3	1.11E-01	1.13E-01	1.10E-01	1.10E-01	1.08E-01	1.10E-01	1.11E-01	1.13E-01	1.11E-01
K_2O	4.95E-03	5.01E-03	5.02E-03	4.78E-03	4.94E-03	4.99E-03	4.85E-03	4.94E-03	4.87E-03
La_2O_3	9.43E-04	9.48E-04	9.81E-04	9.41E-04	9.23E-04	9.99E-04	9.50E-04	9.60E-04	9.76E-04
Li_2O	4.47E-02	4.37E-02	4.61E-02	4.45E-02	4.22E-02	4.50E-02	4.33E-02	1.12E-02	4.42E-02
MgO	2.72E-03	2.83E-03	2.87E-03	2.79E-03	2.75E-03	2.76E-03	2.82E-03	2.81E-03	2.98E-03
MnO	1.12E-02	1.10E-02	1.15E-02	1.11E-02	1.12E-02	1.14E-02	1.11E-02	1.13E-02	1.14E-02
MoO_3	1.32E-05	1.35E-05	1.35E-05	1.30E-05	1.29E-05	1.35E-05	1.36E-05	1.34E-05	1.33E-05
Na_2O	1.38E-01	1.55E-01	1.54E-01	1.50E-01	1.22E-01	1.50E-01	1.24E-01	1.43E-01	1.49E-01
Nd_2O_3	8.11E-04	8.04E-04	8.06E-04	8.10E-04	8.01E-04	8.35E-04	8.01E-04	8.12E-04	8.30E-04
NiO	2.57E-03	2.66E-03	2.60E-03	2.61E-03	2.49E-03	2.57E-03	2.57E-03	2.59E-03	2.54E-03
P_2O_5	3.01E-03	2.95E-03	3.10E-03	3.00E-03	3.03E-03	3.06E-03	2.98E-03	3.12E-03	3.04E-03
PbO	6.08E-03	6.12E-03	6.16E-03	6.10E-03	5.94E-03	6.09E-03	6.06E-03	6.20E-03	6.01E-03
PdO	1.50E-08	1.54E-08	1.58E-08	1.49E-08	1.49E-08	1.57E-08	1.54E-08	1.52E-08	1.51E-08
Pr_2O_3	2.35E-04	2.40E-04	2.46E-04	2.33E-04	2.38E-04	2.38E-04	2.47E-04	2.35E-04	2.35E-04
Rb_2O	1.59E-06	1.64E-06	1.68E-06	1.60E-06	1.61E-06	1.61E-06	1.58E-06	1.62E-06	1.64E-06
Rh_2O_3	1.70E-05	1.75E-05	1.80E-05	1.71E-05	1.72E-05	1.74E-05	1.73E-05	1.74E-05	1.78E-05
RuO_2	4.09E-04	4.12E-04	4.22E-04	4.18E-04	4.12E-04	4.19E-04	4.17E-04	4.21E-04	4.07E-04
Sb_2O_5	2.95E-06	2.94E-06	2.96E-06	2.84E-06	2.78E-06	2.95E-06	2.86E-06	2.90E-06	2.87E-06
SeO_2	2.93E-06	2.87E-06	2.97E-06	2.94E-06	2.92E-06	3.01E-06	3.02E-06	2.93E-06	2.95E-06
SiO_2	4.73E-01	4.66E-01	4.79E-01	4.81E-01	5.16E-01	4.83E-01	5.09E-01	5.20E-01	4.82E-01
SO_3	5.79E-04	5.89E-04	5.81E-04	5.74E-04	5.63E-04	5.79E-04	5.62E-04	5.51E-04	5.52E-04
SrO	2.31E-04	2.30E-04	2.29E-04	2.21E-04	2.23E-04	2.36E-04	2.25E-04	2.29E-04	2.25E-04

Table I.3. Averages of Simulated IHLW Chemical Composition Component Mass Fractions ($\bar{g}_{ij}^{MFPV}$) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type for Tank AY-102/C-106. Values reported for each batch are averages of simulated mass fractions for eight samples per batch with one chemical analysis per sample. (cont.)

IHLW Comp. *j*	Average IHLW Component Mass Fractions for MFPV Batch Numbers *i* = 10 to 18								
	10	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**
Ta_2O_5	1.46E-06	1.50E-06	1.50E-06	1.48E-06	1.45E-06	1.50E-06	1.49E-06	1.50E-06	1.49E-06
TeO_2	8.04E-05	8.02E-05	7.92E-05	8.17E-05	8.20E-05	8.18E-05	8.25E-05	8.34E-05	8.13E-05
TiO_2	1.71E-04	1.74E-04	1.76E-04	1.76E-04	1.78E-04	1.73E-04	1.73E-04	1.74E-04	1.80E-04
TlO	3.22E-06	3.32E-06	3.34E-06	3.23E-06	3.26E-06	3.24E-06	3.23E-06	3.33E-06	3.28E-06
V_2O_5	5.20E-05	5.45E-05	5.43E-05	5.24E-05	5.20E-05	5.32E-05	5.35E-05	5.52E-05	5.41E-05
WO_3	2.13E-04	2.20E-04	2.22E-04	2.14E-04	2.15E-04	2.24E-04	2.16E-04	2.16E-04	2.17E-04
Y_2O_3	8.90E-05	9.01E-05	9.21E-05	9.12E-05	8.98E-05	9.13E-05	8.90E-05	9.12E-05	8.74E-05
ZnO	1.36E-04	1.39E-04	1.39E-04	1.38E-04	1.37E-04	1.37E-04	1.36E-04	1.41E-04	1.36E-04
ZrO_2	2.74E-05	2.75E-05	2.82E-05	2.77E-05	2.68E-05	2.76E-05	2.81E-05	2.74E-05	2.74E-05
Rads[(a)]	2.59E-03	2.64E-03	2.69E-03	2.58E-03	2.50E-03	2.65E-03	2.51E-03	2.57E-03	2.49E-03
Total[(b)]	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00

(a) The total mass fractions of all radionuclide oxides, as listed specifically in Table I.5.
(b) Mass fractions in the table are rounded to two three significant figures. Before rounding, the mass fractions for each batch sum to a total of 1.00 as shown. However, the rounded values may not sum exactly to 1.00.

I.2 Simulated Data Used to Illustrate Calculating Means and Standard Deviations of IHLW Radionuclide Compositions and Inventories

Simulated data were used in Section 6.2.2 to illustrate calculations with Eqs. (4.1.2), (4.1.3), and (4.1.4) for radionuclides. The radionuclide concentrations (g/L)[(a)] and radionuclide oxide mass fractions were generated in the same way as the chemical composition elements and component mass fractions described in Section I.1. The resulting simulated data were used "as is", with no attempt to apply realistic detection limits to small simulated radionuclide concentration values.

Tables I.4 and I.5 respectively list the simulated average radionuclide concentrations and radionuclide oxide mass fractions for the 18 IHLW MFPV batches associated with an HLW waste type from Tank AY-102/C-106.

(a) The form in which the G2 data were supplied by the WTP Project was more conducive to obtaining radionuclide concentrations in units of g/L rather than the units of μCi/mL = mCi/L planned for radiochemical analyses of radionuclide concentrations. In a future revision of this report, realistic simulated radionuclide concentration data in units of μCi/mL = mCi/L will be generated, summarized in this section, and used in the illustrations located in the main body of the report.

Table I.4. Averages of Simulated Radionuclide Concentrations ($\bar{c}_{iq}^{MFPV}$, g/L) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type for Tank AY-102/C-106. Values reported for each batch are averages of simulated concentrations for eight samples per batch with one radiochemical analysis per sample.

Radio-nuclide *q*	Average Radionuclide Concentrations (g/L) for MFPV Batch Numbers *i* = 1 to 9								
	1	2	3	4	5	6	7	8	9
^{227}Ac	2.81E-10	2.72E-10	2.78E-10	2.74E-10	2.76E-10	2.72E-10	2.83E-10	2.72E-10	2.70E-10
^{241}Am	3.87E-03	3.89E-03	3.91E-03	3.89E-03	3.82E-03	3.81E-03	3.97E-03	3.61E-03	4.01E-03
^{243}Am	4.72E-06	4.92E-06	4.95E-06	4.62E-06	4.86E-06	4.84E-06	4.74E-06	4.72E-06	4.72E-06
^{113}Cd	4.64E-08	4.76E-08	4.64E-08	4.46E-08	4.57E-08	4.55E-08	4.65E-08	4.40E-08	4.5E-08
^{242}Cm	7.24E-09	7.06E-09	7.34E-09	7.09E-09	7.12E-09	6.99E-09	7.00E-09	6.79E-09	6.95E-09
^{243}Cm	3.83E-08	3.94E-08	3.75E-08	3.74E-08	3.68E-08	3.78E-08	3.65E-08	3.77E-08	3.66E-08
^{244}Cm	5.25E-07	5.12E-07	4.89E-07	4.97E-07	4.94E-07	5.11E-07	4.91E-07	4.90E-07	5.13E-07
^{60}Co	7.16E-10	7.35E-10	7.16E-10	7.14E-10	6.93E-10	7.03E-10	7.08E-10	7.09E-10	7.18E-10
^{134}Cs	7.89E-08	7.96E-08	7.92E-08	7.96E-08	8.10E-08	7.85E-08	7.97E-08	7.74E-08	8.02E-08
^{137}Cs	2.19E-02	2.16E-02	2.15E-02	2.10E-02	2.08E-02	2.10E-02	2.11E-02	2.06E-02	2.08E-02
^{152}Eu	4.46E-07	4.47E-07	4.52E-07	4.38E-07	4.33E-07	4.53E-07	4.44E-07	4.45E-07	4.39E-07
^{154}Eu	2.48E-05	2.43E-05	2.44E-05	2.43E-05	2.39E-05	2.51E-05	2.46E-05	2.41E-05	2.35E-05
^{155}Eu	7.14E-06	7.18E-06	7.21E-06	7.14E-06	7.08E-06	7.15E-06	6.98E-06	6.87E-06	7.18E-06
^{129}I	6.92E-05	6.80E-05	6.96E-05	6.70E-05	6.58E-05	6.75E-05	6.64E-05	6.53E-05	6.59E-05
^{93}Nb	2.23E-08	2.24E-08	2.31E-08	2.28E-08	2.24E-08	2.26E-08	2.30E-08	2.22E-08	2.23E-08
^{59}Ni	2.79E-03	2.72E-03	2.72E-03	2.77E-03	2.66E-03	2.61E-03	2.73E-03	2.62E-03	2.53E-03
^{63}Ni	3.30E-04	3.22E-04	3.27E-04	3.26E-04	3.16E-04	3.43E-04	3.37E-04	3.26E-04	3.13E-04
^{237}Np	1.01E-02	1.00E-02	1.03E-02	9.96E-03	9.97E-03	9.90E-03	1.02E-02	9.55E-03	9.82E-03
^{231}Pa	2.38E-08	2.24E-08	2.30E-08	2.35E-08	2.27E-08	2.34E-08	2.37E-08	2.28E-08	2.24E-08
^{238}Pu	5.34E-05	5.18E-05	5.27E-05	5.08E-05	5.03E-05	5.01E-05	5.18E-05	5.09E-05	5.17E-05
^{239}Pu	3.95E-02	4.04E-02	3.96E-02	3.85E-02	3.84E-02	4.04E-02	4.02E-02	3.82E-02	3.91E-02
^{240}Pu	1.99E-03	1.94E-03	1.93E-03	1.94E-03	1.90E-03	1.95E-03	2.03E-03	1.98E-03	1.94E-03
^{241}Pu	5.98E-05	5.96E-05	5.74E-05	5.79E-05	5.72E-05	6.09E-05	5.75E-05	5.87E-05	5.84E-05
^{242}Pu	1.95E-05	1.98E-05	1.96E-05	1.94E-05	1.96E-05	2.02E-05	1.91E-05	1.88E-05	1.93E-05
^{226}Ra	6.76E-09	6.55E-09	6.87E-09	6.69E-09	6.58E-09	6.63E-09	6.80E-09	6.72E-09	6.75E-09
^{228}Ra	2.30E-10	2.36E-10	2.36E-10	2.33E-10	2.27E-10	2.28E-10	2.29E-10	2.30E-10	2.28E-10
^{125}Sb	2.34E-09	2.22E-09	2.24E-09	2.25E-09	2.16E-09	2.26E-09	2.33E-09	2.24E-09	2.14E-09
^{79}Se	3.00E-06	3.05E-06	2.91E-06	3.00E-06	2.92E-06	3.00E-06	2.95E-06	2.97E-06	2.83E-06
^{151}Sm	1.49E-04	1.43E-04	1.45E-04	1.45E-04	1.42E-04	1.47E-04	1.47E-04	1.46E-04	1.47E-04
^{126}Sn	6.54E-05	6.49E-05	6.35E-05	6.24E-05	6.06E-05	6.23E-05	6.41E-05	6.15E-05	6.35E-05
^{90}Sr	5.50E-02	5.51E-02	5.39E-02	5.24E-02	5.40E-02	5.49E-02	5.38E-02	5.02E-02	5.47E-02
^{99}Tc	9.40E-04	9.27E-04	9.17E-04	9.29E-04	9.41E-04	9.52E-04	9.54E-04	9.25E-04	9.24E-04
^{229}Th	1.75E-09	1.74E-09	1.73E-09	1.66E-09	1.66E-09	1.76E-09	1.75E-09	1.65E-09	1.72E-09
^{232}Th	9.62E-01	9.49E-01	9.67E-01	9.43E-01	9.34E-01	9.63E-01	9.51E-01	9.27E-01	9.55E-01
^{232}U	9.32E-11	9.28E-11	9.04E-11	9.20E-11	9.08E-11	9.46E-11	9.61E-11	8.79E-11	9.01E-11
^{233}U	9.25E-07	9.44E-07	9.30E-07	9.31E-07	9.09E-07	9.23E-07	9.45E-07	9.14E-07	9.08E-07
^{234}U	3.41E-04	3.36E-04	3.37E-04	3.26E-04	3.38E-04	3.42E-04	3.41E-04	3.22E-04	3.40E-04
^{235}U	2.05E-02	2.08E-02	2.07E-02	2.16E-02	1.98E-02	1.97E-02	2.06E-02	1.97E-02	2.07E-02
^{236}U	2.03E-03	1.98E-03	2.07E-03	2.07E-03	2.00E-03	2.07E-03	2.11E-03	2.03E-03	2.05E-03
^{238}U	4.86E+00	4.82E+00	4.76E+00	4.75E+00	4.71E+00	4.73E+00	4.71E+00	4.61E+00	4.77E+00
^{Tot}U[(a)]	1.41E-05	1.47E-05	1.43E-05	1.46E-05	1.41E-05	1.42E-05	1.44E-05	1.43E-05	1.45E-05
^{93}Zr	2.27E-03	2.33E-03	2.29E-03	2.31E-03	2.25E-03	2.28E-03	2.30E-03	2.22E-03	2.29E-03

(a) This represents all other isotopes of U not specifically listed.

