PNWD-3099
WTP-RPT-013

X%/Y% Tolerance Interval Approach to Determine Sample Sizes and Demonstrate IHLW or ILAW Produced Over a Waste Type is Compliant with Chemical Durability Specifications

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Prepared for Bechtel National, Inc.
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Battelle, Pacific Northwest Division
Richland, Washington 99352

Completeness of Testing

This report describes the results of work and testing specified by Subtask 3 of Test Specification 24590-WTP-TSP-RT-01-002 and Test Plan 24590-WTP-TP-RT-01-003 (PNWD number TP-RPP-WTP-097). The work and any associated testing followed the quality assurance requirements outlined in the Test Specification/ 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
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G. Todd Wright, Manager — Date
Research and Technology

Summary

The River Protection Project—Waste Treatment Plant (RPP-WTP) will produce immobilized high-level waste (IHLW) and immobilized low-activity waste (ILAW) from Hanford tank wastes. The IHLW and ILAW must comply with specifications established in the contract governing the vitrification work (BNI 2001). IHLW must also comply with specifications in the Waste Acceptance Product Specifications (WAPS) developed by the Department of Energy (DOE 1996). The RPP-WTP Project strategies for complying with applicable IHLW and ILAW specifications are presented in the Waste Compliance Plan (WCP) (CHG 2001a) and the Products and Secondary Wastes Plan (PSWP) (CHG 2001b). Many of the RPP-WTP Project compliance strategies are statistical in nature, because sources of variation and uncertainty will be quantified and accounted for in demonstrating compliance with the specifications.

The RPP-WTP Project compliance strategies for IHLW and ILAW have both *process control* and *reporting* aspects. Process control aspects of the compliance strategies focus on making and controlling each process batch so it will yield compliant IHLW or ILAW. The reporting aspects of the compliance strategies focus on reporting and demonstrating IHLW or ILAW produced from a given HLW or LAW *waste type* (see **Definitions**, as well as additional discussions in the WCP and PSWP) is compliant. Thus, *process control* addresses each batch, whereas *reporting* addresses the glass produced over the course of a given waste type. This report presents and illustrates the details of a statistical approach for one aspect of the reporting compliance strategies, namely demonstrating that IHLW or ILAW produced over the course of a HLW or LAW waste type is compliant with chemical durability specifications. These specifications involve three chemical durability tests, namely the Product Consistency Test (PCT) for IHLW and ILAW, the Vapor Hydration Test (VHT) for ILAW, and the Toxicity Characteristic Leaching Procedure (TCLP) for IHLW and ILAW. The statistical approaches for process control aspects of the IHLW and ILAW compliance strategies, as well as the reporting aspects not considered in this report, will be addressed in future reports.

This report develops and illustrates statistical X%/Y% upper tolerance interval (X%/Y% UTI) formulas and related methods for calculating *sample sizes* (see **Definitions**) for use in demonstrating IHLW or ILAW produced from a given waste type is compliant with chemical durability specifications. In this report, an X%/Y% UTI has the general form

$$\text{X\%/Y\% UTI} = \tilde{\mu} + k\tilde{\sigma}\,, \tag{S.1}$$

where $\tilde{\mu}$ is an estimate of the mean release rate for glass produced from a waste type, $\tilde{\sigma}$ is an estimate of the variation of release rates for glass produced from a waste type, and k is an X%/Y% UTI multiplier. An X%/Y% UTI provides for stating with X% confidence that at least Y% of the IHLW or ILAW produced from a HLW or LAW waste type satisfies a chemical durability specification limit (e.g., an upper limit on the PCT boron release). Rather than selecting X and Y then calculating an X%/Y% UTI, the proposed approach is to calculate the values of X and Y that yield an X%/Y% UTI equal to a chemical durability specification limit. The resulting calculated X and Y values are thus the levels of compliance achieved over a waste

type. The RPP-WTP Project will have to select minimally acceptable values of X and Y; however, it is envisioned that values of X and Y greater than 95, 99, or even higher will be achieved.

The X%/Y% UTI formulas in this report were developed in a general manner to be applicable for demonstrating compliance with PCT, VHT, or TCLP specifications for either IHLW or ILAW produced from a given HLW or LAW waste type. The X%/Y% UTI approach directly addresses existing RPP-WTP Project reporting compliance strategies for PCT (IHLW and ILAW) and VHT (ILAW) as described in the WCP (CHG 2001a) and PSWP (CHG 2001b). The compliance strategy is still being developed for specifications involving TCLP, so it is not clear at this time whether an X%/Y% UTI approach will be needed. If so, the X%/Y% UTI formulas in this report will apply for TCLP as well as PCT and VHT.

Although the X%/Y% UTI formulas are generally applicable for PCT, VHT, or TCLP, X%/Y% UTI calculations must be performed in the release rate (or transformed release rate) units used in the model to predict PCT, VHT, or TCLP release rate as a function of glass composition. Calculations of X%/Y% UTIs in this report assume the natural logarithm of release rate is modeled, which is the case for preliminary PCT and TCLP models developed at the Vitreous State Laboratory (Gan and Pegg 2001a, Gan and Pegg 2001b). X%/Y% UTI calculations for release models using other transformations (e.g., VHT or other PCT or TCLP models) can be performed in the future as the release models are developed further.

X%/Y% UTI formulas are developed and presented in this report for the general situation in which:

- samples (glass samples or vitrified process samples) are collected at $n > 1$ times over the course of a waste type, $m \geq 1$ samples are collected at each time, and $r \geq 1$ chemical analyses are performed on each sample

- the resulting analyzed glass compositions (possibly adjusted and renormalized to address biases and reduce imprecision) are substituted into release-composition models to obtain predicted release rates[a]

- the resulting $N = n \cdot m \cdot r$ predicted release rates are then used to calculate the X%/Y% UTI.

In addition to variation in release rates due to variation in glass composition over a waste type, the predicted release rates will be subject to sampling, analytical, and model prediction uncertainties. These three uncertainties are referred to as *nuisance uncertainties*, because they inflate the source of variation of interest (variation in true release rates over a waste type). The nuisance uncertainties inflate the magnitudes of X%/Y% UTIs, so methods to reduce and adjust for nuisance uncertainties were investigated. A no-adjustment method was also investigated for

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[a] If release rates are mathematically transformed to develop release-composition models, the predicted values will be in the transformed units. For example, PCT models often relate the natural logarithm of release (in g/m^2) to glass composition, so that predicted values have units of $\ln(g/m^2)$. In such a case, an X%/Y% UTI would also be calculated in the transformed $\ln(g/m^2)$ units. However, the inverse transformation can always be applied to obtain predicted values or the X%/Y% UTI in the original units.

comparison purposes. The following specific approaches were investigated:

- No reduction or adjustment for nuisance uncertainties ($m = 1$, $r = 1$)
- Reduction (by averaging) but no adjustment for nuisance uncertainties ($m > 1$ and/or $r > 1$)
- Reduction (by averaging) and adjustment for nuisance uncertainties ($m > 1$ and/or $r > 1$)
- Reduction (if $m > 1$ and/or $r > 1$) and adjustment for nuisance uncertainties, as well as removing (subtracting) the reduced sampling and/or analytical uncertainties using one of two removal methods.

The first removal method subtracts estimates of sampling and analytical uncertainties obtained from production data, whereas the second method subtracts estimates obtained during qualification activities. However, the removal methods were found not to reduce X%/Y% UTIs. Hence, the work focused on the approaches in the first three bullets above.

The magnitude of an X%/Y% UTI depends on the mean predicted release rate (or transformed release rate) over glass produced from an HLW or LAW waste type ($\tilde{\mu}$ in (S.1)), as well as the UTI half-width (UTIHW) that accounts for the sources of variation and uncertainty ($k\tilde{\sigma}$ in (S.1)). The UTIHW depends on many input parameters, including:

- values of n, m, and r
- magnitude of the variation in release rates over a waste type, expressed in release rate units[a] ($\hat{\sigma}_g$)
- magnitudes of sampling and analytical uncertainties, expressed in release rate units[a] ($\hat{\sigma}_s$ and $\hat{\sigma}_a$)
- degrees of freedom associated with a release-composition model (df_m)
- magnitude of the average model prediction uncertainty for a given sampling time, expressed in release rate units[a] ($\bar{\hat{\sigma}}_m$)
- values of X (percent confidence) and Y (percent of glass from a waste type in compliance)
- the reduction and adjustment methods used.

The magnitudes of the sources of variation and uncertainty are not known at this time. However, one objective of this work was to provide a basis for the RPP-WTP Project to decide on the values of n, m, r, and df_m. This report presents the results of X%/Y% UTIHW calculations for combinations of appropriate values for the input parameters. Knowledge of the expected PCT performance (for IHLW or ILAW) or VHT performance (for ILAW) will indicate how small UTIHWs must be to demonstrate compliance. This indication will in turn provide a basis for the RPP-WTP Project to decide what values of n, m, r, and df_m will be required, after estimates of $\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$ applicable for each IHLW or ILAW waste type are developed.

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[a] If a model is developed for a mathematical transformation of release rate, then $\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$ are expressed in transformed release rate units.

The X%/Y% UTIHW = $k\tilde{\sigma}$ calculations performed for various combinations of input parameters provide for making the following preliminary conclusions:

- Over the ranges of the parameters studied, those with the most influence on the magnitudes of adjusted X%/Y% UTIHWs are $\hat{\sigma}_g >> n >> \hat{\sigma}_a > m > r > df_m$. The parameters with the least influence are $\hat{\sigma}_s$ and $\bar{\hat{\sigma}}_m$. The parameters with the most influence on the magnitudes of unadjusted X%/Y% UTIHWs are $\hat{\sigma}_g >> \bar{\hat{\sigma}}_m > n > \hat{\sigma}_a > m > r > df_m$, with only $\hat{\sigma}_s$ having little influence. The parameter $\bar{\hat{\sigma}}_m$ impacts the results more for unadjusted than adjusted X%/Y% UTIHWs because the nuisance uncertainties are not adjusted for in the former approach.

- Sampling and analytical uncertainties, and thus X%/Y% UTIHWs, are reduced by averaging model-predicted release rates (or transformed release rates) over $m > 1$ replicate samples at each sampling time and $r > 1$ replicate analyses of each sample. However, sufficient reduction may occur with $m > 1$ and $r = 1$, because taking $m > 1$ samples provides for reducing both sampling and analytical uncertainties via averaging. It may even be possible to demonstrate compliance without reducing sampling and analytical uncertainties, in which case choosing $m = 1$ and $r = 1$ would be allowable. The following chart summarizes the minimum and maximum percentage reductions in X%/Y% UTIHWs obtained in calculations for the reduction cases: (i) $m = 1$, $r = 3$, (ii) $m = 3$, $r = 1$, and (iii) $m = 3$, $r = 3$ compared to the no-reduction case $m = 1$, $r = 1$.

Minimum and Maximum Percentage Reductions in Unadjusted and Adjusted X%/Y% UTIHWs for *m* > 1 and/or *r* > 1 Compared to *m* = 1 and *r* = 1					
		Unadjusted for Nuisance Uncertainties		**Adjusted for Nuisance Uncertainties**	
m	***r***	**Min %**	**Max %**	**Min %**	**Max %**
1	3	0.19	37.4	-0.08	23.0
3	1	0.38	38.0	-0.21	23.5
3	3	0.45	55.4	-0.26	35.0

  The chart shows that having $m > 1$ and/or $r > 1$ can reduce unadjusted X%/Y% UTIHWs by up to 55%, and adjusted X%/Y% UTIHWs by up to 35%. In a few cases when $m > 1$ and/or $r > 1$, adjusted X%/Y% UTIHWs can be slightly larger than when $m = 1$ and $r = 1$ (indicated by the negative minimum percentage reduction values). In almost all cases, however, choosing $m > 1$ and/or $r > 1$ reduces adjusted X%/Y% UTIHWs.

- Adjusting the k multiplier for nuisance uncertainties reduces UTIHWs, with the amount of reduction increasing as the magnitudes of nuisance uncertainties increase. After first reducing sampling and analytical uncertainties where possible, adjusting for nuisance uncertainties resulted in 6% to 76% reductions in both 95%/95% and 99%/99% UTIHWs over the combinations of input parameters considered.

- Removing (subtracting) sampling and analytical uncertainties increases UTIHWs, because the reduction in $\tilde{\sigma}$ is less than the increase in k due to an associated penalty. Hence, removing (subtracting) sampling and/or analytical uncertainties is not recommended.

- The X%/Y% UTIHW values calculated for combinations of input parameters can be viewed as multiples k^* of σ_g rather than as multiples k of $\tilde{\sigma}$. Here, σ_g denotes the true variation in release rates for glass produced from a waste type, whereas $\tilde{\sigma}$ denotes an estimate of σ_g inflated by nuisance uncertainties (so that $\tilde{\sigma} > \sigma_g$). The k^* values range from 2.04 to 5.40 for X%/Y% = 95%/95% and from 3.00 to 8.05 for X%/Y% = 99%/99%, when reducing (if possible) and adjusting for nuisance uncertainties. These results indicate "two standard deviations" may provide 95%/95% protection at best, and potentially much worse protection. Hence, the "two standard deviations" compliance suggestion included in WAPS 1.3 (DOE 1996) could lead to indefensible values of the percent confidence (X) or the percent of glass produced from a waste type (Y) satisfying the specification. The X%/Y% UTI approach in this report provides for obtaining defensible values of X and Y.

In summary, we recommend an X%/Y% UTI approach for demonstrating compliance over a waste type that: (i) reduces sampling and analytical nuisance uncertainties by averaging over $m > 1$ replicate samples at each sampling time and/or $r > 1$ replicate chemical analyses per sample, and (ii) adjusts the k multiplier for nuisance uncertainties regardless of whether it is possible ($m > 1$ and/or $r > 1$) or not possible ($m = 1$ and $r = 1$) to reduce nuisance uncertainties by averaging. The details of the methods to implement these recommendations are provided in this report.

A simulated example was constructed to illustrate using the X%/Y% UTI formulas to demonstrate compliance with the WAPS 1.3 specification (on PCT releases) for IHLW. The example used $n = 10$ samples over the waste type, $m = 2$ samples per sampling time, and $r = 2$ chemical analyses per sample. Averaging over duplicate samples and analyses reduced sampling and analytical nuisance uncertainties. Compared to the method that does not adjust for nuisance uncertainties, adjusting for the nuisance uncertainties (using the approach developed and presented in this report) reduced the X%/Y% UTI by 48.4% for the 95%/95% case and 28.8% for the 99%/99% case. The percent reduction is smaller for the 99%/99% UTI because it has a larger value. For this example, X and Y values over 99.9 were achieved, which indicates very high confidence that essentially all of the glass produced from the waste type would satisfy the specification limit. This example and the results of UTIHW calculations suggest that as few as 10-20 sampling times (during glass production from a given waste type) may be sufficient to demonstrate compliance when IHLW or ILAW release rates are much lower than specification limits.

The report also discusses future work needed to update and eventually finalize the X%/Y% UTI compliance strategy and corresponding numbers of sampling times (n), samples per sampling time (m), and chemical analyses per sample (r). This future work includes: deciding on minimum acceptable values of X and Y; estimating variation over each HLW and LAW waste type as well as sampling and analytical uncertainties; developing PCT-, VHT-, and TCLP-composition databases, models, and uncertainty expressions; and developing algorithms to detect bias, bias-correct, and normalize glass compositions to reduce inaccuracies (bias) and imprecision. Finally, because the X%/Y% UTI formulas developed in this report are new, a statistical simulation study must be performed as part of future work to verify that the formulas yield the claimed Y% content at least X% of the time. Ideally, the simulation study should simulate both property-composition model development data sets and models, as well as data such as will be obtained during RPP-WTP production of IHLW or ILAW over a waste type.

Acknowledgments

The work summarized in this report was performed as part of Subtask 3 of the work scope *Statistics for Waste Form Qualification*, with test plan 24590-WTP-TP-RT-01-003, Rev. 0 and test specification 24590-WTP-TSP-RT-01-002, Rev. 0.

The work is an adaptation and extension of work performed by G.F. Piepel, D.L. Eggett, and C.M. Anderson of Pacific Northwest National Laboratory from 1991 to1992 for West Valley Nuclear Services Co., Inc. That work was documented only in project reports that were not cleared for public release and reference. The work contained in this report is a substantial extension of the previous work for West Valley. The lists of **Acronyms and Abbreviations** and **Definitions** were adapted from CHG (2001a), with some additions and deletions.

The authors acknowledge and thank the following Battelle staff members for reviewing and providing comments on the draft report: Denny Weier (statistical review), Nancy Foote (editorial review), Dean Kurath (project chief scientist review), and Taffy Almeida and Barry Sachs (quality assurance reviews). We also gratefully acknowledge RPP-WTP Project review comments from the WTP Process Engineering group, Tommy Edwards (SRTC), and Kevin Brown (SRTC). We also thank Chrissy Charron (Battelle) for formatting and preparing the report.

Quality Assurance

The work and results in this report were performed according to requirements in the project QA plan (PNNL 2000) for IHLW work that must be compliant with QARD (DOE 1998) and ILAW work that must be compliant with NQA-1 (NQA-1, 1989) and NQA 2A part 2.7 (NQA-2A, 1990). The project QA plan calls for using procedures from the Nuclear Quality Assurance Requirements and Description (NQARD 2001), which comply with IHLW and ILAW requirements.

Acronyms and Abbreviations

ANOVA	Analysis of variance
ASTM	American Society for Testing and Materials
DOE	U.S. Department of Energy
DWPF	Defense Waste Processing Facility
EA	Environmental assessment
HLW	High-level waste
IHLW	Immobilized high-level waste
ILAW	Immobilized low-activity waste
LAW	Low-activity waste
MFPV	Melter feed preparation vessel
MFV	Melter feed vessel
MSE	Mean squared error
NQARD	*Nuclear Quality Assurance Requirements and Description* (NQARD 2001)
PCT	Product consistency test
PNNL	Pacific Northwest National Laboratory
PSWP	Products and Secondary Wastes Plan
QA	Quality Assurance
QARD	*Quality Assurance Requirements and Description for the Civilian Radioactive Waste Management Program* (DOE 1998)
RPP-WTP	River Protection Project-Waste Treatment Plant
RSD	Relative standard deviation
SD	Standard deviation
SRTC	Savannah River Technology Center
SUCI	Simultaneous upper confidence interval
TCLP	Toxicity Characteristic Leaching Procedure
UCI	Upper confidence interval
UTI	Upper tolerance interval
UTIHW	Upper tolerance interval half-width
VHT	Vapor Hydration Test
WAPS	*Waste Acceptance Product Specifications for Vitrified High-Level Waste Forms* (DOE 1996)
WFQ	Waste form qualification
WCP	Waste Form Compliance Plan
WQR	Waste Form Qualification Report

Notation

δ	Noncentrality parameter of the non-central t-distribution
df_m	Degrees of freedom associated with a property-composition model fitted by least squares regression
f	Degrees of freedom associated with $\tilde{\sigma}$
k	Multiplier used in a tolerance interval formula
$\tilde{\mu}$	Estimate of the mean release rate for IHLW or ILAW produced from a waste type
M	Number of data points used to fit a release-composition model
m	Number of process samples or glass samples collected at a specific sampling time over the course of glass production corresponding to a waste type
N	$N = n \cdot m \cdot r$, the total number of results from collecting samples at $n > 1$ times during a waste type, collecting $m \geq 1$ samples at each sampling time, and analyzing each sample $r \geq 1$ times
n	Number of sampling times or periods over the course of glass production corresponding to a waste type
r	Number of chemical analyses per sample
$\hat{\sigma}_g$	Estimate of the standard deviation associated with variation in release rates over the course of a waste type, due to variation in glass composition produced from a waste type
$\hat{\sigma}_s$	Estimate of the standard deviation associated with the variation in release rates due to sampling uncertainty
$\hat{\sigma}_a$	Estimate of the standard deviation associated with the variation in release rates due to analytical uncertainty
$\hat{\sigma}_m(\boldsymbol{x})$	Estimate of the standard deviation due to uncertainty in a model prediction for glass composition $\boldsymbol{x}$
$\bar{\hat{\sigma}}_m$	Estimate of the average standard deviation in model predictions for compositions resulting from replicate samples and replicate analyses of samples at a given sampling time
$\tilde{\sigma}$	Estimate of the standard deviation of release rates from IHLW or ILAW produced from a waste type, inflated by any nuisance uncertainties not subtracted

Definitions

Cold Commissioning	Activities conducted in the full-scale production facility prior to initiation of radioactive operations to verify configuration or function of integrated systems. Also known as cold startup.
Compliance Strategy	Concise description of the strategy for complying with one or more of the waste acceptance product specifications (WAPS) or contract specifications.
Hot Commissioning	Activities conducted in the full-scale production facility with initial radioactive feeds to verify configuration or function of integrated systems. Also known as hot startup.
Nuisance uncertainties	Uncertainties in addition to the variation in IHLW or ILAW produced from a HLW or LAW waste type, specifically: sampling, analytical, and model prediction uncertainties.
Process Control Strategy	The strategy for operating or controlling the HLW or LAW vitrification process during production operations, but distinctly separate from *compliance strategy*.
Production Operations	Activities in a vitrification facility to produce IHLW or ILAW.
Property-composition model	An equation for predicting a glass property (for example, PCT normalized boron release) as a function of glass composition.
Qualification Activities	Activities conducted in advance of Production Operations (through Hot Commissioning) that provide evidence supporting waste form qualification. Generally, the detailed methods and results of these activities are documented in the HLW waste form qualification report (WQR) and the ILAW Qualification Document (ILAW QD).
Sample Size	A generic term referring to the number of: sampling periods, samples per sampling period, chemical analyses per sample, measurements, etc. This term does not refer to the physical size of samples to be taken.
Uncertainty	Lack of knowledge about a true, fixed state of affairs (for example, analytical *uncertainty* in chemical analyses of any given glass sample). See also *Variation*.
Variation	Real changes in a variable over time or space (for example, *variation* in glass composition between and within waste types). See also *Uncertainty*.
Waste form	Radioactive waste materials in a borosilicate glass matrix.
Waste type	The waste material fed to each vitrification plant, the composition and properties of which remain relatively constant over an extended period of time during waste form production (DOE 1996).

X% Simultaneous Upper Confidence Interval (SUCI)	An X% SUCI provides X% confidence the true release rates for all model predictions are less than the corresponding X% SUCI values.
X% Upper Confidence Interval (UCI)	An X% UCI provides X% confidence the true mean release rate for glass produced from a waste type is less than the UCI.
X%/Y% Upper Tolerance Interval (UTI)	An X%/Y% UTI provides X% confidence that at least Y% of the glass produced from a waste type has release rates less than the UTI.

Contents

Tables

Figures

1.0 Introduction

The River Protection Project—Waste Treatment Plant (RPP-WTP) will convert high-level waste (HLW) and low-activity waste (LAW) stored in tanks at the Hanford site near Richland, Washington to solid, vitrified waste forms (borosilicate glass). The immobilized high-level waste (IHLW) and immobilized low-activity waste (ILAW) must comply with specifications established in the contract governing the vitrification work (BNI 2001). IHLW must also comply with specifications in the Waste Acceptance Product Specifications (WAPS) developed by the Department of Energy Office of Civilian Radioactive Waste Management (DOE 1996). The RPP-WTP Project strategies for complying with applicable IHLW and ILAW specifications are presented in the Waste Compliance Plan (WCP) (CHG 2001a) and the Products and Secondary Wastes Plan (PSWP) (CHG 2001b).

Several WAPS and contract specifications set upper limits on various properties of IHLW or ILAW. Specifications of this type addressed by the work in this report include:

- **WAPS 1.3**, which requires IHLW to have 7-day, 90°C Product Consistency Test (PCT) normalized elemental releases of B, Li, and Na less than the corresponding releases for the Defense Waste Processing Facility (DWPF) environmental assessment (EA) glass. The PCT is described in ASTM (1998). Jantzen et al. (1993) discuss the EA glass and its PCT releases. PCT normalized elemental releases for the EA glass, as reported in Table 6 of Jantzen et al. (1993), are 8.35 g/m^2 for B, 4.78 g/m^2 for Li, and 6.67 g/m^2 for Na.[a]

- **Contract specification 2.2.2.17.2**, which requires ILAW to have 7-day, 90°C PCT normalized elemental releases of B, Na, and Si less than 2.0 g/m^2.

- **Contract specification 2.2.2.17.3**, which requires ILAW to have 25-day, 200°C Vapor Hydration Test (VHT) releases less than 50 g/m^2/day. The VHT is discussed in Appendix A of CHG (2001b).

The RPP-WTP Project compliance strategy for each of these specifications has *process control* and *reporting* aspects. Process control aspects of the compliance strategies focus on controlling each process batch so it will yield compliant IHLW or ILAW. The reporting aspects of the compliance strategies focus on demonstrating IHLW or ILAW produced from a given HLW or LAW *waste type* (see **Definitions**, as well as additional discussions in the WCP and PSWP) is compliant. Thus, *process control* addresses each batch, whereas *reporting* addresses the glass produced over the course of a given waste type.

A common aspect of the RPP-WTP Project *reporting* compliance strategies for the preceding specifications is that a *statistical interval* approach will be used to demonstrate that immobilized waste produced from a given waste type has property values less than the specified upper limit. The RPP-WTP Project chose to use the general term *statistical interval* in the WCP

[a] Jantzen et al. (1993) provide PCT normalized elemental releases from the 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 rounded to two decimal places.

and PSWP because the waste form qualification (WFQ) work to select and develop the specific type of statistical intervals for specific compliance situations had not yet been performed. Still, the general term was chosen to indicate that variations and uncertainties will be addressed in the compliance strategies.

The RPP-WTP Project strategies for complying with delisting requirements and land disposal restrictions are still being developed. Upper limits on Toxicity Characteristic Leaching Procedure (TCLP) results may need to be satisfied, and statistical interval approaches would be applicable if included as part of reporting strategies to demonstrate IHLW or ILAW produced from a waste type is compliant.

The RPP-WTP Project compliance strategies for other specifications with lower or upper limits on glass properties or characteristics also call for statistical interval approaches (see the WCP and PSWP for additional discussion). The specification numbers for IHLW and ILAW follow, with a brief description given in parentheses for each specification:

- IHLW—WAPS 3.8.2 (heat generation rate), WAPS 3.9.2 (gamma and neutron dose rates)
- ILAW—Contract Specification 2.2.2.2 (waste loading)

However, the type or implementation of statistical interval appropriate for these specifications could be different than the statistical tolerance interval approach presented in this report for chemical durability specifications. For example, methods to calculate heat generation rate or dose rate will be different than methods to model and predict chemical durability. Hence, these other specifications must be addressed in separate, future reports.

Still other specifications prescribe lower or upper limits for a property or characteristic of IHLW or ILAW, for which the RPP-WTP Project compliance strategies do not include a statistical interval approach. For such specifications, the IHLW and ILAW are expected to easily meet the prescribed lower or upper limit. In such cases, statistical methods and intervals are not necessary, because variations and uncertainties are expected to be much smaller than the difference between waste form property or characteristic values and specification-prescribed limits.

The WCP and PSWP compliance strategies for the PCT and VHT chemical durability specifications do not definitively specify the type of statistical interval approach to be used to demonstrate IHLW or ILAW produced from a given HLW or LAW waste is compliant. A *statistical tolerance interval* approach has been chosen as defensible and appropriate for demonstrating compliance for IHLW or ILAW produced from a waste type.[a] A statistical *X%/Y% upper tolerance interval* (X%/Y% UTI) allows stating with high confidence (X%) that at least some high percentage (Y%) of a distribution is less than an upper limit. Hence, an X%/Y% UTI is well suited to demonstrating the immobilized waste (IHLW or ILAW) produced from a given *waste type* (HLW or LAW) has chemical releases less than the upper limit provided in a specification. This report: (1) develops and presents X%/Y% UTI tolerance interval formulas, (2) uses the formulas to investigate the consequences of different parameters affecting the size of

[a] See Section 1.2 for a discussion of why a statistical tolerance interval is defensible and appropriate for demonstrating compliance for glass produced from a waste type.

the X%/Y% UTIs, and (3) illustrates using the X%/Y% UTI formulas with a simulated data set to demonstrate compliance with the WAPS 1.3 specification for IHLW produced from a waste type.

In the balance of this introductory section, Section 1.1 presents and discusses the IHLW and ILAW chemical durability (PCT and VHT) specifications. Section 1.2 summarizes the RPP-WTP Project compliance strategies for these specifications. Section 1.3 elaborates on the objectives of the work and results included in this report.

In the balance of the report, Section 2 defines and discusses several aspects of statistical tolerance intervals. Section 3 develops and presents the formulas for calculating X%/Y% UTIs for the PCT and VHT release situations addressed in this report. Section 4 presents the results of applying the X%/Y% UTI formulas for many combinations of input parameters to provide guidance to the RPP-WTP Project on answering questions about sample sizes, precision, and other issues. However, the input parameter values used for the calculations in Section 4 assume that the natural logarithm of release is modeled as a function of glass composition. Preliminary models for PCT (IHLW and ILAW) and TCLP (IHLW) are in terms of ln(release), while preliminary models for VHT (ILAW) utilize a different transformation of release (Gan and Pegg 2001a, Gan and Pegg 2001b). Section 5 illustrates the application of the X%/Y% UTI formulas to a simulated data set meant to represent PCT releases of IHLW over the course of a waste type. Section 6 discusses work and results that must be conducted during qualification activities to provide future required inputs for applying the X%/Y% UTI method to demonstrate PCT and VHT compliance during IHLW and ILAW production operations.

1.1 IHLW and ILAW Chemical Durability Specifications

The chemical durability specification for IHLW is WAPS 1.3, *Specification for Product Consistency*. This specification is copied verbatim from the WAPS (DOE 1996), and shown in italics following.

1.3 Specification for 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..*

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.

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.

There are two chemical durability specifications for ILAW, namely contract specifications 2.2.2.17.2, *Product Consistency Test*, and 2.2.2.17.3, *Vapor Hydration Test*. These specifications are copied verbatim from the contract (BNI 2001), and are shown in italics as follows.

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 PCT 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 PCT shall be conducted on waste form samples that are statistically representative of the production glass.

2.2.2.17.3 Vapor Hydration Test (VHT)

The glass corrosion rate shall be measured using a 25 day VHT run at 200°C as defined in the DOE concurred upon Products and Secondary Waste 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 VHT shall be conducted on waste form samples that are statistically representative of the production glass.

Several aspects of the two ILAW chemical durability specifications and the IHLW specification are discussed in the following subsections. Discussion of Piepel and Mellinger (1990) on some aspects of a previous version of WAPS 1.3 forms the basis for parts of the following discussion.

1.1.1 Qualification versus Production Operations

None of the IHLW or ILAW chemical durability specifications are explicit about what is required for compliance as part of *qualification activities* (see **Definitions**) versus what is required as part of *production operations* (see **Definitions**). However, it is generally assumed that qualification activities are required by all the specifications. Less clear is to what extent each specification requires process control activities during production in addition to reporting during or after production. It is generally assumed that a compliance strategy must have both *process control* and *reporting* aspects. These issues are being addressed by the RPP-WTP Project, and are not discussed further in this report. The focus of this report is on one aspect of the reporting compliance strategy for chemical durability specifications on IHLW and ILAW. Statistical approaches for qualification or process control aspects of the compliance strategies for chemical durability specifications will be addressed in future, separate reports.

1.1.2 Quenched versus Representative-Cooled Samples

The ILAW specifications require qualification testing of glass samples subjected to representative waste form cooling curves, whereas the IHLW specification does not mention such qualification testing. Still, it is safe to assume that some qualification testing of representatively cooled IHLW compositions are required. Also, although not explicitly stated in the IHLW or ILAW specifications, it is generally assumed the specifications minimally require qualification testing of air-quenched glass samples. The specifications do not address whether chemical releases reported during production must be based on air-quenched glass, representatively cooled glass, or both. The methods developed in this report will apply to either situation, so this issue is not discussed further.

1.1.3 Benchmark Glass versus Specified Limits

The IHLW chemical durability specification ties the acceptance criterion to the DWPF EA benchmark glass (Jantzen et al. 1993), so that different upper limits apply for B, Li, and Na normalized releases from the PCT. The ILAW chemical durability specifications set specific numeric limits for both the PCT and VHT. Hence, the same upper limit applies for B, Na, and Si PCT normalized releases from ILAW. Normalized elemental releases of B, Li, Na, and to a lesser extent Si, are typically highly correlated, although not necessarily with a slope of one. Hence, having either the same or different upper limits for the various normalized elemental releases from the PCT can result in more or less restrictive constraints for the various normalized elemental releases. The methods discussed in this report are independent of the limit to be satisfied. Hence, the natures of the PCT and VHT limits to be achieved do not impact the work.

1.1.4 Process versus Product Samples as Basis for Compliance During Production

The IHLW chemical durability specification clearly allows for compliance during production to be based on either process samples or product samples. The ILAW specifications are less clear, and could be interpreted to mean that only product samples are an acceptable basis for demonstrating compliance. However, the phrase "*waste form samples that are statistically representative of the production glass*" in Specs. 2.2.2.17.2 and 2.2.2.17.3 could be interpreted as allowing compliance to be based on process samples, as long as they are shown to be statistically representative of the production glass. The work in this report applies whether the data to implement the reporting aspects of the strategy are from process or product samples, so this issue is not addressed further.

1.1.5 Measured versus Predicted Basis for Compliance

The IHLW chemical durability specification allows for demonstrating compliance by measured or predicted PCT results. The term *predicted* rather than *projected* is used in this report because the RPP-WTP Project compliance strategy involves developing property-composition models to *predict* chemical durability of waste glasses as functions of their compositions. The term *project* is reserved for use in the context of WAPS 1.1.1 and 1.2.1, and contract specifications 2.2.2.6.1 and 2.2.2.7.1, which require *projecting* chemical and radionuclide compositions prior to production.

The ILAW chemical durability specifications do not explicitly allow the use of predicted chemical durability values for demonstrating compliance during production. However, that may be due to the lack of clarity in the specifications regarding what is expected or allowed as part of qualification activities versus production operations to demonstrate compliance.

It is assumed in this report that both the IHLW and ILAW chemical durability specifications allow the use of property-composition models to predict PCT and VHT chemical releases and thus demonstrate compliance.

1.1.6 Statistical Acceptance Criteria

The IHLW chemical durability specification requires a statistical acceptance criterion:

> "*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*."

The specification also suggests one acceptable statistical approach:

> "*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*."

Several ambiguities in this requirement and suggested acceptable approach are addressed in Section 1.1.7. However, first note that ILAW chemical durability specifications do not mention a statistical basis for demonstrating compliance (although they do mention waste form samples must be statistically representative of the production glass). Although a statistical basis for demonstrating compliance is not explicitly mentioned in contract specifications 2.2.2.17.2 and 2.2.2.17.3, it is generally agreed that an acceptable compliance strategy must statistically account for applicable variations and uncertainties. Variations and uncertainties to be accounted for include variations in waste glass composition over a waste type, as well as uncertainties due to sampling, chemical analyses, property-composition models, chemical durability testing, or any other measurements involved in demonstrating compliance.

1.1.7 Ambiguities in WAPS 1.3 Statistical Aspects and a Historical Perspective

The following WAPS 1.3 text from WAPS 1.3.1

"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."

has several aspects that are ambiguous, which are discussed under the following headings. Quotes are used to denote specific phrases from the specification that are discussed.

"Statistical Significance"—The phrase "*statistical significance of the reported data*" included in WAPS 1.3 is not well defined. Data are what they are, neither significant nor non-significant. Only inferences (i.e., decisions or conclusions) based on the data can be referred to as statistically significant or not. Hence, it should be assumed that WAPS 1.3 intends that a producer report (rather than define) the statistical significance of conclusions (either during qualification activities or production operations) indicating the waste form has normalized elemental releases lower than those of the EA glass.

"Mean PCT Results for Each Waste Type"—This phrase is fairly clear, apparently referring to the mean (i.e., average) PCT results (normalized elemental releases for B, Li, and Na) for IHLW produced from a given waste type. Issues exist with regard to properly computing the mean, depending on the structure of the available data. However, those are issues with the proper implementation of a compliance strategy, not with the specification itself.

"Standard Deviation"—The term *standard deviation* in "*two standard deviations below the mean PCT results of the EA glass*" is ambiguous, because the answer to "Standard deviation of what?" is not clear. In other words, it is not clear what variations and uncertainties (see **Definitions**) are intended to be included in the standard deviation. The applicable variations and uncertainties will depend on the particular situation. For example, consider a qualification activity demonstrating the PCT results from testing a single glass are below the corresponding EA glass results. Applicable uncertainties are those related to making the glass sample, determining its composition, performing the PCT, and chemically analyzing the resulting leachate. If the PCT normalized elemental releases for a given glass are to be predicted from property-composition models rather than by performing a PCT, then model uncertainty is also involved. If the goal is to demonstrate compliance for HLW glass produced over the course of a waste type, then the approach must account for variation in PCT results that follow from variation in glass composition over the waste type. Calculating standard deviations with multiple sources of variation and uncertainty requires advanced statistical methods. The resulting total standard deviation can be too small if all applicable sources of variation and uncertainty are not included, which could impact the statistical significance of conclusions made about compliance with the specification.

Unfortunately, because of the phrasing of "*two standard deviations below the mean PCT results of the EA glass*", the standard deviation can be incorrectly interpreted as being associated with the "*mean PCT results of the EA glass*". The uncertainties in the mean PCT normalized elemental releases of the EA glass should certainly be accounted for in comparisons versus PCT results of glass in qualification activities or production operations. However, it would be incorrect in such comparisons to ignore the applicable variations and uncertainties in the PCT results from the qualification activities or production operations. Thus, although not clearly stated in WAPS 1.3, it may be surmised the primary focus of *standard deviation* mentioned there is on the variations and uncertainties associated with PCT results of HLW glass in qualification activities or production operations.

<u>"Two Standard Deviations"</u>—It is not immediately clear why the "*one acceptable method*" included in WAPS 1.3.1 specifies <u>two</u> standard deviations. However, reasonable suppositions can be made based on the history of the development of WAPS 1.3. A preliminary version of WAPS 1.3, "Specification for Radionuclide Release Properties" included in DOE (1990) required that sufficient testing of waste form samples be performed to demonstrate with 95% confidence that at least 95% of the production waste glass from a waste type would yield leach test results less than 1.0 g/m^2-day, averaged over a 28-day Materials Characterization Center-1 (MCC-1) leach test (MCC 1983). Ultimately, the MCC-1 leach test was replaced by the PCT because of the shorter time required for the latter (7 days) compared to the former (28 days). The 95%/95% tolerance interval criterion contained in this preliminary version of WAPS 1.3 is well-defined and defensible, with similar criteria used by the U. S. Nuclear Regulatory Commission and other agencies. However, it was not clear why the well-defined 95%/95% criterion was deleted, and replaced in the final WAPS 1.3 with "*two standard deviations*". A likely explanation follows.

Statistical theory for the normal (Gaussian) distribution is sometimes misapplied by considering *95% confidence* as synonymous with *two standard deviations*. This relationship is nearly true in the case of a normal distribution with known mean and standard deviation, where a 95% two-sided confidence interval is given by the mean ± 1.96 standard deviations. However, to demonstrate HLW (or LAW) glass produced over the course of a waste type has PCT releases less than specified limits, only a one-sided statistical interval is required, not a two-sided interval. Further, the distribution of PCT results for glass produced from a waste type is not known. Statistics such as the mean and standard deviation of the distribution must be estimated from data. Also, making a high-confidence statement about a high percentage of the distribution of PCT results for glass produced from a waste type requires a *statistical tolerance interval*, not a *confidence interval*. The number of standard deviations needed to form a statistical tolerance interval is typically larger than the number of standard deviations needed to form a confidence interval. Further, because the distribution and its parameters must be estimated, the number of standard deviations for a tolerance interval depends on several quantities. The development details of one-sided statistical tolerance intervals for compliance with IHLW and ILAW chemical durability specifications are discussed in Section 3.

“Mean PCT Results of the EA Glass”—This phrase is somewhat ambiguous, in that the basis is not clear for calculating the mean of PCT results for the EA glass. If the EA glass and qualification or production glass samples were tested concurrently by the PCT multiple times, the mean over the results of the multiple PCTs on the EA glass could be calculated. However, the phrase “mean PCT results of the EA glass” can also be interpreted as referring to the B, Li, and Na normalized release values reported in Table 6 of Jantzen et al. (1993). Those values are means calculated over many PCT results for the EA glass. Thus, the intended interpretation of the phrase “mean PCT results of the EA glass” in WAPS 1.3 is not completely clear. Further, the specification does not indicate whether the uncertainties in the mean PCT results must be accounted for in making comparisons with PCT results from qualification activities or production operations.

In summary, several ambiguities exist in how the WAPS 1.3 specification for IHLW should be interpreted, and in what contract specifications 2.2.2.17.2 and 2.2.2.17.3 for ILAW require. The safest and most defensible approach is to assume that all of these chemical durability specifications require accounting for applicable variations and uncertainties with statistical methods appropriate for a given qualification activity or for production implementation. As discussed in the following Section 1.2, a statistical tolerance interval approach is a defensible approach for demonstrating that compliance was achieved for glass produced from a given HLW or LAW waste type.

1.2 RPP-WTP Compliance Strategies for Durability Specifications

The RPP-WTP Project strategy to comply with WAPS 1.3 for IHLW is described in the WCP (CHG 2001a), while the strategy for complying with contract specifications 2.2.2.17.2 and 2.2.2.17.3 for ILAW are described in the PSWP (CHG 2001b). All the details of the IHLW compliance strategy are not yet decided, and may or may not end up differing from the details of the ILAW compliance strategy. However, the compliance strategies for IHLW and ILAW are generally similar because they involve process control aspects as well as reporting aspects. Process control involves the use of process samples and information to demonstrate each process batch is acceptable prior to sending it to the melter. Reporting chemical durability compliance involves the use of process or product samples (depending on the specific IHLW or ILAW strategy) to demonstrate compliance over the course of a waste type.

This report focuses on the reporting compliance strategy aspect of demonstrating that PCT and VHT chemical releases from IHLW or ILAW produced from a HLW or LAW waste type meet the limits specified in WAPS 1.3 and contract specifications 2.2.2.17.2 and 2.2.2.17.3. A statistical X%/Y% UTI was selected as an appropriate type of statistical interval for demonstrating compliance over a waste type. An X%/Y% UTI provides for stating with high (X%) confidence that at least a high percentage (Y%) of the IHLW or ILAW produced from a waste type has true PCT or VHT releases less than a specification limit.

A statistical X% upper confidence interval (UCI) approach would not be appropriate for demonstrating compliance over a waste type. An X% UCI would provide X% confidence that the true mean PCT (or other leach test) release over a waste type is less than a specification limit.

However, the mean of a distribution of results over a waste type being less than a specification limit would allow for up to half of a symmetric distribution of results to violate the limit. It would be difficult to defend a compliance strategy in which up to one-half of the IHLW or ILAW produced from a waste type could violate a specification limit. Hence, an X% UCI compliance approach is not appropriate for demonstrating IHLW or ILAW produced over the course of a waste type is compliant.[a]

External reviews of a draft of this report raised the question of using an X% simultaneous upper confidence interval (SUCI) approach based on a release-composition model, and how it would compare to the X%/Y% UTI approach. An %X SUCI would provide X% confidence that the true mean values corresponding to ALL model predictions are less than the corresponding SUCI values for the predictions. The X% SUCI theory makes no assumption about a statistical distribution associated with the multiple model predictions for which simultaneous X% confidence is desired. However, in the RPP-WTP HLW and LAW vitrification applications, the multiple predictions will be associated with the distribution of releases associated with glass compositions produced over an HLW or LAW waste type, as well as sampling, analytical and model uncertainties. An X% SUCI would thus provide X% confidence that the true mean release values for ALL (i.e., 100% of) model predictions for glass produced from a waste type would be less than the corresponding SUCI values. Hence, there would be X% confidence that the true mean release values would be less than the acceptance limit for 100% of glasses produced from a waste type for which the corresponding SUCI values are less than the limit. This is a stronger statement than an X%/Y% UTI statement, which provides X% confidence that at least Y% of true mean release values for glass produced from a waste type are less than a specification limit. That is, making a SUCI statement about all glass produced from a waste type (assuming it all satisfies the applicable release limit) is a stronger statement than making a UTI statement about a high percentage of glass produced from a waste type. This is one way to understand that an X% SUCI is expected to be larger than a corresponding X%/Y% UTI. Section 5.3 discusses the relationship between X%/Y% UTIs and X% SUCIs for a specific example.

In summary, an X%/Y% UTI-based compliance strategy provides high (X%) confidence than a high (Y%) percentage of glass produced from a waste type will be compliant. In other words, the X%/Y% UTI approach allows a small chance of a small fraction of IHLW or ILAW produced over a HLW or LAW waste type to be non-compliant. The X%/Y% UTI approach is much more defensible than an X% UCI approach, which could allow up to half of the glass produced from a waste type to be non-compliant. However, the X%/Y% UTI approach will not provide as much "protection" as an X% SUCI approach that would require all glass produced from a waste type to be compliant with high confidence. The X%/Y% UTI approach is still highly defensible, without the potentially high additional cost associated with the X% SUCI

[a] An X% UCI approach may be the most appropriate approach for situations where there is only uncertainty as opposed to variation (see **Definitions**). In situations where there is a single true value (versus a distribution of values) that can only be estimated with uncertainty (e.g., sampling, analytical, or measurement uncertainties), an X% UCI would probably be the best approach. However, because there is variation over the course of a waste type (i.e., a distribution of results), an X%/Y% UTI approach is more appropriate for that situation.

approach. However, future work is required to verify that the X%/Y% approach and methods recommended later in this report will provide the nominal values of X and Y. This matter is discussed in Sections 3.7 and 6.6.

The steps for implementing the X%/Y% UTI approach for the reporting aspect of the IHLW and ILAW compliance strategies are as follows:

1. Develop databases of PCT and VHT release rates for glass compositions covering the glass composition regions of interest for IHLW and ILAW.

2. Develop PCT and VHT release models as functions of glass composition using the databases from Step 1.

3. Collect product (glass) samples or process (slurry) samples over the course of a waste type. Specifically, collect samples at $n > 1$ times over the production period corresponding to a waste type, and collect $m \geq 1$ samples at each of the n times.

4. Analyze $r \geq 1$ times the chemical composition of each glass sample or slurry sample.

5. Substitute the analyzed glass compositions into the PCT or VHT release-composition models (from Step 2) to obtain predicted releases (in the transformed or untransformed release units used to develop the models).

6. Calculate and report the mean and standard deviation over the waste type of each predicted release (in transformed or untransformed units) using statistical methods that account for the multiple sources of variation and uncertainty (i.e., variation over a waste type, sampling uncertainty, chemical analysis uncertainty, and property-composition model uncertainty). The multiple sources of variation and uncertainty are discussed in Section 2.3. As an example, the mean and standard deviation of predicted ln(release rate) values would be calculated and reported for B, Li, and Na releases from the PCT, where the PCT-composition models are developed in terms of natural logarithms of release rates.

7. Calculate values of X and Y so the X%/Y% one-sided upper tolerance interval for each (transformed or untransformed) release is equal to the corresponding (transformed or untransformed) specification release limit.

8. Report the tolerance interval conclusions that with high confidence (X%) at least some high percentage (Y%) of the distribution of release values for glass produced over the course of a waste type are less than or equal to each specification limit.

Steps 1 and 2 are performed prior to production operations, whereas Steps 3 to 8 are performed during and after production operations for a given waste type. During production operations, additional activities comprising the process control aspects of the IHLW and ILAW compliance strategies will also be performed. The statistical approach to process control activities will be addressed in future documents. The presumption is that every process batch will be found acceptable according to the process control activities prior to implementing the reporting strategy activities described in the preceding Steps 3 to 8.

This report discusses complying with specifications over the period of production corresponding to a waste type. However, that may be a period of one year or longer for some waste types, in which case there may be a need to demonstrate compliance over shorter periods of production. For example, the RPP-WTP Project may need to transfer and have the DOE accept filled IHLW and ILAW canisters on a regular basis. The X%/Y% UTI methodology presented in this report can be applied to demonstrate compliance over shorter periods of production as well as over a period of production corresponding to a waste type. The values of *n*, *m*, and *r* would need to be determined to obtain the desired minimum values of X and Y over the shorter periods of production for which compliance is to be demonstrated.

This report focuses on statistical methods and formulas to implement Steps 6, 7, and 8 described previously. These methods and formulas also provide a basis for assessing the sample sizes *n*, *m*, and *r* required to demonstrate compliance. Section 1.3 describes the objectives of the work and the report in more detail.

1.3 Objectives of the Work and Report

The general objective for the work summarized in this report is to develop and apply the statistical methods needed to implement the reporting aspects of the RPP-WTP Project compliance strategies for IHLW and ILAW chemical durability specifications. More specifically, the general objective is to develop and apply statistical methods to demonstrate that the chemical releases of IHLW or ILAW produced from a given waste type satisfy the requirements of WAPS 1.3 (for IHLW) and contract specifications 2.2.2.17.2 and 2.2.2.17.3 (for ILAW). The specific objectives for this work and report are to:

A. Develop statistical X%/Y% UTI methods and formulas appropriate for RPP-WTP Project strategies to comply with IHLW and ILAW durability specifications. Three X%/Y% UTI approaches to account for the source of variation of interest and nuisance uncertainties are addressed: (i) no adjustment or removal of nuisance uncertainties, (ii) adjustment but no removal of nuisance uncertainties, and (iii) adjustment for nuisance uncertainties and removal of sampling and analytical uncertainties when possible. The “source of variation of interest” is variation in PCT or VHT release results due to variation in IHLW or ILAW composition over a HLW or LAW waste type. Nuisance uncertainties are sampling uncertainty, chemical analysis uncertainty, and property-composition model uncertainty.

B. Use the X%/Y% UTI formulas to calculate UTI half-widths for combinations of input parameters within ranges expected to be appropriate for the RPP-WTP. The input parameters include X, Y, magnitudes of applicable variations and uncertainties, the number of sample times over a waste type (*n*), the number of samples per sampling time (*m*), and the number of chemical analyses per sample (*r*).

C. Assess the benefits of X%/Y% UTIs that reduce, adjust for, and possibly remove nuisance uncertainties (which unnecessarily inflate UTIs).

D. Consider possible average values of IHLW and ILAW releases over a waste type and calculated X%/Y% UTI half-widths, and compare to the release upper limits specified in the WAPS and contract specifications. These comparisons indicate how durable IHLW or ILAW produced by the RPP-WTP must be to satisfy the applicable specification(s).

E. Present calculated X%/Y% UTI half-widths in tabular format to facilitate assessing:
   (i) the number of sampling times (n) over the course of a waste type, the number of samples (m) at a given sampling time, and the number of chemical analyses per sample (r) required to meet the goal of demonstrating compliance over a waste type while simultaneously achieving cost efficiency
   (ii) the values of X (percent confidence) and Y (percentage of the IHLW or ILAW satisfying a given specification limit) that are likely to be achieved by the RPP-WTP for IHLW or ILAW produced from a given HLW or LAW waste type.

F. Present an example illustrating how the X%/Y% UTI formula can be used during production operations to demonstrate that IHLW or ILAW produced from a given waste type complies with durability specifications.

The tolerance interval calculations performed and included in this report to address Objectives B to F should be viewed as computational exercises. These exercises are intended to demonstrate the use of the X%/Y% UTI formulas and to provide information concerning the impact of parameters (such as X, Y, sample sizes, and magnitudes of variations and uncertainties) that influence the UTIs.

2.0 Tolerance Interval Preliminaries

This section discusses several issues associated with developing and interpreting statistical tolerance intervals. These discussions provide the background and framework necessary for developing statistical tolerance intervals appropriate for RPP-WTP compliance needs.

2.1 Types of Statistical Tolerance Intervals

Two types of tolerance intervals are discussed in the statistics literature, *Y-expectation tolerance intervals* and *Y-content tolerance intervals*. A *Y-expectation tolerance interval* will contain Y% of the population of a random variable on average or in the long run (i.e., sometimes more, sometimes less). On the other hand, a *Y-content tolerance interval* will contain at least Y% of the population. Both types of tolerance intervals achieve their respective population content with a specified X% confidence level.

Tolerance intervals can be two-sided, one-sided lower, or one-sided upper. A one-sided upper, Y-content tolerance interval is appropriate for demonstrating compliance with any specification that stipulates an upper limit (e.g., WAPS 1.3 for IHLW and Specifications 2.2.2.17.2 and 2.2.2.17.3 for ILAW).

The remainder of this report focuses on one-sided upper X%-confidence/Y%-content tolerance intervals. Such tolerance intervals are referred to as *X%/Y% upper tolerance intervals* (abbreviated as X%/Y% UTI). With this convention, an X%/Y% UTI provides X% confidence that at least Y% of the population of interest is below a specified upper limit. Both X and Y are percentages and, therefore, have values between 0 and 100. In general practice, X and Y typically are chosen to have values between 90 and 100. For RPP-WTP applications, possibly X and Y should be between 95 and 100, to demonstrate compliance with higher levels of confidence and population content. Note that neither X nor Y can equal 100, because it is not possible to capture 100% of a population with 100% confidence given real-world variations and uncertainties. The interested reader is referred to Hahn and Meeker (1991) for further information on statistical tolerance intervals.

2.2 Infinite Population Approach

An X%/Y% UTI makes an X% confidence statement about at least Y% of the population of PCT or VHT releases for glass produced from a given HLW or LAW waste type. The question then arises, "What is the *population*?" In order to define the population, the *population units* must be defined. Two approaches are discussed, but in both the population corresponds to the waste glass produced from a given HLW or LAW waste type.

One approach is to define a canister of glass as the population unit for a reporting compliance strategy based on glass samples taken from canisters produced from a waste type. In this case, an X%/Y% UTI would demonstrate with X% confidence that at least Y% of the IHLW or ILAW canisters produced from a waste type are acceptable. Similarly, a melter feed preparation vessel (MFPV) batch or melter feed vessel (MFV) batch could be defined as the population unit for a reporting compliance strategy based on slurry samples taken from the MFPV or MFV. In this case, an X%/Y% UTI would demonstrate with X% confidence that at least Y% of the MFPV or MFV batches yield acceptable product over the course of a waste type.

A second approach is to define a small quantity of melter feed slurry or canistered glass as the population unit. With this approach, there is an essentially infinite population of small slurry or glass sample population units for IHLW or ILAW produced from a waste type. Thus, an X%/Y% UTI would demonstrate with 95% confidence that: (i) at least 95% of the glass produced is acceptable (in the case of glass samples as the basis for compliance), or (ii) at least 95% of the melter feed slurry produced acceptable product (in the case of slurry samples as the basis for compliance).

The second approach will be easier and require less sampling than the first approach because:

- Statistical techniques for infinite populations are easier to implement and often require less sampling than statistical techniques for finite populations. The second approach provides an essentially infinite population of units (small quantities of melter feed slurry or glass), whereas the first approach provides only a finite collection of MFPV batches, MFV batches, or glass canisters.

- The second approach avoids the issues of variation within the population unit that occur with the first approach (i.e., variability within an MFPV batch, MFV batch, or within a canister). It also avoids the need to define and determine whether a MFPV batch, MFV batch, or canister is acceptable given such variability. Statistical methods could certainly be applied to such problems, and may be needed to implement a process control strategy based on MFPV or MFV samples. However, the relevant point is that these issues do not need to be addressed with the second approach to demonstrating that glass produced from a waste type complies with chemical durability specifications.

- Future work and reports will address statistical approaches for process control aspects of the IHLW and ILAW compliance strategies. In that future work, the goal will be to demonstrate that each process control batch (e.g., MFPV batch) will yield compliant IHLW or ILAW. In that work, it will be necessary to consider each batch as comprised of an essentially infinite number of possible results from sampling, chemical analysis, and leach test predictions. Hence, using the second approach based on infinite population theory will provide consistency in process control and reporting aspects of the compliance strategies.

Hence, statistical methods to develop X%/Y% UTIs for infinite populations are employed in Section 3.

2.3 Multiple Sources of Variation and Uncertainty

Most of the statistics literature on tolerance intervals is for situations where a random variable of interest has a specific distribution and the goal is to make a confidence statement about some specified proportion of the distribution. Computing a tolerance interval for such situations is straightforward, assuming the variable has a single source of variation that follows a normal (Gaussian) distribution or one of a few other selected distributions. First, a random sample of N units from the population is collected and the value of the variable of interest is determined (without uncertainty in the simplest scenario) for each unit sampled. Then, the sample mean and standard deviation are computed from the N values, and are combined with a tolerance interval multiplier to yield the tolerance interval.

For example, an X%/Y% UTI for a normal distribution is obtained using the formula $\bar{x} + ks$, where $\bar{x}$ is the sample mean, s is the sample standard deviation, and k is the X%/Y% tolerance interval multiplier (which depends on the sample size N and the values of X and Y chosen). The statistical theory and calculation process is straightforward because the assumption is that values of the variable are determined without uncertainty for the N samples.

A few papers in the statistical literature [Hahn (1982); Jaech (1984); Mee (1984); Mulrow et al. (1988)] address situations where the variable of interest varies (the source of variation of interest), but is measured with one source of uncertainty. Having a source of variation and a source of uncertainty complicates the problem, because the usual technique discussed in the previous paragraph would yield an X%/Y% UTI on the uncertain measured values. The resulting X%/Y% UTI would be too wide, because the calculations would incorporate the measurement uncertainty in addition to the population source of variation. Several solutions to the problem have been proposed in the statistics literature, depending on what is known about the measurement uncertainty or what can be learned about it from replicate measurements on population units.

The problem of computing an X%/Y% UTI to demonstrate compliance with IHLW and ILAW chemical durability specifications over an HLW or LAW waste type is complicated by the existence of several sources of uncertainty in addition to the source of variation of interest. The source of variation of interest is the variation in the true release rates of glass produced from a given waste type. However, the true PCT or VHT release rates will not be known; only model predictions of them based on chemical analyses of slurry or glass samples will be available. Hence, the additional sources of uncertainty include:

- Sampling uncertainty (and material inhomogeneity) at a particular time during production. Under the second approach, described in Section 2.2, the sampling uncertainty does not include variation within an MFPV batch, MFV batch, or within a canister because the population unit is a small quantity of slurry or glass.

- Analytical uncertainty in glass compositions, or analytical-plus-calculational uncertainties in estimating glass compositions from chemical analyses of MFPV or MFV samples. If bias detection and correction methods are applied to chemical analyses, only short-term within-lab analytical uncertainty needs to be addressed. However, uncertainty in the composition of the representative, certified standard glass used for bias detection and correction should be included. If bias detection and correction are not employed, long-term within-lab and lab-to-lab uncertainties must be included in addition to short-term within-lab uncertainty. In this report, we assume that chemical analyses of glass composition are unbiased or have been bias-corrected.

- Uncertainties in predictions from models relating release rates to glass composition.

Because these uncertainties undesirably inflate the width of an X%/Y% UTI, they are henceforth referred to as *nuisance uncertainties*. It is possible to reduce, possibly remove, or adjust for the sampling and/or analytical nuisance uncertainties before computing an X%/Y% UTI. The sampling uncertainty may be reduced by collecting more than one sample at each sampling time (i.e., $m > 1$) and averaging the results of replicate samples. Similarly, analytical uncertainty may be reduced by performing more than one chemical analysis of each sample (i.e., $r > 1$) and averaging the results of replicate chemical analyses. Methods for reducing, possibly removing, or adjusting for sampling and/or analytical uncertainties in computing X%/Y% UTIs are presented in Section 3 of this report. The uncertainty due to modeling PCT or VHT releases as a function of composition cannot be separated from the variation in releases over a waste type because the same model will be used over the course of a waste type. Therefore, model uncertainty is included in all uncertainty estimates used to compute tolerance intervals.

If information about the relative magnitudes of the source of variation of interest and the total of nuisance uncertainties is available, then X%/Y% UTI formulas can be developed to adjust the tolerance interval multiplier k for this information. The adjustment approach considered in this report is an adaptation and combination of ideas from Jaech (1984) and Mee (1984). The adjustment approach is discussed further in Section 3.

2.4 Interpretation of Tolerance Intervals

The goal of a statistical X%/Y% UTI is to make an X% confidence statement about at least Y% of the distribution of true population values. In the RPP-WTP situation, the goal is to make a statement with X% confidence that at least Y% of the glass produced from a waste type has true PCT or VHT chemical release values less than a specified limit. It is not possible to know the true glass composition or to know the true PCT or VHT release values for a given glass composition. Instead, we must work with sampled and chemically analyzed glass compositions and model-predicted PCT or VHT releases, which are subject to uncertainties. Nonetheless, the intent and interpretation of an X%/Y% UTI in this report is an X% confidence statement about at least Y% of the distribution of true PCT or VHT release values for glass produced from an HLW or LAW waste type.

Because the X%/Y% UTI formulas developed in this report are based on predicted (from property-composition models) values of PCT or VHT for sampled and analyzed compositions, misinterpretations are possible. For example, an X%/Y% UTI can be misinterpreted as providing X% confidence that at least Y% of the *predicted* releases for the sampled and analyzed compositions must be below a specified release limit. Piepel and Mellinger (1990) noted the distinction between an UTI being a statement about *true* instead of *predicted* releases is an important one. The goal is to make a statement about the true state of affairs (PCT or VHT releases) for a high percentage of the IHLW or ILAW produced from a given waste type (the population). The goal is not to make a statement about a high percentage of the predicted PCT or VHT results obtained for samples and chemical analyses of glass compositions. Predicted PCT or VHT results for sampled and analyzed compositions are used to develop X%/Y% UTIs, but still the X%/Y% UTIs are statements (inferences) about the true results (i.e., true PCT and VHT responses to true glass compositions).

2.5 Normal Distribution Theory for Tolerance Intervals

The methods for computing X%/Y% UTIs presented in this report are based on normal (Gaussian) distribution theory. The majority of the statistical literature on tolerance intervals is for normally distributed populations. Because tolerance intervals are confidence statements about a specified proportion of the population, the shape of the distribution greatly affects tolerance interval values. Therefore, the X%/Y% UTIs discussed in this report are sensitive to the normality assumption (Goodman and Madansky 1962). However, as long as the population distribution is symmetric and the tails of the distribution are short, the tolerance intervals are relatively robust to the normality assumption. If the distribution is skewed or long-tailed, tolerance intervals based on the normal distribution are inappropriate. Methods exist for computing tolerance intervals for populations whose distributions are known but are not normally distributed (e.g. lognormal, chi-square, exponential). These methods could be applied if warranted by the results of RPP-WTP qualification activities.

If the distribution of the population is not known, non-parametric (distribution-free) methods can be used to compute tolerance intervals (Conover 1980, pp. 117-121; Natrella 1966, pp. 2-15). Although non-parametric tolerance intervals are generally not difficult to compute, they usually require a much larger sample size than tolerance intervals based on the normal distribution (Hahn 1970). For example, a minimum of 59 samples (e.g., MFPV, MFV, or glass) over a waste type would be required to obtain a 95%/95% one-sided distribution-free tolerance interval (Conover 1980). If only one sample is taken from each of 59 MFPV batches, MFV batches, or canisters (assuming that many are available for a waste type) and only one analysis per sample, such a tolerance interval would be for the distribution of true release rates inflated by the nuisance uncertainties (sampling, analytical, and property-composition model). The literature search conducted for this work did not turn up any applicable methods for obtaining distribution-free tolerance intervals with nuisance variations reduced or removed. However, it would be straightforward to: (i) average model-predicted chemical durability results from replicate samples and/or analyses to reduce those sources of nuisance uncertainty, and (ii) use the average values to calculate a non-parametric UTI according to the standard procedure discussed by Conover (1980) and Natrella (1966). The method of averaging over replicate samples and analyses to reduce those sources of nuisance uncertainty is also used to develop normality-based X%/Y% UTIs in Section 3.

The normality assumption seems to be reasonable for the sources of variation and uncertainty that affect PCT and VHT releases in the proposed RPP-WTP Project compliance strategy. The reasonableness of the normality assumption for variation of release rates from glass produced from a waste type, as well as for sampling, analytical, and modeling uncertainties, must be verified as data from qualification activities and cold commissioning are collected. Qualification activities also must assess what the distribution of PCT or VHT releases would be if there is a trend or shift in glass composition during processing of a given waste type. Such a trend or shift may produce non-normally distributed results over a waste type. It will then be important to assess the performance of X%/Y% UTIs based on normal distribution theory. Ultimately, as long as all of the predicted PCT or VHT releases for process or glass samples taken over the course of a waste type are acceptable, it may be of little practical consequence that the X and Y values based on normal distribution theory may not be exactly correct due to the trend or shift. Still, this issue should be assessed during qualification activities.

3.0 X%/Y% Upper Tolerance Interval Formula Development and Calculations

In this section, X%/Y% UTI formulas are developed for the RPP-WTP strategy to demonstrate and report that IHLW or ILAW produced from a HLW or LAW waste type complies with chemical durability specifications. Section 3.1 presents the general formula X%/Y% UTI = $\tilde{\mu} + k\tilde{\sigma}$ and explains the notation. Section 3.2 introduces more specific notation and discusses the role of property-composition models in the X%/Y% UTI formulas for IHLW and ILAW chemical durability specifications. Section 3.3 presents the formula for $\tilde{\mu}$. Section 3.4 presents the $\tilde{\sigma}$ formula for the case where all sources of variation and uncertainty are included, with sampling and analytical uncertainties reduced by averaging when possible. Section 3.5 presents the $\tilde{\sigma}$ formula for the case where nuisance uncertainties are removed, if possible. Section 3.6 discusses two options for the *k* multiplier used in the X%/Y% UTI formula. Section 3.6 also proposes a modified form of one of the *k* multipliers that is more useful in comparing multiplier values to the theoretical minimum values. Section 3.7 summarizes the X%/Y% UTI formulas used in this report. Section 3.8 discusses the method for obtaining values of X and Y so the X%/Y% UTI equals the release limit[a] given in a particular IHLW or ILAW durability specification.