Table I.4. Averages of Simulated Radionuclide Concentrations ($\bar{c}_{iq}^{MFPV}$, g/L) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type for Tank AY-102/C-106. Values reported for each batch are averages of simulated concentrations for eight samples per batch with one radiochemical analysis per sample. (cont.)

Radio-nuclide *q*	Average Radionuclide Concentrations (g/L) for MFPV Batch Numbers *i* = 10 to 18								
	10	11	12	13	14	15	16	17	18
^{227}Ac	2.78E-10	2.78E-10	2.71E-10	2.82E-10	2.69E-10	2.64E-10	2.64E-10	2.66E-10	2.80E-10
^{241}Am	3.90E-03	3.86E-03	3.95E-03	3.98E-03	3.84E-03	3.90E-03	3.86E-03	3.85E-03	4.00E-03
^{243}Am	4.76E-06	4.88E-06	4.82E-06	4.85E-06	4.99E-06	4.94E-06	4.84E-06	4.75E-06	4.78E-06
^{113}Cd	4.50E-08	4.43E-08	4.46E-08	4.37E-08	4.50E-08	4.30E-08	4.41E-08	4.33E-08	4.35E-08
^{242}Cm	7.03E-09	7.06E-09	6.71E-09	7.10E-09	7.10E-09	7.12E-09	7.02E-09	6.90E-09	7.15E-09
^{243}Cm	3.87E-08	3.85E-08	3.80E-08	3.75E-08	3.60E-08	3.92E-08	3.68E-08	3.68E-08	3.77E-08
^{244}Cm	5.24E-07	5.12E-07	5.11E-07	5.22E-07	5.15E-07	5.03E-07	5.29E-07	5.01E-07	5.03E-07
^{60}Co	7.10E-10	6.87E-10	7.14E-10	6.78E-10	6.81E-10	6.79E-10	6.72E-10	6.78E-10	6.96E-10
^{134}Cs	6.35E-08	5.20E-08	4.42E-08	4.01E-08	3.80E-08	3.71E-08	3.63E-08	3.42E-08	3.58E-08
^{137}Cs	1.59E-02	1.18E-02	9.22E-03	7.85E-03	7.11E-03	6.53E-03	6.23E-03	6.05E-03	6.08E-03
^{152}Eu	4.42E-07	4.39E-07	4.52E-07	4.33E-07	4.22E-07	4.44E-07	4.25E-07	4.37E-07	4.42E-07
^{154}Eu	2.45E-05	2.49E-05	2.36E-05	2.37E-05	2.48E-05	2.38E-05	2.47E-05	2.41E-05	2.44E-05
^{155}Eu	7.07E-06	6.97E-06	6.82E-06	7.18E-06	6.97E-06	6.86E-06	6.72E-06	7.00E-06	6.86E-06
^{129}I	6.46E-05	6.70E-05	6.64E-05	6.68E-05	6.38E-05	6.60E-05	6.40E-05	6.24E-05	6.49E-05
^{93}Nb	2.27E-08	2.29E-08	2.31E-08	2.30E-08	2.27E-08	2.20E-08	2.26E-08	2.26E-08	2.28E-08
^{59}Ni	2.72E-03	2.66E-03	2.78E-03	2.72E-03	2.73E-03	2.74E-03	2.73E-03	2.70E-03	2.74E-03
^{63}Ni	3.30E-04	3.41E-04	3.23E-04	3.26E-04	3.36E-04	3.31E-04	3.28E-04	3.18E-04	3.33E-04
^{237}Np	1.01E-02	9.99E-03	1.01E-02	1.02E-02	9.87E-03	1.03E-02	9.73E-03	9.98E-03	1.01E-02
^{231}Pa	2.19E-08	2.26E-08	2.30E-08	2.25E-08	2.30E-08	2.32E-08	2.28E-08	2.26E-08	2.30E-08
^{238}Pu	5.38E-05	5.08E-05	5.15E-05	5.25E-05	5.19E-05	5.41E-05	5.15E-05	5.19E-05	5.11E-05
^{239}Pu	4.06E-02	4.03E-02	3.86E-02	3.97E-02	3.94E-02	3.95E-02	3.98E-02	3.86E-02	3.91E-02
^{240}Pu	2.00E-03	2.00E-03	2.01E-03	1.94E-03	1.96E-03	2.01E-03	1.95E-03	2.02E-03	1.98E-03
^{241}Pu	5.95E-05	5.85E-05	6.05E-05	5.66E-05	5.82E-05	6.08E-05	5.76E-05	5.84E-05	5.78E-05
^{242}Pu	1.96E-05	2.01E-05	1.97E-05	1.91E-05	1.97E-05	1.98E-05	1.97E-05	1.92E-05	2.03E-05
^{226}Ra	6.80E-09	6.98E-09	6.95E-09	6.85E-09	6.61E-09	6.80E-09	6.75E-09	6.78E-09	6.92E-09
^{228}Ra	2.31E-10	2.40E-10	2.37E-10	2.43E-10	2.44E-10	2.43E-10	2.39E-10	2.30E-10	2.41E-10
^{125}Sb	2.20E-09	2.19E-09	2.18E-09	2.17E-09	2.10E-09	2.19E-09	2.12E-09	2.12E-09	2.15E-09
^{79}Se	2.89E-06	3.08E-06	2.89E-06	2.94E-06	2.83E-06	2.87E-06	2.91E-06	2.93E-06	2.75E-06
^{151}Sm	1.45E-04	1.49E-04	1.51E-04	1.46E-04	1.42E-04	1.45E-04	1.43E-04	1.41E-04	1.49E-04
^{126}Sn	6.29E-05	6.23E-05	6.38E-05	6.53E-05	6.08E-05	6.21E-05	6.24E-05	6.26E-05	6.47E-05
^{90}Sr	5.46E-02	5.53E-02	5.48E-02	5.34E-02	5.51E-02	5.61E-02	5.46E-02	5.32E-02	5.27E-02
^{99}Tc	9.27E-04	9.04E-04	9.45E-04	9.23E-04	8.89E-04	9.21E-04	8.91E-04	8.60E-04	9.24E-04
^{229}Th	1.72E-09	1.65E-09	1.63E-09	1.63E-09	1.63E-09	1.66E-09	1.61E-09	1.62E-09	1.65E-09
^{232}Th	9.98E-01	9.75E-01	9.54E-01	9.72E-01	9.26E-01	9.62E-01	9.45E-01	9.43E-01	9.61E-01
^{232}U	9.25E-11	8.96E-11	8.76E-11	8.36E-11	8.53E-11	8.94E-11	8.75E-11	8.38E-11	8.68E-11
^{233}U	8.92E-07	8.77E-07	9.26E-07	8.68E-07	8.67E-07	8.79E-07	8.67E-07	8.41E-07	8.90E-07
^{234}U	3.47E-04	3.43E-04	3.44E-04	3.43E-04	3.33E-04	3.39E-04	3.40E-04	3.25E-04	3.39E-04
^{235}U	2.04E-02	2.12E-02	2.07E-02	2.08E-02	2.07E-02	2.07E-02	2.03E-02	2.05E-02	2.10E-02
^{236}U	2.05E-03	2.04E-03	2.05E-03	2.06E-03	2.04E-03	2.10E-03	2.04E-03	2.05E-03	2.10E-03
^{238}U	4.78E+00	4.89E+00	4.92E+00	4.85E+00	4.72E+00	4.89E+00	4.61E+00	4.69E+00	4.59E+00
^{Tot}U[(a)]	1.42E-05	1.40E-05	1.45E-05	1.47E-05	1.41E-05	1.43E-05	1.42E-05	1.37E-05	1.45E-05
^{93}Zr	2.28E-03	2.27E-03	2.24E-03	2.29E-03	2.30E-03	2.24E-03	2.31E-03	2.21E-03	2.31E-03

(a) This represents all other isotopes of U not specifically listed.

Table I.5. Averages of Simulated IHLW Radionuclide Composition Component Mass Fractions ($\bar{g}_{iq}^{MFPV}$) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type for Tank AY-102/C-106. Values reported for each batch are averages of simulated mass fractions for eight samples per batch with one chemical analysis per sample.