3.1 General Formula and Notation for X%/Y% Upper Tolerance Interval

In this report, the following general formula is used for an X%/Y% UTI

$$\text{UTI} = \tilde{\mu} + k\tilde{\sigma}\,, \tag{3.1}$$

where $\tilde{\mu}$ is an estimate of the population mean, $\tilde{\sigma}$ is an estimate of the population standard deviation, and *k* denotes the tolerance interval multiplier that is implicitly a function of X, Y, the degrees of freedom *f* associated with $\tilde{\sigma}$ (which is discussed in more detail in Section 4), and other parameters (such as sample sizes and relative magnitudes of standard deviations associated with sources of variation and uncertainty). As discussed in Section 2.4, the goal is to develop an X%/Y% UTI for the population of true PCT or VHT release values for IHLW or ILAW produced from a given HLW or LAW waste type. However, as noted in Section 1.2, because the RPP-WTP Project compliance strategy involves working with property-composition model predictions of sampled and chemically analyzed material, nuisance uncertainties inflate the population of interest. Methods for reducing, adjusting, and possibly removing some nuisance uncertainties are discussed in subsequent subsections of Section 3.

[a] If a model is in terms of a transformed release rate, then the X%/Y% UTI and the specification limit are also expressed in the transformed units.

Also of importance is the upper tolerance interval half-width (UTIHW):

$$\text{UTIHW} = k\,\tilde{\sigma}\,. \tag{3.2}$$

The UTI formula in (3.1) is relevant when data are available to compute an X%/Y% UTI and demonstrate compliance with IHLW or ILAW chemical durability specifications. However, the UTIHW formula in (3.2) is relevant for assessing the required numbers of samples and analyses (n, m, and r), the required precision, and other issues.

The general notation of $\tilde{\mu}$ and $\tilde{\sigma}$ is used in (3.1) and (3.2) because the nature of the RPP-WTP application results in $\tilde{\mu}$ and $\tilde{\sigma}$ being more complicated than for a basic X%/Y% UTI. In a basic X%/Y% UTI, $\tilde{\mu}$ and $\tilde{\sigma}$ would be the sample mean and sample standard deviation, respectively, calculated from N measured property values (see the first two paragraphs of Section 2.3). Sections 3.3, 3.4, and 3.5 develop and present formulas for $\tilde{\mu}$ and $\tilde{\sigma}$ considered in this work. The X%/Y% UTI multiplier k in (3.1) and (3.2) is also more complicated than for a basic X%/Y% UTI and is discussed in Section 3.6. Section 3.7 summarizes the X%/Y% UTI formulas developed in this work to address the production situation discussed in Section 1.2 and summarized as follows.

(i) Process or product samples are collected at $n > 1$ times (randomly selected) over the course of production corresponding to a waste type. If the reporting compliance strategy as well as the process control compliance strategy relies on process samples (such as is currently planned for IHLW), samples from every process batch will be available. The data from all such batches (sampling times) could be used to implement the X%/Y% UTI reporting strategy, or a random subset of n of them could be used if doing so would provide a cost benefit. If the reporting compliance strategy relies on product samples (e.g., shard samples), then samples would be taken n times over the course of a waste type. Although the statistical theory is based on random samples, sampling systematically at n times over the course of a waste type would not have a practical impact. Finally, as long as waste types yield more than a few batches or canisters, the inclusion or non-inclusion of samples during the transition period between waste types should not have a major impact on the results.[a] Of course, it is assumed that the glass made from both the old and new waste type is acceptable, so that glass made during the transition is acceptable.

(ii) At each sampling time, $m \geq 1$ samples are collected.

(iii) Each sample is chemically analyzed $r \geq 1$ times to yield an estimate of IHLW or ILAW composition. Let $\boldsymbol{x}_{ijk}$ denote the k^{th} chemical composition analysis of the j^{th} sample collected at the i^{th} time over the course of a waste type. Here, $\boldsymbol{x}_{ijk}$ represents a glass composition,

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[a] We mention this because the RPP-WTP may decide to sample more frequently during the transition between two waste types than during the middle and end of a waste type. Such a practice would involve non-random or non-systematic sampling over glass produced from a waste type. The impacts of such sampling practices on X%/Y% UTIs will need to be investigated. However, the impact may not be of practical concern as long as the glass composition and its release properties are not significantly different for successive waste types.

based on chemical analysis of a glass sample or on chemical analysis of a vitrified slurry sample from the MFPV or MFV.

(iv) A property-composition model relating a PCT or VHT release rate to chemical composition of IHLW or ILAW is applied to each of the $N = n{\cdot}m{\cdot}r$ estimates of composition. Let $\hat{y}_{ijk} = \hat{y}\,(\boldsymbol{x}_{ijk})$ denote the prediction from the property-composition model for the k^{th} chemical composition analysis of the j^{th} sample collected at the i^{th} time over the course of a waste type. If a property-composition model is for a transformation of a release rate, then $\hat{y}_{ijk}$ is in transformed units.

(v) The resulting $N = n{\cdot}m{\cdot}r$ predicted durability property values $\hat{y}_{ijk}$ are used to calculate the X%/Y% UTI according to the applicable specific formula. We assume that the results at each sampling period will be monitored so that any outliers are detected, thus enabling the collection of additional samples or additional analyses if needed. However, it may be that the RPP-WTP Project will choose the values of n, m, and r to permit discarding one or two outlying results without the need for additional sampling or chemical analyses.

The details of Step 5 applicable for specific cases are discussed in Sections 3.3 to 3.8. First, Section 3.2 introduces notation and discusses the role of property-composition models in the X%/Y% UTI formulas.

3.2 Role of Property-Composition Models in the Chemical Durability X%/Y% UTI Formulas

Property-composition models play a major role in the RPP-WTP Project strategies for complying with IHLW and ILAW chemical durability specifications. In particular, as described in Step (iv) of Section 3.1, property-composition models will be directly involved in calculating X%/Y% UTIs. It is helpful for the following discussion to introduce the mathematical notation for a property-composition model

$$\hat{y}_{ijk} = \boldsymbol{b}'\,\boldsymbol{w}_{ijk}\,, \tag{3.3}$$

where $\hat{y}_{ijk}$ is as previously defined, $\boldsymbol{b}$ denotes a vector of model coefficients, and $\boldsymbol{w}_{ijk} = f(\boldsymbol{x}_{ijk})$ denotes a vector that represents the model form as a function of the glass composition vector $\boldsymbol{x}_{ijk}$ previously defined. Note that boldface is used to denote vectors. For simplicity of notation in the rest of this section, the subscript "*ijk*" is dropped.

A widely used property-composition model form involves the identity function $\boldsymbol{w} = f(\boldsymbol{x}) = \boldsymbol{x}$. This model form is referred to as the Scheffé linear mixture model (Cornell 1990), which is given by

$$\hat{y} = \boldsymbol{b}'\,\boldsymbol{w} = \boldsymbol{b}'\,\boldsymbol{x} = b_1 x_1 + b_2 x_2 + \cdots + b_q x_q\,. \tag{3.4}$$

where $\boldsymbol{b} = [b_1, b_2, \ldots, b_q]'$ and $\boldsymbol{x} = [x_1, x_2, \ldots, x_q]'$ so that $x_1 + x_2 + \ldots + x_q = 1$. However, $\hat{y} = \boldsymbol{b}'\boldsymbol{w}$ may represent any model form linear in the coefficients, including model forms containing nonlinear terms in the x_i. For example, the Scheffé quadratic mixture model form (Cornell 1990) is given by

$$\hat{y} = \boldsymbol{b}'\boldsymbol{w} = \sum_{i=1}^{q} b_i x_i + \sum_{i=1}^{q-1} \sum_{j=i+1}^{q} b_{ij} x_i x_j \; . \tag{3.5}$$

where $\boldsymbol{b} = [b_1, b_2, \ldots, b_q, b_{12}, \ldots, b_{q-1,q}]'$ and $\boldsymbol{w} = [x_1, x_2, \ldots, x_q, x_1 x_2, \ldots, x_{q-1} x_q]'$. Reduced forms of (3.5) containing the linear terms and an appropriate subset of quadratic terms such as proposed by Piepel et al. (2001) can also be very useful and are linear in the coefficients.

Property-composition models for PCT are typically developed with $y = \ln(r_i^{PCT})$ as the response variable, where r_i^{PCT} denotes the PCT normalized release of an element i of interest (e.g., B, Li, and Na for IHLW, and B, Na, and Si for ILAW). The preliminary PCT-composition models developed by VSL (Gan and Pegg 2001a, Gan and Pegg 2001b) are for $\ln(r_i^{PCT})$. Preliminary VHT-composition models developed by VSL (Gan and Pegg 2001b) involve $y = \ln(\ln(1/(1 - r))$ as the transformed response, where r denotes the fraction of sample transformed by the VHT. However, VHT models using other transformations may be developed in the future. The following paragraph explains why the natural logarithm of PCT releases (g/m^2) is used in developing property-composition models. The same reasons would apply if future VHT-composition models were developed in terms of $\ln(r_i^{VHT})$, except that VHT releases are measured in terms of g/m^2-day.

The natural logarithm transformation of PCT normalized elemental releases (in g/m^2) is used for several reasons. First, experience has shown that linear mixture and other mixture model forms fit PCT release data better after a logarithmic transformation. Second, ordinary least squares regression requires the experimental error variance be the same for the response values of all data points. However, this requirement is typically not directly met for PCT normalized releases, which can vary over one to two orders of magnitude in many PCT-composition data sets. Experimental error variances tend to increase proportionally to the magnitude of the PCT normalized elemental release. Logarithm transformations of such data stabilize (make relatively constant) the experimental error variances. Third, the natural logarithm is used rather than the common logarithm because of the strong approximate relationship $SD\,[ln(r_i^{PCT})] \approx RSD\,(r_i^{PCT})$ where r_i^{PCT} is measured in g/m^2. Hence, a standard deviation (SD) of ln(release) is approximately equal to the relative standard deviation (RSD) of release. This relationship, which only holds for the natural logarithm, is very useful in interpreting models fitted to data. Finally, note that while predicted PCT values are in $\ln(g/m^2)$ units, the exponential transformation can be applied to the predicted values to convert them to normalized elemental releases in the original g/m^2 units.

Additional discussion of property-composition models and uncertainties in their predictions is provided in Appendix A.

3.3 Formula for $\tilde{\mu}$, the Estimate of Mean Release from Glass Produced from a Waste Type

This section develops and presents the formula for $\tilde{\mu}$ from the general X%/Y% UTI formula (3.1). Recall that $\tilde{\mu}$ is an estimate of the true mean release from glass produced from a waste type.

Given the data structure discussed in Section 1.2 and at the end of Section 3.1, we denote by $\hat{y}_{ijk}$ the predicted (via a property-composition model) response value for the k^{th} chemical analysis (in IHLW or ILAW composition units) for the j^{th} sample at the i^{th} sampling time for glass produced from a waste type. Then,

$$\bar{\hat{y}}_{i..} = \frac{1}{m} \sum_{j=1}^{m} \left[\frac{1}{r} \sum_{k=1}^{r} \hat{y}_{ijk} \right], \; i = 1, 2, \ldots, n \tag{3.6a}$$

denotes the average of the $\hat{y}_{ijk}$ values corresponding to the m replicate samples at the i^{th} sampling time and r replicate chemical analyses of each sample at the i^{th} sampling time. In $\bar{\hat{y}}_{i..}$, the dots in the j and k subscript locations, along with the bar over $\hat{y}$, denote averaging over those subscripts. The n sampling times over the course of a waste type result in n values of $\bar{\hat{y}}_{i..}$, $i = 1, 2, \ldots, n$. This notation and (3.6a) can still be used even if $m = 1$ and/or $r = 1$.

Equation (3.6a) assumes the data are balanced (i.e., the same number m of samples are taken at each of the n sampling times over a waste type, and the same number r of chemical analyses are made on each sample). If the data are not balanced, the number of samples at the i^{th} sampling time is denoted m_i, and the number of chemical analyses for the j^{th} sample at the i^{th} sampling time is denoted r_{ij}. Then, equation (3.6a) becomes

$$\bar{\hat{y}}_{i..} = \frac{1}{m_i} \sum_{j=1}^{m_i} \left[\frac{1}{r_{ij}} \sum_{k=1}^{r_{ij}} \hat{y}_{ijk} \right], \; i = 1, 2, \ldots, n \, , \tag{3.6b}$$

where all quantities are as previously defined.

Now, $\tilde{\mu}$ can be written as:

$$\tilde{\mu} = \frac{1}{n} \sum_{i=1}^{n} \bar{\hat{y}}_{i..} \, , \tag{3.7}$$

where $\bar{\hat{y}}_{i..}$ is given by (3.6a) or (3.6b). Hence, $\tilde{\mu}$ is the average of the n values $\bar{\hat{y}}_{i..}$.

3.4 Formula for $\tilde{\sigma}$ Including All Sources of Variation and Uncertainty, With Reductions of Sampling and Analytical Nuisance Uncertainties

This section develops and presents one possible formula for $\tilde{\sigma}$ from the general X%/Y% UTI formula (3.1). The specific formula in this section includes the source of variation of interest (variation in PCT or VHT releases due to IHLW or ILAW composition variation over a HLW or LAW waste type) and the nuisance uncertainties (uncertainties due to sampling, chemical analysis, and the property-composition model) as discussed in Section 2.3. However, the nuisance uncertainties are effectively reduced by averaging the results from $m > 1$ samples at a given sampling time, and averaging the results from $r > 1$ chemical analyses per sample.

Using the expression (3.3) for a prediction $\hat{y}_{ijk}$ from a property-composition model, the estimated variance of such a prediction is given by

$$\widehat{Var}(\hat{y}_{ijk}) = \widehat{Var}(\boldsymbol{b}'\boldsymbol{w}_{ijk}) \tag{3.8}$$

where $\hat{y}_{ijk}$, $\boldsymbol{b}$, and $\boldsymbol{w}_{ijk}$ are as defined previously. To simplify the presentation immediately following, the "*ijk*" subscripts will be dropped from $\hat{y}_{ijk}$ and $\boldsymbol{x}_{ijk}$.

Regardless of the form of the property-composition model $\hat{y} = \boldsymbol{b}'\boldsymbol{w}$, both $\boldsymbol{b}$ and $\boldsymbol{w}$ are subject to uncertainty when the model is used to make property predictions for estimated IHLW or ILAW compositions. The regression coefficient vector $\boldsymbol{b}$ is subject to uncertainty because it is calculated from an experimental property-composition database. The glass composition vector $\boldsymbol{x}$, and hence $\boldsymbol{w} = f(\boldsymbol{x})$, is subject to variation in glass composition over the course of IHLW or ILAW production for a given waste type, and is also subject to sampling and analytical uncertainties.

The regression coefficient vector $\boldsymbol{b}$ is determined prior to, and thus independently of, obtaining (during production operations) the $\boldsymbol{x}$ compositions that will be used to calculate an X%/Y% UTI (or its half-width UTIHW). Because both $\boldsymbol{b}$ and $\boldsymbol{x}$ have inherent variation and/or uncertainties, error propagation theory for independent random variables can be applied to determine how $\boldsymbol{b}$ and $\boldsymbol{x}$ contribute to $\mathrm{Var}(\hat{y})$. According to this theory (Hahn and Shapiro 1968, Section 7.2), if A and B are independent random variables or vectors, and if f is a function of these two random variables or vectors, $f(A, B)$, then

$$\mathrm{Var}[f(A,B)] \approx \left[\frac{\partial f}{\partial A}\right]^2 \mathrm{Var}(A) + \left[\frac{\partial f}{\partial B}\right]^2 \mathrm{Var}(B)\,. \tag{3.9}$$

For this situation, $f(\boldsymbol{b}, \boldsymbol{w}) = \boldsymbol{b}'\boldsymbol{w}$. Therefore, $\dfrac{\partial f}{\partial \boldsymbol{b}} = \boldsymbol{w}$ and $\dfrac{\partial f}{\partial \boldsymbol{w}} = \boldsymbol{b}'$ are the necessary first partial derivatives. Then, expanding (3.8) according to (3.9) yields

$$\widehat{\text{Var}}(\hat{y}) = \widehat{\text{Var}}(\boldsymbol{b}'\boldsymbol{w}) \cong \boldsymbol{w}'\widehat{\text{Var}}(\boldsymbol{b})\,\boldsymbol{w} + \boldsymbol{b}'\widehat{\text{Var}}(\boldsymbol{w})\,\boldsymbol{b} \tag{3.10}$$

where $\widehat{\text{Var}}(\boldsymbol{b})$ and $\widehat{\text{Var}}(\boldsymbol{w})$ are estimated variance-covariance matrices of $\boldsymbol{b}$ and $\boldsymbol{w}$, respectively. The quantity $\widehat{\text{Var}}(\boldsymbol{b})$ results from the least squares regression development of a given property-composition model. The last term in (3.10) can be used indirectly rather than directly. Hence, it is not necessary to obtain $\widehat{\text{Var}}(\boldsymbol{w})$, which would be very complicated given multiple sources of composition uncertainty.

Formula (3.10) indicates that property-composition model uncertainty and glass composition variation and uncertainties contribute to the overall variance in the predicted y-values. For brevity, the terms on the right hand side of (3.10) are represented as $\boldsymbol{w}'\widehat{\text{Var}}(\boldsymbol{b})\boldsymbol{w} = \hat{\sigma}_m^2$ and $\boldsymbol{b}'\widehat{\text{Var}}(\boldsymbol{w})\boldsymbol{b} = \hat{\sigma}_c^2$. In this notation, m refers to the property-composition model uncertainty and c refers to the glass composition variation and uncertainty. However, both components of variance are in squared units of predictions resulting from the property-composition model. For example, if PCT models were developed for $\ln(r_i^{PCT})$ in units of $\ln(\text{g/m}^2)$, then $\hat{\sigma}_m^2$ and $\hat{\sigma}_c^2$ would both be in units of $[\ln(\text{g/m}^2)]^2$.

The glass composition variation and uncertainty component $\hat{\sigma}_c^2$ encompasses the variation in release rates due to the variation in glass composition over a waste type, the sampling uncertainty, and the analytical uncertainty. This situation is represented by writing

$$\hat{\sigma}_c^2 = \hat{\sigma}_g^2 + \hat{\sigma}_s^2 + \hat{\sigma}_a^2, \tag{3.11}$$

where the $\hat{\sigma}_i^2$ notation represents an estimate of the variance (squared standard deviation) for the i^{th} source of variation or uncertainty. In this notation, g refers to glass variation over a waste type, s refers to sampling uncertainty, and a refers to analytical uncertainty. Appendix B provides additional discussion of how multivariate composition variation and uncertainties are propagated through a property-composition model to yield univariate variation and uncertainty components as in (3.11).

Equation (3.10) can now be written as

$$\widehat{\text{Var}}(\hat{y}_{ijk}) = \hat{\sigma}_m^2(\boldsymbol{x}_{ijk}) + \hat{\sigma}_c^2 = \hat{\sigma}_m^2(\boldsymbol{x}_{ijk}) + \hat{\sigma}_g^2 + \hat{\sigma}_s^2 + \hat{\sigma}_a^2\,. \tag{3.12}$$

In this notation, $\hat{\sigma}_g^2$ quantifies the variation of interest, while $\hat{\sigma}_s^2$, $\hat{\sigma}_a^2$, and $\hat{\sigma}_m^2(\boldsymbol{x}_{ijk})$ quantify the nuisance uncertainties. The notation $\hat{\sigma}_m^2(\boldsymbol{x}_{ijk})$ indicates that the model prediction uncertainty depends on the glass composition $\boldsymbol{x}_{ijk}$, as discussed in Appendix A. Although $\hat{\sigma}_g^2$, $\hat{\sigma}_s^2$, and $\hat{\sigma}_a^2$ quantify glass composition variation and uncertainties, they are expressed in $\hat{y}_{ijk}$ units. The same is true of $\hat{\sigma}_m^2(\boldsymbol{x}_{ijk})$. Hence, when $\hat{y}_{ijk}$ represents a property-composition model prediction of $\ln(r_i^{PCT})$, $\hat{\sigma}_g^2$, $\hat{\sigma}_s^2$, $\hat{\sigma}_a^2$, and $\hat{\sigma}_m^2(\boldsymbol{x}_{ijk})$ are expressed in units of $[\ln(\mathrm{g/m^2})]^2$. Appendix C discusses how statistical analysis of variance (ANOVA) and statistical least squares regression methods can be used to obtain the estimates of variation and uncertainties in (3.12). Appendix C also discusses Satterthwaite's formula (Satterthwaite 1946) for approximating the degrees of freedom associated with a linear combination of variation and uncertainty components.

Finally, it is now possible to express $\tilde{\sigma}^2$ as:

$$\tilde{\sigma}^2 = \widehat{\mathrm{Var}}(\bar{\bar{y}}_{i..}) = \bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \frac{\hat{\sigma}_s^2}{m} + \frac{\hat{\sigma}_a^2}{mr} \qquad (3.13a)$$

where

$$\bar{\hat{\sigma}}_m^2 = (1/mr)\sum_{j=1}^{m}\sum_{k=1}^{r}\hat{\sigma}_m^2(\boldsymbol{x}_{ijk}). \qquad (3.13b)$$

The difference between (3.12) and (3.13a) is that in (3.13a), the estimates of nuisance uncertainties due to sampling $\hat{\sigma}_s^2$ and analytical $\hat{\sigma}_a^2$ have been reduced because $\bar{\bar{y}}_{i..}$ averages over the *m* replicate samples and *r* replicate chemical analyses of each sample for a given sampling time *i* over a waste type. Note in (3.13a) that $r > 1$ reduces only the analytical uncertainty, whereas $m > 1$ reduces both sampling uncertainty and analytical uncertainty. If $m = 1$ and $r = 1$, no reduction in sampling and analytical uncertainties occurs.

Detailed formulas for $\tilde{\sigma}^2$ based on (3.13a) are presented in Appendixes D to G. The specific formulas depend on the values of the sample sizes (*n*, *m*, and *r*), with different cases covered in Appendix D ($m > 1$, $r > 1$), Appendix E ($m = 1$, $r > 1$), Appendix F ($m > 1$, $r = 1$, and Appendix G ($m = 1$, $r = 1$). The square root of the appropriate implementation of (3.13a) from Appendices D to G gives the formula for $\tilde{\sigma}$ that is needed in the X%/Y% UTI and UTIHW formulas in (3.1) and (3.2).

3.5 Formula for $\tilde{\sigma}$ when Sampling and Analytical Uncertainties Are Removed where Possible

This section develops and presents the formula for $\tilde{\sigma}$ from the general X%/Y% UTI formula (3.1) when sampling and analytical nuisance uncertainties are removed where possible. The specific formula in this section includes the source of variation of interest (variation in PCT or VHT releases due to IHLW or ILAW composition variation over a waste type) and the nuisance uncertainties (uncertainties due to sampling, chemical analysis, and the property-composition model) as discussed in Section 2.3. As in Section 3.4, the nuisance uncertainties are effectively reduced by averaging the results from $m > 1$ samples at a given sampling time, and averaging the results from $r > 1$ chemical analyses per sample. However, in this section sampling and analytical nuisance uncertainties are removed (where possible) in forming $\tilde{\sigma}$.

The estimates $\hat{\sigma}_s^2$, $\hat{\sigma}_a^2$, and $\bar{\hat{\sigma}}_m^2$ are nuisance uncertainties relative to the source of variation of interest, σ_g^2. When $\hat{\sigma}_s^2$, $\hat{\sigma}_a^2$, and $\bar{\hat{\sigma}}_m^2$ are included in $\widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..})$ as in (3.13a) of Section 3.4, an inflated $\tilde{\sigma}^2$ value is obtained relative to the source of variation of interest, σ_g^2. For this reason, we now discuss the possibility of removing (subtracting) some of these nuisance uncertainties from $\widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..})$ to obtain a less-inflated estimate of the variance, $\tilde{\sigma}^2$. In turn, this approach may yield an X%/Y% UTI with a shorter half-width.

Although $\bar{\hat{\sigma}}_m^2$ (and thus $\hat{\sigma}_m^2(\boldsymbol{x}_{ijk})$) is a nuisance uncertainty, it cannot be eliminated from the overall variance estimate. Recall that $\hat{\sigma}_m^2(\boldsymbol{x}_{ijk})$ represents the uncertainty in the prediction from a property-composition model for glass composition $\boldsymbol{x}_{ijk}$. It is assumed the same PCT or VHT property-composition model will be used to calculate the $\hat{y}_{ijk}$ values for the $\boldsymbol{x}_{ijk}$ compositions of samples collected during production of glass made from a waste type. Hence, if the fitted model tends to predict somewhat high (or low) for the subregion of glass compositions produced over a waste type, all the predictions $\hat{y}_{ijk}$ will tend to be high (or low). This is the nature of regression model uncertainties, because only one set of data is developed and used to fit a model one time for a given property. Least squares regression theory provides for quantifying the uncertainty in model predictions based on differences in results that would occur from collecting many data sets, fitting the model form to each data set, and using the different fitted models to make predictions. However, in practice only one data set and one fitted model are obtained for a given property, and that model is used repeatedly. Hence, although the regression model uncertainty can be quantified, it is not appropriate to eliminate it from the overall variance estimate.

Two approaches are considered for removing (subtracting) from $\widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..})$ the reduced nuisance uncertainties for sampling ($\hat{\sigma}_s^2/m$) and chemical analyses ($\hat{\sigma}_a^2/mr$). The first approach is based on applying statistical ANOVA methodology to the data values obtained over a waste type. These data values are the $\hat{y}_{ijk}$ values corresponding to n sampling times, m samples at each time, and r chemical analyses per sample. With the ANOVA approach, only those nuisance uncertainty components that can be estimated from the $\hat{y}_{ijk}$ values resulting from model predictions for replicate samples and/or replicate chemical analyses may be subtracted from $\widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..})$ to determine $\tilde{\sigma}^2$.

<u>If $m > 1$ and $r > 1$</u>

In this case, both σ_s^2 and σ_a^2 can be estimated from the $\hat{y}_{ijk}$ values. Then, the reduced uncertainty estimates $\hat{\sigma}_s^2/m$ and $\hat{\sigma}_a^2/mr$ can be removed from $\widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..})$ as expressed in (3.13a), yielding:

$$\tilde{\sigma}^2 = \widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..}) - \frac{\hat{\sigma}_s^2}{m} - \frac{\hat{\sigma}_a^2}{mr} = \bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 . \tag{3.14a}$$

If $m > 1$ and $r = 1$

In this case, a joint estimate $\widehat{\sigma_s^2 + \sigma_a^2}$ can be obtained and then $(\widehat{\sigma_s^2 + \sigma_a^2})/m$ removed from $\widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..})$ as expressed in (3.13a), yielding:

$$\tilde{\sigma}^2 = \widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..}) - \left(\frac{\widehat{\sigma_s^2 + \sigma_a^2}}{m}\right) = \bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 . \tag{3.14b}$$

If $m = 1$ and $r > 1$

In this case, σ_s^2 cannot be estimated separately from σ_g^2. Hence, only $\hat{\sigma}_a^2$ can be estimated and then $\hat{\sigma}_a^2/r$ removed from $\widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..})$ as expressed in (3.13a), yielding:

$$\tilde{\sigma}^2 = \widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..}) - \frac{\hat{\sigma}_a^2}{r} = \bar{\hat{\sigma}}_m^2 + \widehat{\sigma_g^2 + \sigma_s^2} . \tag{3.14c}$$

If $m = 1$ and $r = 1$

In this case, neither σ_s^2 nor σ_a^2 can be estimated separately from σ_g^2, so it is not possible to subtract or reduce either nuisance uncertainty. Thus,

$$\tilde{\sigma}^2 = \widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..}) = \bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \hat{\sigma}_s^2 + \hat{\sigma}_a^2 , \tag{3.14d}$$

which is just (3.13a) with $m = 1$ and $r = 1$ substituted.

The second approach to removing nuisance uncertainties requires that prior and independent estimates of the nuisance uncertainties are available. Then, the reduced forms of these prior and independent estimates may be subtracted from $\widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..})$ to determine $\tilde{\sigma}^2$. The term "prior and independent" is with respect to the IHLW or ILAW production data used to calculate an X%/Y% UTI. Such estimates of nuisance uncertainties would be obtained during qualification activities, and then subtracted when calculating X%/Y% UTIs during production operations. Of course, with this approach it must be assumed the nuisance uncertainties have similar magnitudes during production operations as they did when quantified during qualification activities. This second approach does not require the nuisance uncertainty components to be estimable from the $\hat{y}_{ijk}$ values in order to subtract the corresponding independent estimates from $\widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..})$. This means that m and/or r can equal one and the sampling and analytical nuisance uncertainties can still be removed.

Formulas analogous to (3.14a), (3.14b), (3.14c), and (3.14d) are given below for cases where prior, independent estimates $\tilde{\sigma}_s^2$ and $\tilde{\sigma}_a^2$ of σ_s^2 and σ_a^2 are available for removal from $\widehat{\mathrm{Var}}(\bar{\hat{y}}_{i..})$. Note that "tildes" are used to denote independent (pre-production) estimates, whereas "hats" are used to denote production estimates.

If $m > 1$ and $r > 1$

$$\tilde{\sigma}^2 = \widehat{\text{Var}}(\bar{\hat{y}}_{i..}) - \frac{\tilde{\sigma}_s^2}{m} - \frac{\tilde{\sigma}_a^2}{mr} = \bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \frac{\hat{\sigma}_s^2}{m} + \frac{\hat{\sigma}_a^2}{mr} - \frac{\tilde{\sigma}_s^2}{m} - \frac{\tilde{\sigma}_a^2}{mr} \quad (3.15a)$$

If $m > 1$ and $r = 1$

$$\tilde{\sigma}^2 = \widehat{\text{Var}}(\bar{\hat{y}}_{i..}) - \frac{\tilde{\sigma}_s^2}{m} - \frac{\tilde{\sigma}_a^2}{m} = \bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \frac{\widehat{\sigma_s^2 + \sigma_a^2}}{m} - \frac{\tilde{\sigma}_s^2}{m} - \frac{\tilde{\sigma}_a^2}{m} \quad (3.15b)$$

If $m = 1$ and $r > 1$

$$\tilde{\sigma}^2 = \widehat{\text{Var}}(\bar{\hat{y}}_{i..}) - \tilde{\sigma}_s^2 - \frac{\tilde{\sigma}_a^2}{r} = \bar{\hat{\sigma}}_m^2 + \widehat{\sigma_g^2 + \sigma_s^2} + \frac{\hat{\sigma}_a^2}{r} - \tilde{\sigma}_s^2 - \frac{\tilde{\sigma}_a^2}{r} \quad (3.15c)$$

If $m = 1$ and $r = 1$

$$\tilde{\sigma}^2 = \widehat{\text{Var}}(\bar{\hat{y}}_{i..}) - \tilde{\sigma}_s^2 - \tilde{\sigma}_a^2 = \bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \hat{\sigma}_s^2 + \hat{\sigma}_a^2 - \tilde{\sigma}_s^2 - \tilde{\sigma}_a^2 \quad (3.15d)$$

Because the prior, independent estimates $\tilde{\sigma}_s^2$ and $\tilde{\sigma}_a^2$ will not be the same as the ANOVA estimates $\hat{\sigma}_s^2$ and $\hat{\sigma}_a^2$ (or $\widehat{\sigma_s^2 + \sigma_a^2}$) calculated from production data, removed uncertainty terms do not cancel in the above formulas as they do in (3.14a), (3.14b), and (3.14c).

Detailed formulas for $\tilde{\sigma}^2$ based on (3.14) or (3.15) are presented in Appendixes D to G. The specific formulas depend on the values of the sample sizes (*n*, *m*, and *r*), with different cases covered in Appendix D ($m > 1$, $r > 1$), Appendix E ($m = 1$, $r > 1$), Appendix F ($m > 1$, $r = 1$, and Appendix G ($m = 1$, $r = 1$). The square root of the appropriate implementation of either (3.14) or (3.15) from Appendices D to G gives the formula for $\tilde{\sigma}$ that is needed in the X%/Y% UTI and UTIHW formulas in (3.1) and (3.2).

3.6 The *k* Multiplier

According to formula (3.1), an X%/Y% UTI = $\tilde{\mu} + k\tilde{\sigma}$. Thus, *k* is the number of standard deviations $\tilde{\sigma}$ added to $\tilde{\mu}$ to obtain an X%/Y% UTI. However, the value and interpretation of *k* depends on the specific form of $\tilde{\sigma}$. In general, $\tilde{\sigma}$ will be an inflated estimate of σ_g, the standard deviation of the distribution of true PCT or VHT values for glass made from a waste type. The value and interpretation of *k* also depends on the statistical theory applied to develop an X%/Y% UTI (see Appendix H).

One approach is to select $k = k_0$ corresponding to $\tilde{\sigma}$ given by the square root of (3.13a), to obtain an X%/Y% UTI on the distribution of $\bar{\hat{y}}_{i..}$ values. This distribution has the variation over a waste type (σ_g^2) inflated by reduced sampling, reduced analytical, and modeling uncertainties (σ_s^2/m, σ_a^2/rm, and $\bar{\sigma}_m^2$). Section 2.4 discussed that the goal is to develop an X%/Y% UTI on the true release rates for glass produced from a waste type, not on the $\bar{\hat{y}}_{i..}$ values, which are averages of model-predicted values based on samples and chemical analyses. However, an

X%/Y% UTI approach and k_0 value based on the distribution of $\bar{\bar{y}}_{i..}$ values is discussed here (and the theory developed in Section H.2 of Appendix H) to show the advantages of the following approach.

As discussed in Section 2.4, we desire to develop an X%/Y% UTI on the true release rates for glass produced from a waste type. An approach for doing so is developed in Section H.1 of Appendix H. This approach assumes the ratio σ_g/σ_2 is known, where

$$\sigma_2 = \sqrt{\bar{\sigma}_m^2 + \sigma_g^2 + \frac{\sigma_s^2}{m} + \frac{\sigma_a^2}{mr}} \tag{3.16}$$

The ratio σ_g/σ_2 is used to adjust the value of $k = k_1$ smaller to compensate for $\tilde{\sigma}$ being an inflated estimate of σ_g (see Section H.1 of Appendix H for the details). Such an adjustment is not made in obtaining k_0, so that $k_1 < k_0$ and thus $\tilde{\mu} + k_1\tilde{\sigma} < \tilde{\mu} + k_0\tilde{\sigma}$. X%/Y% UTIs based on k_1 are tentatively recommended for RPP-WTP use in demonstrating IHLW or ILAW produced from a waste type complies with chemical durability specifications. Formulas for k_0 and k_1 are given in Section 3.7. The recommendation is only tentative at this time pending verification of the approach as discussed in Section 6.6.

The value of k_1 will be smaller than it would be if $\tilde{\sigma}$ were not an inflated estimate of σ_g. This aspect of the k_1 multiplier follows from the theoretical development of the X%/Y% UTI formula given in Section H.1 of Appendix H.

Results in Section 4 show that the k_1 values for many adjusted X%/Y% UTIHWs are smaller than the theoretical minimum multiplier values of 1.645 for 95%/95% UTIs and 2.327 for 99%/99% UTIs. These theoretical minimums apply for the distribution of interest (the distribution of true PCT or VHT values over a waste type) being normally distributed with known mean μ_g and known standard deviation σ_g. The difference is that these theoretical minimum values for the tolerance interval multiplier are multipliers of the standard deviation σ_g, whereas in (3.1) and (3.2) k (either k_0 or k_1) is the multiplier for the standard deviation $\tilde{\sigma}$, an inflated estimate of σ_g. Re-expressing the UTI formula (3.1) as follows provides for a more meaningful comparison of k multipliers to the theoretical minimum values:

$$\text{UTI} = \tilde{\mu} + k\tilde{\sigma} = \tilde{\mu} + k\left(\frac{\tilde{\sigma}}{\sigma_g}\right)\sigma_g = \tilde{\mu} + k^*\sigma_g, \tag{3.17}$$

where $k^* = k(\tilde{\sigma}/\sigma_g)$. Thus, k^* inflates the k value by a factor $(\tilde{\sigma}/\sigma_g)$ that represents the ratio by which $\tilde{\sigma}$ overestimates σ_g. In practice, the ratio $(\tilde{\sigma}/\sigma_g)$ will not be known because the true value σ_g will not be known. However, in calculational exercises where the values of various input parameters are assumed known, it is possible to determine k^* from k (either k_0 or k_1). Such calculation exercises are presented in Section 4 of this report, where both *k* and the more meaningful k^* values are summarized and compared.

3.7 X%/Y% Upper Tolerance Interval Formulas

The preceding sections summarize the approaches to calculate X%/Y% UTI = $\tilde{\mu}+k\tilde{\sigma}$ values with or without adjustment of *k* for nuisance uncertainties, and with or without subtraction of nuisance uncertainties in $\tilde{\sigma}$. The theoretical development of X%/Y% UTIs with adjustment for nuisance uncertainties, with or without subtraction of nuisance uncertainties, is given in Section H.1 of Appendix H. The theoretical development of X%/Y% UTIs without adjustment for nuisance uncertainties, with or without subtraction of nuisance uncertainties, is given in Section H.2 of Appendix H. Formulas specific to the two approaches are given in Sections H.1 and H.2 of Appendix H. Formulas that apply to both approaches are given in Appendices D to G for particular combinations of values of *m* (number of samples at each sampling time) and *r* (number of chemical analyses of each sample).

Section H.3 describes why adjusted X%/Y% UTIs are always smaller without subtraction of nuisance uncertainties. Section H.4 of Appendix H describes why adjusted X%/Y% UTIs without subtraction of nuisance uncertainties are always smaller than unadjusted X%/Y% UTIs with subtraction of nuisance uncertainties. Hence, for the calculations in Sections 4 and 5, we focus on two approaches: (1) adjusted X%/Y% UTIs without subtraction of nuisance uncertainties, and (2) unadjusted X%/Y% UTIs without subtraction of nuisance uncertainties. Both approaches reduce sampling and analytical nuisance uncertainties by averaging over data from replicate samples and/or analyses per sample. The applicable formulas for calculating X%/Y% UTIs with the two approaches are scattered in various parts of the report, and so are summarized in this section for convenience.

<u>Recommended Approach: Adjusted X%/Y% UTIs Without Subtracting Nuisance Uncertainties</u>

This approach provides X%/Y% UTIs on the <u>true</u> release rates (possibly transformed) for glass produced from a waste type. This approach is recommended because it yields smaller X%/Y% UTI values than all other approaches considered. This recommendation is made tentatively, because future work is required to verify that this approach will provide at least the nominal values of X and Y. The work required for this verification is discussed in Section 6.6. The formulas for calculating adjusted X%/Y% UTIs without subtracting nuisance uncertainties follow.

$$\text{Adjusted X\%/Y\% UTI} = \tilde{\mu}+k_1\tilde{\sigma} \tag{3.18a}$$

where

$$\tilde{\mu}=\frac{1}{n}\sum_{i=1}^{n}\bar{\bar{y}}_{i..} \tag{3.18b}$$

$$\tilde{\sigma} = \sqrt{\bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \frac{\hat{\sigma}_s^2}{m} + \frac{\hat{\sigma}_a^2}{rm}} = \sqrt{\bar{\hat{\sigma}}_m^2 + \frac{1}{rm} MS_g} \tag{3.18c}$$

$$k_1 = \frac{t_1(X, Y, f, \delta_1)}{\sqrt{n}} \tag{3.18d}$$

$$\delta_1 = z_{1-\beta} \sqrt{n} \frac{\sigma_g}{\sigma_2} \tag{3.18e}$$

and

$$f \approx \frac{\left[\bar{\hat{\sigma}}_m^2 + \frac{1}{rm} MS_g\right]^2}{\frac{\left(\bar{\hat{\sigma}}_m^2\right)^2}{\mathrm{df}_m} + \frac{\left[\frac{MS_g}{rm}\right]^2}{\mathrm{df}_g}} . \tag{3.18f}$$

The quantities appearing in these equations have been defined previously in Section 3 or are defined in Appendix H. In (3.18f), $\bar{\hat{\sigma}}_m^2$ is given by (3.13b) and MS_g, df_m, and df_g are described in Appendix D. When $m = 1$ and/or $r = 1$, the formulas (3.18c) and (3.18f) reduce to the corresponding formulas in Appendices E, F, and G.

Comparison Approach: Unadjusted X%/Y% UTIs Without Subtracting Nuisance Uncertainties

This approach provides X%/Y% UTIs on the predicted release rates (possibly transformed) for glass produced from a waste type, where the predictions are subject to sampling, analytical, and model-prediction nuisance uncertainties. This approach does not adjust the *k* multiplier for nuisance uncertainties, and thus serves to demonstrate the benefits of adjusting X%/Y% UTIs for nuisance uncertainties using the recommended approach. Hence, the unadjusted approach is not recommended for use, but is presented for comparison with the recommended adjusted approach. The formulas for calculating unadjusted X%/Y% UTIs without subtracting nuisance uncertainties follow.

$$\text{Unadjusted X\%/Y\% UTI} = \tilde{\mu} + k_0 \tilde{\sigma} \tag{3.19a}$$

where

$$\tilde{\mu} = \frac{1}{n} \sum_{i=1}^{n} \bar{\hat{y}}_{i..} \tag{3.19b}$$

$$\tilde{\sigma} = \sqrt{\bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \frac{\hat{\sigma}_s^2}{m} + \frac{\hat{\sigma}_a^2}{rm}} = \sqrt{\bar{\hat{\sigma}}_m^2 + \frac{1}{rm} MS_g} \tag{3.19c}$$

$$k_0 = \frac{t_0(X, Y, f, \delta_0)}{\sqrt{n}} \tag{3.19d}$$

$$\delta_0 = z_{1-\beta}\sqrt{n} \tag{3.19e}$$

and

$$f \approx \frac{\left[\bar{\hat{\sigma}}_m^2 + \frac{1}{rm} MS_g\right]^2}{\frac{\left(\bar{\hat{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{rm}\right]^2}{df_g}}\ . \tag{3.19f}$$

The quantities appearing in these equations have been defined previously in Section 3 or are defined in Appendix H. In (3.19f), $\bar{\hat{\sigma}}_m^2$ is given by (3.13b) and MS_g, df_m, and df_g are described in Appendix D. When $m = 1$ and/or $r = 1$, the formulas (3.19c) and (3.19f) reduce to the corresponding formulas in Appendices E, F, and G.

3.8 Determining the X and Y UTI Values Achieved for a Given Compliance Situation

During RPP-WTP production operations for IHLW and ILAW, the X%/Y% UTI formula will be applied to demonstrate compliance with the PCT (IHLW and ILAW) and VHT (ILAW) durability specifications. Specifically, Step 7 of Section 1.2 indicates values of X and Y will be calculated so that the X%/Y% UTI for each release rate is equal to the corresponding specification release limit (in untransformed or transformed units as applicable). Such calculated values of X and Y can be considered as the achieved values of the percent confidence (X) and minimum percent of the glass produced within a waste type satisfying the specification (Y). For any given waste type, it is expected that X and Y should both exceed 95.

Equation (3.1) indicates the value of an X%/Y% UTI depends on the multiplying factor k, which is implicitly a function of X, Y, and other parameters. Holding the other parameters constant, an X%/Y% UTI can be viewed as a function of X and Y. Thus, the values of X and Y associated with a fixed value of UTI (e.g., a release limit in a specification) are not unique. In fact, an infinite number of X and Y pairs are associated with any given value of UTI. Specific implementations of the general formula (3.1) can be solved for X given UTI and Y, or for Y given UTI and X. Thus, for a fixed UTI value and a selected value of X, the corresponding value of Y (call it Y*) can be determined. Alternatively, for a fixed UTI value and a selected value of Y, the corresponding value of X (call it X*) can be determined.

After the RPP-WTP completes production of IHLW or ILAW for a given waste type, it is proposed that values of X and Y corresponding to UTI = L (the applicable limit corresponding to a PCT or VHT specification, in untransformed or transformed units as appropriate) be obtained as follows. First, set X = 95 and calculate Y*. Then if Y* is significantly greater than 95, X can be set to higher values (e.g., 99) and the corresponding value of Y* calculated. This process continues until suitably high values of X and Y = Y* are obtained, so that it can be stated with as high as possible X% confidence that at least as high as possible Y% of the glass produced over a waste type satisfies the specification. A similar process would be followed by setting Y to successively higher values and calculating X*. The RPP-WTP Project must choose to report the final (X, Y*) combination, the final (X*, Y) combination, or both, to summarize the achieved values of X and Y for PCT or VHT performance of that waste type. It would be simplest and maybe most appropriate to report the final (X, Y*) combination. In the case of PCT, where limits exist for several elemental releases, the calculations must be performed for each elemental release and its limit. This procedure and the results are illustrated for the example considered in Section 5.

4.0 X%/Y% Tolerance Interval Half-Width Calculations for Ranges of Input Parameters

This section describes and presents the results of a computational exercise to generate UTIHW values $k_1\tilde{\sigma}$ and $k_0\tilde{\sigma}$ according to the equations in Section 3.7. Values of variation and uncertainty components within reasonable ranges are used to calculate $\tilde{\sigma}$. The multiplying factors k_1 and k_0 are calculated based on the values of X, Y, and other parameters as discussed in Section 3.7.

4.1 Ranges of Input Parameters

In order to calculate UTIHWs, values must be supplied for various input parameters. These input parameters include estimates of the variation and uncertainty components ($\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$), values for the sample sizes mentioned in Section 1.2 (n, m, and r), and values for the confidence and population coverage percentages (X and Y, respectively). One additional input parameter needed to calculate the UTIHWs is the degrees of freedom associated with $\bar{\hat{\sigma}}_m$, denoted df_m. By definition df_m = df[$\hat{\sigma}_m(\boldsymbol{x})$] = df[$\bar{\hat{\sigma}}_m$] = $M - p$, where M is the number of data points used to fit the property-composition model, and p is the number of fitted parameters in the model. Hence, UTIHWs indirectly depend on M and p through df_m. Table 4.1 shows the different values used in this computational exercise for each of the input parameters. The values for the input parameters were chosen to represent reasonable ranges for the input parameters based on past experience. Also, the values of the variation and uncertainty components ($\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$) assume a chemical durability is modeled in terms of the natural logarithm transformation of release rate. In the preliminary models for PCT and VHT (Gan and Pegg 2001a, Gan and Pegg 2001b), only the PCT models use natural logarithm transformations. Hence, the calculated UTIHW values in Section 4 are only applicable for PCT compliance. Similar computations can be performed in the future for VHT compliance after VHT-composition models and the associated transformation are further developed.

The values of the variation and uncertainty components ($\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$) in Table 4.1 are absolute (not relative) values in PCT ln(release rate) units. However, as discussed in Section 3.2, these values can also be thought of as relative standard deviations (RSDs) in original PCT units. For example, the values of $\hat{\sigma}_g$ = 0.10, 0.25, and 0.50 can be interpreted as RSDs in original PCT units (g/m^2). Such RSD interpretations were considered in selecting the values of $\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$ shown in Table 4.1.

Table 4.1. Input Parameter Values for UTIHW Calculations

Input Parameter	Values Used
$\hat{\sigma}_g$	0.10, 0.25, 0.50
n	10, 30, 50
$\hat{\sigma}_s$	0.05, 0.10
m	1, 3
$\hat{\sigma}_a$	0.05, 0.20, 0.50
r	1, 3
$\bar{\hat{\sigma}}_m$ [(a)]	0.20, 0.40
df_m [(b)]	20, 40
X%/Y%	95%/95%, 99%/99%

(a) See Appendix A for further discussion of the interpretation of $\bar{\hat{\sigma}}_m$, which depends on the compositions $\boldsymbol{x}_{ijk}$ for which model predictions are made. However, the dependence of $\bar{\hat{\sigma}}_m$ on the $\boldsymbol{x}_{ijk}$ cannot be accounted for in calculating UTIHW values for combinations of input parameters without a specific model. Hence, for this computational exercise $\bar{\hat{\sigma}}_m$ is treated as having the same value for each sampling time i over a waste type.

(b) The degrees of freedom for the property-composition model (df_m) is equal to the number of data points used to fit the model (M) minus the number of fitted coefficients in the model (p). Hence, $df_m = M - p$.

4.2 Calculated X%/Y% Tolerance Interval Half-Widths

This section presents the results of calculating UTIHW values for the combinations of input parameters listed in Table 4.1. However, before presenting and discussing those results, we discuss observations about UTIHWs that are helpful in viewing and assessing the results.

An UTIHW can be viewed in two ways. First, an UTIHW literally is the half-width of an X%/Y% UTI. Hence, it is the amount added to a $\tilde{\mu}$ value from (3.18b) or (3.19b) to obtain an X%/Y% UTI value. Second, an UTIHW can be viewed as the minimum distance a $\tilde{\mu}$ value must be below a specification limit (e.g., in natural logarithm units for PCT) in order to satisfy the specification. Table 4.2 lists the IHLW and ILAW PCT specification limits and some possible $\tilde{\mu}$ values in original and natural logarithm units. The differences between the specification limits and possible $\tilde{\mu}$ values indicate how large UTIHW values can be and still result in meeting PCT specification limits for certain levels of average PCT performance over a waste type. For example, consider the IHLW PCT normalized boron release limit of 8.35 g/m^2, which is 2.122 in ln(g/m^2) units as shown in Table 4.2. Now, suppose that over the IHLW produced from a given waste type the average PCT normalized boron release was 2.0 g/m^2, which is 0.693 in ln(g/m^2) units. Then, the UTIHW (which depends on X and Y) would have to be less than 2.122 − 0.693 = 1.429 in order to satisfy the limit.

Table 4.2. PCT Specification Limits and Selected Average Performance Values in Original and Natural Log Units

		Specification Limit	**ln(Specification Limit)**		**Average Performance**	**ln(Average Performance)**
IHLW PCT	**B**	8.35 g/m^2	2.122 ln(g/m^2)	**PCT**		
	Li	4.78 g/m^2	1.564 ln(g/m^2)		0.5 g/m^2	-0.693 ln(g/m^2)
	Na	6.67 g/m^2	1.898 ln(g/m^2)		1.0 g/m^2	0.0 ln(g/m^2)
ILAW PCT	**B**	2 g/m^2	0.693 ln(g/m^2)		2.0 g/m^2	0.693 ln(g/m^2)
	Na	2 g/m^2	0.693 ln(g/m^2)		4.0 g/m^2	1.386 ln(g/m^2)
	Si	2 g/m^2	0.693 ln(g/m^2)			

Tables 4.3 and 4.4 summarize the calculated UTIHW values for X%/Y% = 95%/95%, and Tables 4.5 and 4.6 summarize the calculated UTIHW values for X%/Y% = 99%/99%. Tables 4.3 and 4.5 contain the results for the "no-adjustment and no-subtraction" approach, while Tables 4.4 and 4.6 contain the results for the "adjustment and no-subtraction" approach. These approaches were described in Section 3.7. Each of these tables summarizes the UTIHW values calculated for the combinations of input parameter values in Table 4.1. The sample sizes (n, m, and r) and model degrees of freedom (df_m) vary across the columns of each table, while the standard deviations $\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$ vary down the rows of each table. The UTIHW results presented in Tables 4.3 to 4.6 do not remove nuisance uncertainties. The methods for removing sampling and/or analytical nuisance uncertainties by either the ANOVA approach or the independent-estimates approach (as discussed in Section 3.5) were used to calculate UTIHW values. However, the "subtraction" UTIHW results are not summarized in tables because they are always worse (larger) than UTIHWs fromthe adjustment approach without subtracting nuisance uncertainties, as discussed in Sections H.3 and H.4. Appendix I presents additional details corresponding to the 95%/95% UTIHW calculations shown in Tables 4.3 and 4.4. Similar details are available corresponding to the 99%/99% UTIHW calculations shown in Tables 4.5 and 4.6, but were not included in Appendix I for space considerations.

Table 4.3. 95%/95% Upper Tolerance Interval Half-Width Values
Without Adjustment for Nuisance Uncertainties

			(a)	df_m	20	20	20	20	20	20	20	20	20	20	20	20
				n	10	10	10	10	30	30	30	30	50	50	50	50
(b)				m	1	1	3	3	1	1	3	3	1	1	3	3
$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\bar{\hat{\sigma}}_m$	r	1	3	1	3	1	3	1	3	1	3	1	3
0.10	0.05	0.05	0.20		0.561	0.553	0.545	0.543	0.511	0.505	0.500	0.498	0.499	0.494	0.489	0.487
			0.40		1.022	1.019	1.016	1.015	0.952	0.950	0.948	0.947	0.935	0.933	0.931	0.930
		0.20	0.20		0.748	0.615	0.607	0.562	0.643	0.549	0.543	0.512	0.617	0.532	0.527	0.500
			0.40		1.104	1.044	1.041	1.023	1.009	0.967	0.965	0.952	0.986	0.949	0.946	0.935
		0.50	0.20		1.499	0.942	0.935	0.680	1.189	0.782	0.777	0.594	1.116	0.743	0.738	0.573
			0.40		1.620	1.211	1.207	1.072	1.374	1.084	1.081	0.987	1.313	1.053	1.050	0.966
	0.10	0.05	0.20		0.598	0.590	0.557	0.554	0.537	0.531	0.508	0.506	0.522	0.517	0.496	0.495
			0.40		1.037	1.034	1.021	1.020	0.962	0.960	0.951	0.950	0.944	0.942	0.934	0.933
		0.20	0.20		0.784	0.653	0.619	0.575	0.668	0.576	0.552	0.521	0.640	0.556	0.535	0.507
			0.40		1.122	1.060	1.046	1.028	1.022	0.979	0.969	0.956	0.997	0.959	0.950	0.938
		0.50	0.20		1.519	0.973	0.946	0.692	1.205	0.804	0.785	0.603	1.131	0.763	0.745	0.581
			0.40		1.638	1.230	1.214	1.077	1.386	1.098	1.086	0.991	1.324	1.065	1.054	0.970
0.25	0.05	0.05	0.20		0.819	0.811	0.803	0.801	0.693	0.688	0.682	0.680	0.662	0.657	0.652	0.650
			0.40		1.140	1.136	1.132	1.131	1.035	1.032	1.029	1.028	1.009	1.006	1.004	1.003
		0.20	0.20		0.980	0.867	0.860	0.820	0.809	0.728	0.723	0.694	0.767	0.694	0.689	0.663
			0.40		1.235	1.167	1.163	1.141	1.101	1.054	1.051	1.035	1.067	1.025	1.023	1.009
		0.50	0.20		1.638	1.143	1.137	0.922	1.293	0.928	0.924	0.768	1.212	0.876	0.872	0.730
			0.40		1.739	1.345	1.340	1.199	1.459	1.178	1.175	1.076	1.390	1.136	1.134	1.045
	0.10	0.05	0.20		0.853	0.845	0.815	0.812	0.717	0.712	0.690	0.689	0.684	0.679	0.660	0.658
			0.40		1.159	1.155	1.138	1.137	1.048	1.045	1.033	1.032	1.020	1.018	1.007	1.007
		0.20	0.20		1.009	0.900	0.871	0.831	0.831	0.752	0.731	0.702	0.787	0.715	0.696	0.670
			0.40		1.254	1.186	1.169	1.147	1.114	1.067	1.055	1.040	1.079	1.037	1.027	1.013
		0.50	0.20		1.657	1.169	1.146	0.933	1.307	0.947	0.930	0.775	1.225	0.894	0.878	0.737
			0.40		1.755	1.363	1.347	1.206	1.471	1.191	1.179	1.081	1.400	1.148	1.138	1.049
0.50	0.05	0.05	0.20		1.478	1.473	1.468	1.467	1.174	1.170	1.167	1.166	1.102	1.099	1.096	1.095
			0.40		1.603	1.599	1.595	1.594	1.362	1.359	1.356	1.355	1.302	1.299	1.297	1.296
		0.20	0.20		1.580	1.508	1.503	1.478	1.249	1.196	1.193	1.175	1.172	1.123	1.120	1.103
			0.40		1.689	1.628	1.624	1.604	1.423	1.380	1.377	1.362	1.357	1.318	1.315	1.302
		0.50	0.20		2.063	1.690	1.686	1.543	1.610	1.332	1.329	1.222	1.505	1.248	1.245	1.147
			0.40		2.120	1.784	1.780	1.657	1.735	1.492	1.489	1.400	1.641	1.419	1.417	1.337
	0.10	0.05	0.20		1.499	1.494	1.475	1.474	1.189	1.186	1.172	1.171	1.116	1.113	1.101	1.100
			0.40		1.620	1.617	1.601	1.600	1.374	1.371	1.360	1.359	1.313	1.310	1.300	1.300
		0.20	0.20		1.599	1.528	1.510	1.485	1.264	1.211	1.198	1.180	1.185	1.137	1.124	1.108
			0.40		1.705	1.645	1.630	1.610	1.435	1.392	1.381	1.366	1.368	1.329	1.319	1.306
		0.50	0.20		2.079	1.709	1.692	1.549	1.621	1.345	1.333	1.227	1.515	1.260	1.249	1.151
			0.40		2.134	1.800	1.786	1.663	1.745	1.503	1.493	1.405	1.651	1.430	1.420	1.340

(a) df_m = degrees of freedom for property-composition model (see Appendix A), n = the number of sampling times over a waste type, m = the number of samples at each sampling time, and r = the number of chemical analyses per sample.

(b) $\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$ are as defined in Section 3.4.

Table 4.3. 95%/95% Upper Tolerance Interval Half-Width Values Without Adjustment for Nuisance Uncertainties (cont'd)

			(a)	df_m	40	40	40	40	40	40	40	40	40	40	40	40
				n	10	10	10	10	30	30	30	30	50	50	50	50
(b)				m	1	1	3	3	1	1	3	3	1	1	3	3
$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\bar{\hat{\sigma}}_m$	r	1	3	1	3	1	3	1	3	1	3	1	3
0.10	0.05	0.05	0.20		0.541	0.532	0.523	0.520	0.487	0.481	0.474	0.472	0.473	0.467	0.461	0.459
			0.40		0.965	0.961	0.957	0.956	0.886	0.883	0.880	0.879	0.866	0.863	0.860	0.859
		0.20	0.20		0.739	0.600	0.591	0.542	0.632	0.530	0.524	0.488	0.604	0.512	0.506	0.474
			0.40		1.061	0.992	0.988	0.966	0.959	0.907	0.904	0.887	0.933	0.885	0.882	0.867
		0.50	0.20		1.497	0.937	0.930	0.668	1.188	0.776	0.771	0.580	1.114	0.736	0.731	0.557
			0.40		1.605	1.179	1.175	1.025	1.356	1.046	1.043	0.932	1.292	1.011	1.008	0.908
	0.10	0.05	0.20		0.582	0.573	0.536	0.533	0.517	0.511	0.484	0.482	0.500	0.494	0.470	0.468
			0.40		0.984	0.979	0.963	0.962	0.901	0.897	0.885	0.884	0.879	0.876	0.865	0.864
		0.20	0.20		0.776	0.640	0.604	0.556	0.658	0.560	0.534	0.498	0.628	0.539	0.515	0.483
			0.40		1.082	1.011	0.994	0.972	0.974	0.922	0.909	0.892	0.946	0.898	0.886	0.871
		0.50	0.20		1.518	0.968	0.940	0.681	1.203	0.799	0.778	0.590	1.129	0.756	0.738	0.566
			0.40		1.623	1.200	1.181	1.031	1.369	1.061	1.048	0.937	1.304	1.024	1.012	0.912
0.25	0.05	0.05	0.20		0.811	0.804	0.796	0.793	0.684	0.679	0.673	0.671	0.652	0.647	0.642	0.640
			0.40		1.102	1.097	1.093	1.091	0.989	0.986	0.983	0.982	0.960	0.957	0.954	0.953
		0.20	0.20		0.975	0.861	0.853	0.813	0.804	0.720	0.715	0.685	0.761	0.685	0.680	0.653
			0.40		1.204	1.131	1.127	1.103	1.064	1.011	1.008	0.990	1.027	0.979	0.976	0.960
		0.50	0.20		1.637	1.140	1.134	0.917	1.291	0.924	0.920	0.761	1.210	0.872	0.868	0.722
			0.40		1.726	1.320	1.316	1.166	1.444	1.149	1.146	1.037	1.372	1.104	1.101	1.002
	0.10	0.05	0.20		0.846	0.838	0.807	0.805	0.710	0.704	0.682	0.680	0.675	0.670	0.649	0.648
			0.40		1.122	1.118	1.100	1.098	1.004	1.001	0.988	0.987	0.973	0.970	0.958	0.957
		0.20	0.20		1.005	0.894	0.865	0.824	0.826	0.745	0.723	0.694	0.781	0.707	0.687	0.661
			0.40		1.224	1.152	1.134	1.109	1.079	1.026	1.013	0.995	1.041	0.993	0.981	0.965
		0.50	0.20		1.656	1.166	1.143	0.928	1.305	0.944	0.926	0.769	1.223	0.890	0.874	0.729
			0.40		1.742	1.340	1.322	1.173	1.456	1.163	1.150	1.042	1.384	1.117	1.105	1.007
0.50	0.05	0.05	0.20		1.476	1.471	1.467	1.465	1.172	1.169	1.165	1.164	1.100	1.097	1.094	1.093
			0.40		1.587	1.583	1.579	1.578	1.343	1.340	1.337	1.336	1.281	1.278	1.275	1.274
		0.20	0.20		1.578	1.506	1.502	1.477	1.248	1.194	1.191	1.173	1.170	1.121	1.118	1.101
			0.40		1.675	1.613	1.609	1.588	1.407	1.362	1.359	1.343	1.339	1.298	1.295	1.281
		0.50	0.20		2.063	1.689	1.685	1.541	1.609	1.330	1.327	1.220	1.504	1.246	1.243	1.145
			0.40		2.112	1.772	1.768	1.643	1.726	1.477	1.475	1.383	1.631	1.403	1.401	1.317
	0.10	0.05	0.20		1.497	1.492	1.474	1.472	1.188	1.184	1.170	1.169	1.114	1.111	1.098	1.097
			0.40		1.605	1.601	1.585	1.584	1.356	1.353	1.342	1.341	1.292	1.290	1.279	1.278
		0.20	0.20		1.598	1.527	1.508	1.484	1.263	1.210	1.196	1.178	1.184	1.135	1.122	1.105
			0.40		1.692	1.630	1.615	1.594	1.419	1.374	1.363	1.348	1.350	1.309	1.299	1.285
		0.50	0.20		2.078	1.708	1.691	1.548	1.620	1.344	1.332	1.225	1.515	1.259	1.248	1.149
			0.40		2.126	1.788	1.774	1.649	1.736	1.489	1.479	1.388	1.640	1.414	1.404	1.321

(a) df_m = degrees of freedom for property-composition model (see Appendix A), n = the number of sampling times over a waste type, m = the number of samples at each sampling time, and r = the number of chemical analyses per sample.

(b) $\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$ are as defined in Section 3.4.

Table 4.4. 95%/95% Upper Tolerance Interval Half-Width Values
With Adjustment for Nuisance Uncertainties

			(a)	df_m	20	20	20	20	20	20	20	20	20	20	20	20
				n	10	10	10	10	30	30	30	30	50	50	50	50
(b)				m	1	1	3	3	1	1	3	3	1	1	3	3
$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\bar{\hat{\sigma}}_m$	r	1	3	1	3	1	3	1	3	1	3	1	3
0.10	0.05	0.05	0.20		0.305	0.304	0.302	0.302	0.252	0.252	0.252	0.252	0.237	0.237	0.238	0.238
			0.40		0.407	0.406	0.405	0.405	0.313	0.313	0.313	0.313	0.285	0.285	0.285	0.285
		0.20	0.20		0.348	0.317	0.315	0.306	0.267	0.255	0.255	0.252	0.245	0.238	0.237	0.237
			0.40		0.425	0.411	0.411	0.407	0.319	0.315	0.314	0.313	0.288	0.286	0.286	0.285
		0.50	0.20		0.506	0.390	0.389	0.332	0.344	0.287	0.286	0.261	0.301	0.258	0.258	0.241
			0.40		0.536	0.449	0.448	0.418	0.371	0.330	0.329	0.317	0.324	0.294	0.294	0.287
	0.10	0.05	0.20		0.314	0.312	0.305	0.304	0.254	0.254	0.252	0.252	0.237	0.237	0.237	0.237
			0.40		0.410	0.409	0.406	0.406	0.314	0.314	0.313	0.313	0.286	0.285	0.285	0.285
		0.20	0.20		0.356	0.326	0.318	0.308	0.271	0.258	0.256	0.253	0.247	0.239	0.238	0.237
			0.40		0.429	0.415	0.412	0.408	0.321	0.316	0.315	0.314	0.289	0.286	0.286	0.285
		0.50	0.20		0.510	0.397	0.391	0.335	0.346	0.290	0.287	0.262	0.303	0.261	0.259	0.241
			0.40		0.540	0.453	0.449	0.419	0.373	0.331	0.330	0.317	0.325	0.296	0.294	0.287
0.25	0.05	0.05	0.20		0.659	0.657	0.655	0.654	0.547	0.547	0.546	0.546	0.519	0.518	0.518	0.518
			0.40		0.707	0.707	0.706	0.705	0.598	0.598	0.598	0.598	0.568	0.568	0.569	0.569
		0.20	0.20		0.701	0.672	0.670	0.659	0.563	0.552	0.551	0.547	0.528	0.521	0.521	0.519
			0.40		0.728	0.713	0.712	0.708	0.602	0.599	0.599	0.598	0.567	0.567	0.568	0.568
		0.50	0.20		0.849	0.741	0.740	0.687	0.631	0.580	0.580	0.557	0.577	0.539	0.539	0.524
			0.40		0.846	0.754	0.753	0.720	0.648	0.610	0.610	0.600	0.594	0.570	0.570	0.567
	0.10	0.05	0.20		0.668	0.666	0.658	0.657	0.551	0.550	0.547	0.547	0.520	0.520	0.518	0.518
			0.40		0.711	0.710	0.707	0.707	0.599	0.599	0.598	0.598	0.568	0.568	0.568	0.568
		0.20	0.20		0.709	0.681	0.673	0.662	0.566	0.555	0.552	0.548	0.530	0.523	0.521	0.519
			0.40		0.733	0.717	0.714	0.709	0.604	0.600	0.599	0.599	0.568	0.567	0.567	0.568
		0.50	0.20		0.853	0.747	0.742	0.689	0.633	0.583	0.581	0.558	0.578	0.541	0.540	0.525
			0.40		0.849	0.758	0.754	0.722	0.650	0.612	0.610	0.601	0.595	0.571	0.570	0.567
0.50	0.05	0.05	0.20		1.377	1.376	1.375	1.375	1.090	1.090	1.089	1.089	1.022	1.022	1.021	1.021
			0.40		1.308	1.307	1.306	1.306	1.091	1.091	1.091	1.091	1.036	1.036	1.035	1.035
		0.20	0.20		1.400	1.384	1.383	1.377	1.100	1.093	1.093	1.090	1.029	1.024	1.024	1.022
			0.40		1.332	1.315	1.314	1.308	1.099	1.094	1.093	1.092	1.040	1.037	1.037	1.036
		0.50	0.20		1.499	1.424	1.423	1.392	1.147	1.111	1.111	1.097	1.063	1.037	1.037	1.027
			0.40		1.442	1.357	1.356	1.323	1.143	1.109	1.108	1.096	1.067	1.045	1.045	1.038
	0.10	0.05	0.20		1.382	1.381	1.377	1.376	1.092	1.092	1.090	1.090	1.023	1.023	1.022	1.022
			0.40		1.313	1.312	1.308	1.307	1.093	1.093	1.091	1.091	1.037	1.036	1.036	1.036
		0.20	0.20		1.405	1.389	1.385	1.379	1.102	1.095	1.093	1.091	1.031	1.025	1.024	1.022
			0.40		1.336	1.320	1.316	1.310	1.101	1.095	1.094	1.092	1.041	1.038	1.037	1.036
		0.50	0.20		1.502	1.428	1.425	1.394	1.149	1.113	1.112	1.097	1.064	1.038	1.037	1.027
			0.40		1.446	1.362	1.358	1.325	1.145	1.110	1.109	1.097	1.068	1.046	1.045	1.038

(a) df_m = degrees of freedom for property-composition model (see Appendix A), n = the number of sampling times over a waste type, m = the number of samples at each sampling time, and r = the number of chemical analyses per sample.