Radionuclide Component q	Average IHLW Radionuclide Component Mass Fractions for Batch Numbers i = 1 to 9								
	1	2	3	4	5	6	7	8	9
$^{227}Ac_2O_3$	1.17E-13	1.12E-13	1.16E-13	1.10E-13	1.10E-13	1.12E-13	1.19E-13	1.07E-13	1.08E-13
$^{241}Am_2O_3$	1.60E-06	1.59E-06	1.62E-06	1.56E-06	1.52E-06	1.57E-06	1.65E-06	1.42E-06	1.60E-06
$^{243}Am_2O_3$	1.95E-09	2.02E-09	2.06E-09	1.85E-09	1.93E-09	1.99E-09	1.97E-09	1.85E-09	1.88E-09
^{113}CdO	1.99E-11	2.02E-11	2.00E-11	1.85E-11	1.89E-11	1.94E-11	2.01E-11	1.79E-11	1.88E-11
$^{242}Cm_2O_3$	2.98E-12	2.89E-12	3.05E-12	2.84E-12	2.83E-12	2.87E-12	2.91E-12	2.67E-12	2.77E-12
$^{243}Cm_2O_3$	1.58E-11	1.61E-11	1.56E-11	1.50E-11	1.46E-11	1.55E-11	1.52E-11	1.48E-11	1.46E-11
$^{244}Cm_2O_3$	2.16E-10	2.10E-10	2.03E-10	1.99E-10	1.96E-10	2.10E-10	2.04E-10	1.92E-10	2.04E-10
^{60}CoO	3.40E-13	3.47E-13	3.43E-13	3.30E-13	3.18E-13	3.33E-13	3.39E-13	3.21E-13	3.30E-13
$^{134}Cs_2O$	3.14E-11	3.14E-11	3.17E-11	3.07E-11	3.10E-11	3.11E-11	3.20E-11	2.93E-11	3.08E-11
$^{137}Cs_2O$	8.70E-06	8.52E-06	8.61E-06	8.10E-06	7.95E-06	8.30E-06	8.44E-06	7.80E-06	7.97E-06
$^{152}Eu_2O_3$	1.94E-10	1.93E-10	1.98E-10	1.85E-10	1.81E-10	1.96E-10	1.94E-10	1.84E-10	1.84E-10
$^{154}Eu_2O_3$	1.07E-08	1.05E-08	1.07E-08	1.02E-08	1.00E-08	1.09E-08	1.08E-08	9.93E-09	9.87E-09
$^{155}Eu_2O_3$	3.09E-09	3.09E-09	3.15E-09	3.00E-09	2.96E-09	3.09E-09	3.05E-09	2.83E-09	3.00E-09
^{129}I	2.59E-08	2.54E-08	2.63E-08	2.44E-08	2.38E-08	2.52E-08	2.51E-08	2.33E-08	2.39E-08
$^{93}Nb_2O_5$	1.20E-11	1.19E-11	1.25E-11	1.19E-11	1.16E-11	1.21E-11	1.24E-11	1.13E-11	1.15E-11
^{59}NiO	1.33E-06	1.29E-06	1.31E-06	1.28E-06	1.22E-06	1.24E-06	1.31E-06	1.19E-06	1.17E-06
^{63}NiO	1.55E-07	1.50E-07	1.55E-07	1.49E-07	1.43E-07	1.61E-07	1.60E-07	1.46E-07	1.42E-07
$^{237}Np_2O_5$	4.45E-06	4.37E-06	4.54E-06	4.24E-06	4.21E-06	4.32E-06	4.53E-06	3.99E-06	4.16E-06
$^{231}PaO_2$	1.02E-11	9.52E-12	9.93E-12	9.76E-12	9.36E-12	9.97E-12	1.02E-11	9.26E-12	9.24E-12
$^{238}PuO_2$	2.27E-08	2.19E-08	2.26E-08	2.10E-08	2.07E-08	2.12E-08	2.22E-08	2.06E-08	2.13E-08
$^{239}PuO_2$	1.68E-05	1.71E-05	1.70E-05	1.59E-05	1.57E-05	1.71E-05	1.73E-05	1.55E-05	1.61E-05
$^{240}PuO_2$	8.44E-07	8.21E-07	8.29E-07	7.99E-07	7.77E-07	8.25E-07	8.71E-07	8.03E-07	7.97E-07
$^{241}PuO_2$	2.54E-08	2.52E-08	2.46E-08	2.39E-08	2.35E-08	2.58E-08	2.47E-08	2.38E-08	2.40E-08
$^{242}PuO_2$	8.27E-09	8.36E-09	8.41E-09	8.02E-09	8.03E-09	8.55E-09	8.20E-09	7.60E-09	7.90E-09
^{226}RaO	2.72E-12	2.62E-12	2.78E-12	2.61E-12	2.55E-12	2.65E-12	2.76E-12	2.57E-12	2.62E-12
^{228}RaO	9.25E-14	9.39E-14	9.54E-14	9.08E-14	8.78E-14	9.14E-14	9.27E-14	8.80E-14	8.83E-14
$^{125}Sb_2O_5$	1.16E-12	1.09E-12	1.12E-12	1.08E-12	1.03E-12	1.11E-12	1.16E-12	1.05E-12	1.02E-12
$^{79}SeO_2$	1.58E-09	1.60E-09	1.55E-09	1.54E-09	1.48E-09	1.57E-09	1.57E-09	1.49E-09	1.44E-09
$^{151}Sm_2O_3$	6.46E-08	6.19E-08	6.35E-08	6.12E-08	5.93E-08	6.37E-08	6.43E-08	6.04E-08	6.17E-08
$^{126}SnO_2$	3.07E-08	3.03E-08	3.01E-08	2.85E-08	2.75E-08	2.92E-08	3.04E-08	2.76E-08	2.89E-08
^{90}SrO	2.43E-05	2.42E-05	2.40E-05	2.25E-05	2.30E-05	2.42E-05	2.40E-05	2.11E-05	2.33E-05
$^{99}TcO_2$	4.66E-07	4.57E-07	4.59E-07	4.48E-07	4.50E-07	4.71E-07	4.78E-07	4.37E-07	4.43E-07
$^{229}ThO_2$	7.48E-13	7.41E-13	7.46E-13	6.88E-13	6.84E-13	7.50E-13	7.54E-13	6.73E-13	7.10E-13
$^{232}ThO_2$	4.10E-04	4.03E-04	4.16E-04	3.91E-04	3.84E-04	4.10E-04	4.10E-04	3.77E-04	3.94E-04
$^{232}U_3O_8$	4.14E-14	4.09E-14	4.05E-14	3.97E-14	3.89E-14	4.19E-14	4.31E-14	3.71E-14	3.87E-14
$^{233}U_3O_8$	4.10E-10	4.16E-10	4.16E-10	4.01E-10	3.89E-10	4.08E-10	4.23E-10	3.86E-10	3.89E-10
$^{234}U_3O_8$	1.51E-07	1.48E-07	1.51E-07	1.41E-07	1.45E-07	1.51E-07	1.52E-07	1.36E-07	1.46E-07
$^{235}U_3O_8$	9.07E-06	9.15E-06	9.27E-06	9.28E-06	8.45E-06	8.72E-06	9.23E-06	8.33E-06	8.88E-06
$^{236}U_3O_8$	9.01E-07	8.73E-07	9.25E-07	8.92E-07	8.53E-07	9.13E-07	9.42E-07	8.56E-07	8.77E-07
$^{238}U_3O_8$	2.15E-03	2.12E-03	2.12E-03	2.04E-03	2.01E-03	2.08E-03	2.10E-03	1.94E-03	2.04E-03
$^{Tot}U_3O_8$[(a)]	6.25E-09	6.45E-09	6.37E-09	6.26E-09	6.03E-09	6.26E-09	6.43E-09	6.00E-09	6.18E-09
$^{93}ZrO_2$	1.14E-06	1.17E-06	1.17E-06	1.13E-06	1.09E-06	1.14E-06	1.17E-06	1.07E-06	1.11E-06
Total	2.63E-03	2.59E-03	2.61E-03	2.50E-03	2.46E-03	2.56E-03	2.58E-03	2.38E-03	2.50E-03

(a) This represents the oxides all other isotopes of U not specifically listed.

Table I.5. Averages of Simulated IHLW Radionuclide Composition Component Mass Fractions ($\bar{g}_{iq}^{MFPV}$) for 18 IHLW MFPV Batches Corresponding to an HLW Waste Type for Tank AY-102/C-106. Values reported for each batch are averages of simulated mass fractions for eight samples per batch with one chemical analysis per sample. (cont.)

Radionuclide Component	Average IHLW Radionuclide Component Mass Fractions for Batch Numbers *i* = 10 to 18								
q	10	11	12	13	14	15	16	17	18
$^{227}Ac_2O_3$	1.14E-13	1.15E-13	1.14E-13	1.15E-13	1.10E-13	1.10E-13	1.10E-13	1.12E-13	1.16E-13
$^{241}Am_2O_3$	1.59E-06	1.59E-06	1.65E-06	1.62E-06	1.56E-06	1.61E-06	1.59E-06	1.61E-06	1.64E-06
$^{243}Am_2O_3$	1.95E-09	2.00E-09	2.02E-09	1.97E-09	2.02E-09	2.04E-09	1.99E-09	1.99E-09	1.96E-09
^{113}CdO	1.91E-11	1.89E-11	1.93E-11	1.84E-11	1.89E-11	1.84E-11	1.89E-11	1.88E-11	1.85E-11
$^{242}Cm_2O_3$	2.87E-12	2.91E-12	2.81E-12	2.89E-12	2.88E-12	2.95E-12	2.89E-12	2.89E-12	2.93E-12
$^{243}Cm_2O_3$	1.58E-11	1.58E-11	1.59E-11	1.52E-11	1.46E-11	1.62E-11	1.52E-11	1.54E-11	1.55E-11
$^{244}Cm_2O_3$	2.14E-10	2.11E-10	2.14E-10	2.12E-10	2.08E-10	2.08E-10	2.18E-10	2.10E-10	2.06E-10
^{60}CoO	3.35E-13	3.25E-13	3.44E-13	3.17E-13	3.18E-13	3.24E-13	3.19E-13	3.27E-13	3.29E-13
$^{134}Cs_2O$	2.50E-11	2.06E-11	1.78E-11	1.57E-11	1.49E-11	1.48E-11	1.44E-11	1.38E-11	1.42E-11
$^{137}Cs_2O$	6.26E-06	4.67E-06	3.71E-06	3.07E-06	2.78E-06	2.60E-06	2.47E-06	2.44E-06	2.40E-06
$^{152}Eu_2O_3$	1.90E-10	1.90E-10	1.99E-10	1.85E-10	1.80E-10	1.94E-10	1.84E-10	1.93E-10	1.91E-10
$^{154}Eu_2O_3$	1.05E-08	1.08E-08	1.04E-08	1.02E-08	1.06E-08	1.03E-08	1.07E-08	1.06E-08	1.05E-08
$^{155}Eu_2O_3$	3.04E-09	3.01E-09	3.00E-09	3.07E-09	2.97E-09	2.98E-09	2.91E-09	3.08E-09	2.96E-09
^{129}I	2.40E-08	2.51E-08	2.53E-08	2.47E-08	2.35E-08	2.48E-08	2.40E-08	2.37E-08	2.42E-08
$^{93}Nb_2O_5$	1.21E-11	1.23E-11	1.25E-11	1.22E-11	1.19E-11	1.19E-11	1.21E-11	1.23E-11	1.22E-11
^{59}NiO	1.28E-06	1.27E-06	1.35E-06	1.28E-06	1.28E-06	1.31E-06	1.30E-06	1.31E-06	1.30E-06
^{63}NiO	1.54E-07	1.60E-07	1.54E-07	1.51E-07	1.55E-07	1.56E-07	1.54E-07	1.52E-07	1.56E-07
$^{237}Np_2O_5$	4.40E-06	4.37E-06	4.47E-06	4.40E-06	4.25E-06	4.51E-06	4.26E-06	4.44E-06	4.40E-06
$^{231}PaO_2$	9.28E-12	9.62E-12	9.94E-12	9.47E-12	9.64E-12	9.95E-12	9.71E-12	9.79E-12	9.77E-12
$^{238}PuO_2$	2.27E-08	2.15E-08	2.22E-08	2.20E-08	2.17E-08	2.31E-08	2.19E-08	2.24E-08	2.16E-08
$^{239}PuO_2$	1.71E-05	1.71E-05	1.67E-05	1.67E-05	1.65E-05	1.69E-05	1.69E-05	1.67E-05	1.66E-05
$^{240}PuO_2$	8.44E-07	8.49E-07	8.66E-07	8.13E-07	8.19E-07	8.57E-07	8.28E-07	8.73E-07	8.36E-07
$^{241}PuO_2$	2.51E-08	2.48E-08	2.61E-08	2.37E-08	2.43E-08	2.59E-08	2.44E-08	2.52E-08	2.45E-08
$^{242}PuO_2$	8.26E-09	8.53E-09	8.47E-09	7.99E-09	8.22E-09	8.44E-09	8.35E-09	8.29E-09	8.57E-09
^{226}RaO	2.71E-12	2.79E-12	2.83E-12	2.71E-12	2.61E-12	2.74E-12	2.71E-12	2.77E-12	2.77E-12
^{228}RaO	9.21E-14	9.60E-14	9.66E-14	9.60E-14	9.64E-14	9.78E-14	9.59E-14	9.38E-14	9.65E-14
$^{125}Sb_2O_5$	1.08E-12	1.08E-12	1.09E-12	1.06E-12	1.02E-12	1.09E-12	1.05E-12	1.07E-12	1.06E-12
$^{79}SeO_2$	1.51E-09	1.62E-09	1.54E-09	1.53E-09	1.46E-09	1.52E-09	1.53E-09	1.57E-09	1.44E-09
$^{151}Sm_2O_3$	6.23E-08	6.44E-08	6.65E-08	6.25E-08	6.05E-08	6.34E-08	6.19E-08	6.23E-08	6.45E-08
$^{126}SnO_2$	2.93E-08	2.92E-08	3.04E-08	3.03E-08	2.81E-08	2.93E-08	2.93E-08	2.99E-08	3.03E-08
^{90}SrO	2.39E-05	2.44E-05	2.45E-05	2.33E-05	2.39E-05	2.48E-05	2.41E-05	2.38E-05	2.32E-05
$^{99}TcO_2$	4.56E-07	4.47E-07	4.76E-07	4.51E-07	4.34E-07	4.58E-07	4.42E-07	4.33E-07	4.57E-07
$^{229}ThO_2$	7.28E-13	7.04E-13	7.07E-13	6.87E-13	6.86E-13	7.14E-13	6.90E-13	7.04E-13	7.02E-13
$^{232}ThO_2$	4.22E-04	4.15E-04	4.13E-04	4.09E-04	3.88E-04	4.12E-04	4.03E-04	4.08E-04	4.08E-04
$^{232}U_3O_8$	4.07E-14	3.97E-14	3.94E-14	3.66E-14	3.72E-14	3.98E-14	3.88E-14	3.78E-14	3.84E-14
$^{233}U_3O_8$	3.93E-10	3.88E-10	4.17E-10	3.80E-10	3.78E-10	3.91E-10	3.84E-10	3.79E-10	3.93E-10
$^{234}U_3O_8$	1.52E-07	1.52E-07	1.55E-07	1.50E-07	1.45E-07	1.51E-07	1.51E-07	1.46E-07	1.50E-07
$^{235}U_3O_8$	8.95E-06	9.37E-06	9.29E-06	9.07E-06	9.00E-06	9.19E-06	8.99E-06	9.21E-06	9.29E-06
$^{236}U_3O_8$	8.98E-07	9.02E-07	9.21E-07	9.02E-07	8.89E-07	9.34E-07	9.03E-07	9.23E-07	9.28E-07
$^{238}U_3O_8$	2.10E-03	2.16E-03	2.21E-03	2.11E-03	2.05E-03	2.17E-03	2.04E-03	2.10E-03	2.02E-03
$^{Tot}U_3O_8$[(a)]	6.22E-09	6.16E-09	6.49E-09	6.40E-09	6.11E-09	6.35E-09	6.27E-09	6.16E-09	6.39E-09
$^{93}ZrO_2$	1.14E-06	1.14E-06	1.15E-06	1.14E-06	1.14E-06	1.13E-06	1.16E-06	1.13E-06	1.16E-06
Total	2.59E-03	2.64E-03	2.69E-03	2.58E-03	2.50E-03	2.65E-03	2.51E-03	2.57E-03	2.49E-03

(a) This represents the oxides of all other isotopes of U not specifically listed.

To illustrate using Eqs. (4.2.1) and (4.2.2) for calculating means and standard deviations of IHLW radionuclide inventories, it was necessary to simulate masses of glass in 75 IHLW canisters calculated as corresponding to 18 IHLW MFPV batches associated with an HLW waste type from Tank AY-102/C-106. These masses of glass in the 75 IHLW canisters, which are listed in Table I.6, were created by generating randomly distributed disturbances with mean 0 and standard deviation 1.7831×10^4 g and adding them to the mean mass of glass in an IHLW canister = of 3.089×10^6 g. The mean and standard deviation values were based on data from Andre (2004).

Table I.6. Simulated Masses of Glass ($m_d^{Canister}$, g) in the 75 IHLW Canisters Corresponding to 18 IHLW MFPV Batches for an AY-102/C-106 HLW Waste Type

IHLW Canister d	Mass of Glass (g)	IHLW Canister d	Mass of Glass (g)	IHLW Canister d	Mass of Glass (g)
1	3.0321E+06	26	3.1699E+06	51	3.1631E+06
2	3.0306E+06	27	3.1493E+06	52	3.1176E+06
3	3.0960E+06	28	3.0468E+06	53	3.1442E+06
4	3.0702E+06	29	3.0180E+06	54	3.0089E+06
5	3.1046E+06	30	3.0225E+06	55	3.1642E+06
6	3.0273E+06	31	2.9977E+06	56	3.0029E+06
7	2.9645E+06	32	3.1396E+06	57	3.0547E+06
8	3.0508E+06	33	3.0518E+06	58	3.2364E+06
9	3.0265E+06	34	3.1300E+06	59	3.1574E+06
10	3.0745E+06	35	3.0209E+06	60	3.1191E+06
11	3.0202E+06	36	3.0861E+06	61	3.1572E+06
12	3.0029E+06	37	3.1747E+06	62	3.0562E+06
13	3.0888E+06	38	3.1192E+06	63	3.1061E+06
14	2.9965E+06	39	3.1601E+06	64	3.0713E+06
15	3.0907E+06	40	3.1603E+06	65	3.0630E+06
16	3.0168E+06	41	2.9113E+06	66	3.0263E+06
17	3.0791E+06	42	3.0578E+06	67	2.9823E+06
18	3.0667E+06	43	3.0590E+06	68	3.1071E+06
19	3.0516E+06	44	3.0400E+06	69	3.2576E+06
20	2.9708E+06	45	3.1255E+06	70	3.1142E+06
21	3.1278E+06	46	3.0029E+06	71	2.9023E+06
22	2.9795E+06	47	3.1273E+06	72	2.9702E+06
23	3.0797E+06	48	2.9301E+06	73	3.1550E+06
24	3.1246E+06	49	3.0795E+06	74	3.0980E+06
25	3.0057E+06	50	3.0242E+06	75	2.9971E+06

I.3 Simulated Data Used to Illustrate Product Consistency Test (PCT) Compliance for IHLW from a Single MFPV Batch

Simulated data were used in Section 6.3.1 to illustrate calculations with Eqs. (4.3.4) to (4.3.7) to demonstrate PCT compliance for IHLW from a single MFPV batch. The data were generated as described in Section I.1, with the values in Tables I.7 and I.8 corresponding to the concentrations (g/L) for 8 samples with 1 chemical analysis and 1 radiochemical analysis each for the first of the 18 MFPV batches corresponding to an AY-102/C-106 HLW waste type. The concentrations for chemical composition analytes are listed in Table I.7, and the radionuclide concentrations are listed in Table I.8.

Table I.7. Simulated Concentrations (c_{1jl}^{MFPV}, g/L) of Chemical Composition Analytes for Eight Samples from the First IHLW MFPV Batch for an AY-102/C-106 HLW Waste Type[(a)]

IHLW Analyte *j*	Sample Number, *l*							
	1	2	3	4	5	6	7	8
Ag	4.56E-02	4.61E-02	4.49E-02	4.77E-02	4.39E-02	4.45E-02	4.32E-02	4.87E-02
Al	3.32E+01	3.22E+01	3.42E+01	3.42E+01	3.58E+01	3.20E+01	3.69E+01	3.56E+01
As	5.04E-02	5.35E-02	5.24E-02	4.49E-02	5.74E-02	5.31E-02	5.18E-02	5.22E-02
B	6.08E+01	7.28E+01	7.08E+01	6.65E+01	6.64E+01	6.59E+01	6.94E+01	6.70E+01
Ba	1.42E+00	1.22E+00	1.43E+00	1.38E+00	1.37E+00	1.47E+00	1.50E+00	1.36E+00
Be	1.16E-02	1.07E-02	9.99E-03	1.17E-02	1.16E-02	1.25E-02	1.22E-02	1.24E-02
Bi	2.51E-01	2.31E-01	2.49E-01	2.74E-01	2.65E-01	2.66E-01	2.46E-01	2.82E-01
Ca	1.18E+01	1.24E+01	1.14E+01	1.16E+01	1.12E+01	1.09E+01	1.17E+01	9.84E+00
Cd	1.90E-01	1.79E-01	1.72E-01	1.79E-01	1.92E-01	1.78E-01	1.74E-01	1.87E-01
Ce	2.72E+00	3.00E+00	2.70E+00	3.06E+00	3.01E+00	2.80E+00	2.94E+00	2.95E+00
Cl	2.50E-01	2.70E-01	2.57E-01	2.52E-01	2.36E-01	2.59E-01	2.76E-01	2.44E-01
Cr	8.49E-07	8.87E-07	9.48E-07	9.12E-07	9.37E-07	8.63E-07	9.07E-07	8.99E-07
Cs	2.34E+00	2.25E+00	2.38E+00	2.51E+00	2.42E+00	2.37E+00	2.46E+00	2.46E+00
Cu	7.92E-02	8.10E-02	7.51E-02	7.78E-02	8.27E-02	7.78E-02	7.79E-02	8.45E-02
F	3.67E-01	3.99E-01	4.05E-01	3.88E-01	3.84E-01	4.04E-01	4.11E-01	3.78E-01
Fe	4.44E-01	4.97E-01	4.81E-01	5.18E-01	5.20E-01	5.13E-01	4.95E-01	4.56E-01
K	2.14E+02	1.95E+02	1.92E+02	2.15E+02	2.16E+02	2.00E+02	2.05E+02	1.97E+02
La	1.87E-03	1.85E-03	1.75E-03	1.95E-03	1.92E-03	1.79E-03	1.87E-03	1.97E-03
Li	5.75E+00	5.53E+00	5.51E+00	5.57E+00	5.45E+00	5.17E+00	5.69E+00	5.43E+00
Mg	2.08E+00	2.12E+00	2.27E+00	2.30E+00	2.21E+00	2.21E+00	2.11E+00	2.19E+00
Mn	1.60E-01	1.61E-01	1.59E-01	1.42E-01	1.63E-01	1.49E-01	1.54E-01	1.56E-01
Mo	5.34E+01	5.52E+01	5.77E+01	5.37E+01	5.48E+01	6.21E+01	5.80E+01	5.36E+01
Na	4.61E+00	4.75E+00	4.44E+00	4.30E+00	4.51E+00	4.65E+00	4.34E+00	4.52E+00
Nd	2.47E+01	2.44E+01	2.28E+01	2.33E+01	2.27E+01	2.34E+01	2.34E+01	2.28E+01
Ni	2.27E-02	2.46E-02	2.31E-02	2.46E-02	2.42E-02	2.43E-02	2.32E-02	2.22E-02

(a) Similar data were obtained for 17 other batches to calculate the averages in Table I.1.

Table I.7. Simulated Concentrations (c_{1jl}^{MFPV}, g/L) of Chemical Composition Analytes for Eight Samples from the First IHLW MFPV Batch for an AY-102/C-106 HLW Waste Type[(a)] (cont.)

IHLW Analyte *j*	Sample Number, *l*							
	1	2	3	4	5	6	7	8
P	3.59E+00	3.85E+00	3.52E+00	3.20E+00	3.43E+00	3.64E+00	3.27E+00	3.69E+00
Pb	1.57E+01	1.61E+01	1.56E+01	1.68E+01	1.49E+01	1.52E+01	1.67E+01	1.42E+01
Pd	3.81E-05	3.64E-05	3.73E-05	3.71E-05	3.81E-05	3.43E-05	3.73E-05	3.84E-05
Pr	5.50E-01	5.40E-01	5.58E-01	5.46E-01	5.09E-01	5.65E-01	5.66E-01	5.09E-01
Rb	4.10E-03	4.00E-03	3.96E-03	3.85E-03	3.95E-03	4.29E-03	4.00E-03	3.83E-03
Rh	3.73E-02	3.69E-02	4.01E-02	3.42E-02	3.66E-02	3.69E-02	3.69E-02	4.25E-02
Ru	8.56E-01	8.57E-01	9.15E-01	8.45E-01	8.90E-01	8.75E-01	8.41E-01	8.62E-01
Sb	5.49E-03	5.80E-03	5.93E-03	5.77E-03	6.49E-03	6.23E-03	6.18E-03	5.76E-03
Se	5.68E-03	5.53E-03	5.63E-03	5.63E-03	5.78E-03	5.82E-03	5.52E-03	5.46E-03
Si	6.09E+02	6.06E+02	6.13E+02	5.87E+02	5.68E+02	5.51E+02	6.04E+02	5.43E+02
S	6.43E-01	6.34E-01	6.59E-01	6.56E-01	5.97E-01	6.20E-01	6.14E-01	6.15E-01
Sr	5.03E-01	4.74E-01	5.02E-01	5.22E-01	5.11E-01	5.40E-01	4.99E-01	5.23E-01
Ta	3.25E-03	3.36E-03	3.41E-03	3.33E-03	3.23E-03	3.54E-03	3.15E-03	3.07E-03
Te	1.66E-01	1.74E-01	1.72E-01	1.77E-01	1.85E-01	1.66E-01	1.92E-01	1.88E-01
Ti	2.75E-01	2.90E-01	2.67E-01	2.64E-01	2.61E-01	2.53E-01	2.81E-01	2.65E-01
Tl	7.78E-03	7.70E-03	8.32E-03	8.51E-03	8.11E-03	7.89E-03	8.14E-03	8.39E-03
V	7.65E-02	7.96E-02	8.04E-02	7.52E-02	7.96E-02	8.21E-02	7.35E-02	7.49E-02
W	4.32E-01	4.63E-01	4.44E-01	4.42E-01	4.77E-01	4.99E-01	4.76E-01	4.78E-01
Y	1.88E-01	2.19E-01	1.76E-01	1.90E-01	1.90E-01	1.73E-01	1.92E-01	1.86E-01
Zn	2.66E-01	2.81E-01	2.95E-01	2.92E-01	3.01E-01	2.71E-01	3.22E-01	2.75E-01
Zr	5.46E-02	5.39E-02	5.29E-02	4.99E-02	5.46E-02	5.79E-02	5.27E-02	5.21E-02

(a) Similar data were obtained for 17 other batches to calculate the averages in Table I.1.

Table I.8. Simulated Concentrations (c_{1ql}^{MFPV}, g/L) of Radionuclides for Eight Samples from the First IHLW MFPV Batch for an AY-102/C-106 HLW Waste Type[(a)]