(b) $\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$ are as defined in Section 3.4.

Table 4.4. 95%/95% Upper Tolerance Interval Half-Width Values
With Adjustment for Nuisance Uncertainties (cont'd)

(b)			(a)	df_m	40	40	40	40	40	40	40	40	40	40	40	40
				n	10	10	10	10	30	30	30	30	50	50	50	50
				m	1	1	3	3	1	1	3	3	1	1	3	3
$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\bar{\hat{\sigma}}_m$	r	1	3	1	3	1	3	1	3	1	3	1	3
0.10	0.05	0.05	0.20		0.298	0.296	0.294	0.293	0.244	0.243	0.243	0.243	0.229	0.228	0.228	0.228
			0.40		0.394	0.393	0.392	0.392	0.301	0.301	0.301	0.301	0.273	0.273	0.273	0.273
		0.20	0.20		0.345	0.312	0.310	0.298	0.265	0.250	0.249	0.244	0.242	0.232	0.231	0.229
			0.40		0.416	0.400	0.399	0.394	0.312	0.304	0.304	0.302	0.280	0.275	0.275	0.273
		0.50	0.20		0.505	0.389	0.388	0.328	0.344	0.286	0.285	0.257	0.301	0.257	0.257	0.237
			0.40		0.533	0.443	0.442	0.408	0.369	0.324	0.324	0.308	0.322	0.289	0.289	0.277
	0.10	0.05	0.20		0.308	0.306	0.297	0.296	0.248	0.247	0.244	0.244	0.231	0.230	0.228	0.228
			0.40		0.399	0.398	0.394	0.394	0.303	0.303	0.301	0.301	0.275	0.274	0.273	0.273
		0.20	0.20		0.353	0.322	0.313	0.302	0.269	0.254	0.250	0.246	0.245	0.235	0.232	0.229
			0.40		0.421	0.405	0.401	0.396	0.314	0.306	0.304	0.302	0.282	0.276	0.275	0.274
		0.50	0.20		0.510	0.396	0.390	0.331	0.346	0.289	0.286	0.258	0.302	0.260	0.257	0.238
			0.40		0.537	0.447	0.443	0.409	0.371	0.326	0.324	0.308	0.323	0.290	0.289	0.278
0.25	0.05	0.05	0.20		0.653	0.651	0.649	0.648	0.541	0.540	0.539	0.539	0.512	0.511	0.511	0.510
			0.40		0.690	0.689	0.688	0.687	0.579	0.578	0.578	0.578	0.547	0.547	0.547	0.547
		0.20	0.20		0.698	0.668	0.666	0.654	0.560	0.547	0.546	0.541	0.524	0.516	0.515	0.512
			0.40		0.715	0.697	0.696	0.690	0.588	0.581	0.581	0.579	0.552	0.548	0.548	0.547
		0.50	0.20		0.848	0.739	0.738	0.683	0.631	0.578	0.578	0.553	0.576	0.537	0.537	0.520
			0.40		0.841	0.744	0.743	0.706	0.644	0.600	0.600	0.585	0.590	0.559	0.559	0.550
	0.10	0.05	0.20		0.663	0.661	0.652	0.652	0.545	0.544	0.541	0.540	0.514	0.514	0.511	0.511
			0.40		0.695	0.694	0.689	0.689	0.581	0.580	0.579	0.579	0.548	0.548	0.547	0.547
		0.20	0.20		0.706	0.677	0.669	0.657	0.563	0.551	0.547	0.543	0.527	0.518	0.516	0.513
			0.40		0.720	0.702	0.698	0.692	0.590	0.583	0.582	0.579	0.553	0.549	0.548	0.547
		0.50	0.20		0.852	0.746	0.740	0.686	0.633	0.581	0.579	0.555	0.578	0.540	0.538	0.521
			0.40		0.845	0.749	0.745	0.708	0.646	0.602	0.600	0.585	0.591	0.561	0.559	0.550
0.50	0.05	0.05	0.20		1.376	1.375	1.374	1.373	1.088	1.088	1.087	1.087	1.020	1.020	1.019	1.019
			0.40		1.297	1.295	1.294	1.294	1.078	1.078	1.077	1.077	1.021	1.021	1.020	1.020
		0.20	0.20		1.399	1.383	1.382	1.376	1.099	1.092	1.091	1.089	1.028	1.022	1.022	1.020
			0.40		1.322	1.304	1.303	1.297	1.088	1.081	1.081	1.078	1.027	1.023	1.022	1.021
		0.50	0.20		1.499	1.423	1.422	1.391	1.147	1.110	1.110	1.095	1.063	1.036	1.036	1.025
			0.40		1.438	1.349	1.348	1.313	1.138	1.100	1.099	1.085	1.062	1.035	1.035	1.025
	0.10	0.05	0.20		1.381	1.380	1.375	1.375	1.091	1.090	1.088	1.088	1.022	1.021	1.020	1.020
			0.40		1.302	1.301	1.296	1.296	1.080	1.080	1.078	1.078	1.022	1.022	1.021	1.021
		0.20	0.20		1.403	1.387	1.383	1.378	1.101	1.094	1.092	1.089	1.029	1.024	1.022	1.021
			0.40		1.327	1.309	1.305	1.299	1.090	1.083	1.081	1.079	1.029	1.024	1.023	1.021
		0.50	0.20		1.502	1.427	1.424	1.392	1.148	1.112	1.111	1.096	1.064	1.037	1.036	1.025
			0.40		1.441	1.354	1.350	1.314	1.140	1.102	1.100	1.085	1.063	1.036	1.035	1.025

(a) df_m = degrees of freedom for property-composition model (see Appendix A), n = the number of sampling times over a waste type, m = the number of samples at each sampling time, and r = the number of chemical analyses per sample.

(b) $\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$ are as defined in Section 3.4.

Table 4.5. 99%/99% Upper Tolerance Interval Half-Width Values
Without Adjustment for Nuisance Uncertainties

			(a)	df_m	20	20	20	20	20	20	20	20	20	20	20	20
				n	10	10	10	10	30	30	30	30	50	50	50	50
(b)				m	1	1	3	3	1	1	3	3	1	1	3	3
$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\bar{\hat{\sigma}}_m$	r	1	3	1	3	1	3	1	3	1	3	1	3
0.10	0.05	0.05	0.20		0.859	0.847	0.836	0.832	0.784	0.778	0.772	0.770	0.768	0.762	0.757	0.756
			0.40		1.588	1.585	1.583	1.582	1.500	1.499	1.498	1.497	1.480	1.479	1.478	1.478
		0.20	0.20		1.168	0.943	0.929	0.861	0.968	0.833	0.825	0.786	0.923	0.808	0.801	0.769
			0.40		1.691	1.611	1.607	1.589	1.554	1.512	1.510	1.500	1.523	1.489	1.487	1.480
		0.50	0.20		2.503	1.509	1.497	1.051	1.817	1.180	1.173	0.897	1.672	1.107	1.100	0.862
			0.40		2.552	1.856	1.849	1.646	2.069	1.648	1.644	1.530	1.960	1.601	1.597	1.504
	0.10	0.05	0.20		0.916	0.903	0.853	0.849	0.817	0.809	0.781	0.779	0.795	0.788	0.765	0.763
			0.40		1.604	1.600	1.587	1.586	1.508	1.506	1.499	1.499	1.486	1.484	1.480	1.479
		0.20	0.20		1.230	1.006	0.950	0.879	1.006	0.870	0.837	0.796	0.955	0.839	0.811	0.777
			0.40		1.717	1.631	1.614	1.594	1.569	1.522	1.513	1.503	1.535	1.497	1.490	1.482
		0.50	0.20		2.540	1.564	1.515	1.072	1.841	1.215	1.184	0.910	1.693	1.137	1.110	0.873
			0.40		2.582	1.886	1.859	1.654	2.088	1.666	1.650	1.534	1.976	1.616	1.602	1.507
0.25	0.05	0.05	0.20		1.291	1.278	1.264	1.260	1.044	1.036	1.027	1.024	0.988	0.981	0.974	0.971
			0.40		1.745	1.738	1.732	1.730	1.584	1.581	1.577	1.576	1.548	1.545	1.542	1.541
		0.20	0.20		1.576	1.377	1.364	1.293	1.222	1.097	1.089	1.045	1.144	1.034	1.027	0.989
			0.40		1.893	1.786	1.779	1.746	1.670	1.608	1.604	1.585	1.619	1.567	1.564	1.548
		0.50	0.20		2.752	1.867	1.857	1.474	1.979	1.408	1.401	1.158	1.817	1.307	1.301	1.088
			0.40		2.760	2.075	2.068	1.836	2.199	1.778	1.774	1.637	2.072	1.710	1.707	1.591
	0.10	0.05	0.20		1.351	1.338	1.284	1.280	1.081	1.073	1.040	1.037	1.020	1.013	0.984	0.982
			0.40		1.773	1.767	1.741	1.739	1.600	1.597	1.583	1.581	1.561	1.558	1.546	1.545
		0.20	0.20		1.629	1.434	1.383	1.313	1.256	1.133	1.101	1.058	1.173	1.066	1.038	1.000
			0.40		1.924	1.815	1.789	1.755	1.688	1.625	1.610	1.590	1.634	1.581	1.569	1.553
		0.50	0.20		2.786	1.914	1.873	1.493	2.001	1.438	1.411	1.170	1.837	1.334	1.310	1.098
			0.40		2.789	2.107	2.079	1.847	2.217	1.797	1.780	1.643	2.088	1.726	1.712	1.596
0.50	0.05	0.05	0.20		2.466	2.457	2.449	2.446	1.793	1.788	1.782	1.780	1.650	1.645	1.640	1.639
			0.40		2.522	2.515	2.508	2.506	2.050	2.046	2.042	2.041	1.943	1.940	1.936	1.935
		0.20	0.20		2.648	2.520	2.511	2.467	1.911	1.828	1.823	1.794	1.756	1.681	1.677	1.651
			0.40		2.672	2.565	2.559	2.523	2.144	2.078	2.073	2.051	2.024	1.967	1.963	1.944
		0.50	0.20		3.509	2.846	2.838	2.582	2.475	2.040	2.035	1.868	2.262	1.871	1.867	1.718
			0.40		3.438	2.840	2.834	2.617	2.626	2.249	2.245	2.109	2.447	2.116	2.112	1.994
	0.10	0.05	0.20		2.503	2.495	2.462	2.459	1.817	1.812	1.790	1.789	1.672	1.667	1.648	1.646
			0.40		2.552	2.545	2.518	2.516	2.069	2.065	2.048	2.047	1.960	1.956	1.942	1.940
		0.20	0.20		2.683	2.556	2.524	2.480	1.934	1.852	1.831	1.802	1.777	1.703	1.684	1.658
			0.40		2.701	2.596	2.569	2.533	2.162	2.096	2.080	2.057	2.040	1.983	1.969	1.949
		0.50	0.20		3.536	2.878	2.849	2.594	2.493	2.062	2.043	1.876	2.278	1.891	1.874	1.725
			0.40		3.463	2.869	2.843	2.627	2.643	2.267	2.251	2.116	2.461	2.131	2.118	2.000

(a) df_m = degrees of freedom for property-composition model (see Appendix A), n = the number of sampling times over a waste type, m = the number of samples at each sampling time, and r = the number of chemical analyses per sample.

(b) $\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$ are as defined in Section 3.4.

Table 4.5. 99%/99% Upper Tolerance Interval Half-Width Values Without Adjustment for Nuisance Uncertainties (cont'd)

			(a)	df_m	40	40	40	40	40	40	40	40	40	40	40	40
				n	10	10	10	10	30	30	30	30	50	50	50	50
(b)				m	1	1	3	3	1	1	3	3	1	1	3	3
$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\bar{\hat{\sigma}}_m$	r	1	3	1	3	1	3	1	3	1	3	1	3
0.10	0.05	0.05	0.20		0.806	0.791	0.778	0.773	0.725	0.716	0.707	0.704	0.706	0.698	0.690	0.687
			0.40		1.439	1.434	1.429	1.427	1.337	1.334	1.330	1.329	1.312	1.309	1.306	1.305
		0.20	0.20		1.144	0.903	0.887	0.808	0.940	0.787	0.777	0.727	0.892	0.759	0.751	0.707
			0.40		1.579	1.475	1.469	1.440	1.430	1.362	1.358	1.338	1.393	1.334	1.331	1.313
		0.50	0.20		2.499	1.495	1.483	1.020	1.813	1.165	1.157	0.861	1.667	1.090	1.083	0.823
			0.40		2.511	1.771	1.763	1.523	2.024	1.552	1.547	1.393	1.910	1.499	1.495	1.362
	0.10	0.05	0.20		0.872	0.857	0.799	0.794	0.768	0.758	0.721	0.718	0.742	0.734	0.702	0.699
			0.40		1.463	1.458	1.436	1.434	1.354	1.350	1.335	1.334	1.327	1.324	1.311	1.310
		0.20	0.20		1.208	0.971	0.910	0.830	0.982	0.831	0.792	0.741	0.928	0.797	0.763	0.719
			0.40		1.611	1.503	1.478	1.448	1.450	1.380	1.364	1.343	1.411	1.350	1.336	1.318
		0.50	0.20		2.536	1.551	1.501	1.042	1.837	1.201	1.169	0.876	1.688	1.121	1.093	0.836
			0.40		2.543	1.805	1.775	1.533	2.044	1.574	1.555	1.400	1.927	1.518	1.501	1.367
0.25	0.05	0.05	0.20		1.271	1.257	1.243	1.239	1.022	1.013	1.004	1.001	0.964	0.956	0.948	0.945
			0.40		1.644	1.637	1.629	1.627	1.471	1.466	1.462	1.460	1.429	1.425	1.421	1.420
		0.20	0.20		1.563	1.360	1.346	1.274	1.209	1.078	1.070	1.023	1.128	1.013	1.006	0.965
			0.40		1.813	1.692	1.684	1.645	1.579	1.502	1.497	1.472	1.522	1.456	1.451	1.430
		0.50	0.20		2.749	1.858	1.848	1.459	1.976	1.398	1.392	1.142	1.813	1.297	1.291	1.070
			0.40		2.726	2.011	2.004	1.750	2.161	1.705	1.700	1.538	2.030	1.631	1.627	1.487
	0.10	0.05	0.20		1.333	1.319	1.264	1.260	1.061	1.053	1.018	1.015	0.998	0.991	0.960	0.957
			0.40		1.677	1.670	1.640	1.638	1.492	1.488	1.469	1.467	1.447	1.443	1.427	1.426
		0.20	0.20		1.617	1.419	1.366	1.294	1.243	1.116	1.083	1.037	1.159	1.047	1.017	0.977
			0.40		1.847	1.726	1.696	1.656	1.601	1.523	1.504	1.479	1.541	1.474	1.458	1.436
		0.50	0.20		2.783	1.906	1.864	1.478	1.998	1.429	1.402	1.154	1.833	1.324	1.300	1.080
			0.40		2.756	2.045	2.015	1.761	2.180	1.727	1.707	1.546	2.047	1.650	1.634	1.494
0.50	0.05	0.05	0.20		2.461	2.453	2.444	2.441	1.788	1.783	1.777	1.776	1.645	1.640	1.635	1.634
			0.40		2.480	2.473	2.466	2.464	2.004	1.999	1.995	1.993	1.892	1.888	1.884	1.883
		0.20	0.20		2.644	2.515	2.507	2.463	1.908	1.824	1.818	1.789	1.752	1.677	1.672	1.646
			0.40		2.635	2.525	2.518	2.481	2.103	2.033	2.028	2.005	1.979	1.918	1.914	1.893
		0.50	0.20		3.507	2.842	2.835	2.578	2.473	2.037	2.032	1.864	2.260	1.868	1.863	1.713
			0.40		3.417	2.808	2.801	2.578	2.604	2.214	2.209	2.067	2.422	2.077	2.073	1.947
	0.10	0.05	0.20		2.499	2.490	2.457	2.454	1.813	1.807	1.786	1.784	1.667	1.662	1.643	1.641
			0.40		2.511	2.504	2.476	2.474	2.024	2.019	2.002	2.000	1.910	1.906	1.890	1.889
		0.20	0.20		2.679	2.552	2.519	2.475	1.930	1.848	1.826	1.797	1.772	1.698	1.679	1.653
			0.40		2.666	2.556	2.529	2.492	2.122	2.053	2.035	2.011	1.996	1.935	1.920	1.899
		0.50	0.20		3.534	2.875	2.846	2.590	2.491	2.058	2.039	1.872	2.276	1.887	1.870	1.720
			0.40		3.442	2.837	2.811	2.589	2.620	2.232	2.216	2.073	2.437	2.093	2.079	1.953

(a) df_m = degrees of freedom for property-composition model (see Appendix A), n = the number of sampling times over a waste type, m = the number of samples at each sampling time, and r = the number of chemical analyses per sample.

(b) $\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$ are as defined in Section 3.4.

Table 4.6. 99%/99% Upper Tolerance Interval Half-Width Values
With Adjustment for Nuisance Uncertainties

			(a)	df_m	20	20	20	20	20	20	20	20	20	20	20	20
				n	10	10	10	10	30	30	30	30	50	50	50	50
(b)				m	1	1	3	3	1	1	3	3	1	1	3	3
$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\bar{\hat{\sigma}}_m$	r	1	3	1	3	1	3	1	3	1	3	1	3
0.10	0.05	0.05	0.20		0.456	0.454	0.452	0.452	0.378	0.379	0.380	0.380	0.357	0.359	0.361	0.361
			0.40		0.606	0.605	0.605	0.605	0.472	0.473	0.473	0.473	0.434	0.434	0.435	0.435
		0.20	0.20		0.523	0.473	0.470	0.456	0.392	0.378	0.378	0.378	0.358	0.353	0.353	0.357
			0.40		0.626	0.610	0.609	0.606	0.472	0.471	0.471	0.472	0.428	0.430	0.431	0.433
		0.50	0.20		0.787	0.596	0.593	0.497	0.505	0.420	0.419	0.384	0.437	0.376	0.375	0.354
			0.40		0.799	0.660	0.659	0.617	0.538	0.482	0.482	0.471	0.468	0.431	0.431	0.428
	0.10	0.05	0.20		0.467	0.464	0.455	0.454	0.378	0.378	0.379	0.379	0.354	0.354	0.358	0.359
			0.40		0.608	0.608	0.605	0.605	0.471	0.471	0.472	0.473	0.431	0.432	0.434	0.434
		0.20	0.20		0.537	0.487	0.475	0.460	0.397	0.381	0.379	0.378	0.361	0.353	0.353	0.356
			0.40		0.631	0.614	0.610	0.606	0.474	0.471	0.471	0.472	0.428	0.429	0.430	0.433
		0.50	0.20		0.794	0.607	0.597	0.502	0.508	0.425	0.421	0.385	0.439	0.379	0.376	0.354
			0.40		0.805	0.666	0.661	0.618	0.541	0.484	0.483	0.471	0.469	0.432	0.431	0.428
0.25	0.05	0.05	0.20		1.029	1.025	1.021	1.019	0.819	0.818	0.817	0.817	0.770	0.770	0.770	0.770
			0.40		1.061	1.060	1.059	1.059	0.901	0.901	0.902	0.902	0.859	0.860	0.861	0.861
		0.20	0.20		1.110	1.054	1.050	1.030	0.843	0.826	0.825	0.819	0.781	0.772	0.772	0.770
			0.40		1.092	1.069	1.068	1.061	0.897	0.899	0.899	0.901	0.847	0.854	0.855	0.859
		0.50	0.20		1.371	1.183	1.181	1.082	0.944	0.868	0.867	0.834	0.849	0.796	0.796	0.776
			0.40		1.293	1.135	1.133	1.080	0.953	0.904	0.903	0.897	0.868	0.844	0.844	0.850
	0.10	0.05	0.20		1.047	1.043	1.027	1.025	0.824	0.823	0.819	0.818	0.772	0.771	0.770	0.770
			0.40		1.066	1.065	1.061	1.060	0.899	0.899	0.901	0.901	0.856	0.856	0.860	0.860
		0.20	0.20		1.124	1.071	1.056	1.036	0.847	0.830	0.826	0.821	0.783	0.774	0.773	0.771
			0.40		1.099	1.075	1.070	1.063	0.898	0.898	0.898	0.900	0.845	0.851	0.854	0.858
		0.50	0.20		1.377	1.195	1.185	1.087	0.947	0.873	0.869	0.835	0.851	0.799	0.797	0.777
			0.40		1.300	1.142	1.135	1.082	0.956	0.905	0.904	0.897	0.869	0.844	0.844	0.849
0.50	0.05	0.05	0.20		2.291	2.289	2.287	2.286	1.662	1.661	1.660	1.660	1.528	1.527	1.527	1.527
			0.40		2.039	2.037	2.035	2.034	1.634	1.634	1.633	1.633	1.539	1.539	1.539	1.539
		0.20	0.20		2.335	2.304	2.302	2.292	1.678	1.667	1.666	1.662	1.538	1.531	1.530	1.528
			0.40		2.084	2.053	2.051	2.040	1.645	1.637	1.637	1.634	1.542	1.540	1.540	1.539
		0.50	0.20		2.508	2.378	2.377	2.319	1.747	1.694	1.694	1.672	1.586	1.549	1.549	1.534
			0.40		2.294	2.133	2.132	2.068	1.710	1.659	1.658	1.641	1.576	1.548	1.548	1.541
	0.10	0.05	0.20		2.300	2.298	2.290	2.290	1.665	1.665	1.662	1.661	1.530	1.529	1.527	1.527
			0.40		2.049	2.046	2.038	2.038	1.636	1.636	1.634	1.634	1.540	1.540	1.539	1.539
		0.20	0.20		2.343	2.313	2.305	2.295	1.681	1.670	1.667	1.663	1.540	1.533	1.531	1.528
			0.40		2.093	2.062	2.054	2.043	1.647	1.639	1.637	1.635	1.543	1.540	1.540	1.539
		0.50	0.20		2.513	2.385	2.379	2.322	1.749	1.697	1.695	1.673	1.588	1.551	1.550	1.535
			0.40		2.300	2.142	2.134	2.071	1.713	1.661	1.659	1.642	1.577	1.549	1.548	1.541

(a) df_m = degrees of freedom for property-composition model (see Appendix A), n = the number of sampling times over a waste type, m = the number of samples at each sampling time, and r = the number of chemical analyses per sample.

(b) $\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$ are as defined in Section 3.4.

Table 4.6. 99%/99% Upper Tolerance Interval Half-Width Values With Adjustment for Nuisance Uncertainties (cont'd)

(b)			(a)	df_m	40	40	40	40	40	40	40	40	40	40	40	40
				n	10	10	10	10	30	30	30	30	50	50	50	50
				m	1	1	3	3	1	1	3	3	1	1	3	3
$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\bar{\hat{\sigma}}_m$	r	1	3	1	3	1	3	1	3	1	3	1	3
0.10	0.05	0.05	0.20		0.436	0.433	0.429	0.428	0.357	0.356	0.356	0.356	0.335	0.335	0.335	0.335
			0.40		0.572	0.571	0.570	0.570	0.440	0.440	0.440	0.440	0.401	0.401	0.401	0.401
		0.20	0.20		0.516	0.459	0.455	0.436	0.385	0.364	0.363	0.357	0.350	0.338	0.337	0.335
			0.40		0.603	0.580	0.579	0.573	0.451	0.443	0.443	0.441	0.406	0.402	0.402	0.401
		0.50	0.20		0.786	0.592	0.590	0.487	0.504	0.417	0.416	0.374	0.436	0.372	0.372	0.343
			0.40		0.792	0.644	0.642	0.591	0.533	0.468	0.467	0.447	0.463	0.417	0.417	0.404
	0.10	0.05	0.20		0.452	0.448	0.434	0.433	0.362	0.361	0.357	0.357	0.337	0.336	0.335	0.335
			0.40		0.578	0.577	0.572	0.571	0.442	0.442	0.440	0.440	0.402	0.402	0.401	0.401
		0.20	0.20		0.530	0.476	0.461	0.442	0.391	0.370	0.365	0.359	0.354	0.341	0.338	0.335
			0.40		0.610	0.586	0.581	0.574	0.454	0.445	0.443	0.441	0.408	0.403	0.402	0.401
		0.50	0.20		0.793	0.604	0.594	0.492	0.507	0.422	0.418	0.376	0.438	0.376	0.373	0.345
			0.40		0.798	0.651	0.645	0.593	0.536	0.471	0.468	0.448	0.464	0.419	0.417	0.404
0.25	0.05	0.05	0.20		1.014	1.010	1.005	1.004	0.803	0.802	0.800	0.800	0.753	0.752	0.751	0.751
			0.40		1.014	1.012	1.010	1.010	0.849	0.849	0.849	0.848	0.804	0.804	0.805	0.805
		0.20	0.20		1.102	1.042	1.038	1.015	0.834	0.813	0.811	0.804	0.772	0.758	0.757	0.753
			0.40		1.057	1.026	1.024	1.014	0.860	0.852	0.851	0.849	0.807	0.804	0.804	0.804
		0.50	0.20		1.369	1.179	1.176	1.072	0.943	0.864	0.863	0.823	0.848	0.791	0.790	0.765
			0.40		1.282	1.109	1.107	1.041	0.943	0.877	0.876	0.855	0.856	0.815	0.814	0.805
	0.10	0.05	0.20		1.034	1.030	1.012	1.010	0.810	0.809	0.803	0.802	0.757	0.756	0.752	0.752
			0.40		1.022	1.020	1.013	1.012	0.851	0.850	0.849	0.849	0.804	0.804	0.804	0.804
		0.20	0.20		1.116	1.060	1.044	1.022	0.840	0.819	0.814	0.806	0.775	0.762	0.759	0.754
			0.40		1.066	1.035	1.027	1.017	0.863	0.854	0.852	0.850	0.808	0.805	0.804	0.804
		0.50	0.20		1.376	1.190	1.180	1.078	0.946	0.868	0.864	0.825	0.850	0.794	0.791	0.766
			0.40		1.288	1.117	1.110	1.044	0.945	0.880	0.877	0.856	0.858	0.816	0.815	0.805
0.50	0.05	0.05	0.20		2.287	2.285	2.283	2.282	1.658	1.657	1.656	1.656	1.523	1.522	1.522	1.522
			0.40		2.008	2.006	2.003	2.003	1.600	1.599	1.598	1.598	1.502	1.501	1.501	1.501
		0.20	0.20		2.331	2.300	2.298	2.287	1.674	1.663	1.662	1.658	1.535	1.526	1.526	1.523
			0.40		2.058	2.023	2.021	2.008	1.617	1.605	1.604	1.600	1.511	1.504	1.504	1.502
		0.50	0.20		2.507	2.376	2.374	2.315	1.746	1.692	1.691	1.668	1.585	1.547	1.546	1.530
			0.40		2.281	2.111	2.109	2.040	1.698	1.635	1.634	1.611	1.562	1.522	1.522	1.508
	0.10	0.05	0.20		2.296	2.294	2.286	2.285	1.661	1.660	1.657	1.657	1.525	1.525	1.523	1.523
			0.40		2.018	2.016	2.007	2.006	1.603	1.603	1.600	1.599	1.504	1.503	1.502	1.501
		0.20	0.20		2.339	2.309	2.301	2.290	1.678	1.666	1.663	1.659	1.537	1.529	1.527	1.524
			0.40		2.068	2.033	2.024	2.012	1.620	1.608	1.605	1.601	1.513	1.506	1.505	1.502
		0.50	0.20		2.512	2.383	2.376	2.318	1.748	1.695	1.692	1.670	1.587	1.549	1.547	1.531
			0.40		2.288	2.120	2.112	2.043	1.700	1.638	1.635	1.612	1.564	1.524	1.522	1.508

(a) df_m = degrees of freedom for property-composition model (see Appendix A), n = the number of sampling times over a waste type, m = the number of samples at each sampling time, and r = the number of chemical analyses per sample.

(b) $\hat{\sigma}_g$, $\hat{\sigma}_s$, $\hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$ are as defined in Section 3.4.

The UTIHW values in Tables 4.3 to 4.6 can be used to answer several questions of interest. The questions of interest and their answers follow.

1. What is the benefit to using the approach that adjusts X%/Y% UTIHWs for nuisance uncertainties compared to the approach that does not adjust for nuisance uncertainties? The adjusted 95%/95% UTIHWs in Table 4.4 range from 6.3% to 75.5% smaller than the corresponding unadjusted 95%/95% UTIHWs in Table 4.3. The adjusted 99%/99% UTIHWs in Table 4.6 range from 6.5% to 76.2% smaller than the corresponding unadjusted 99%/99% UTIHWs in Table 4.5. Hence, there can be substantial benefit to adjusting UTIHWs (and thus UTIs) for nuisance uncertainties.

2. Is there practical value to collecting replicate samples at each sampling time over a waste type and/or performing replicate chemical analyses of samples? If so, under what conditions? The primary value of replicate samples and replicate analyses per sample (i.e., $m > 1$ and/or $r > 1$) comes from reducing the sampling and analytical nuisance uncertainties by averaging over replicate samples and/or analyses. Hence, $\hat{\sigma}_s^2$ and $\hat{\sigma}_a^2$ are reduced to $\hat{\sigma}_s^2/m$ and $\hat{\sigma}_a^2/rm$, which reduces $\tilde{\sigma}$. When $\tilde{\sigma}$ is reduced: (i) unadjusted UTIHW = $k_0\tilde{\sigma}$ values will always be reduced, and (ii) adjusted UTIHW = $k_1\tilde{\sigma}$ values will generally be reduced except in a few cases when k_1 increases more than $\tilde{\sigma}$ decreases. When unadjusted and adjusted UTIHWs are reduced, the reduction may vary from negligible to substantial depending on the values of $\hat{\sigma}_s^2$, $\hat{\sigma}_a^2$, m, and r. Table 4.7 summarizes the ranges of percentage reductions of unadjusted and adjusted UTIHWs for the cases: (i) $m = 1$, $r = 3$, (ii) $m = 3$, $r = 1$, and (iii) $m = 3$, $r = 3$ compared to the case $m = 1$, $r = 1$.

Table 4.7. Minimum and Maximum Percentage Reductions in Unadjusted and Adjusted X%/Y% UTIHWs for $m > 1$ and/or $r > 1$ Compared to $m = 1$ and $r = 1$

		Unadjusted for Nuisance Uncertainties		**Adjusted for Nuisance Uncertainties**	
m	***r***	**Min %**	**Max %**	**Min %**	**Max %**
1	3	0.19	37.4	-0.08	23.0
3	1	0.38	38.0	-0.21	23.5
3	3	0.45	55.4	-0.26	35.0

Table 4.7 shows that having $m > 1$ and/or $r > 1$ can reduce unadjusted X%/Y% UTIHWs by up to 55%, and adjusted X%/Y% UTIHWs by up to 35%. In a few cases when $m > 1$ and/or $r > 1$, adjusted X%/Y% UTIHWs can be slightly larger than when $m = 1$ and $r = 1$ (indicated by the negative minimum percentage reduction values). In almost all cases, however, choosing $m > 1$ and/or $r > 1$ reduces adjusted X%/Y% UTIHWs.