IHLW Radionuclide q	Sample Number, l							
	1	2	3	4	5	6	7	8
^{227}Ac	2.86E-10	2.62E-10	2.79E-10	2.86E-10	2.87E-10	2.91E-10	2.82E-10	2.77E-10
^{241}Am	3.98E-03	4.05E-03	3.73E-03	3.90E-03	3.85E-03	3.53E-03	3.87E-03	4.09E-03
^{243}Am	4.89E-06	4.59E-06	4.50E-06	5.05E-06	4.82E-06	4.57E-06	4.65E-06	4.69E-06
^{113}Cd	4.54E-08	4.76E-08	4.27E-08	5.09E-08	4.61E-08	4.67E-08	4.84E-08	4.38E-08
^{242}Cm	7.07E-09	7.36E-09	7.54E-09	6.68E-09	7.54E-09	6.93E-09	7.17E-09	7.60E-09
^{243}Cm	3.61E-08	3.70E-08	3.88E-08	4.15E-08	3.55E-08	3.92E-08	3.79E-08	4.02E-08
^{244}Cm	5.42E-07	5.40E-07	5.21E-07	5.53E-07	5.14E-07	5.14E-07	5.35E-07	4.82E-07
^{60}Co	7.43E-10	7.35E-10	7.24E-10	7.62E-10	6.60E-10	7.21E-10	7.09E-10	6.71E-10
^{134}Cs	7.99E-08	7.18E-08	8.11E-08	8.32E-08	8.36E-08	8.03E-08	7.57E-08	7.54E-08
^{137}Cs	2.24E-02	2.36E-02	2.31E-02	2.10E-02	2.09E-02	2.13E-02	2.09E-02	2.21E-02
^{152}Eu	4.01E-07	4.59E-07	4.33E-07	4.38E-07	4.76E-07	4.35E-07	4.68E-07	4.55E-07
^{154}Eu	2.47E-05	2.51E-05	2.27E-05	2.36E-05	2.62E-05	2.62E-05	2.58E-05	2.37E-05
^{155}Eu	7.51E-06	6.75E-06	7.11E-06	6.23E-06	7.44E-06	7.82E-06	6.79E-06	7.44E-06
^{129}I	6.95E-05	7.22E-05	6.27E-05	7.01E-05	7.20E-05	6.89E-05	6.85E-05	6.96E-05
^{93}Nb	2.32E-08	2.06E-08	2.05E-08	2.43E-08	2.24E-08	2.32E-08	2.25E-08	2.17E-08
^{59}Ni	2.89E-03	2.85E-03	2.78E-03	2.74E-03	2.75E-03	2.94E-03	2.76E-03	2.62E-03
^{63}Ni	3.08E-04	3.31E-04	3.30E-04	3.38E-04	3.32E-04	3.26E-04	3.29E-04	3.49E-04
^{237}Np	9.94E-03	1.04E-02	1.02E-02	1.09E-02	9.79E-03	9.63E-03	1.00E-02	1.03E-02
^{231}Pa	2.38E-08	2.29E-08	2.36E-08	2.47E-08	2.54E-08	2.23E-08	2.31E-08	2.44E-08
^{238}Pu	5.33E-05	5.25E-05	4.96E-05	5.27E-05	5.29E-05	5.31E-05	5.77E-05	5.50E-05
^{239}Pu	4.22E-02	4.17E-02	3.81E-02	4.15E-02	3.98E-02	4.15E-02	3.40E-02	3.69E-02
^{240}Pu	1.93E-03	1.90E-03	2.14E-03	1.87E-03	1.89E-03	1.99E-03	2.19E-03	1.97E-03
^{241}Pu	6.04E-05	6.14E-05	6.37E-05	5.79E-05	5.90E-05	5.61E-05	5.90E-05	6.10E-05
^{242}Pu	1.80E-05	1.87E-05	2.08E-05	2.05E-05	2.09E-05	1.97E-05	1.84E-05	1.88E-05
^{226}Ra	6.81E-09	6.59E-09	6.65E-09	6.48E-09	7.36E-09	7.04E-09	6.42E-09	6.73E-09
^{228}Ra	2.41E-10	2.39E-10	2.19E-10	2.32E-10	2.21E-10	2.44E-10	2.21E-10	2.27E-10
^{125}Sb	2.27E-09	2.25E-09	2.59E-09	2.26E-09	2.23E-09	2.30E-09	2.36E-09	2.42E-09
^{79}Se	2.95E-06	2.88E-06	2.92E-06	3.09E-06	2.87E-06	3.20E-06	3.13E-06	2.98E-06
^{151}Sm	1.46E-04	1.40E-04	1.50E-04	1.36E-04	1.59E-04	1.51E-04	1.52E-04	1.54E-04
^{126}Sn	6.34E-05	6.47E-05	6.41E-05	6.82E-05	6.47E-05	6.83E-05	6.68E-05	6.28E-05
^{90}Sr	5.96E-02	5.46E-02	5.61E-02	5.15E-02	5.56E-02	5.23E-02	5.43E-02	5.60E-02
^{99}Tc	9.38E-04	9.78E-04	1.05E-03	9.39E-04	8.91E-04	9.50E-04	8.58E-04	9.17E-04
^{229}Th	1.76E-09	1.87E-09	1.64E-09	1.72E-09	1.75E-09	1.75E-09	1.77E-09	1.75E-09
^{232}Th	9.29E-01	9.73E-01	9.97E-01	9.56E-01	9.81E-01	9.38E-01	8.58E-01	1.06E+00
^{232}U	9.27E-11	9.07E-11	9.09E-11	9.38E-11	9.52E-11	8.73E-11	9.74E-11	9.78E-11
^{233}U	9.06E-07	9.23E-07	9.00E-07	9.06E-07	9.23E-07	8.48E-07	1.03E-06	9.59E-07
^{234}U	3.40E-04	3.50E-04	3.52E-04	3.45E-04	3.49E-04	3.42E-04	3.32E-04	3.17E-04
^{235}U	2.10E-02	1.99E-02	2.09E-02	2.22E-02	1.95E-02	2.01E-02	1.96E-02	2.06E-02
^{236}U	1.98E-03	1.98E-03	2.16E-03	2.11E-03	1.94E-03	2.02E-03	2.11E-03	1.98E-03
^{238}U	5.03E+00	5.28E+00	4.64E+00	4.76E+00	4.83E+00	4.77E+00	4.73E+00	4.84E+00
^{Tot}U	1.50E-05	1.38E-05	1.42E-05	1.41E-05	1.45E-05	1.45E-05	1.33E-05	1.36E-05
^{93}Zr	2.21E-03	2.47E-03	2.33E-03	2.19E-03	2.05E-03	2.58E-03	2.20E-03	2.09E-03

(a) Similar data were obtained for 17 other batches to calculate the averages in Table I.4.

Appendix J

Simulated Data Used to Illustrate ILAW Compliance Methods

Appendix J: Simulated Data Used to Illustrate ILAW Compliance Methods

This appendix presents the simulated data used to illustrate in Section 7 the immobilized low-activity waste (ILAW) compliance methods that were presented in Section 5. These simulated data are based on data from tank-waste samples, glass-formulation development work, melter testing, realistic estimates of variations and uncertainties, G2 software (Deng 2004; Vora 2004) simulations of the Waste Treatment Plant (WTP) low-activity waste (LAW) vitrification process, and statistical simulations to include realistic uncertainties. Hence, the data included in this appendix have been "constructed" from various inputs and methods to provide, as much as is possible at this time, a realistic simulation of data that will be collected during operation of the WTP ILAW facility

J.1 Simulated Data Used to Illustrate Calculating Means and Standard Deviations of ILAW Chemical Compositions

Simulated data were used in Section 7.1.2 to illustrate calculations of means, standard deviations, and percent relative standard deviations (%RSDs) of ILAW chemical compositions (mass fractions). Ideally, simulated data would have been generated for all of the inputs appearing in Eqs. (5.1.2), (5.1.5), and (5.1.6), such as elemental and radionuclide concentrations of Concentrate Receipt Vessel (CRV) samples, CRV and Melter Feed Process Vessel (MFPV) volumes, masses of glass-forming chemicals (GFCs) added to the MFPV, and others. However, not all of the needed inputs were available in the Excel spreadsheet (Vienna 2004b) containing results from Run 3.1vv of the G2 dynamic simulation flowsheet (Deng 2004; Vora 2004) for ILAW resulting from Tank AP-101. Further, G2 does not simulate multiple LAW CRV samples, analyses per sample, or volume determinations, and thus the simulated data from G2 do not include CRV mixing/sampling, analytical, volume, or other applicable uncertainties that affect ILAW composition. Because of the complicated WTP ILAW compliance strategy and equations for calculating ILAW composition associated with an ILAW MFPV batch, it was not possible at the time of this work to augment the G2 outputs with the various uncertainties affecting ILAW composition. However, simulated data representative of all applicable uncertainties in the WTP LAW vitrification process as well as batch-to-batch variations simulated by G2 will be generated and used in illustrations in the final version of this report scheduled for 2007.

The simulated data used in this version of the report, as presented in this section, consist of mass fractions for chemical-composition components (oxides and halogens) for each of 25 ILAW MFPV batches corresponding to LAW from Tank AP-101. The 25 ILAW MFPV batches are assumed to correspond to an LAW waste type for illustration purposes in this report. Mass fractions for chemical-composition components (oxides and halogens) are listed in Table J.1. These mass fractions reflect only batch-to-batch variations as simulated by G2 and do not include any contributions from the uncertainties affecting ILAW compositions, as described in the previous paragraph.

Table J.1. Mass Fractions (g_{ij}^{MFPV}) of Chemical Composition Components (Oxides and Halogens) over 25 ILAW MFPV Batches (Vienna 2004b) Corresponding to LAW Tank AP-101

ILAW Comp. *j*	ILAW Component Mass Fractions by ILAW MFPV Batch Number *i* = 1 to 9								
	1	2	3	4	5	6	7	8	9
Ag_2O	8.93E-07	9.00E-07	9.03E-07	9.09E-07	9.11E-07	9.15E-07	9.18E-07	9.20E-07	9.22E-07
Al_2O_3	5.89E-02	5.89E-02	5.89E-02	5.89E-02	5.89E-02	5.89E-02	5.89E-02	5.89E-02	5.89E-02
As_2O_5	3.23E-06	3.27E-06	3.28E-06	3.31E-06	3.32E-06	3.34E-06	3.35E-06	3.36E-06	3.37E-06
B_2O_3	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02
BaO	3.77E-07	3.77E-07	3.77E-07	3.77E-07	3.78E-07	3.78E-07	3.78E-07	3.78E-07	3.78E-07
BeO	3.13E-06	3.12E-06	3.12E-06	3.11E-06	3.11E-06	3.10E-06	3.10E-06	3.10E-06	3.10E-06
Bi_2O_3	1.89E-06	1.88E-06	1.88E-06	1.88E-06	1.87E-06	1.87E-06	1.87E-06	1.87E-06	1.86E-06
CaO	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02
CdO	1.92E-06	1.92E-06	1.92E-06	1.91E-06	1.91E-06	1.91E-06	1.91E-06	1.91E-06	1.91E-06
Ce_2O_3	8.34E-08	8.35E-08	8.36E-08	8.37E-08	8.37E-08	8.38E-08	8.39E-08	8.39E-08	8.39E-08
Cl	1.59E-03	1.59E-03	1.58E-03	1.58E-03	1.58E-03	1.57E-03	1.57E-03	1.57E-03	1.57E-03
Cr_2O_3	2.45E-04	2.46E-04	2.47E-04	2.47E-04	2.47E-04	2.48E-04	2.48E-04	2.49E-04	2.49E-04
Cs_2O	2.82E-10	2.81E-10	2.81E-10	2.80E-10	2.79E-10	2.79E-10	2.78E-10	2.78E-10	2.78E-10
CuO	1.95E-06	1.96E-06	1.96E-06	1.96E-06	1.96E-06	1.96E-06	1.96E-06	1.96E-06	1.96E-06
F	2.31E-03	2.30E-03	2.29E-03	2.29E-03	2.28E-03	2.28E-03	2.27E-03	2.27E-03	2.27E-03
Fe_2O_3	5.83E-02	5.83E-02	5.83E-02	5.83E-02	5.83E-02	5.83E-02	5.83E-02	5.83E-02	5.83E-02
K_2O	2.96E-02	2.95E-02	2.94E-02	2.93E-02	2.93E-02	2.92E-02	2.91E-02	2.91E-02	2.91E-02
La_2O_3	1.29E-06	1.29E-06	1.30E-06	1.30E-06	1.30E-06	1.30E-06	1.30E-06	1.30E-06	1.30E-06
Li_2O	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02
MgO	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02
MnO	1.21E-06	1.21E-06	1.20E-06	1.20E-06	1.20E-06	1.19E-06	1.19E-06	1.19E-06	1.19E-06
MoO_3	1.86E-05	1.85E-05	1.85E-05	1.85E-05	1.84E-05	1.84E-05	1.84E-05	1.84E-05	1.84E-05
Na_2O	1.62E-01	1.62E-01	1.62E-01	1.62E-01	1.62E-01	1.63E-01	1.63E-01	1.63E-01	1.63E-01
Nd_2O_3	6.00E-06	6.07E-06	6.09E-06	6.15E-06	6.17E-06	6.21E-06	6.23E-06	6.25E-06	6.27E-06
NiO	3.12E-05	3.17E-05	3.19E-05	3.22E-05	3.23E-05	3.26E-05	3.28E-05	3.29E-05	3.30E-05

Table J.1. Mass Fractions (g_{ij}^{MFPV}) of Chemical Composition Components (Oxides and Halogens) over 25 ILAW MFPV Batches (Vienna 2004b) Corresponding to LAW Tank AP-101 (cont.)

ILAW Comp. *j*	ILAW Component Mass Fractions by ILAW MFPV Batch Number *i* = 1 to 9								
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
P_2O_5	1.71E-03	1.73E-03	1.74E-03	1.76E-03	1.77E-03	1.78E-03	1.79E-03	1.79E-03	1.80E-03
PbO	3.10E-05	3.13E-05	3.15E-05	3.17E-05	3.18E-05	3.20E-05	3.21E-05	3.22E-05	3.23E-05
PdO	2.05E-07	2.09E-07	2.11E-07	2.15E-07	2.16E-07	2.18E-07	2.20E-07	2.21E-07	2.23E-07
Pr_2O_3	3.60E-08	3.64E-08	3.65E-08	3.68E-08	3.69E-08	3.71E-08	3.72E-08	3.73E-08	3.74E-08
Rb_2O	3.58E-06	3.57E-06	3.56E-06	3.56E-06	3.55E-06	3.54E-06	3.54E-06	3.54E-06	3.53E-06
Rh_2O_3	7.09E-07	7.24E-07	7.30E-07	7.42E-07	7.46E-07	7.55E-07	7.61E-07	7.64E-07	7.69E-07
RuO_2	1.34E-05	1.37E-05	1.38E-05	1.40E-05	1.41E-05	1.43E-05	1.44E-05	1.44E-05	1.45E-05
SiO_2	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01
Ta_2O_5	1.26E-07	1.26E-07	1.27E-07	1.27E-07	1.27E-07	1.27E-07	1.27E-07	1.28E-07	1.28E-07
TeO_2	3.57E-07	3.64E-07	3.67E-07	3.73E-07	3.75E-07	3.80E-07	3.83E-07	3.84E-07	3.87E-07
TiO_2	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02
Tl_2O	1.04E-07	1.06E-07	1.07E-07	1.08E-07	1.08E-07	1.10E-07	1.10E-07	1.11E-07	1.11E-07
SO_3	3.22E-03	3.22E-03	3.22E-03	3.22E-03	3.22E-03	3.22E-03	3.22E-03	3.21E-03	3.22E-03
Sb_2O_3	6.88E-08	6.95E-08	6.98E-08	7.04E-08	7.06E-08	7.10E-08	7.13E-08	7.14E-08	7.17E-08
SeO_2	9.36E-06	9.49E-06	9.55E-06	9.65E-06	9.69E-06	9.77E-06	9.81E-06	9.84E-06	9.89E-06
SrO	1.21E-05	1.23E-05	1.25E-05	1.26E-05	1.27E-05	1.29E-05	1.30E-05	1.30E-05	1.31E-05
V_2O_5	1.54E-06	1.55E-06	1.55E-06	1.56E-06	1.56E-06	1.56E-06	1.56E-06	1.56E-06	1.57E-06
WO_3	2.82E-05	2.81E-05	2.80E-05	2.79E-05	2.78E-05	2.77E-05	2.77E-05	2.77E-05	2.76E-05
Y_2O_3	1.89E-06	1.93E-06	1.95E-06	1.98E-06	1.99E-06	2.02E-06	2.03E-06	2.04E-06	2.05E-06
ZnO	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02
ZrO_2	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02
Rads[(a)]	2.32E-04	2.32E-04	2.33E-04	2.33E-04	2.33E-04	2.33E-04	2.34E-04	2.34E-04	2.34E-04
Total	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00

(a) The total mass fractions of all radionuclide oxides, as listed specifically in Table J.2.

Table J.1. Mass Fractions (g_{ij}^{MFPV}) of Chemical Composition Components (Oxides and Halogens) over 25 ILAW MFPV Batches (Vienna 2004b) Corresponding to LAW Tank AP-101 (cont.)

ILAW Comp. *j*	ILAW Component Mass Fractions by ILAW MFPV Batch Number *i* = 10 to 18								
	10	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**
Ag_2O	9.24E-07	9.26E-07	9.27E-07	9.28E-07	9.29E-07	9.29E-07	9.30E-07	9.30E-07	9.32E-07
Al_2O_3	5.89E-02	5.89E-02	5.89E-02	5.89E-02	5.89E-02	5.89E-02	5.89E-02	5.89E-02	5.89E-02
As_2O_5	3.38E-06	3.39E-06	3.39E-06	3.40E-06	3.40E-06	3.40E-06	3.41E-06	3.41E-06	3.42E-06
B_2O_3	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02
BaO	3.78E-07	3.78E-07	3.78E-07	3.78E-07	3.78E-07	3.78E-07	3.78E-07	3.78E-07	3.78E-07
BeO	3.09E-06	3.09E-06	3.09E-06	3.09E-06	3.09E-06	3.09E-06	3.08E-06	3.08E-06	3.08E-06
Bi_2O_3	1.86E-06	1.86E-06	1.86E-06	1.86E-06	1.86E-06	1.86E-06	1.86E-06	1.86E-06	1.85E-06
CaO	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02
CdO	1.91E-06	1.90E-06	1.90E-06	1.90E-06	1.90E-06	1.90E-06	1.90E-06	1.90E-06	1.90E-06
Ce_2O_3	8.40E-08	8.40E-08	8.40E-08	8.40E-08	8.40E-08	8.40E-08	8.40E-08	8.40E-08	8.41E-08
Cl	1.56E-03	1.56E-03	1.56E-03	1.56E-03	1.56E-03	1.56E-03	1.56E-03	1.56E-03	1.55E-03
Cr_2O_3	2.49E-04	2.49E-04	2.49E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04
Cs_2O	2.78E-10	2.77E-10	2.77E-10	2.77E-10	2.77E-10	2.76E-10	2.76E-10	2.76E-10	2.76E-10
CuO	1.96E-06	1.96E-06	1.96E-06	1.96E-06	1.96E-06	1.96E-06	1.96E-06	1.96E-06	1.96E-06
F	2.26E-03	2.26E-03	2.26E-03	2.26E-03	2.25E-03	2.25E-03	2.25E-03	2.25E-03	2.25E-03
Fe_2O_3	5.83E-02	5.83E-02	5.83E-02	5.83E-02	5.83E-02	5.83E-02	5.83E-02	5.83E-02	5.83E-02
K_2O	2.90E-02	2.90E-02	2.90E-02	2.89E-02	2.89E-02	2.89E-02	2.89E-02	2.89E-02	2.88E-02
La_2O_3	1.30E-06	1.31E-06	1.31E-06	1.31E-06	1.31E-06	1.31E-06	1.31E-06	1.31E-06	1.31E-06
Li_2O	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02
MgO	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02
MnO	1.19E-06	1.19E-06	1.18E-06	1.18E-06	1.18E-06	1.18E-06	1.18E-06	1.18E-06	1.18E-06
MoO_3	1.83E-05	1.83E-05	1.83E-05	1.83E-05	1.83E-05	1.83E-05	1.83E-05	1.83E-05	1.83E-05
Na_2O	1.63E-01	1.63E-01	1.63E-01	1.63E-01	1.63E-01	1.63E-01	1.63E-01	1.63E-01	1.63E-01
Nd_2O_3	6.28E-06	6.31E-06	6.32E-06	6.33E-06	6.33E-06	6.34E-06	6.34E-06	6.35E-06	6.36E-06
NiO	3.31E-05	3.33E-05	3.33E-05	3.34E-05	3.35E-05	3.35E-05	3.35E-05	3.35E-05	3.37E-05

Table J.1. Mass Fractions (g_{ij}^{MFPV}) of Chemical Composition Components (Oxides and Halogens) over 25 ILAW MFPV Batches (Vienna 2004b) Corresponding to LAW Tank AP-101 (cont.)

ILAW Comp. *j*	ILAW Component Mass Fractions by ILAW MFPV Batch Number *i* = 10 to 18								
	10	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**
P_2O_5	1.80E-03	1.81E-03	1.81E-03	1.82E-03	1.82E-03	1.82E-03	1.82E-03	1.82E-03	1.83E-03
PbO	3.24E-05	3.25E-05	3.26E-05	3.26E-05	3.26E-05	3.27E-05	3.27E-05	3.27E-05	3.28E-05
PdO	2.23E-07	2.25E-07	2.25E-07	2.26E-07	2.27E-07	2.27E-07	2.27E-07	2.27E-07	2.29E-07
Pr_2O_3	3.75E-08	3.76E-08	3.77E-08	3.77E-08	3.78E-08	3.78E-08	3.78E-08	3.78E-08	3.79E-08
Rb_2O	3.53E-06	3.53E-06	3.52E-06	3.52E-06	3.52E-06	3.52E-06	3.52E-06	3.51E-06	3.51E-06
Rh_2O_3	7.72E-07	7.77E-07	7.79E-07	7.82E-07	7.83E-07	7.84E-07	7.86E-07	7.86E-07	7.90E-07
RuO_2	1.46E-05	1.47E-05	1.47E-05	1.48E-05	1.48E-05	1.48E-05	1.48E-05	1.48E-05	1.49E-05
SiO_2	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01
Ta_2O_5	1.28E-07	1.28E-07	1.28E-07	1.28E-07	1.28E-07	1.28E-07	1.28E-07	1.28E-07	1.28E-07
TeO_2	3.88E-07	3.91E-07	3.92E-07	3.93E-07	3.94E-07	3.95E-07	3.95E-07	3.95E-07	3.98E-07
TiO_2	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02
Tl_2O	1.12E-07	1.12E-07	1.12E-07	1.13E-07	1.13E-07	1.13E-07	1.13E-07	1.13E-07	1.14E-07
SO_3	3.22E-03	3.21E-03	3.21E-03	3.21E-03	3.21E-03	3.21E-03	3.21E-03	3.21E-03	3.21E-03
Sb_2O_3	7.18E-08	7.21E-08	7.22E-08	7.23E-08	7.24E-08	7.24E-08	7.25E-08	7.25E-08	7.27E-08
SeO_2	9.91E-06	9.96E-06	9.98E-06	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.00E-05	1.01E-05
SrO	1.31E-05	1.32E-05	1.33E-05	1.33E-05	1.33E-05	1.34E-05	1.34E-05	1.34E-05	1.35E-05
V_2O_5	1.57E-06	1.57E-06	1.57E-06	1.57E-06	1.57E-06	1.57E-06	1.57E-06	1.57E-06	1.57E-06
WO_3	2.76E-05	2.75E-05	2.75E-05	2.75E-05	2.75E-05	2.74E-05	2.74E-05	2.74E-05	2.74E-05
Y_2O_3	2.06E-06	2.07E-06	2.08E-06	2.09E-06	2.09E-06	2.09E-06	2.10E-06	2.10E-06	2.11E-06
ZnO	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02
ZrO_2	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02
Rads[(a)]	2.35E-04	2.34E-04	2.34E-04	2.34E-04	2.34E-04	2.34E-04	2.34E-04	2.34E-04	2.35E-04
Total	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00+00	1.00E+00

(a) The total mass fractions of all radionuclide oxides, as listed specifically in Table J.2.

Table J.1. Mass Fractions (g_{ij}^{MFPV}) of Chemical Composition Components (Oxides and Halogens) over 25 ILAW MFPV Batches (Vienna 2004b) Corresponding to LAW Tank AP-101 (cont.)

ILAW Comp. *j*	ILAW Component Mass Fractions by ILAW MFPV Batch Number *i* = 19 to 25						
	19	20	21	22	23	24	25
Ag_2O	9.33E-07	9.43E-07	9.47E-07	9.52E-07	9.57E-07	9.59E-07	9.64E-07
Al_2O_3	5.89E-02	5.90E-02	5.90E-02	5.90E-02	5.90E-02	5.90E-02	5.90E-02
As_2O_5	3.42E-06	3.47E-06	3.49E-06	3.51E-06	3.53E-06	3.54E-06	3.57E-06
B_2O_3	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02	9.28E-02
BaO	3.78E-07	3.79E-07	3.79E-07	3.79E-07	3.79E-07	3.80E-07	3.80E-07
BeO	3.08E-06	3.07E-06	3.06E-06	3.06E-06	3.05E-06	3.05E-06	3.04E-06
Bi_2O_3	1.85E-06	1.84E-06	1.84E-06	1.84E-06	1.83E-06	1.83E-06	1.83E-06
CaO	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02	4.98E-02
CdO	1.90E-06	1.89E-06	1.89E-06	1.89E-06	1.89E-06	1.88E-06	1.88E-06
Ce_2O_3	8.41E-08	8.42E-08	8.43E-08	8.44E-08	8.45E-08	8.46E-08	8.46E-08
Cl	1.55E-03	1.54E-03	1.54E-03	1.53E-03	1.53E-03	1.53E-03	1.52E-03
Cr_2O_3	2.50E-04	2.51E-04	2.52E-04	2.52E-04	2.53E-04	2.53E-04	2.54E-04
Cs_2O	2.76E-10	2.75E-10	2.74E-10	2.73E-10	2.73E-10	2.72E-10	2.72E-10
CuO	1.96E-06	1.96E-06	1.97E-06	1.97E-06	1.97E-06	1.97E-06	1.97E-06
F	2.25E-03	2.23E-03	2.23E-03	2.22E-03	2.21E-03	2.21E-03	2.20E-03
Fe_2O_3	5.83E-02	5.83E-02	5.83E-02	5.84E-02	5.84E-02	5.84E-02	5.84E-02
K_2O	2.88E-02	2.86E-02	2.85E-02	2.84E-02	2.84E-02	2.83E-02	2.82E-02
La_2O_3	1.31E-06	1.31E-06	1.31E-06	1.32E-06	1.32E-06	1.32E-06	1.32E-06
Li_2O	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02	1.20E-02
MgO	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02
MnO	1.18E-06	1.17E-06	1.17E-06	1.16E-06	1.16E-06	1.16E-06	1.15E-06
MoO_3	1.83E-05	1.82E-05	1.82E-05	1.81E-05	1.81E-05	1.81E-05	1.80E-05
Na_2O	1.63E-01	1.63E-01	1.63E-01	1.63E-01	1.63E-01	1.63E-01	1.63E-01
Nd_2O_3	6.37E-06	6.46E-06	6.50E-06	6.55E-06	6.60E-06	6.62E-06	6.66E-06
NiO	3.37E-05	3.43E-05	3.46E-05	3.49E-05	3.52E-05	3.53E-05	3.56E-05

Table J.1. Mass Fractions (g_{ij}^{MFPV}) of Chemical Composition Components (Oxides and Halogens) over 25 ILAW MFPV Batches (Vienna 2004b) Corresponding to LAW Tank AP-101 (cont.)

ILAW Comp. *j*	ILAW Component Mass Fractions by ILAW MFPV Batch Number *i* = 19 to 25						
	19	**20**	**21**	**22**	**23**	**24**	**25**
P_2O_5	1.83E-03	1.86E-03	1.87E-03	1.89E-03	1.90E-03	1.91E-03	1.92E-03
PbO	3.28E-05	3.33E-05	3.35E-05	3.37E-05	3.39E-05	3.40E-05	3.42E-05
PdO	2.29E-07	2.35E-07	2.38E-07	2.41E-07	2.43E-07	2.45E-07	2.48E-07
Pr_2O_3	3.79E-08	3.84E-08	3.86E-08	3.89E-08	3.91E-08	3.92E-08	3.94E-08
Rb_2O	3.51E-06	3.49E-06	3.48E-06	3.48E-06	3.47E-06	3.46E-06	3.46E-06
Rh_2O_3	7.92E-07	8.12E-07	8.21E-07	8.32E-07	8.42E-07	8.46E-07	8.56E-07
RuO_2	1.50E-05	1.53E-05	1.55E-05	1.57E-05	1.59E-05	1.60E-05	1.61E-05
SiO_2	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01	4.38E-01
Ta_2O_5	1.28E-07	1.29E-07	1.29E-07	1.30E-07	1.30E-07	1.30E-07	1.30E-07
TeO_2	3.98E-07	4.09E-07	4.13E-07	4.19E-07	4.23E-07	4.25E-07	4.30E-07
TiO_2	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02	1.53E-02
Tl_2O	1.14E-07	1.16E-07	1.17E-07	1.19E-07	1.20E-07	1.20E-07	1.22E-07
SO_3	3.21E-03	3.21E-03	3.21E-03	3.21E-03	3.21E-03	3.21E-03	3.21E-03
Sb_2O_3	7.28E-08	7.38E-08	7.42E-08	7.47E-08	7.52E-08	7.54E-08	7.59E-08
SeO_2	1.01E-05	1.03E-05	1.03E-05	1.04E-05	1.05E-05	1.06E-05	1.06E-05
SrO	1.35E-05	1.38E-05	1.40E-05	1.42E-05	1.43E-05	1.44E-05	1.45E-05
V_2O_5	1.57E-06	1.58E-06	1.58E-06	1.59E-06	1.59E-06	1.59E-06	1.60E-06
WO_3	2.74E-05	2.72E-05	2.71E-05	2.70E-05	2.69E-05	2.69E-05	2.68E-05
Y_2O_3	2.11E-06	2.17E-06	2.19E-06	2.22E-06	2.25E-06	2.26E-06	2.28E-06
ZnO	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02
ZrO_2	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02	2.90E-02
Rads[(a)]	2.35E-04	2.35E-04	2.36E-04	2.36E-04	2.36E-04	2.37E-04	2.36E-04
Total	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00

(a) The total mass fractions of all radionuclide oxides, as listed specifically in Table J.2.