As expected, the reduction in UTIHW values is greatest when the nuisance uncertainties reduced by replication ($\hat{\sigma}_s^2$ and $\hat{\sigma}_a^2$) take larger values. For example, consider the adjusted 95%/95% UTIHW values listed on the second page of Table 4.4 for $\hat{\sigma}_g = 0.10$, $\hat{\sigma}_s = 0.10$,

$\hat{\sigma}_a = 0.50$, $\hat{\sigma}_m = 0.20$, $df_m = 40$, and $n = 10$. The adjusted 95%/95% UTIHW value is reduced from 0.510 when $m = 1$ and $r = 1$, to: (i) 0.396 when $m = 1$ and $r = 3$, (ii) 0.390 when $m = 3$ and $r = 1$, and (iii) 0.331 when $m = 3$ and $r = 3$. Note that $m = 3$ and $r = 1$ will almost always yield a reduction in UTIHW at least as large as $m = 1$ and $r = 3$. With the former, both $\hat{\sigma}_s^2$ and $\hat{\sigma}_a^2$ are reduced by a factor of 3, whereas with the latter only $\hat{\sigma}_a^2$ is reduced by a factor of 3. Having both $m = 3$ and $r = 3$ reduces UTIHW still further, but the reduction is much smaller, and may not be worth the extra sampling and chemical analysis costs.

Whether it will be necessary to choose $m > 1$ and/or $r > 1$ in order to demonstrate compliance with PCT specifications will depend on the target PCT releases, magnitudes of variations and uncertainties, and other aspects for each HLW and LAW waste type. However, if the PCT target values for a waste type are substantially below the specification limits, and variation over a waste type and nuisance uncertainties do not eliminate too much of the margins, it may be sufficient to choose $m = 1$ and/or $r = 1$ to demonstrate compliance over a waste type. This situation is likely to be the case for the IHLW PCT specification (WAPS 1.3), where the target PCT releases are expected to be up to an order of magnitude below the specification limits.

3. <u>Does removing (subtracting) sampling and analytical nuisance uncertainties substantially reduce the size of UTIHWs? If so, under what conditions?</u> It is important to keep in mind that if it is possible to subtract sampling and/or analytical nuisance uncertainties, it is the reduced versions ($\hat{\sigma}_s^2/m$ and $\hat{\sigma}_a^2/rm$) that are being subtracted. Hence, if $m > 1$ and/or $r > 1$, the potential is less to benefit from subtracting nuisance uncertainties because they will have been reduced already. However, this issue ends up being irrelevant, because subtracting nuisance uncertainties never yields smaller UTIHWs than when UTIHWs are adjusted for nuisance uncertainties without subtracting nuisance uncertainties (see Sections H.3 and H.4 of Appendix H).

4. <u>How many sampling times over a waste type are required (i.e., what value of *n* should be selected)?</u> This question cannot be answered for the RPP-WTP IHLW and ILAW plants at this time because the answer depends on: (i) specifics of compliance strategies, (ii) magnitudes of variations over waste types, (iii) magnitudes of sampling and analytical uncertainties, (iv) property-composition models and prediction uncertainties, and (v) the target values of PCT releases for each waste type, among other things. However, because target values for PCT releases are expected to be substantially below specification limits, as few as 10 to 20 sampling times over a waste type (or other shorter period of production) may be sufficient to demonstrate compliance with the PCT specifications for IHLW and ILAW, as discussed in Section 1.1.

5. <u>Which input parameters have the most influence on the values of UTIHWs and which have the least influence?</u> For the adjusted UTIHWs in Tables 4.4 and 4.6, the parameters with the most influence on the magnitudes of UTIHWs are $\hat{\sigma}_g$, *m*, *n*, $\hat{\sigma}_a$, and *r*, and the parameters with the least influence are df_m, $\hat{\sigma}_s$, and $\overline{\sigma}_m$. Keep in mind that these conclusions are based on the ranges the parameters were varied over (as listed in Table 4.1). As an example, $\hat{\sigma}_g$

took three values over a relatively wide range and is the source of variation of interest in constructing UTIs. Hence, it is not surprising it has the largest influence on UTIHWs. As another example, $\hat{\sigma}_s$ took only two values over a small range, so it is not surprising that it was one of the least influential parameters. It makes sense that df_m and $\bar{\hat{\sigma}}_m$ are among the least influential parameters, because model uncertainty cannot be reduced as can sampling and analytical uncertainties. Hence, model uncertainty contributes to the magnitude of every UTIHW, although the ranges of values considered for df_m and $\hat{\sigma}_m$ did not have a large impact on the magnitudes of UTIHWs.

6. <u>How do the values of *k* compare to 2 (which is based on the "two standard deviations" mentioned in WAPS 1.3)?</u> Table 4.8 lists the minimum and maximum k and k^* values (see Section 3.6) associated with the 95%/95% and 99%/99% adjusted and unadjusted UTIHWs listed in Tables 4.3 to 4.6. As described in Section 3.6, some k_1 values corresponding to adjusted UTIHWs are much smaller than the theoretical minimum tolerance multiplier values of 1.645 for 95%/95% UTIs and 2.327 for 99%/99% UTIs. However, these theoretical minimums are actually k^* values using the notation introduced in Section 3.6. Table 4.8 summarizes the minimum and maximum k^* values corresponding to the UTIHWs in Tables 4.3 to 4.6. The minimum k^* values are all larger than the theoretical minimum values, sometimes much larger. For adjusted 95%/95% UTIHWs, k^* has a minimum of 2.038, which is slightly larger than the "two standard deviations" mentioned in WAPS 1.3. For adjusted 99%/99% UTIHWs, k^* has a minimum of 3.002, which is well above the "two standard deviations" mentioned in WAPS 1.3. The fact that the maximum k^* values for the adjusted 95%/95% UTIHWs are significantly greater than 2.0 indicates that, in some situations, the "two standard deviations" mentioned in WAPS 1.3 would provide far less than 95% confidence that at least 95% of the IHLW produced during a waste type would satisfy the specification. Hence, the adjusted X%/Y% UTI approach recommended in Section 3.7 is preferred over the "two standard deviation" approach. The adjusted X%/Y% UTI approach has been developed to achieve the minimum acceptable values of X and Y chosen by the RPP-WTP Project. However, as noted previously and discussed in more detail in Section 6.6, additional work is required to verify that the adjusted X%/Y% UTI approach achieves its nominal X and Y values.

Table 4.8. Minimum and Maximum Values of k and k^* for 95%/95% and 99%/99% UTIHWs in Tables 4.3 to 4.6

Method	95%/95% UTIHWs				99%/99% UTIHWs			
	k		k^*		k		k^*	
	Min	Max	Min	Max	Min	Max	Min	Max
Unadjusted	1.986	2.803	2.185	16.377	2.934	4.768	3.267	25.822
Adjusted	0.493	2.548	2.038	5.396	0.708	4.238	3.002	8.046

5.0 Example Illustrating Use of the X%/Y% Upper Tolerance Interval Formula to Demonstrate Compliance

Actual representative data are not available to illustrate calculating an X%/Y% UTI to demonstrate compliance over a waste type. Instead, a simulated data set of predicted PCT boron release values was constructed and used to illustrate the tolerance interval approach to demonstrating compliance over a waste type. The example with simulated data uses an X%/Y% UTI adjusted for nuisance uncertainties (see Section 3.7) to demonstrate that IHLW produced from a hypothetical HLW waste type complies with the WAPS 1.3 PCT normalized boron release specification for IHLW (DOE 1996).

5.1 Description of the Simulated Data Set

The Minitab software package (Minitab 2000) was used to generate a set of simulated predicted $\ln(r_B^{PCT})$ values. The simulated data were constructed to follow a nested design structure with n = 10 sampling times over glass produced from a waste type, m = 2 samples per sampling time, and r = 2 chemical analyses per sample. Thus, a total of 40 predicted $\ln(r_B^{PCT})$ values were generated.[a] The details of how the simulated data were generated are discussed in the following paragraph. The example problem also required a hypothetical value for the degrees of freedom for the $\ln(r_B^{PCT})$ property-composition model, which was chosen to be df_m = 40 (an option considered earlier in Table 4.1). The df_m value is hypothetical in that no property-composition model was actually used. During the time the major part of this work was performed, the RPP-WTP Project had not publicly released any PCT (or VHT) property-composition models[b], and use of a model developed outside the project was considered inappropriate. Hence, $\ln(r_B^{PCT})$ model predicted values were simulated directly.

The predicted $\ln(r_B^{PCT})$ values were produced using Minitab capabilities for generating normal (Gaussian) distribution random deviates. Specifically, data were generated according to the nested model:

$$\ln(r_B^{PCT})_{\mathrm{ijk}} = \mathrm{mean} + g_i + s_{j(i)} + a_{k(ij)} \tag{5.1}$$

where mean = -0.51 ln (g/m^2) and each variation and uncertainty term has a normal distribution with mean zero and standard deviation [denoted N(0, σ)] as follows: $g_i \sim$ N(0, 0.25), $s_{j(i)} \sim$ N(0, 0.05), and $a_{k(ij)} \sim$ N(0, 0.20). The target values for the standard deviations of g, s, and a (σ_g, σ_s,

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[a] The values n = 10, m = 2, and r = 2 have no special significance. We wanted to keep the simulated data set relatively small, and include replicate samples and chemical analyses, so these values of n, m, and r were selected. There is insufficient information at this time to select the values of n, m, and r to be used in the RPP-WTP IHLW and ILAW vitrification facilities.

[b] Preliminary PCT, VHT, and other models for IHLW and ILAW are available in documents by Gan and Pegg (2001a) and Gan and Pegg (2001b), but these documents became available only after the work and report were substantially completed.

and σ_a) were chosen from the values used earlier in Table 4.1. Ideally, (5.1) should also contain a term representing random prediction errors from a fitted $\ln(r_B^{PCT})$ property-composition model. However, prediction errors made with a given property-composition model will have certain correlations, depending on the magnitude of variation over a waste type and magnitudes of sampling and analytical uncertainties. There was insufficient information to simulate model prediction errors with the proper correlation structure, so prediction errors were not generated and included in the simulated $\ln(r_B^{PCT})$ values resulting from (5.1). However, an assumed model prediction uncertainty value of $\bar{\hat{\sigma}}_m$ = 0.20 was used to calculate X%/Y% UTIs.

Based on applying statistical variance propagation methods, the target total standard deviation for the simulated data was 0.3240 ln(g/m^2) using the formula $\sqrt{\hat{\sigma}_g^2 + \hat{\sigma}_s^2 + \hat{\sigma}_a^2}$, or 0.2784 ln(g/m^2) using the formula that incorporates reductions $\sqrt{\hat{\sigma}_g^2 + \frac{\hat{\sigma}_s^2}{m} + \frac{\hat{\sigma}_a^2}{rm}}$. As discussed at the end of Section 3.2, this standard deviation in ln(g/m^2) units may be interpreted as approximately the relative standard deviation in g/m^2 units. Hence, in original PCT normalized boron release units, the target mean was 0.60 g/m^2, while the total and reduced total standard deviations were 0.19 and 0.16 g/m^2, respectively. These target values for mean and standard deviation were considered feasible based on past experience.

The data set of 40 simulated predicted $\ln(r_B^{PCT})$ values generated by Minitab is listed in Table 5.1. This set of values has a mean of –0.6070 ln(g/m^2) and a total standard deviation of 0.3333 ln(g/m^2)[(a)] using the formula without reductions and 0.3010 using the formula that incorporates reductions. These statistics in ln(g/m^2) units translate to a mean, total standard deviation, and reduced total standard deviation in original units of 0.5450, 0.182, and 0.164 g/m^2, respectively. The histogram of the data in Figure 5.1 indicates the simulated data do approximate a normal distribution. Normality was an assumption made in developing the X%/Y% UTI methodology presented in Section 3 (also see Appendix H).

[(a)] The total standard deviation was obtained by first estimating the separate variance components, then summing the separate estimates and taking the square root.

Table 5.1. Simulated Predicted ln(PCT Boron Releases)

Glass	Sample	Analysis	Predicted $\ln(r_B^{PCT})$
1	1	1	-0.73003
1	1	2	-0.91363
1	2	1	-0.86659
1	2	2	-1.08912
2	1	1	-0.23729
2	1	2	-0.28561
2	2	1	-0.17396
2	2	2	-0.28885
3	1	1	-0.47658
3	1	2	-0.74071
3	2	1	-0.63283
3	2	2	-0.66132
4	1	1	-0.70626
4	1	2	-0.25107
4	2	1	-0.28256
4	2	2	-0.32189
5	1	1	-0.65554
5	1	2	-0.13095
5	2	1	-0.56595
5	2	2	-0.46276
6	1	1	-0.51416
6	1	2	-0.26314
6	2	1	-0.18057
6	2	2	-0.11377
7	1	1	-1.15004
7	1	2	-0.99747
7	2	1	-0.85085
7	2	2	-0.93776
8	1	1	-0.46174
8	1	2	-0.30681
8	2	1	-0.34563
8	2	2	-0.43648
9	1	1	-1.06460
9	1	2	-0.82185
9	2	1	-1.09805
9	2	2	-1.12229
10	1	1	-0.69738
10	1	2	-0.77265
10	2	1	-0.59509
10	2	2	-1.07436

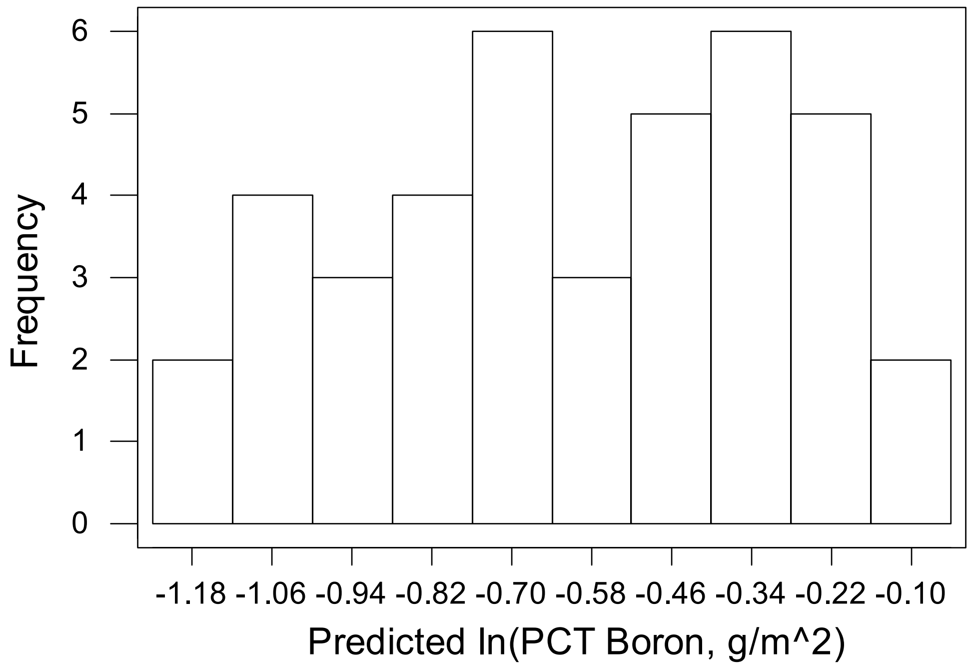

Figure 5.1. Histogram of Simulated Predicted $\ln(r_B^{PCT})$ Releases

5.2 X%/Y% UTI Results for the Simulated Example

The software package SAS (SAS 2001) was used to calculate UTIHWs from the 40 simulated predicted $\ln(r_B^{PCT})$ values listed in Table 5.1. The calculations were accomplished in two stages. First, a SAS program involving PROC NESTED (the first program in Section J.2 of Appendix J) was used to calculate the ANOVA mean squares associated with glass (over a waste type), samples, and analyses. As suggested by the name, PROC NESTED calculates mean squares according to the desired nested data structure. After the mean squares were calculated, another SAS program (the second program in Section J.2) was used to calculate the UTIHWs. The second program applies the formulas for the adjusted X%/Y% UTI approach recommended in Section 3.7 to the calculated mean squares values and to the input parameter values n, m, r, df_m, and $\bar{\hat{\sigma}}_m$ mentioned in Section 5.1. The second program calculates unadjusted and adjusted X%/Y% UTIs as discussed in Sections 3.6 and 3.7. X%/Y% UTIs were computed for X%/Y% = 95%/95%, 99%/99%, and the cases X*%/99% and 99%/Y*% so the UTI equals the limiting value of $\ln(r_B^{PCT\,EA}) = \ln(8.35) = 2.122$ for IHLW (obtained from Jantzen et al. 1993).

A printout from the first SAS program is given in Table 5.2. The printout was edited slightly to include the terminology used in this report, but none of the numerical results were edited. According to the SAS output, the calculated values for the mean squares are $MS_g = 0.355376$, $MS_s = 0.020090$, and $MS_a = 0.027234$. The SAS printout also indicates the

Table 5.2. Output from SAS Program to Calculate Mean Squares for Subsequent Use in Calculating X%/Y% UTIs

The SAS System

The NESTED Procedure

Coefficients of Expected Mean Squares

Source	glass	samples	analysis
glass	4	2	1
samples	0	2	1
analysis	0	0	1

Nested Random Effects Analysis of Variance for Variable ln(PCT-B)

Variance Source	DF	Sum of Squares	F Value	Pr > F	Error Term
Total	39	3.943964			
glass	9	3.198384	17.69	<.0001	samples
samples	10	0.200896	0.74	0.6825	analysis
analysis	20	0.544684			

Nested Random Effects Analysis of Variance for Variable ln(PCT-B)

Variance Source	Mean Square	Variance Component	Percent of Total
Total	0.101127	0.111056	100.0000
glass	0.355376	0.083822	75.4770
samples	0.020090	-0.003572	0.0000
analysis	0.027234	0.027234	24.5230

The NESTED Procedure

ln(PCT-B) Mean	-0.60695475
Standard Error of ln(PCT-B) Mean	0.09425709

ANOVA estimates for the sampling and analytical variance components are $\hat{\sigma}_s^2$ = -0.003572 and $\hat{\sigma}_a^2$ = 0.027234, respectively. Of course, variance estimates cannot be negative, but such a result can occur when trying to separately estimate variance components of different magnitudes based on limited data. Hence, the variance estimate for sampling must be set to zero. Other statistical methods for estimating variance components that do not yield negative values are available in the statistical literature and software, but are not considered in this report because the UTI results do not differ much from the ANOVA results after setting $\hat{\sigma}_s^2$ = 0.0.

The second, third, and fourth SAS programs in Section J.2 of Appendix J were used to calculate X%/Y% UTIs as previously described, and the results are given in Table 5.3. The first portion of Table 5.3 contains the results for X%/Y% = 95%/95% and 99%/99%. The second and third portions of the table contain the results when either X or Y is selected, then the achieved value of the other (Y or X) is calculated so that the UTI equals the specification limit (as discussed in Section 3.8). Because the simulated example is intended to involve IHLW, the specification limit for PCT boron release is 8.35 g/m^2 (WAPS 1.3 in DOE (1996), Jantzen 1993). The specification limit in natural logarithm units is ln(8.35) = 2.122 ln(g/m^2). Results in Table 5.3 are presented with and without adjustment for nuisance uncertainties as discussed in Section 3.7. The results in Table 5.3 include the calculated value of $\tilde{\sigma}$, the degrees of freedom f associated with $\tilde{\sigma}$, the multiplying factors k_1 and k_0, and the calculated X%/Y% UTI values. These values were obtained according to formulas (3.18) and (3.19) in Section 3.7.

The 95%/95% and 99%/99% UTIs in Table 5.3 have values in ln(g/m^2) units that are well below the specification limit for PCT boron release of 2.122 ln(g/m^2). The adjusted UTIs are noticeably smaller than the unadjusted UTIs, thus illustrating the value of the adjustment approach developed in this report. Table 5.3 also lists the X*%/Y% and X%/Y*% values yielding calculated UTIs equal to the ln(r_B^{PCT}) specification limit of 2.122. It was possible to select both X and Y as high as 99.99% and determine Y* and X* with values larger than 99.9%. Hence, in this simulated (but still realistic) example, there is at least 99.9% confidence that at least 99.9% of the IHLW produced from the waste type satisfies the boron release limit associated with WAPS 1.3.

Table 5.3. X%/Y% Upper Tolerance Intervals for Simulated Data

X	Y	Adjustment[a]	$\tilde{\sigma}$	f	k	UTI
Both X and Y Selected						
95	95	No	0.359	18.1	2.527	0.300
95	95	Yes	0.359	18.1	2.122	0.155
99	99	No	0.359	18.1	4.017	0.835
99	99	Yes	0.359	18.1	3.347	0.594
X Selected and Achieved Value of Y Determined						
99.99	99.931	No	0.359	18.1	7.603	2.122
99.99	99.996	Yes	0.359	18.1	7.603	2.122
Y Selected and Achieved Value of X Determined						
99.931	99.99	No	0.359	18.1	7.603	2.122
99.996	99.99	Yes	0.359	18.1	7.603	2.122

(a) *No* or *Yes* respectively indicates that the unadjusted approach or the adjusted approach discussed in Sections 3.6 and 3.7 was used.

The results in Table 5.3 represent just one example of the X%/Y% UTI calculation process. Other examples could be obtained using the SAS programs with other values for n, m, r, and df_m, as well as for $\hat{\sigma}_g, \hat{\sigma}_s, \hat{\sigma}_a$, and $\bar{\hat{\sigma}}_m$. This process would require that new simulated predicted $\ln(r_B^{PCT})$ data sets be generated according to appropriate data structures, as was done using Minitab for the example problem presented here.

5.3 Comparison to Other Statistical Intervals

Text in Section 1.2 generally describes why the X%/Y% UTI approach was chosen over the X% UCI and X% SUCI approaches. It is instructive to apply the latter two approaches to the simulated data in Table 5.1, and compare the resulting statistical intervals to the X%/Y% UTIs in Table 5.3. Specifically, we compare the adjusted and unadjusted 95%/95% UTIs to the 95% UCI and the 95% SUCI for the $n \times m \times r$ data structure described in Section 1.2.

The formula for an 95% UCI in this application is

$$95\%\ \mathrm{UCI} = \tilde{\mu} + t_{0.95}(f)\frac{\tilde{\sigma}}{\sqrt{n}}, \tag{5.2}$$

where $t_{0.95}(f)$ is the 95$^{\text{th}}$ percentile of Student's t-distribution with f degrees of freedom, $\tilde{\mu}$ is given by (3.7), and $\tilde{\sigma}$ is given by (3.13a). The degrees of freedom f is the same as given by formulas in Appendices D to G.

The formula for an 95% SUCI in this application is

$$95\%\ \mathrm{SUCI} = \bar{\hat{y}}_{i..} + \sqrt{pF_{0.90}(p, M-p)}\ \bar{\hat{\sigma}}_m, \tag{5.3}$$

where $F_{0.90}(p, M\text{-}p)$ is the 90$^{\text{th}}$ percentile of the F-distribution with p numerator degrees of freedom and $M\text{-}p$ denominator degrees of freedom, $\bar{\hat{y}}_{i..}$ is given by (3.6), and $\bar{\hat{\sigma}}_m$ is given by (3.13b). Recall that p is the number of parameters estimated in a release-composition model, and M is the number of data points used to estimate the parameters. Equation (5.3) is an adaptation of the two-sided formula given by Miller (1981, p. 111) that uses the notation in this report. Because a one-sided interval is desired, $F_{0.95}(p, M\text{-}p)$ in the two-sided formula given by Miller becomes $F_{0.90}(p, M\text{-}p)$ in (5.3). Finally, note that (5.3) does not explicitly depend on $\hat{\sigma}_g, \hat{\sigma}_s$, or $\hat{\sigma}_a$, because the SUCI theory does not address any underlying distribution associated with multiple model predictions. These standard deviations are accounted for indirectly in the SUCI formula through the variation and uncertainty in the $\bar{\hat{y}}_{i..}$ ($i = 1, 2, \ldots, n$) values.

An X% SUCI accounts for model uncertainty when making multiple predictions with a model. As seen in (5.3), the X% SUCI formula is highly dependent on the number of model parameters (p) estimated from data. As p increases, X% SUCI values increase. Hence, as p

increases, the potential for an X% SUCI to be larger than an X%/Y% UTI increases. For small p values, an X% SUCI may be close in magnitude to an X%/Y% UTI, depending on the values of X and Y. Ultimately, whether an X% SUCI is only slightly larger or much larger than an X%/Y% UTI depends on several parameters, especially $\bar{\hat{\sigma}}_m$, p, X, and Y.

Equation (5.3) provides 95% simultaneous confidence for UCIs on all possible predictions. However, in order to obtain a single SUCI value, we focus on the 95% simultaneous UCI (i.e., SUCI) corresponding to $\bar{\hat{y}}_{i..}(\text{largest})$. Here, $\bar{\hat{y}}_{i..}(\text{largest})$ denotes the largest of the $\bar{\hat{y}}_{1..}, \bar{\hat{y}}_{2..}, \ldots, \bar{\hat{y}}_{n..}$ and has corresponding uncertainty $\bar{\hat{\sigma}}_m$. Because there is no model for this example to compute $\bar{\hat{\sigma}}_m$ in (5.3), we use $\bar{\hat{\sigma}}_m = 0.20$ as was done for the X%/Y% UTI calculations in Section 5.2.

The formulas in (5.2) and (5.3) were applied to the simulated predicted PCT boron release values [in ln(g/m^2) units] given Table 5.1. Table 5.4 compares the 95% UCI and 95% SUCI values to the adjusted and unadjusted 95%/95% UTI values, assuming a PCT-composition model in terms of ln(g/m^2). Table 5.4 contains results for:

Case 1: $\tilde{\mu}$ = -0.6070 ln(g/m^2) as used in Sections 5.1 and 5.2

Case 2: $\tilde{\mu}$ = 1.3863 ln(g/m^2) corresponding to an untransformed mean PCT boron release value of 4.0 g/m^2.

Cases 1 and 2 allow comparing the values of the different statistical intervals for situations where there is either a small or large mean PCT boron release for glass produced from a waste type. The data for Case 2 were obtained by adding 1.3863 – (-0.6070) = 1.9933 to each predicted value in Table 5.1. Finally, recall that $n = 10$, $m = 2$, and $r = 2$ for this example.

Table 5.4 contains results for 95% SUCIs with $p = 2$ and $p = 15$ to illustrate how the value of p influences the magnitudes of 95% SUCIs. Models for PCT and VHT release models are expected to have at least 12 to 20 parameters estimated from data, so the results for $p = 15$ are more representative for WTP applications than the results for $p = 2$.

The statistical interval results in Table 5.4 show, for both Case 1 and Case 2:

- The 95% UCIs are much smaller than the unadjusted and adjusted 95%/95% UTIs.
- The unadjusted and adjusted 95%/95% UTIs are noticeably smaller than the 95% SUCIs with $p = 15$. These results illustrate how the magnitudes of X% SUCIs increase with increasing p in order to provide simultaneous X% confidence on an infinite number of model predictions.
- The 95% SUCIs with $p = 2$ are larger than the adjusted 95%/95% UTIs, but smaller than the unadjusted 95%/95% UTIs. However, the 95% SUCIs are much closer to the adjusted 95%/95% UTIs for $p = 2$ than for $p = 15$. This result occurs because a smaller multiplier in the SUCI formula is required to provide simultaneous confidence for an infinite number of model predictions when $p = 2$ compared to when $p = 15$.

Note for Case 2, the adjusted 95%/95% UTI = 2.148 is just barely less than the specification limit of $\ln(r_B^{PCT\ EA}) = 2.122$, while the unadjusted 95%/95% UTI = 2.293 is just barely above the specification limit. On the other hand, the 95% SUCI (p = 15) = 2.746 is well over the $\ln(r_B^{PCT\ EA}) = 2.122$ limit. Hence, the adjusted 95%/95% UTI would provide for demonstrating compliance over this hypothetical waste type, whereas the unadjusted 95%/95% UTI would not. The 95% SUCI with p = 15 would not provide for demonstrating compliance over this hypothetical waste type.

Table 5.4. Comparison of 95%/95% UTI, 95% UCI, and 95% SUCI Values

Statistical Interval	**Standard Deviation**	**Degrees of Freedom**	**Multiplier for $\tilde{\sigma}$** [(a)]	**Interval Value** [(b)]	**X%/Y% for Equivalent UTI** [(c)]	
					X	**Y***
Case 1: $\tilde{\mu}$ = -0.6070 ln(g/m^2) for 95%/95% UTI and 95% UCI, $\bar{\hat{y}}_{i..}$ (largest) = -0.2464 for 95% SUCI						
Adjusted 95%/95% UTI	$\tilde{\sigma} = 0.359$	$f = 18.1$	$k_1 = 2.122$	0.155	95	95
Unadjusted 95%/95% UTI	$\tilde{\sigma} = 0.359$	$f = 18.1$	$k_0 = 2.527$	0.300	95	97.93
95% UCI	$\tilde{\sigma} = 0.359$	$f = 18.1$	$t_{0.95}(f)/\sqrt{n} = 0.548$	-0.410	95	50.01
95% SUCI	$\bar{\hat{\sigma}}_m = 0.20$	$p = 15$ M-$p = 40$	$\sqrt{pF_{0.90}(p, M-p)} = 4.994$	0.752	95	99.94
95% SUCI	$\bar{\hat{\sigma}}_m = 0.20$	$p = 2$ M-$p = 40$	$\sqrt{pF_{0.90}(p, M-p)} = 2.209$	0.195	95	96.04
Case 2: $\tilde{\mu}$ = 1.3863 ln(g/m^2) for 95%/95% UTI and 95% UCI, $\bar{\hat{y}}_{i..}$ (largest) = 1.7469 for 95% SUCI						
Adjusted 95%/95% UTI	$\tilde{\sigma} = 0.359$	$f = 18.1$	$k_1 = 2.122$	2.148	95	95
Unadjusted 95%/95% UTI	$\tilde{\sigma} = 0.359$	$f = 18.1$	$k_0 = 2.527$	2.293	95	97.93
95% UCI	$\tilde{\sigma} = 0.359$	$f = 18.1$	$t_{0.95}(f)/\sqrt{n} = 0.548$	1.583	95	50.01
95% SUCI	$\bar{\hat{\sigma}}_m = 0.20$	$p = 15$ M-$p = 40$	$\sqrt{pF_{0.90}(p, M-p)} = 4.994$	2.746	95	99.94
95% SUCI	$\bar{\hat{\sigma}}_m = 0.20$	$p = 2$ M-$p = 40$	$\sqrt{pF_{0.90}(p, M-p)} = 2.209$	2.189	95	96.04

(a) $n = 10$, $t_{0.95}(18.1) = 1.734$, $F_{0.90}(15, 40) = 1.66$, $F_{0.90}(2, 40) = 2.44$.
(b) The 95%/95% UTI, 95% UCI, and 95% SUCI values are in terms of ln(g/m^2) values.
(c) The unadjusted 95%/95% UTI, 95% UCI, and 95% SUCI values were evaluated as if they were adjusted X%/Y% UTIs to see what Y* value (percent of glass produced from a waste type) is achieved for X = 95%.

The last column of Table 5.4 lists the Y* values that yield adjusted 95/Y* UTIs equal to the statistical intervals. Of course, Y* must be 95 for the adjusted 95%/95% UTIs, but will take different values for the unadjusted 95/Y* UTIs and the 95% UCIs and 95% SUCIs. For both Cases 1 and 2[(a)], the unadjusted 95%/95% UTI is equivalent to an adjusted 95%/97.93% UTI, with the 97.93% content larger than 95% as expected. The 95% UCI is equivalent to an adjusted

95%/50.01% UTI for Cases 1 and 2[a], with the 50.01% of glass from a waste type acceptable much smaller than 95%. This result is strong evidence that an X% UCI compliance strategy approach could be very hard to defend. For Cases 1 and 2[a], the 95% SUCI ($p = 15$) is equivalent to an adjusted 95%/99.94% UTI, with the 99.94% content larger than 95% as expected. This result illustrates the extent to which the X% SUCI approach yields stronger statistical interval statements when p is larger than does the X%/Y% UTI approach (as previously discussed in Section 1.2). Finally, the 95% SUCI ($p = 2$) is equivalent to an adjusted 95%/96.04% UTI for Cases 1 and 2[a], with the 96.04% content only somewhat larger than 95%. This result illustrates the extent to which the difference between adjusted X%/Y% UTIs and X% SUCIs decreases as p decreases.

[a] The Y* values are the same for Cases 1 and 2 of the unadjusted X%/Y% UTI, the X% UCI, and the X% SUCI because the data for the two cases differ only by the mean value.

6.0 Work and Inputs Needed for Future Application of the X%/Y% UTI Method and Relationships to Planned RPP-WTP Qualification Activities

The adjusted X%/Y% UTI methodology discussed in this report is proposed to demonstrate IHLW or ILAW produced from an HLW or LAW waste type complies with chemical durability specifications. The X%/Y% UTI methodology requires several inputs that must be developed by the RPP-WTP Project as part of qualification activities for IHLW and ILAW. Some of the inputs and subsequent applications of the tolerance interval methodology are to support other qualification activities, while other inputs and methodology applications are to support production activities. Subsections 6.1 to 6.5 discuss the inputs needed for future applications of the tolerance interval methodology developed in this report. Subsection 6.6 discusses the need to perform a simulation study to verify that the adjusted X%/Y% UTI approach and formulas provide the nominal values of X and Y.