J.2 Simulated Data Used to Illustrate Calculating Means and Standard Deviations of ILAW Radionuclide Compositions and Inventories

Simulated data were used in Section 7.2.2 to illustrate calculations of means, standard deviations, and %RSDs of ILAW radionuclide compositions (mass fractions) and inventories. Ideally, simulated data would have been generated for all of the inputs appearing in Eqs. (5.1.2), (5.1.5), and (5.1.6), such as elemental and radionuclide concentrations of CRV samples, CRV and MFPV volumes, masses of GFCs added to the MFPV, and others. However, not all of the needed inputs were available in the Excel spreadsheet (Vienna 2004b) containing results from Run 3.1vv of the G2 dynamic simulation flowsheet (Deng 2004; Vora 2004) for ILAW resulting from Tank AP-101. Further, G2 does not simulate multiple LAW CRV samples, analyses per sample, or volume determinations, and thus the simulated data from G2 do not include CRV mixing/sampling, analytical, volume, or other applicable uncertainties that affect ILAW composition. Because of the complicated WTP ILAW compliance strategy and equations for calculating ILAW composition associated with an ILAW MFPV batch, it was not possible at the time of this work to augment the G2 outputs with the various uncertainties affecting ILAW composition. However, simulated data representative of all applicable uncertainties in the WTP LAW vitrification process as well as batch-to-batch variations simulated by G2 will be generated and used in illustrations in the final version of this report scheduled for 2007.

The simulated data used in this version of the report, as presented in this section, consist of mass fractions for radionuclide composition components (oxides) for each of 25 ILAW MFPV batches corresponding to LAW from Tank AP-101. The 25 ILAW MFPV batches are assumed to correspond to an LAW waste type for illustration purposes in this report. Mass fractions for radionuclide composition components (oxides) are listed in Table J.2. These mass fractions reflect only batch-to-batch variations as simulated by G2 and do not include any contributions from the uncertainties affecting ILAW compositions, as described in the previous paragraph.

To illustrate using Eqs. (5.2.1) and (5.2.2) for calculating means and standard deviations of ILAW radionuclide inventories, it was necessary to simulate masses of glass in 41 ILAW containers calculated as corresponding to 25 ILAW MFPV batches associated with an assumed LAW waste type from Tank AP-101. These masses of glass in the 41 ILAW containers, which are listed in Table J.3, were created by generating randomly distributed disturbances with mean 0 and standard deviation 8.0508×10^4 g and adding them to the mean mass of glass in an ILAW container = 5.911×10^6 g. The mean and standard deviation values were based on data from Andre (2004).

Table J.2. Mass Fractions (g_{iq}^{MFPV}) of Radionuclide Composition Components (Oxides) over 25 ILAW MFPV Batches (Vienna 2004b) Corresponding to LAW Tank AP-101

Radio-nuclide Comp. *q*	ILAW Radionuclide Component Mass Fractions by ILAW MFPV Batch Number *i* = 1 to 9								
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
$^{227}Ac_2O_3$	5.90E-15	5.87E-15	5.86E-15	5.84E-15	5.83E-15	5.80E-15	5.81E-15	5.79E-15	5.78E-15
$^{241}Am_2O_3$	6.66E-11	6.69E-11	6.70E-11	6.72E-11	6.73E-11	6.75E-11	6.76E-11	6.76E-11	6.77E-11
$^{243}Am_2O_3$	6.13E-14	6.17E-14	6.18E-14	6.21E-14	6.22E-14	6.24E-14	6.25E-14	6.26E-14	6.27E-14
^{113}CdO	8.31E-11	8.29E-11	8.29E-11	8.27E-11	8.27E-11	8.25E-11	8.25E-11	8.24E-11	8.24E-11
$^{243}Cm_2O_3$	5.13E-16	5.14E-16	5.14E-16	5.14E-16	5.15E-16	5.15E-16	5.15E-16	5.15E-16	5.00E-16
$^{244}Cm_2O_3$	5.16E-14	5.25E-14	5.29E-14	5.36E-14	5.39E-14	5.44E-14	5.48E-14	5.50E-14	5.53E-14
^{60}CoO	1.76E-12	1.77E-12	1.77E-12	1.78E-12	1.78E-12	1.78E-12	1.78E-12	1.79E-12	1.79E-12
$^{134}Cs_2O$	2.21E-16	2.21E-16	2.21E-16	2.14E-16	2.14E-16	2.14E-16	2.14E-16	2.14E-16	2.14E-16
$^{137}Cs_2O$	8.06E-11	8.03E-11	8.02E-11	7.99E-11	7.98E-11	7.96E-11	7.95E-11	7.94E-11	7.93E-11
$^{152}Eu_2O_3$	9.00E-12	9.01E-12	9.01E-12	9.01E-12	9.00E-12	9.00E-12	9.00E-12	9.00E-12	9.00E-12
$^{154}Eu_2O_3$	7.10E-11	7.24E-11	7.30E-11	7.41E-11	7.45E-11	7.53E-11	7.59E-11	7.62E-11	7.67E-11
$^{155}Eu_2O_3$	2.00E-11	2.04E-11	2.06E-11	2.09E-11	2.10E-11	2.13E-11	2.14E-11	2.15E-11	2.17E-11
^{129}I	2.69E-07	2.69E-07	2.69E-07	2.68E-07	2.68E-07	2.68E-07	2.67E-07	2.67E-07	2.67E-07
$^{93}Nb_2O_5$	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11
^{59}NiO	1.90E-08	1.93E-08	1.95E-08	1.97E-08	1.98E-08	2.00E-08	2.01E-08	2.02E-08	2.03E-08
^{63}NiO	2.37E-09	2.41E-09	2.43E-09	2.46E-09	2.47E-09	2.49E-09	2.51E-09	2.52E-09	2.53E-09
$^{237}Np_2O_5$	1.57E-07	1.60E-07	1.61E-07	1.64E-07	1.65E-07	1.67E-07	1.68E-07	1.69E-07	1.70E-07
$^{231}Pa_2O_5$	3.23E-11	3.23E-11	3.23E-11	3.23E-11	3.23E-11	3.22E-11	3.22E-11	3.22E-11	3.22E-11
$^{238}PuO_2$	5.99E-12	6.10E-12	6.15E-12	6.23E-12	6.26E-12	6.33E-12	6.37E-12	6.39E-12	6.43E-12
$^{239}PuO_2$	1.13E-08	1.15E-08	1.15E-08	1.17E-08	1.18E-08	1.19E-08	1.19E-08	1.20E-08	1.21E-08
$^{240}PuO_2$	6.38E-10	6.50E-10	6.55E-10	6.63E-10	6.67E-10	6.74E-10	6.78E-10	6.81E-10	6.85E-10
$^{241}PuO_2$	1.27E-11	1.30E-11	1.31E-11	1.33E-11	1.33E-11	1.35E-11	1.36E-11	1.36E-11	1.37E-11
$^{242}PuO_2$	4.19E-12	4.27E-12	4.30E-12	4.36E-12	4.38E-12	4.43E-12	4.46E-12	4.48E-12	4.51E-12
^{226}RaO	5.69E-14	5.70E-14	5.70E-14	5.70E-14	5.71E-14	5.71E-14	5.71E-14	5.71E-14	5.72E-14
^{228}RaO	1.90E-13	1.89E-13	1.89E-13	1.88E-13	1.88E-13	1.87E-13	1.87E-13	1.86E-13	1.86E-13
$^{125}Sb_2O_5$	1.02E-11	1.01E-11	1.01E-11	1.01E-11	1.01E-11	1.00E-11	1.00E-11	1.00E-11	1.00E-11
$^{79}SeO_2$	1.28E-08	1.29E-08	1.29E-08	1.29E-08	1.29E-08	1.29E-08	1.29E-08	1.30E-08	1.30E-08
$^{151}Sm_2O_3$	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07
$^{126}SnO_2$	7.15E-08	7.16E-08	7.16E-08	7.16E-08	7.16E-08	7.16E-08	7.17E-08	7.17E-08	7.17E-08
^{90}SrO	4.37E-09	4.45E-09	4.48E-09	4.54E-09	4.57E-09	4.61E-09	4.64E-09	4.66E-09	4.69E-09
$^{99}TcO_2$	3.58E-06	3.57E-06	3.57E-06	3.56E-06	3.56E-06	3.55E-06	3.55E-06	3.55E-06	3.54E-06
$^{229}ThO_2$	1.09E-11	1.08E-11	1.08E-11	1.07E-11	1.07E-11	1.07E-11	1.07E-11	1.07E-11	1.06E-11
$^{232}ThO_2$	1.12E-04	1.11E-04	1.11E-04	1.11E-04	1.10E-04	1.10E-04	1.10E-04	1.10E-04	1.10E-04
$^{232}U_3O_8$	5.92E-13	5.89E-13	5.88E-13	5.85E-13	5.84E-13	5.83E-13	5.81E-13	5.81E-13	5.80E-13
$^{233}U_3O_8$	5.92E-09	5.89E-09	5.88E-09	5.85E-09	5.84E-09	5.83E-09	5.82E-09	5.81E-09	5.80E-09
$^{234}U_3O_8$	7.44E-09	7.51E-09	7.54E-09	7.60E-09	7.63E-09	7.67E-09	7.70E-09	7.71E-09	7.74E-09
$^{235}U_3O_8$	8.61E-07	8.69E-07	8.73E-07	8.79E-07	8.81E-07	8.86E-07	8.89E-07	8.91E-07	8.94E-07
$^{236}U_3O_8$	4.06E-08	4.12E-08	4.14E-08	4.19E-08	4.21E-08	4.24E-08	4.26E-08	4.28E-08	4.30E-08
$^{238}U_3O_8$	1.12E-04	1.13E-04	1.14E-04	1.14E-04	1.15E-04	1.15E-04	1.16E-04	1.16E-04	1.16E-04
$^{93}ZrO_2$	3.11E-06	3.11E-06	3.11E-06	3.11E-06	3.10E-06	3.10E-06	3.10E-06	3.10E-06	3.10E-06
Total	2.32E-04	2.32E-04	2.33E-04	2.33E-04	2.33E-04	2.33E-04	2.34E-04	2.34E-04	2.34E-04

Table J.2. Mass Fractions (g_{iq}^{MFPV}) of Radionuclide Composition Components (Oxides) over 25 ILAW MFPV Batches (Vienna 2004b) Corresponding to LAW Tank AP-101 (cont.)

Radio-nuclide Comp. q	ILAW Radionuclide Component Mass Fractions by ILAW MFPV Batch Number i = 10 to 18								
	10	11	12	13	14	15	16	17	18
$^{227}Ac_2O_3$	5.78E-15	5.76E-15	5.76E-15	5.76E-15	5.75E-15	5.75E-15	5.75E-15	5.74E-15	5.74E-15
$^{241}Am_2O_3$	6.78E-11	6.79E-11	6.79E-11	6.80E-11	6.80E-11	6.80E-11	6.80E-11	6.80E-11	6.81E-11
$^{243}Am_2O_3$	6.27E-14	6.29E-14	6.29E-14	6.30E-14	6.30E-14	6.30E-14	6.30E-14	6.30E-14	6.31E-14
^{113}CdO	8.23E-11	8.23E-11	8.23E-11	8.22E-11	8.22E-11	8.21E-11	8.21E-11	8.21E-11	8.20E-11
$^{243}Cm_2O_3$	5.00E-16	5.00E-16	5.00E-16	5.01E-16	5.01E-16	5.01E-16	5.02E-16	5.02E-16	5.02E-16
$^{244}Cm_2O_3$	5.54E-14	5.57E-14	5.59E-14	5.61E-14	5.61E-14	5.62E-14	5.63E-14	5.63E-14	5.66E-14
^{60}CoO	1.79E-12	1.79E-12	1.79E-12	1.79E-12	1.79E-12	1.79E-12	1.79E-12	1.79E-12	1.79E-12
$^{134}Cs_2O$	2.14E-16	2.14E-16	2.14E-16	2.14E-16	2.15E-16	2.15E-16	2.15E-16	2.15E-16	2.15E-16
$^{137}Cs_2O$	7.93E-11	7.92E-11	7.91E-11	7.91E-11	7.90E-11	7.90E-11	7.89E-11	7.89E-11	7.88E-11
$^{152}Eu_2O_3$	9.00E-12	9.00E-12	9.00E-12	9.00E-12	9.00E-12	9.00E-12	9.00E-12	9.00E-12	9.00E-12
$^{154}Eu_2O_3$	7.69E-11	7.74E-11	7.76E-11	7.79E-11	7.80E-11	7.81E-11	7.82E-11	7.82E-11	7.86E-11
$^{155}Eu_2O_3$	2.17E-11	2.19E-11	2.19E-11	2.20E-11	2.20E-11	2.21E-11	2.21E-11	2.21E-11	2.22E-11
^{129}I	2.67E-07	2.67E-07	2.67E-07	2.66E-07	2.66E-07	2.66E-07	2.66E-07	2.66E-07	2.66E-07
$^{93}Nb_2O_5$	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11
^{59}NiO	2.03E-08	2.05E-08	2.05E-08	2.06E-08	2.06E-08	2.06E-08	2.06E-08	2.06E-08	2.07E-08
^{63}NiO	2.54E-09	2.55E-09	2.55E-09	2.56E-09	2.57E-09	2.57E-09	2.57E-09	2.57E-09	2.58E-09
$^{237}Np_2O_5$	1.70E-07	1.71E-07	1.72E-07	1.72E-07	1.73E-07	1.73E-07	1.73E-07	1.73E-07	1.74E-07
$^{231}Pa_2O_5$	3.22E-11	3.22E-11	3.22E-11	3.22E-11	3.22E-11	3.22E-11	3.21E-11	3.21E-11	3.21E-11
$^{238}PuO_2$	6.45E-12	6.48E-12	6.50E-12	6.52E-12	6.53E-12	6.54E-12	6.55E-12	6.55E-12	6.58E-12
$^{239}PuO_2$	1.21E-08	1.22E-08	1.22E-08	1.22E-08	1.22E-08	1.23E-08	1.23E-08	1.23E-08	1.23E-08
$^{240}PuO_2$	6.87E-10	6.91E-10	6.92E-10	6.95E-10	6.96E-10	6.96E-10	6.97E-10	6.98E-10	7.01E-10
$^{241}PuO_2$	1.37E-11	1.38E-11	1.39E-11	1.39E-11	1.39E-11	1.39E-11	1.40E-11	1.40E-11	1.40E-11
$^{242}PuO_2$	4.52E-12	4.55E-12	4.56E-12	4.57E-12	4.58E-12	4.58E-12	4.59E-12	4.59E-12	4.62E-12
^{226}RaO	5.72E-14	5.72E-14	5.72E-14	5.72E-14	5.72E-14	5.72E-14	5.72E-14	5.72E-14	5.72E-14
^{228}RaO	1.86E-13	1.86E-13	1.86E-13	1.85E-13	1.85E-13	1.85E-13	1.85E-13	1.85E-13	1.85E-13
$^{125}Sb_2O_5$	9.99E-12	9.97E-12	9.97E-12	9.95E-12	9.95E-12	9.94E-12	9.94E-12	9.94E-12	9.92E-12
$^{79}SeO_2$	1.30E-08	1.30E-08	1.30E-08	1.30E-08	1.30E-08	1.30E-08	1.30E-08	1.30E-08	1.30E-08
$^{151}Sm_2O_3$	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07
$^{126}SnO_2$	7.17E-08	7.17E-08	7.17E-08	7.17E-08	7.17E-08	7.17E-08	7.17E-08	7.17E-08	7.17E-08
^{90}SrO	4.70E-09	4.73E-09	4.74E-09	4.76E-09	4.76E-09	4.77E-09	4.77E-09	4.78E-09	4.80E-09
$^{99}TcO_2$	3.54E-06	3.54E-06	3.54E-06	3.53E-06	3.53E-06	3.53E-06	3.53E-06	3.53E-06	3.53E-06
$^{229}ThO_2$	1.06E-11	1.06E-11	1.06E-11	1.06E-11	1.06E-11	1.06E-11	1.06E-11	1.06E-11	1.06E-11
$^{232}ThO_2$	1.10E-04	1.09E-04	1.09E-04	1.09E-04	1.09E-04	1.09E-04	1.09E-04	1.09E-04	1.09E-04
$^{232}U_3O_8$	5.79E-13	5.78E-13	5.78E-13	5.77E-13	5.77E-13	5.76E-13	5.76E-13	5.76E-13	5.75E-13
$^{233}U_3O_8$	5.79E-09	5.78E-09	5.78E-09	5.77E-09	5.77E-09	5.76E-09	5.76E-09	5.76E-09	5.75E-09
$^{234}U_3O_8$	7.75E-09	7.78E-09	7.79E-09	7.81E-09	7.81E-09	7.82E-09	7.82E-09	7.82E-09	7.85E-09
$^{235}U_3O_8$	8.95E-07	8.98E-07	8.99E-07	9.01E-07	9.02E-07	9.02E-07	9.03E-07	9.03E-07	9.05E-07
$^{236}U_3O_8$	4.31E-08	4.33E-08	4.34E-08	4.35E-08	4.35E-08	4.35E-08	4.36E-08	4.36E-08	4.38E-08
$^{238}U_3O_8$	1.17E-04	1.17E-04	1.17E-04	1.17E-04	1.17E-04	1.17E-04	1.17E-04	1.17E-04	1.18E-04
$^{93}ZrO_2$	3.10E-06	3.10E-06	3.10E-06	3.10E-06	3.10E-06	3.10E-06	3.10E-06	3.10E-06	3.10E-06
Total	2.35E-04	2.34E-04	2.34E-04	2.34E-04	2.34E-04	2.34E-04	2.34E-04	2.34E-04	2.35E-04

Table J.2. Mass Fractions (g_{iq}^{MFPV}) of Radionuclide Composition Components (Oxides) over 25 ILAW MFPV Batches (Vienna 2004b) Corresponding to LAW Tank AP-101 (cont.)

Radio-nuclide Comp. *q*	ILAW Radionuclide Component Mass Fractions by ILAW MFPV Batch Number *i* = 19 to 25						
	19	**20**	**21**	**22**	**23**	**24**	**25**
$^{227}Ac_2O_3$	5.73E-15	5.69E-15	5.67E-15	5.65E-15	5.64E-15	5.62E-15	5.61E-15
$^{241}Am_2O_3$	6.81E-11	6.85E-11	6.87E-11	6.89E-11	6.91E-11	6.92E-11	6.94E-11
$^{243}Am_2O_3$	6.32E-14	6.36E-14	6.38E-14	6.41E-14	6.43E-14	6.44E-14	6.46E-14
^{113}CdO	8.20E-11	8.18E-11	8.17E-11	8.15E-11	8.14E-11	8.14E-11	8.12E-11
$^{243}Cm_2O_3$	5.02E-16	5.02E-16	5.02E-16	5.02E-16	4.88E-16	4.88E-16	4.87E-16
$^{244}Cm_2O_3$	5.67E-14	5.79E-14	5.84E-14	5.91E-14	5.97E-14	6.00E-14	6.06E-14
^{60}CoO	1.80E-12	1.80E-12	1.81E-12	1.81E-12	1.82E-12	1.82E-12	1.82E-12
$^{134}Cs_2O$	2.15E-16	2.15E-16	2.07E-16	2.07E-16	2.07E-16	2.07E-16	2.07E-16
$^{137}Cs_2O$	7.88E-11	7.84E-11	7.82E-11	7.80E-11	7.79E-11	7.78E-11	7.76E-11
$^{152}Eu_2O_3$	9.00E-12	8.99E-12	8.99E-12	8.99E-12	9.00E-12	9.00E-12	8.99E-12
$^{154}Eu_2O_3$	7.88E-11	8.07E-11	8.15E-11	8.25E-11	8.34E-11	8.38E-11	8.47E-11
$^{155}Eu_2O_3$	2.23E-11	2.28E-11	2.30E-11	2.33E-11	2.36E-11	2.37E-11	2.40E-11
^{129}I	2.66E-07	2.65E-07	2.65E-07	2.64E-07	2.64E-07	2.64E-07	2.63E-07
$^{93}Nb_2O_5$	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11	2.85E-11
^{59}NiO	2.08E-08	2.12E-08	2.14E-08	2.16E-08	2.18E-08	2.19E-08	2.21E-08
^{63}NiO	2.59E-09	2.64E-09	2.66E-09	2.69E-09	2.72E-09	2.73E-09	2.75E-09
$^{237}Np_2O_5$	1.74E-07	1.79E-07	1.80E-07	1.83E-07	1.85E-07	1.86E-07	1.88E-07
$^{231}Pa_2O_5$	3.21E-11	3.21E-11	3.21E-11	3.20E-11	3.20E-11	3.20E-11	3.20E-11
$^{238}PuO_2$	6.59E-12	6.74E-12	6.80E-12	6.88E-12	6.95E-12	6.98E-12	7.05E-12
$^{239}PuO_2$	1.24E-08	1.26E-08	1.27E-08	1.29E-08	1.30E-08	1.31E-08	1.32E-08
$^{240}PuO_2$	7.02E-10	7.18E-10	7.25E-10	7.33E-10	7.41E-10	7.44E-10	7.52E-10
$^{241}PuO_2$	1.41E-11	1.44E-11	1.45E-11	1.47E-11	1.48E-11	1.49E-11	1.51E-11
$^{242}PuO_2$	4.63E-12	4.73E-12	4.78E-12	4.83E-12	4.89E-12	4.91E-12	4.96E-12
^{226}RaO	5.72E-14	5.73E-14	5.74E-14	5.74E-14	5.75E-14	5.75E-14	5.75E-14
^{228}RaO	1.85E-13	1.83E-13	1.83E-13	1.82E-13	1.81E-13	1.81E-13	1.80E-13
$^{125}Sb_2O_5$	9.92E-12	9.85E-12	9.82E-12	9.79E-12	9.76E-12	9.75E-12	9.72E-12
$^{79}SeO_2$	1.30E-08	1.30E-08	1.31E-08	1.31E-08	1.31E-08	1.31E-08	1.31E-08
$^{151}Sm_2O_3$	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07	1.65E-07
$^{126}SnO_2$	7.17E-08	7.17E-08	7.17E-08	7.18E-08	7.18E-08	7.18E-08	7.18E-08
^{90}SrO	4.81E-09	4.91E-09	4.96E-09	5.02E-09	5.07E-09	5.09E-09	5.14E-09
$^{99}TcO_2$	3.53E-06	3.51E-06	3.51E-06	3.50E-06	3.50E-06	3.49E-06	3.49E-06
$^{229}ThO_2$	1.05E-11	1.05E-11	1.04E-11	1.04E-11	1.04E-11	1.04E-11	1.03E-11
$^{232}ThO_2$	1.09E-04	1.08E-04	1.08E-04	1.07E-04	1.07E-04	1.07E-04	1.06E-04
$^{232}U_3O_8$	5.75E-13	5.71E-13	5.69E-13	5.67E-13	5.65E-13	5.64E-13	5.62E-13
$^{233}U_3O_8$	5.75E-09	5.71E-09	5.69E-09	5.67E-09	5.65E-09	5.64E-09	5.62E-09
$^{234}U_3O_8$	7.85E-09	7.96E-09	8.00E-09	8.06E-09	8.11E-09	8.13E-09	8.18E-09
$^{235}U_3O_8$	9.06E-07	9.17E-07	9.22E-07	9.28E-07	9.33E-07	9.36E-07	9.41E-07
$^{236}U_3O_8$	4.38E-08	4.46E-08	4.50E-08	4.54E-08	4.58E-08	4.59E-08	4.63E-08
$^{238}U_3O_8$	1.18E-04	1.19E-04	1.20E-04	1.21E-04	1.21E-04	1.22E-04	1.22E-04
$^{93}ZrO_2$	3.10E-06	3.10E-06	3.10E-06	3.09E-06	3.09E-06	3.09E-06	3.09E-06
Total	2.35E-04	2.35E-04	2.36E-04	2.36E-04	2.36E-04	2.37E-04	2.36E-04

Table J.3. Simulated Masses of Glass ($m_d^{Container}$, g) in the 41 ILAW Containers Corresponding to 25 ILAW MFPV Batches for an AP-101 LAW Waste Type

ILAW Container d	Mass of Glass (g)	ILAW Container d	Mass of Glass (g)
1	5.7930E+06	22	6.0074E+06
2	5.9159E+06	23	5.9476E+06
3	5.9939E+06	24	5.9760E+06
4	5.8558E+06	25	5.7968E+06
5	5.7636E+06	26	5.9635E+06
6	5.9858E+06	27	5.9066E+06
7	5.9125E+06	28	5.8836E+06
8	5.6761E+06	29	5.8816E+06
9	5.8682E+06	30	5.8755E+06
10	5.9478E+06	31	5.7821E+06
11	5.8231E+06	32	5.8391E+06
12	5.9318E+06	33	5.7994E+06
13	5.8061E+06	34	5.9893E+06
14	5.7871E+06	35	5.7801E+06
15	5.8118E+06	36	6.0322E+06
16	5.9733E+06	37	5.8240E+06
17	5.8980E+06	38	5.8485E+06
18	6.0546E+06	39	5.9841E+06
19	6.0554E+06	40	5.9664E+06
20	5.8940E+06	41	5.9944E+06
21	5.7712E+06	(a)	

(a) This cell of the table is intentionally blank.

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