6.1 Minimum Acceptable Values of X and Y for X%/Y% UTIs

Section 1.2 presented several steps of the general strategy for demonstrating, during production operations, that glass produced from a given HLW or LAW waste type complies with an IHLW or ILAW chemical durability specification. Step 7 involves calculating the values of X and Y that yield an X%/Y% UTI equal to the specification limit, and Step 8 involves reporting compliance was achieved. The RPP-WTP Project must decide on the minimum acceptable (i.e., defensible) values of X (% confidence) and Y (% of distribution of releases over a waste type that are less than or equal to a specification limit) for demonstrating compliance. It may be that X and Y must be at least 95 to be defensible to the RPP-WTP Project, DOE, and the public. However, the RPP-WTP Project expects to produce IHLW and ILAW that are more chemically durable than required by factors of 2 to 10 or more. Hence, values of X and Y considerably larger than 95 are likely to be obtained. Still, minimally acceptable values of X and Y must be selected as inputs to a qualification activity that will calculate sample sizes to be used during cold commissioning, hot commissioning, and production operations.

6.2 Estimates of Variations and Uncertainties to Determine Required Sample Sizes

As a part of qualification activities, the RPP-WTP Project will need to determine the

- number of times *n* during production of IHLW or ILAW from a given HLW or LAW waste type that the process or product must be sampled
- number of samples *m* to collect at a given sampling time
- number of chemical analyses *r* to perform on each sample

to demonstrate compliance with PCT and VHT specifications. Section 4 describes the results of calculating X%/Y% UTIHWs for various combinations of values of *n*, *m*, *r*, and other input parameters such as $\hat{\sigma}_g$, $\hat{\sigma}_s$, and $\hat{\sigma}_a$. Those calculations and results can be very helpful in assessing the consequences of possible sample sizes (*n*, *m*, and *r*) and possible magnitudes of variation and uncertainty components.

However, as part of qualification activities, the RPP-WTP Project must determine the values of $\hat{\sigma}_g$, $\hat{\sigma}_s$, and $\hat{\sigma}_a$ expected for IHLW and ILAW to be produced from each HLW and LAW waste type. These values can then be used to perform calculations with the X%/Y% UTI formulas and decide on the values of *n*, *m*, and *r* to use during IHLW and ILAW production operations. It is envisioned that these values of *n*, *m*, and *r* will be used during cold commissioning and hot commissioning to verify their adequacy. Then, either these values or updated values of *n*, *m*, and *r* will be used in production operations. Note the values of *n*, *m*, and *r* may or may not be different for different waste types depending on the values of input parameters such as of $\hat{\sigma}_g$, $\hat{\sigma}_s$, and $\hat{\sigma}_a$.

The estimates of $\hat{\sigma}_g$, $\hat{\sigma}_s$, and $\hat{\sigma}_a$ obtained during qualification activities will be useful for other purposes in addition to determining the required values of *n*, *m*, and *r*. For example, the variation and uncertainty estimates will also be used to make process control and compliance decisions during operation of the IHLW and ILAW facilities.

6.3 Sample Sizes

After the RPP-WTP Project has decided on the minimally defensible values of X and Y, and has estimated the magnitudes of variations and uncertainties relevant to the specific IHLW or ILAW compliance strategy, the recommended unadjusted X%/Y% UTI formulas presented in Equation (3.18) of Section 3.7 can be used to calculate sample sizes required during production operations for a given HLW or LAW waste type. These sample sizes include *n* sampling times over a waste type, *m* samples per sampling time, and *r* chemical analyses per sample. It is assumed these required sample sizes will be used during cold commissioning, and updated as needed for hot commissioning or subsequent production operations. In fact, sample size calculations will have to be periodically updated during production operations as magnitudes of variations or uncertainties change (either decrease or increase). Prior to final determination of sample sizes based on the unadjusted X%/Y% UTI approach and formulas, it will be necessary to perform a simulation study to verify that the approach provides the nominal values of X and Y. This subject is discussed further in Section 6.6.

<u>It is extremely important to realize that the sample sizes during production must be selected to satisfy several process control and reporting goals.</u> Demonstrating that IHLW or ILAW produced from a HLW or LAW waste type complies with chemical durability specifications is just one goal, involving reporting compliance. However, there are also process control aspects that are part of the compliance strategy, and process control aspects that are not part of the compliance strategy.

Table 6.1 summarizes in a general way how process and product samples collected during IHLW and ILAW production will be used to satisfy various process control and reporting needs. Table 6.1 is based on the current RPP-WTP compliance strategies for IHLW (CHG 2001a)[(a)] and ILAW (CHG 2001b). Additional explanation of the Table 6.1 information is provided in the following bullets.

- For IHLW, process samples will be used for the process control aspects of the compliance strategy (i.e., demonstrating each batch meets compliance specifications before sending it to the melter) and reporting aspects of the compliance strategy (i.e., demonstrating glass produced from a waste type meets specifications). Process samples during IHLW production will also be used for process control purposes not related to the compliance strategy (i.e., demonstrating each batch meets processing and other requirements not related to compliance specifications before sending the batch to the melter). Only limited IHLW product samples will be collected for confirmation purposes rather than as the primary compliance strategy.

- For ILAW, process samples will be used for process control aspects of the compliance strategy (i.e., demonstrating each batch meets compliance specifications before sending it to the melter) as well as other aspects not part of the compliance strategy (i.e., demonstrating each batch meets processing and other requirements not related to compliance specifications before sending the batch to the melter). Product samples will be used for the reporting aspects of the compliance strategy (i.e., demonstrating glass produced from a waste type meets specifications).

Ultimately, the numbers of process sampling times, samples per sampling time, and chemical analyses per sample will have to be sufficient to satisfy process control (compliance as well as other aspects) as well as reporting compliance goals.

Table 6.1. Goals to be Satisfied by Process and Product Samples for IHLW and ILAW

Goal of Samples	IHLW Samples		ILAW Samples	
	Process	Product	Process	Product
Process control aspects of the compliance strategy	X		X	
Reporting aspects of the compliance strategy	X			X
Process control aspects not part of the compliance strategy	X		X	
Confirmation (limited samples for secondary aspect of compliance strategy)		X		

[(a)] A revision to the IHLW compliance strategy has been developed by the RPP-WTP Project and reviewed by DOE/ORP, but the details remain to be finalized.

6.4 PCT- and VHT-Composition Databases and Models

As discussed in Section 1.2, models relating PCT and VHT releases to glass composition are required to implement the RPP-WTP Project strategy for complying with IHLW and ILAW chemical durability specifications during production operations. Hence, PCT-composition databases (for IHLW and ILAW) and VHT-composition databases (for ILAW) must be developed to cover the glass composition region(s) of interest for IHLW and ILAW. The RPP-WTP Project strategy envisions initially developing *global* property-composition databases and models over wider glass composition regions that apply to several or all HLW or LAW waste types. Then, as waste types and glass composition variation regions for the waste types become better defined, if needed the project will develop *local* property-composition databases for one or more waste types, from which more accurate models can be developed.

The number of data points M used to develop a property-composition model and the distribution of glass compositions over the composition region of interest impact the uncertainties of property-composition model predictions. Because the uncertainties of model predictions impact the width of X%/Y% UTIs, property data must be developed for a sufficient number of compositions covering the IHLW or ILAW region(s) of interest (either a global region or different local regions). The number and coverage of property-composition data points must be sufficient to develop models that yield accurate and sufficiently precise predicted property values over the region(s) for which data were collected. Statistical mixture experiment design methods (Cornell 1990) and software can be applied to: (i) assess how well existing property-composition data cover a composition region of interest, and (ii) select additional compositions for which property data should be obtained.

As part of the PCT-composition and VHT-composition model development efforts, it is extremely important that statistical lack-of-fit and model-validation methods be applied. The statistical theory leading to the vector-matrix equation for uncertainties of regression model predictions [see (A.6) in Appendix A] requires that the model not have a statistically significant lack-of-fit. This theory and vector-matrix equation for model predictions was utilized in developing the formula for an X%/Y% UTI. Any statistically significant lack-of-fits in PCT-composition or VHT-composition models will need to be investigated as to the effect on X%/Y% UTIs obtained using the formulas in this report. Historically, property-composition models for waste glass often explain large fractions of the variation in data used to develop and validate the models (e.g., R^2 and $R^2_{validation}$ values of 0.80 and higher). Despite these larger R^2 and $R^2_{validation}$ values, the models often have statistically significant lack-of-fits. This means that the model predictions differ from measured values for data points (test glasses and their property values) by more than can be explained by experimental variation and property measurement uncertainties. However, usually the case can be made that the model is practically useful despite the statistically significant lack-of-fit. In such a situation, it is important to assess whether the inflated model prediction uncertainties (due to lack-of-fit) obtained from the vector-matrix formula (A.6) are sufficient when used in the X%/Y% UTI formula to yield X%/Y% UTI values that provide close to the desired X%/Y% protection. After PCT-composition and VHT-composition models are available, statistical methods for checking model lack-of-fit and model-validation can be applied. If there is statistically significant lack-of-fit for a model, simulations should be performed to assess whether X%/Y% UTIs provide sufficient values of X%/Y% to demonstrate compliance with specification limits.

6.5 Bias Detection, Correction, and Adjustment Algorithms for Glass Compositions

It is envisioned that property-composition models falling in the general class of mixture experiment models (Cornell 1990) will be used for various aspects of the RPP-WTP compliance strategy, including calculating X%/Y% UTIs as discussed in this report. In mixture experiments, compositions $\boldsymbol{x}$ are traditionally expressed in terms of proportions of the components, so that $0 \leq x_i \leq 1$ and $\Sigma x_i = 1$. Although the results of chemical analyses of glass samples (or vitrified slurry samples) can be expressed in proportions (e.g., mass or mole fractions of oxides), the proportions do not sum exactly to 1. In some previous experiences involving chemical analyses of glasses during the same time period, the average value of Σx_i for a group was close to 1, suggesting no bias in glass composition analyses. However, in many other past experiences, the average value of Σx_i was enough below 1 (compared to the standard deviation of the Σx_i values) that it was clear the glass chemical analysis process was yielding biased results. For example, it is often difficult to completely dissolve all of the SiO_2 in the process for chemically analyzing glasses, so that SiO_2 analyzed values are often underestimated.

Hence, it is recommended that the RPP-WTP Project develop an approach for detecting biases in analyzed glass compositions. Bias detection involves: (i) analyzing a standard glass (with certified composition that is representative of the glass being produced and analyzed) along with the samples of IHLW or ILAW production glass, and (ii) statistically comparing the analyzed and certified compositions of the standard glass given the uncertainties in both compositions. In case a biased analyzed glass composition is detected, the RPP-WTP Project needs a procedure to decide between either bias correcting the analyzed composition, or discarding it and reanalyzing the composition. A bias-correction procedure would adjust the component proportions determined to have statistically significant biases, based on the statistical comparison of the analyzed and certified compositions of the representative standard glass.

Even if an analyzed glass composition is not biased, the sum of its proportions will generally not equal 1. Such imprecision in an analyzed glass composition can induce a bias in property predictions resulting from substituting the analyzed glass composition in property-composition models. Such models are developed with statistical mixture experiment modeling methods for data satisfying $\Sigma x_i = 1$. Deming (1964) showed that adjusting compositions so their proportions sum to 1 (or their percentages sum to 100) yields a more precise estimate of composition. Mandel (1964) illustrated the weighted-least-squares composition-adjustment approach proposed by Deming for a simple three-component alloy example. However, the method could be adapted for application to analyzed waste glass compositions comprised of many components.

In summary, the RPP-WTP Project should develop:

- Standard glasses (IHLW and ILAW) with certified compositions that are representative of the IHLW and ILAW to be produced.

- A procedure for detecting biases in analyzed glass compositions.

- A procedure for deciding between bias-correcting a biased analyzed glass composition or discarding it and reanalyzing the glass.

- A procedure for bias-correcting analyzed glass compositions that are biased but deemed correctable.

- A procedure for adjusting unbiased or bias-corrected analyzed glass compositions so that $\Sigma x_i = 1$ after the adjustments. Such adjusted analyzed glass compositions would then be ready for use in property-composition models.

A procedure addressing the above issues was under initial development by Battelle for the RPP-WTP Project at the time of the completion of this report.

6.6 Simulation Study to Verify X%/Y% UTI Performance

The theoretical development of the adjusted X%/Y% UTI approach in Appendix H is based on adaptation and extension of previous work in the statistical literature to develop tolerance intervals for special situations. In fact, some of this previous literature work adapted and extended work from still earlier literature on statistical tolerance intervals. It has been traditional in such literature to perform large simulation studies to verify that the newly developed tolerance interval method achieves the claimed values of X and Y. Such a large simulation study needs to be performed for the adjusted X%/Y% UTI approach, but was not included in the scope or budget for the work documented in this report. It is important that such a study be performed in the future to ensure that the adjusted X%/Y% UTI approach tentatively recommended in this report provides at least the nominal values of X and Y.

To verify the adjusted X%/Y% UTI approach achieves the claimed X and Y values, the simulation study ideally needs to simulate:

- the source of variation of interest (variation in glass compositions produced from a given waste type)
- sampling and chemical analysis uncertainties associated with obtaining estimates of IHLW or ILAW compositions during production
- the uncertainty related to developing and applying property-composition models used to predict chemical releases from IHLW or ILAW.

The first and second bullets involve generating simulated data sets of glass compositions corresponding to n sampling times over the course of an HLW or LAW waste type, $m \geq 1$

samples per sampling time, and $r \geq 1$ chemical analyses per sample. These steps are somewhat complicated, requiring non-trivial efforts to estimate the covariance structures associated with these three sources of variation and uncertainty in order to generate simulated multivariate glass compositions.

The third bullet involves simulating a property-composition data set and fitting the selected property-composition model form to that simulated data set. One approach is to use a resampling (sometimes called *bootstrap*) approach on the existing data set used to develop the property-composition model of interest. That is, the existing data set of M property-composition data points would be sampled with replacement to generate a set of M data points, which would then be used to fit the property-composition model form. A different kind of resampling (bootstrap) approach would work with the residuals from the given fitted model to generate a new simulated data set and model for each simulation. It is beyond the scope of this report to delve into the advantages and disadvantages of these two resampling approaches. Regardless of the approach chosen, the result would be a new, simulated property-composition model that reflects the uncertainty in the modeling process.

Finally, the new simulated model (third bullet) would be applied to the $n \times m \times r$ simulated IHLW or ILAW compositions (first and second bullets) to generate predicted release values. The adjusted X%/Y% UTI formulas would then be applied to the $n \times m \times r$ predicted release values to calculate adjusted X%/Y% UTIs. It would probably be sufficient to calculate 95%/95% and 99%/99% UTIs, and determine whether the claimed Y = 95 or 99 values are achieved for each simulation. This determination would be based on the assumed true distribution of releases for IHLW or ILAW produced from a given HLW or LAW waste type. We have tentatively outlined the general approach for developing the assumed true distribution for a given HLW or LAW waste type, but it is beyond the scope of this work to discuss the general approach and details.

The simulation process described in the preceding paragraphs would be repeated a large number of times (e.g., 5000). Hence, there would be a large number (e.g., 5000) of 95%/95% UTI values and 99%/99% UTI values. Each one of the 95%/95% UTI and 99%/99% UTI values will be either above or below the 95th percentile or 99th percentile of the assumed true release distribution for IHLW or ILAW produced from a waste type. If at least 95% of the 95%/95% UTIs are above the true 95th percentile, then the adjusted X%/Y% UTI approach will be verified for X = 95 and Y = 95. Similarly, if at least 99% of the 99%/99% UTIs are above the true 99th percentile, then the adjusted X%/Y% UTI approach will be verified for X = 99 and Y = 99. Verification of this sort for the 95/95 and 99/99 combinations should be sufficient to verify the performance of the adjusted X%/Y% UTI approach for RPP-WTP use.

Although the preceding discussion outlines our best current thoughts on the nature of the large simulation study needed, we have considered alternative approaches for the study. One of those approaches would be to simulate $n \times m \times r$ release values directly, such as was done in Section 5 for the simulated example. This approach has the advantage of not having to estimate composition covariance matrices associated with waste type variation, sampling, and chemical analysis. However, it is not clear for this approach how to properly associate model prediction uncertainties with the directly simulated release values. The directly simulated release values will have a nested $n \times m \times r$ structure, which would have to be accounted for along with the magnitudes of the release values in attaching appropriate model uncertainty values to the simulated release values. This step of the simulation process (associating proper model uncertainty estimates to directly simulated release values) was skipped in the Section 5 example because of the difficulty. However, a solution to this issue would have to be developed if this approach were to be used in a large simulation study to verify the adjusted X%/Y% UTI methodology.

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Appendix A: Property-Composition Models and Required Data

Appendix A

Property-Composition Models and Required Data

Property-composition models for PCT (IHLW and ILAW) and VHT (ILAW) will play an important role in developing IHLW and ILAW glass formulations, operating and controlling the IHLW and ILAW plants, and demonstrating compliance with specifications during production operations. For example, property-composition models will play an important role in calculating X%/Y% UTIs for demonstrating compliance with IHLW and ILAW chemical durability specifications over the course of a waste type. Because property-composition models are very important: (i) sufficient property-composition data covering glass composition regions of interest must be collected, and (ii) models must be properly developed, evaluated, and validated using statistical methods and glass science knowledge and experience. After adequate models are developed, statistical methods for quantifying the uncertainty in model predictions must be applied. This appendix provides an overview of least squares regression methods and theory for developing property-composition models and corresponding uncertainty expressions. Hrma et al. (1994) is a good reference showing how these techniques are applied to HLW glass property-composition data.

In order to develop a property-composition model, a database of M glass compositions and corresponding property values must be obtained. Each glass composition can be represented mathematically as a vector having q entries, one for each glass component of interest. These composition vectors are denoted as $\boldsymbol{x} = [x_1, x_2, \ldots, x_q]'$ [(a)], where x_i denotes the mass or mole fraction of component i. (It is assumed that $\Sigma x_i = 1$ for each composition vector $\boldsymbol{x}$, as will be required by mixture experiment model forms used as property-composition models.) A composition data matrix $\boldsymbol{X}$ can be formed by combining the M composition vectors, so that each composition vector becomes a row in the matrix $\boldsymbol{X}$. Thus, $\boldsymbol{X}$ is of dimension $M \times q$.

For each composition vector, there will be a corresponding property value (or a mathematical transformation of a property value, such as a logarithmic transformation). The property or mathematical transformation of a property is denoted by y. Hence, if the natural logarithm of PCT normalized boron release is modeled, then $y = \ln(r_B^{PCT})$. Because there will be M composition vectors, there will also be M of these y-values for each property to be modeled (e.g., PCT normalized releases of B, Li, and Na in the IHLW context). The y-values for a particular property can be combined into a $M \times 1$ response vector $\boldsymbol{y} = [y_1, y_2, \ldots, y_M]'$ where y_j is the property value (possibly mathematically transformed) associated with composition vector $\boldsymbol{x}_j$. Hence, a response vector is associated with each property to be modeled. Note the number M of compositions and corresponding property values may differ from one property to the next, because not all properties may be measured for all glass compositions.

(a) Boldface is used to denote vectors and matrices.

The matrix $\boldsymbol{X}$ and a response vector $\boldsymbol{y}$ for a given property will be used to determine the model coefficients via least squares regression. We assume a model of the general form

$$\boldsymbol{y} = \boldsymbol{W}'\beta + \varepsilon \ , \tag{A.1}$$

where $\boldsymbol{\beta}$ is the vector of true coefficients relating $\boldsymbol{W}$ and $\boldsymbol{y}$, and $\boldsymbol{\varepsilon}$ is a vector of corresponding random errors with mean zero and variance σ_ε^2. The matrix $\boldsymbol{W}$ ($M \times p$) is formed from the composition matrix $\boldsymbol{X}$ ($M \times q$) by expanding each row (composition) of $\boldsymbol{X}$ in the specific form of the model considered. Many models linear in the coefficients $\boldsymbol{\beta}$ are of the general form (A.1). Models linear and quadratic in composition are listed as Equations (3.4) and (3.5) in the main body of the report. In the case of (3.4), $\boldsymbol{W} = \boldsymbol{X}$.

For the general model in (A.1), it can be shown (e.g., Draper and Smith 1998) that the ordinary (unweighted) least squares estimator for $\boldsymbol{\beta}$ is given by

$$\boldsymbol{b} = \left(\boldsymbol{W}'\boldsymbol{W}\right)^{-1}\boldsymbol{W}'\boldsymbol{y} \ . \tag{A.2}$$

Thus, the vector $\boldsymbol{b}$ contains p coefficient estimates referred to as regression coefficients. Because each property has its own response vector $\boldsymbol{y}$, each property will have its own vector $\boldsymbol{b}$ of regression coefficients. After these coefficient vectors are obtained, they can be used to calculate predicted property values for one or more composition vectors.

Because the coefficient vectors are obtained from experimental data, they have some inherent amount of uncertainty. The variance-covariance matrix associated with the regression coefficient vector $\boldsymbol{b}$ quantifies the regression uncertainty, and is denoted by Var($\boldsymbol{b}$). The formula for Var($\boldsymbol{b}$) is provided after the following discussion of assumptions.

For an individual property value y, the property-composition model can be written in the form

$$y = \boldsymbol{\beta}'\boldsymbol{w} + \varepsilon \ , \tag{A.3}$$

where $\boldsymbol{\beta}$ is the true coefficient vector for a particular property, $\boldsymbol{w}$ is the version of a composition vector $\boldsymbol{x}$ expanded in the form of specific model being considered, and $\boldsymbol{\varepsilon}$ is the random error component associated with y. It is assumed that $\boldsymbol{\varepsilon} \sim N(0,\ \sigma_\varepsilon^2)$, so that $y \sim N(\boldsymbol{\beta}'\boldsymbol{w},\ \sigma_\varepsilon^2)$. Under this assumption, the equation for Var($\boldsymbol{b}$) is given by

$$\mathrm{Var}(\boldsymbol{b}) = (\boldsymbol{W}'\boldsymbol{W})^{-1}\,\sigma_\varepsilon^2 \ . \tag{A.4}$$

Typically, the mean square error (MSE) from the regression is used as an estimate $\hat{\sigma}_\varepsilon^2$ of σ_ε^2, provided the model does not have a significant lack-of-fit. Tests for model lack-of-fit must be performed as part of the model evaluation and validation work when developing property composition models. It is beyond the scope of this report to discuss testing for model lack-of-fit and other model evaluation and validation methods, but Draper and Smith (1998) and Montgomery and Peck (1992) provide good discussions of these topics. Note that each property-composition model will have its own associated coefficient vector, and thus its own variance-covariance matrix with a unique associated value σ_{ε}^{2}.

Property predictions are made with the fitted property-composition model

$$\hat{y}(\boldsymbol{x}) = \boldsymbol{b}'\boldsymbol{w}\,, \tag{A.5}$$

where $\hat{y}(\boldsymbol{x})$ denotes the dependence of the prediction on the specific composition $\boldsymbol{x}$ (because $\boldsymbol{w}$ is an expansion of $\boldsymbol{x}$). When $\hat{y}(\boldsymbol{x})$ is considered as a prediction of the mean response at a given composition $\boldsymbol{x}$ (known without uncertainty), the uncertainty in the prediction is given by

$$\widehat{Var}[\hat{y}(\boldsymbol{x})] = \boldsymbol{w}'(\boldsymbol{W}'\boldsymbol{W})^{-1}\boldsymbol{w}\;\;\hat{\sigma}_{\varepsilon}^{2} = \hat{\sigma}_{m}^{2}(\boldsymbol{x})\,. \tag{A.6}$$

Note the uncertainty of a model prediction depends (through $\boldsymbol{w}$) on the composition $\boldsymbol{x}$ at which the prediction is made. It also depends (through $\boldsymbol{W}$) on the composition matrix $\boldsymbol{X}$ used to develop the property-composition model. The notation $\hat{\sigma}_{m}^{2}(\boldsymbol{x})$ is used to indicate the uncertainty of a model prediction at composition $\boldsymbol{x}$. The degrees of freedom associated with $\hat{\sigma}_{m}^{2}(\boldsymbol{x})$ are df($\hat{\sigma}_{m}^{2}$) = df($\boldsymbol{w}'(\boldsymbol{W}'\boldsymbol{W})^{-1}\boldsymbol{w}\,\hat{\sigma}_{\varepsilon}^{2}$) = df($\hat{\sigma}_{\varepsilon}^{2}$) = df(MSE) = $M-p$, because the matrix used to develop the model is $\boldsymbol{W}$ of dimension $M \times p$.

Note that (A.6) provides an expression for the uncertainty in a prediction of a property-composition model at composition $\boldsymbol{x}$ when that composition is known without uncertainty. However, in the RPP-WTP situation, IHLW and ILAW compositions will be estimated with uncertainty from process and/or product samples and chemical analyses of those samples. Hence, the uncertainty in estimated glass compositions must also be considered. This topic is addressed in Appendix B.

Appendix B: Glass Composition Variation and Uncertainty Propagated Through Property-Composition Models

Appendix B

Glass Composition Variation and Uncertainty Propagated Through Property-Composition Models

During IHLW and ILAW production operations, the RPP-WTP will take process and/or product samples to satisfy process control and reporting compliance requirements. Ultimately, the samples will be chemically analyzed and glass compositions $\boldsymbol{x} = [x_1, x_2, \ldots, x_q]'$ will be obtained for each sample. It is assumed these compositions are ultimately expressed as mass or mole fractions, such that $\Sigma x_i = 1$. The data structure for a given IHLW or ILAW waste type is assumed to involve $n > 1$ sampling times over the course of a waste type, $m \geq 1$ samples at each time, and $r \geq 1$ chemical analyses per sample. This appendix addresses how the variation (over the waste type) and uncertainties (due to sampling and chemical analyses) in glass compositions $\boldsymbol{x}$ are quantified and accounted for in relation to property-composition models.

Glass compositions $\boldsymbol{x}$ are multivariate, being of dimension q - 1 for q-component compositions. The dimension of $\boldsymbol{x}$ is q - 1 instead of q because of the so-called mixture constraint that $\Sigma x_i = 1$. This constraint is an important aspect of the forms of property-composition models that will be employed, and hence must be recognized and accounted for in the methods used. Because glass compositions $\boldsymbol{x}$ are multivariate, variations or uncertainties in glass compositions are expressed in terms of variance-covariance matrices $\boldsymbol{V}$, of dimension $q \times q$. A variance-covariance matrix $\boldsymbol{V}$ has the variances of the glass components down the diagonal positions and covariances of pairs of glass components in the off-diagonal positions. A variance-covariance matrix is symmetric, in that $\mathrm{cov}(x_i, x_j) = \mathrm{cov}(x_j, x_i)$.

The total variance-covariance matrix of a composition $\boldsymbol{x}$ is denoted by $\boldsymbol{V_x} = \mathrm{Var}(\boldsymbol{x})$. The total variance-covariance matrix for glass composition can be partitioned into parts

$$\boldsymbol{V_x} = \boldsymbol{V}_g + \boldsymbol{V}_s + \boldsymbol{V}_a \tag{B.1}$$

corresponding to the variance over a waste type ($\boldsymbol{V}_g$), uncertainty corresponding to sampling ($\boldsymbol{V}_s$), and uncertainty corresponding to chemical analysis ($\boldsymbol{V}_a$). It is possible to directly obtain a matrix estimate for a given composition variance-covariance matrix given a sufficient number of experimentally obtained composition vectors $\boldsymbol{x}$ containing the source(s) of variation to be estimated. For example, to estimate $\boldsymbol{V}_a$, a representative glass composition (for IHLW or ILAW) would have to be chemically analyzed multiple times over enough time to capture the various effects that contribute to uncertainty in analyzed compositions. The number of chemical analyses must be larger than the number of glass components, q. Nuclear waste glasses often contain over 50 components, but even the major glass components that affect glass properties number at least 8 to 10. Hence, large numbers of experimentally determined glass compositions can be required to even estimate a composition variance-covariance matrix. Further, work in the statistics literature has shown that to precisely estimate a variance-covariance matrix, very large numbers of data points (compositions in this case) are required. For example, as many as 30 to 50 compositions may be required to adequately estimate a variance-covariance matrix for 10-component compositions. An additional complication is performing multivariate variance component estimation for multiple sources of variation and uncertainty, such as represented in (B.1). Statistical methods and software exist, but are complicated, and require a very large amount of nested compositional data containing the sources of variation and uncertainty of interest.

Fortunately, for the purposes of developing X%/Y% UTIs for PCT or VHT releases, it is not necessary to use multivariate statistical methods to estimate glass composition variance-covariance matrices according to (B.1). Because glass compositions are substituted into a property-composition model to yield predicted PCT or VHT releases, composition variation (over a waste type) and uncertainties (sampling and chemical analysis) can be considered in PCT or VHT release units (or mathematical transformations thereof). Thus, the multivariate variation and uncertainty problem of (B.1) becomes the univariate variation and uncertainty problem

$$\hat{\sigma}_c^2 = \hat{\sigma}_g^2 + \hat{\sigma}_s^2 + \hat{\sigma}_a^2, \tag{B.2}$$

as represented by (3.11) in Section 3.4 of this report. Note the variance components on both sides of (B.2) are in PCT or VHT release units (or mathematical transformations of these units, if used to construct the applicable property-composition model). Of course, it seems a little strange to talk about and quantify composition variations and uncertainties in terms of PCT or VHT release (or transformed release) units. However, to demonstrate compliance with IHLW and ILAW chemical durability specifications over a waste type via X%/Y% UTIs, PCT or VHT release (or transformed release) units are the natural units for the problem.

Consider the IHLW or ILAW production operation situation addressed in this report, namely a set of property-composition model predictions $\hat{y}_{ijk}$ ($i = 1, 2, \ldots, n$; $j = 1, 2, \ldots, m$; $k = 1, 2, \ldots, r$) corresponding to glass composition estimates $\boldsymbol{x}_{ijk}$ from n sampling times over the course of a waste type, with m samples per time and r chemical analyses per sample. Univariate variance component estimation methods can be used to estimate the variance components of (B.2), which in turn can be used to calculate X%/Y% UTIs. The details of these calculations for the sources of variation and uncertainty of interest are discussed in Appendixes C to G.

Appendix C: Estimating Variance Components and Degrees of Freedom

Appendix C

Estimating Variance Components and Degrees of Freedom

As shown in (3.12), $\widehat{\mathrm{Var}}(\hat{y}_{ijk})$ is comprised of variance component estimates $\bar{\hat{\sigma}}_{\boldsymbol{m}}^2$, $\hat{\sigma}_g^2$, $\hat{\sigma}_s^2$, and $\hat{\sigma}_a^2$. For the computational exercise presented in Section 4 of this report, ranges of reasonable estimates (assuming natural log units) were used for $\bar{\hat{\sigma}}_{\boldsymbol{m}}$, $\hat{\sigma}_g$, $\hat{\sigma}_s$, and $\hat{\sigma}_a$. When applicable data are collected during qualification activities and then during production operations, these variance component estimates for the appropriate transformations of PCT and VHT properties will be obtained from that data (see Section 6.2).

The model variance component $\hat{\sigma}_m^2$ can be calculated based on the data set used to develop a property-composition model, as shown in (A.6) of Appendix A. As shown in (A.6), $\hat{\sigma}_m^2$ is sometimes written $\hat{\sigma}_m^2(\boldsymbol{x})$ to denote that its value depends on the glass composition $\boldsymbol{x}$ for which a model prediction is to be made. The quantity $\bar{\hat{\sigma}}_{\boldsymbol{m}}^2$ can be calculated by averaging $\hat{\sigma}_m^2(\boldsymbol{x})$ values as described in (3.13b).

The estimates $\hat{\sigma}_g^2$, $\hat{\sigma}_s^2$, and $\hat{\sigma}_a^2$ can be calculated using the mean squares from an analysis of variance (ANOVA) conducted using predicted property values for the $N = n{\cdot}m{\cdot}r$ glass compositions collected over the course of a waste type. The ANOVA should be conducted according to the balanced nested ANOVA structure that results for glass compositions because of the data generation process described in Steps 3 and 4 of Section 1.2. In the ANOVA, all glass composition factors (glass, samples, and analyses) are viewed as random effects. Appendix B provides further details on $\hat{\sigma}_g^2$, $\hat{\sigma}_s^2$, and $\hat{\sigma}_a^2$. The ANOVA structure associated with glass composition directly affects the way the values of $\hat{\sigma}_g^2$, $\hat{\sigma}_s^2$, and $\hat{\sigma}_a^2$ are used in the formula for $\widehat{\mathrm{Var}}(\hat{y}_{ijk})$. Table C.1 is a general summary of this ANOVA structure (Montgomery 1991).

Table C.1. General Nested ANOVA Model Associated with Glass Compositions

Source	df	Mean Squares	Expected Mean Squares E(MS)
Glass (over a waste type)	$n-1$	MS_g	$E(MS_g) = r\,m\,\sigma_g^2 + r\,\sigma_s^2 + \sigma_a^2$
Samples (at a given location)	$n(m-1)$	MS_s	$E(MS_s) = r\,\sigma_s^2 + \sigma_a^2$
Analyses	$nm(r-1)$	MS_a	$E(MS_a) = \sigma_a^2$

The expected mean squares for each component (glass, samples, and analyses) will be estimable provided its respective degrees of freedom (*df*) value is greater than zero. Thus, estimability depends on the values of *n*, *m*, and *r*. Using the mean square (*MS*) for each component as an estimate of the corresponding expected mean square, the resulting system of equations can be solved to obtain formulas for the estimated components of variation and uncertainty denoted $\hat{\sigma}_g^2$, $\hat{\sigma}_s^2$, and $\hat{\sigma}_a^2$. That is, the system of equations

$$\begin{aligned} MS_g &= r\,m\,\hat{\sigma}_g^2 + r\,\hat{\sigma}_s^2 + \hat{\sigma}_a^2 \\ MS_s &= r\,\hat{\sigma}_s^2 + \hat{\sigma}_a^2 \\ MS_a &= \hat{\sigma}_a^2 \end{aligned} \tag{C.1}$$

is solved for $\hat{\sigma}_g^2$, $\hat{\sigma}_s^2$, and $\hat{\sigma}_a^2$. The resulting formulas are given in Appendixes D through G. In all cases it is assumed that $n > 1$, but m and r may be greater than or equal to 1. Thus, in some cases σ_s^2 and/or σ_a^2 will not be estimable.

As a notational convention, df_{source} will denote the degrees of freedom for the mean squares associated with a particular source of variation or uncertainty. That is, $df_{source} = \mathrm{df}(MS_{source})$. Thus, according to Table C.1, $df_g = n - 1$, $df_s = n(m - 1)$, and $df_a = nm(r - 1)$.

Unlike the other variation and uncertainty components, $\hat{\sigma}_m^2 = \hat{\sigma}_m^2(\boldsymbol{x})$ is not calculated from the ANOVA mean squares. Recall from Appendix A that $\hat{\sigma}_m^2 = \boldsymbol{w}'(\boldsymbol{W}'\boldsymbol{W})^{-1}\boldsymbol{w}\,\hat{\sigma}_\varepsilon^2$, where $\boldsymbol{w}$ is an expansion of $\boldsymbol{x}$ based on the property-composition model, $\boldsymbol{x}$ is any composition vector within the property-composition model's composition region of validity, and $\hat{\sigma}_\varepsilon^2$ represents the MSE from regression. As discussed in Appendix A, the degrees of freedom associated with $\bar{\hat{\sigma}}_m^2$ and $\hat{\sigma}_m^2$ is $\mathrm{df}(\bar{\hat{\sigma}}_m^2) = M - p$. For consistency in notation, $\mathrm{df}(\bar{\hat{\sigma}}_m^2)$ is denoted df_m.

Because $\tilde{\sigma}^2$ is a linear combination of variation and uncertainty estimates (which are in turn linear combinations of mean squares), Satterthwaite's formula (Satterthwaite 1946) is used to calculate the degrees of freedom f associated with $\tilde{\sigma}^2$. Let Ψ be a linear combination of the mean squares $s_1^2, s_2^2, \ldots, s_n^2$

$$\Psi = \sum_{i=1}^{n} a_i s_i^2\,, \tag{C.2}$$

where the coefficients a_i are constants. Satterthwaite's formula for the approximate degrees of freedom f associated with Ψ is

$$f \approx \frac{\psi^2}{\displaystyle\sum_{i=1}^{n} \frac{(a_i s_i^2)^2}{f_i}} \tag{C.3}$$

where f_i represents the degrees of freedom associated with s_i^2.

Satterthwaite (1946) suggested caution using (C.2) and (C.3) when some a_i are negative. This occurs when solving the system of equations (C.1) for individual variance components. However, the X%/Y% UTI approaches considered in this report do not require individual estimates of the variance components, as will be seen in Appendices D to G. Negative a_i also occur when subtracting nuisance uncertainties. Gaylor and Hopper (1969) describe the conditions under which Ψ is approximately distributed as a chi-squared random variable with degrees of freedom f given by (C.3) when some a_i are negative. Their conditions require:

- forming the linear combination of mean squares with positive coefficients (denoted MS_p) and the linear combination of mean squares with negative coefficients (denoted MS_n)

- applying Satterthwaite's formula in (C.3) to obtain the degrees of freedom f_p and f_n associated with MS_p and MS_n, respectively.

Then, the Gaylor and Hopper conditions for applicability of Satterthwaite's formula require that one of the following conditions be satisfied:

$$\frac{E(MS_p)}{E(MS_n)} \geq F_{0.975}(f_n, f_p) \quad \text{if} \quad f_p \leq 10 \tag{C.4}$$

$$\frac{E(MS_p)}{E(MS_n)} \geq F_{0.975}(f_n, f_p) \quad \text{and} \quad f_n \geq \frac{f_p}{2} \quad \text{if} \quad 10 < f_p \leq 100 \tag{C.5}$$

In situations where (C.5) is not satisfied because $f_n < \frac{f_p}{2}$, Satterthwaite's formula is still applicable if one of the following conditions is satisfied:

$$\frac{E(MS_p)}{E(MS_n)} \geq F_{0.99}(f_n, f_p) \quad \text{if} \quad f_p \leq 20 \tag{C.6}$$

$$\frac{E(MS_p)}{E(MS_n)} \geq F_{0.99}(f_n, f_p) \quad \text{and} \quad f_n \geq \frac{f_p}{5} \quad \text{if} \quad 20 < f_p \leq 100 \tag{C.7}$$

In the above equations, E(MS_i) denotes the expected (true) value of MS_i. Gaylor and Hopper also presented alternative conditions to (C.4) through (C.7) in cases where estimates MS_i must be used rather than true values. However, for the calculational exercises of Section 4, the true values are known so (C.4) through (C.7) can be used.

It was not necessary to check the conditions (C.4) to (C.7) in calculating the UTIHWs presented in Tables 4.3 to 4.6 in Section 4.2 because there are no negative coefficients a_i in (C.2). UTIHWs based on subtracting nuisance uncertainties (see Section 3.5) were calculated, but not presented in Section 4 because they are always larger than UTIHWs with adjustments but without subtracting nuisance uncertainties (see Sections H.3 and H.4 of Appendix H). In the calculation of UTIHWs after subtracting nuisance uncertainties, the conditions (C.4) through (C.7) were not satisfied (henceforth referred to as "failures") for several combinations of the input parameters. Specifically, there were 55 failures for the independent-estimates subtraction (INDEPSUB) approach, but only 23 failures for the ANOVA subtraction (ANOVASUB) approach. The reason the number of failures is less with the ANOVASUB approach than the INDEPSUB approach can be explained as follows. First, the condition $10 < f_p \leq 100$ is satisfied for all combinations of input parameters, so that (C.4) never applies. For the INDEPSUB approach, f_n is assumed to be infinite (see Appendices D to G), so that the condition $f_n \geq \frac{f_p}{2}$ in (C.5) is always satisfied. Thus, condition (C.5) fails for the INDEPSUB approach only when $\frac{E(MS_p)}{E(MS_n)} \geq F_{0.975}(f_n, f_p)$ fails, which also implies failure of $\frac{E(MS_p)}{E(MS_n)} \geq F_{0.99}(f_n, f_p)$ in (C.6) and (C.7). Hence, only the ANOVASUB approach can take advantage of conditions (C.6) and (C.7), which reduces the number of failures compared to the INDEPSUB approach. The calculated UTIHW values obtained using the ANOVASUB and INDEPSUB methods are not included in this report due to space considerations.

Appendix D: Equations to Implement X%/Y% Upper Tolerance Intervals for Sampling Plans with m > 1 Samples Per Sampling Time and r > 1 Analyses Per Sample

Appendix D

Equations to Implement X%/Y% Upper Tolerance Intervals for Sampling Plans with *m* > 1 Samples Per Sampling Time and *r* > 1 Analyses Per Sample

When $m > 1$ and $r > 1$, all three variation and uncertainty components are estimable, and Table D.1 is the appropriate ANOVA table. Table D.1 is the same as Table C.1 presented in Appendix C, but is reproduced here for completeness and clarity.

Table D.1. ANOVA Table Appropriate When $m > 1$ and $r > 1$

Source	df	MS	Expected Mean Squares E(MS)
Glass	$n-1$	MS_g	$E(MS_g) = r\,m\,\sigma_g^2 + r\,\sigma_s^2 + \sigma_a^2$
Samples	$n(m-1)$	MS_s	$E(MS_s) = r\,\sigma_s^2 + \sigma_a^2$
Analyses	$nm(r-1)$	MS_a	$E(MS_a) = \sigma_a^2$

The sources of variation and uncertainty (glass, samples, and analyses) mentioned in Table D.1 are described in Section 2.3.

The estimates of the variation and uncertainty components can be written as:

$$\begin{aligned}
\hat{\sigma}_a^2 &= MS_a \\
\hat{\sigma}_s^2 &= \frac{MS_s - \hat{\sigma}_a^2}{r} = \frac{MS_s - MS_a}{r} \\
\hat{\sigma}_g^2 &= \frac{MS_g - (r\,\hat{\sigma}_s^2 + \hat{\sigma}_a^2)}{rm} = \frac{MS_g - MS_s}{rm}
\end{aligned} \tag{D.1}$$

The estimates of the variation and uncertainty components, expressed using the mean squares, can be used to obtain the estimate $\tilde{\sigma}$. Applying Satterthwaite's formula from (C.3) yields f, the degrees of freedom associated with $\tilde{\sigma}$. Three cases are considered: (1) no nuisance (sampling and analytical) uncertainties are subtracted, (2) estimable sampling and/or analytical nuisance uncertainties are subtracted by the ANOVA method, and (3) sampling and analytical nuisance uncertainties are subtracted based on independent estimates. For all three cases, the equations for $\tilde{\sigma}$ and f apply for both unadjusted and adjusted X%/Y% UTIs.

Case 1: No nuisance uncertainties are subtracted

$$\tilde{\sigma} = \sqrt{\bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \frac{\hat{\sigma}_s^2}{m} + \frac{\hat{\sigma}_a^2}{rm}} = \sqrt{\bar{\hat{\sigma}}_m^2 + \frac{1}{rm} MS_g} \tag{D.2}$$

$$f \approx \frac{\left[\bar{\hat{\sigma}}_m^2 + \frac{1}{rm} MS_g\right]^2}{\frac{\left(\bar{\hat{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{rm}\right]^2}{df_g}} \tag{D.3}$$

Case 2: Estimable nuisance uncertainties (both sampling and analysis) are subtracted by the ANOVA method

$$\begin{aligned} \tilde{\sigma} &= \sqrt{\bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \frac{\hat{\sigma}_s^2}{m} + \frac{\hat{\sigma}_a^2}{rm} - \frac{\hat{\sigma}_s^2}{m} - \frac{\hat{\sigma}_a^2}{rm}} = \sqrt{\bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2} \\ &= \sqrt{\bar{\hat{\sigma}}_m^2 + \frac{1}{rm} MS_g - \frac{1}{rm} MS_s} \end{aligned} \tag{D.4}$$

$$f \approx \frac{\left[\bar{\hat{\sigma}}_m^2 + \frac{1}{rm} MS_g - \frac{1}{rm} MS_s\right]^2}{\frac{\left(\bar{\hat{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{rm}\right]^2}{df_g} + \frac{\left[\frac{MS_s}{rm}\right]^2}{df_s}} \tag{D.5}$$

Case 3: Sampling and analysis nuisance uncertainties are subtracted assuming independent estimates are available

$$\begin{aligned} \tilde{\sigma} &= \sqrt{\bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \frac{\hat{\sigma}_s^2}{m} + \frac{\hat{\sigma}_a^2}{rm} - \frac{\tilde{\sigma}_s^2}{m} - \frac{\tilde{\sigma}_a^2}{rm}} \\ &= \sqrt{\bar{\hat{\sigma}}_m^2 + \frac{1}{rm} MS_g - \frac{\tilde{\sigma}_s^2}{m} - \frac{\tilde{\sigma}_a^2}{rm}} \end{aligned} \tag{D.6}$$

$$f \approx \frac{\left[\bar{\hat{\sigma}}_m^2 + \frac{1}{rm} MS_g - \frac{\tilde{\sigma}_s^2}{m} - \frac{\tilde{\sigma}_a^2}{rm}\right]^2}{\frac{\left(\bar{\hat{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{rm}\right]^2}{df_g} + \frac{\left[\frac{\tilde{\sigma}_s^2}{m}\right]^2}{\tilde{f}_s} + \frac{\left[\frac{\tilde{\sigma}_a^2}{rm}\right]^2}{\tilde{f}_a}} \tag{D.7}$$

$$f \approx \frac{\left[\bar{\tilde{\sigma}}_m^2 + \frac{1}{rm} MS_g - \frac{\tilde{\sigma}_s^2}{m} - \frac{\tilde{\sigma}_a^2}{rm}\right]^2}{\frac{\left(\bar{\tilde{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{rm}\right]^2}{df_g}} \tag{D.8}$$

In the formula (D.7) for f above, $\tilde{f}_s$ and $\tilde{f}_a$ are used to represent the degrees of freedom for the independent estimates $\tilde{\sigma}_s^2$ and $\tilde{\sigma}_a^2$, respectively. In (D.8), $\tilde{f}_s$ and $\tilde{f}_a$ are assumed sufficiently large so that $(\tilde{\sigma}_s^2 / m)^2 / \tilde{f}_s$ and $(\tilde{\sigma}_a^2 / rm)^2 / \tilde{f}_a$ are essentially equal to zero. This assumption, and hence (D.8), will be appropriate for the RPP-WTP situation if $\tilde{\sigma}_s^2$ and $\tilde{\sigma}_a^2$ are estimated from a large amount of data during qualification activities. If this assumption is not appropriate, (D.7) can be used. Applications in this report used (D.8).

Appendix E: Equations to Implement X%/Y% Upper Tolerance Intervals for Sampling Plans with *m* = 1 Sample Per Sampling Time and *r* > 1 Analyses Per Sample

Appendix E

Equations to Implement X%/Y% Upper Tolerance Intervals for Sampling Plans with m = 1 Sample Per Sampling Time and r > 1 Analyses Per Sample

When $m = 1$ and $r > 1$, the uncertainty component for sampling is not estimable and is therefore confounded with (i.e., not separable from) the glass variation component. The ANOVA table initially given in Table C.1 now follows the format shown in Table E.1.

Table E.1. ANOVA Table Appropriate When $m = 1$ and $r > 1$

Source	df	*MS*	Expected Mean Squares E(*MS*)
Glass + Samples	$n-1$	MS_g	$E(MS_g) = r(\sigma_g^2 + \sigma_s^2) + \sigma_a^2$
Analyses	$n(r-1)$	MS_a	$E(MS_a) = \sigma_a^2$

The sources of variation and uncertainty (glass, samples, and analyses) mentioned in Table E.1 are described in Section 2.3.

The estimates of the variation and uncertainty components can be written as:

$$
\begin{aligned}
&\hat{\sigma}_a^2 = MS_a \\
&\sigma_s^2 \ \text{ not estimable, confounded with glass variation} \\
&\widehat{\sigma_g^2 + \sigma_s^2} = \frac{MS_g - \hat{\sigma}_a^2}{r} = \frac{MS_g - MS_a}{r}
\end{aligned}
\tag{E.1}
$$

The estimates of the variation and uncertainty components, expressed using the mean squares, can be used to obtain the estimate $\tilde{\sigma}$. Applying Satterthwaite's formula from (C.3) yields f, the degrees of freedom associated with $\tilde{\sigma}$. Three cases are considered: (1) no nuisance (sampling and analytical) uncertainties are subtracted, (2) estimable sampling and/or analytical nuisance uncertainties are subtracted by the ANOVA method, and (3) sampling and analytical nuisance uncertainties are subtracted based on independent estimates. For all three cases, the equations for $\tilde{\sigma}$ and f apply for both unadjusted and adjusted X%/Y% UTIs.

<u>Case 1: No nuisance uncertainties are subtracted</u> (Because sampling uncertainty is unestimable, it is confounded with, and therefore included with, glass variation.)

$$\tilde{\sigma} = \sqrt{\bar{\hat{\sigma}}_m^2 + \widehat{\sigma_g^2 + \sigma_s^2} + \frac{\hat{\sigma}_a^2}{r}} = \sqrt{\bar{\hat{\sigma}}_m^2 + \frac{1}{r} MS_g} \tag{E.2}$$

$$f \approx \frac{\left[\bar{\hat{\sigma}}_m^2 + \frac{1}{r} MS_g\right]^2}{\frac{\left(\bar{\hat{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{r}\right]^2}{df_g}} \tag{E.3}$$

Case 2: Estimable nuisance uncertainty for analysis is subtracted by the ANOVA method

$$\begin{aligned} \tilde{\sigma} &= \sqrt{\bar{\hat{\sigma}}_m^2 + \widehat{\sigma_g^2 + \sigma_s^2} + \frac{\hat{\sigma}_a^2}{r} - \frac{\hat{\sigma}_a^2}{r}} = \sqrt{\bar{\hat{\sigma}}_m^2 + \widehat{\sigma_g^2 + \sigma_s^2}} \\ &= \sqrt{\bar{\hat{\sigma}}_m^2 + \frac{1}{r}(MS_g - MS_a)} \end{aligned} \tag{E.4}$$

$$f \approx \frac{\left[\bar{\hat{\sigma}}_m^2 + \frac{1}{r} MS_g - \frac{1}{r} MS_a\right]^2}{\frac{\left(\bar{\hat{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{r}\right]^2}{df_g} + \frac{\left[\frac{MS_a}{r}\right]^2}{df_a}} \tag{E.5}$$

Case 3: Sampling and analysis nuisance uncertainties are subtracted assuming independent estimates are available

$$\begin{aligned} \tilde{\sigma} &= \sqrt{\bar{\hat{\sigma}}_m^2 + \widehat{\sigma_g^2 + \sigma_s^2} + \frac{\hat{\sigma}_a^2}{r} - \tilde{\sigma}_s^2 - \frac{\tilde{\sigma}_a^2}{r}} \\ &= \sqrt{\bar{\hat{\sigma}}_m^2 + \frac{1}{r} MS_g - \tilde{\sigma}_s^2 - \frac{\tilde{\sigma}_a^2}{r}} \end{aligned} \tag{E.6}$$

$$f \approx \frac{\left[\bar{\hat{\sigma}}_m^2 + \frac{1}{r} MS_g - \tilde{\sigma}_s^2 - \frac{\tilde{\sigma}_a^2}{r}\right]^2}{\frac{\left(\bar{\hat{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{r}\right]^2}{df_g} + \frac{\tilde{\sigma}_s^4}{\tilde{f}_s} + \frac{\left[\frac{\tilde{\sigma}_a^2}{r}\right]^2}{\tilde{f}_a}} \tag{E.7}$$

$$f \approx \frac{\left[\bar{\hat{\sigma}}_m^2 + \frac{1}{r} MS_g - \tilde{\sigma}_s^2 - \frac{\tilde{\sigma}_a^2}{r}\right]^2}{\frac{\left(\bar{\hat{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{r}\right]^2}{df_g}} \tag{E.8}$$

In the formula (E.7) for f above, $\tilde{f}_s$ and $\tilde{f}_a$ are used to represent the degrees of freedom for the independent estimates $\tilde{\sigma}_s^2$ and $\tilde{\sigma}_a^2$, respectively. In (E.8), $\tilde{f}_s$ and $\tilde{f}_a$ are assumed sufficiently large so that $\tilde{\sigma}_s^4 / \tilde{f}_s$ and $(\tilde{\sigma}_a^2 / r)^2 / \tilde{f}_a$ are essentially equal to zero. This assumption, and hence (E.8), will be appropriate for the RPP-WTP situation if $\tilde{\sigma}_s^2$ and $\tilde{\sigma}_a^2$ are estimated from a large amount of data during qualification activities. If this assumption is not appropriate, (E.7) can be used. Applications in this report used (E.8).

Appendix F: Equations to Implement X%/Y% Upper Tolerance Intervals for Sampling Plans with m > 1 Samples Per Sampling Time and r = 1 Analysis Per Sample

Appendix F

Equations to Implement X%/Y% Upper Tolerance Intervals for Sampling Plans with *m* > 1 Samples Per Sampling Time and *r* = 1 Analysis Per Sample

When $m > 1$ and $r = 1$, the uncertainty component for analysis is not estimable and is therefore confounded with (i.e., not separable from) the uncertainty component for samples. The ANOVA table initially given in Table C.1 now follows the format shown in Table F.1.

Table F.1. ANOVA Table Appropriate When $m > 1$ and $r = 1$

Source	df	*MS*	Expected Mean Squares E(*MS*)
Glass	$n-1$	MS_g	$E(MS_g) = m\sigma_g^2 + (\sigma_s^2 + \sigma_a^2)$
Samples + Analysis	$n(m-1)$	MS_s	$E(MS_s) = \sigma_s^2 + \sigma_a^2$

The sources of variation and uncertainty (glass, samples, and analyses) mentioned in Table F.1 are described in Section 2.3.

The estimates of the variation and uncertainty components can be written as:

$$\sigma_a^2 \quad \text{not estimable, confounded with sample uncertainty}$$

$$\widehat{\sigma_s^2 + \sigma_a^2} = MS_s \tag{F.1}$$

$$\hat{\sigma}_g^2 = \frac{MS_g - \widehat{\sigma_s^2 + \sigma_a^2}}{m} = \frac{MS_g - MS_s}{m}$$

The estimates of the variation and uncertainty components, expressed using the mean squares, can be used to obtain the estimate $\tilde{\sigma}$. Applying Satterthwaite's formula from (C.3) yields f, the degrees of freedom associated with $\tilde{\sigma}$. Three cases are considered: (1) no nuisance (sampling and analytical) uncertainties are subtracted, (2) estimable sampling and/or analytical nuisance uncertainties are subtracted by the ANOVA method, and (3) sampling and analytical nuisance uncertainties are subtracted based on independent estimates. For all three cases, the equations for $\tilde{\sigma}$ and f apply for both unadjusted and adjusted X%/Y% UTIs.

<u>Case 1: No nuisance uncertainties are subtracted</u> (Because analysis uncertainty is unestimable, it is confounded with, and therefore included with, sampling variation.)

$$\tilde{\sigma} = \sqrt{\bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \frac{\widehat{\sigma_s^2 + \sigma_a^2}}{m}} = \sqrt{\bar{\hat{\sigma}}_m^2 + \frac{1}{m} MS_g} \tag{F.2}$$

$$f \approx \frac{\left[\bar{\hat{\sigma}}_m^2 + \frac{1}{m} MS_g\right]^2}{\frac{\left(\bar{\hat{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{m}\right]^2}{df_g}} \tag{F.3}$$

Case 2: Estimable nuisance uncertainty for sampling is subtracted by the ANOVA method

(Because analysis uncertainty was confounded with sampling uncertainty and not individually estimable, the combined sampling and analysis uncertainty term is removed from $\tilde{\sigma}$.)

$$\tilde{\sigma} = \sqrt{\bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \frac{\widehat{\sigma_s^2 + \sigma_a^2}}{m} - \frac{\widehat{\sigma_s^2 + \sigma_a^2}}{m}} = \sqrt{\bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2}$$

$$= \sqrt{\bar{\hat{\sigma}}_m^2 + \frac{1}{m}(MS_g - MS_s)} \tag{F.4}$$

$$f \approx \frac{\left[\bar{\hat{\sigma}}_m^2 + \frac{1}{m} MS_g - \frac{1}{m} MS_s\right]^2}{\frac{\left(\bar{\hat{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{m}\right]^2}{df_g} + \frac{\left[\frac{MS_s}{m}\right]^2}{df_s}} \tag{F.5}$$

Case 3: Sampling and analysis nuisance uncertainties are subtracted assuming independent estimates are available

$$\tilde{\sigma} = \sqrt{\bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \frac{\widehat{\sigma_s^2 + \sigma_a^2}}{m} - \frac{\tilde{\sigma}_s^2}{m} - \frac{\tilde{\sigma}_a^2}{m}}$$

$$= \sqrt{\bar{\hat{\sigma}}_m^2 + \frac{1}{m} MS_g - \frac{\tilde{\sigma}_s^2}{m} - \frac{\tilde{\sigma}_a^2}{m}} \tag{F.6}$$

$$f \approx \frac{\left[\bar{\tilde{\sigma}}_m^2 + \frac{1}{m} MS_g - \frac{\tilde{\sigma}_s^2}{m} - \frac{\tilde{\sigma}_a^2}{m}\right]^2}{\frac{\left(\bar{\tilde{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{rm}\right]^2}{df_g} + \frac{\left[\frac{\tilde{\sigma}_s^2}{m}\right]^2}{\tilde{f}_s} + \frac{\left[\frac{\tilde{\sigma}_a^2}{m}\right]^2}{\tilde{f}_a}} \tag{F.7}$$

$$f \approx \frac{\left[\bar{\tilde{\sigma}}_m^2 + \frac{1}{m} MS_g - \frac{\tilde{\sigma}_s^2}{m} - \frac{\tilde{\sigma}_a^2}{m}\right]^2}{\frac{\left(\bar{\tilde{\sigma}}_m^2\right)^2}{df_m} + \frac{\left[\frac{MS_g}{m}\right]^2}{df_g}} \tag{F.8}$$

In the formula (F.7) for f above, $\tilde{f}_s$ and $\tilde{f}_a$ are used to represent the degrees of freedom for the independent estimates $\tilde{\sigma}_s^2$ and $\tilde{\sigma}_a^2$, respectively. In (F.8), $\tilde{f}_s$ and $\tilde{f}_a$ are assumed sufficiently large so that $(\tilde{\sigma}_s^2 / m)^2 / \tilde{f}_s$ and $(\tilde{\sigma}_a^2 / rm)^2 / \tilde{f}_a$ are essentially equal to zero. This assumption, and hence (F.8), will be appropriate for the RPP-WTP situation if $\tilde{\sigma}_s^2$ and $\tilde{\sigma}_a^2$ are estimated from a large amount of data during qualification activities. If this assumption is not appropriate, (F.7) can be used. Applications in this report used (F.8).

Appendix G: Equations to Implement X%/Y% Upper Tolerance Intervals for Sampling Plans with *m* = 1 Sample Per Sampling Time and *r* = 1 Analysis Per Sample

Appendix G

Equations to Implement X%/Y% Upper Tolerance Intervals for Sampling Plans with *m* = 1 Sample Per Sampling Time and *r* = 1 Analysis Per Sample

When $m = 1$ and $r = 1$, the uncertainty components for both sampling and analysis are inestimable and are therefore confounded with (i.e., not separable from) the glass variation component. The general ANOVA table given in Table C.1 appropriately modified for this situation is shown in Table G.1.

Table G.1. ANOVA Table Appropriate When $m = 1$ and $r = 1$

Source	df	*MS*	Expected Mean Squares E(*MS*)
Glass + Samples + Analysis	$n-1$	MS_g	$E(MS_g) = \sigma_g^2 + \sigma_s^2 + \sigma_a^2$

The sources of variation and uncertainty (glass, samples, and analyses) mentioned in Table G.1 are described in Section 2.3.

The estimates of the variation and uncertainty components can be written as:

$$\begin{aligned} &\sigma_a^2 \quad \text{not estimable, confounded with glass variation} \\ &\sigma_s^2 \quad \text{not estimable, confounded with glass variation} \\ &\widehat{\sigma_g^2 + \sigma_s^2 + \sigma_a^2} = MS_g \end{aligned} \tag{G.1}$$

The estimates of the variation and uncertainty components, expressed using the mean squares, can be used to obtain the estimate $\tilde{\sigma}$. Applying Satterthwaite's formula from (C.3) yields *f*, the degrees of freedom associated with $\tilde{\sigma}$. Because no nuisance uncertainties are estimable and removable by the ANOVA method, only two cases are considered: (1) no nuisance (sampling and analytical) uncertainties are subtracted, and (2) sampling and analytical nuisance uncertainties are subtracted based on independent estimates. For all three cases, the equations for $\tilde{\sigma}$ and *f* apply for both unadjusted and adjusted X%/Y% UTIs.

<u>Case 1: No nuisance uncertainties are subtracted</u> (Because neither sampling nor analysis uncertainty components are individually estimable, they are confounded with, and therefore included with, the glass variation component.)

$$\tilde{\sigma} = \sqrt{\bar{\hat{\sigma}}_m^2 + \widehat{\sigma_g^2 + \sigma_s^2 + \sigma_a^2}} = \sqrt{\bar{\hat{\sigma}}_m^2 + MS_g} \tag{G.2}$$

$$f \approx \frac{[\bar{\hat{\sigma}}_m^2 + MS_g]^2}{\frac{\left(\bar{\hat{\sigma}}_m^2\right)^2}{df_m} + \frac{MS_g^2}{df_g}} \tag{G.3}$$

Case 2: Not applicable, because neither the sampling nor analysis nuisance uncertainty is estimable via the ANOVA method when $m = 1$ and $r = 1$. Hence the formulas and results are the same as for the no-subtraction situation in Case 1.

Case 3: Sampling and analysis nuisance uncertainties are subtracted assuming independent estimates are available

$$\begin{aligned} \tilde{\sigma} &= \sqrt{\bar{\hat{\sigma}}_m^2 + \widehat{\sigma_g^2 + \sigma_s^2 + \sigma_a^2} - \tilde{\sigma}_s^2 - \tilde{\sigma}_a^2} \\ &= \sqrt{\bar{\hat{\sigma}}_m^2 + MS_g - \tilde{\sigma}_s^2 - \tilde{\sigma}_a^2} \end{aligned} \tag{G.4}$$

$$f \approx \frac{[\hat{\sigma}_m^2 + MS_g - \tilde{\sigma}_s^2 - \tilde{\sigma}_a^2]^2}{\frac{\left(\hat{\sigma}_m^2\right)^2}{df_m} + \frac{MS_g^2}{df_g} + \frac{\tilde{\sigma}_s^4}{\tilde{f}_s} + \frac{\tilde{\sigma}_a^4}{\tilde{f}_a}} \tag{G.5}$$

$$f \approx \frac{[\hat{\sigma}_m^2 + MS_g - \tilde{\sigma}_s^2 - \tilde{\sigma}_a^2]^2}{\frac{\left(\hat{\sigma}_m^2\right)^2}{df_m} + \frac{MS_g^2}{df_g}} \tag{G.6}$$

In the formula (G.5) for f above, $\tilde{f}_s$ and $\tilde{f}_a$ are used to represent the degrees of freedom for the independent estimates $\tilde{\sigma}_s^2$ and $\tilde{\sigma}_a^2$, respectively. In (G.6), $\tilde{f}_s$ and $\tilde{f}_a$ are assumed sufficiently large so that $\tilde{\sigma}_s^4 / \tilde{f}_s$ and $\tilde{\sigma}_a^4 / \tilde{f}_a$ are essentially equal to zero. This assumption, and hence (G.6), will be appropriate for the RPP-WTP situation if $\tilde{\sigma}_s^2$ and $\tilde{\sigma}_a^2$ are estimated from a large amount of data during qualification activities. If this assumption is not appropriate, (G.5) can be used. Applications in this report used (G.6).

Appendix H: Derivation of X%/Y% One-Sided Upper Tolerance Interval Formulas Without and With Adjustment for Nuisance Uncertainties

Appendix H

Derivation of X%/Y% One-Sided Upper Tolerance Interval Formulas Without and With Adjustment for Nuisance Uncertainties

Two general formulas for calculating an X%/Y% one-sided upper tolerance interval (X/Y UTI) are derived in this appendix. The first formula is for an X%/Y% UTI on the distribution of interest, which is due to variation in true IHLW or ILAW PCT or VHT release rates for glass produced from a given waste type. The second formula is for an X%/Y% UTI on the distribution of interest inflated by sampling, analytical, and model nuisance uncertainties. The first formula is the proposed for use by the RPP-WTP, because the resulting X%/Y% UTIs are smaller as a result of adjusting for the nuisance uncertainties. The second formula is developed so that the reduction in X%/Y% UTIs provided by the first formula can be assessed in the calculations of Sections 4 and 5. Results from the first formula are referred to as *adjusted* X%/Y% UTIs, while results from the second formula are referred to as *unadjusted* X%/Y% UTIs.

As in the main body of the report: (i) the data structure is n sampling times over a waste type, m samples at each sampling time, and r chemical analyses per sample, and (ii) $\hat{y}_{ijk}$ denotes the predicted (possibly transformed) PCT or VHT release of the k^{th} chemical analysis of the j^{th} sample taken at the i^{th} sampling time over the waste type. Hence, the data consist of $N = n{\cdot}m{\cdot}r$ predicted values $\hat{y}_{ijk}$.

The quantities $\bar{\hat{y}}_{i..}$ and $\tilde{\mu}$ defined in Equations (3.6) and (3.7) of Section 3.3 play important roles in deriving the two general formulas for an X%/Y% UTI. Specifically, $\bar{\hat{y}}_{i..}$ is the average of predicted release values (possibly transformed) over replicate samples and/or chemical analyses at a given sampling time for a waste type. Averaging over replicate samples and/or chemical analyses effectively reduces these two sources of nuisance uncertainty. Then, $\tilde{\mu}$ is the average of the $\bar{\hat{y}}_{i..}$ values, $\tilde{\mu} = \frac{1}{n}\sum_{i=1}^{n} \bar{\hat{y}}_{i..}$ as given in Equation (3.7). The notation

$$\sigma_2^2 = \mathrm{Var}(\bar{\hat{y}}_{i..}) = \bar{\sigma}_m^2 + \sigma_g^2 + \frac{\sigma_s^2}{m} + \frac{\sigma_a^2}{rm} \tag{H.1}$$

is defined for subsequent use, where $\bar{\sigma}_m^2 = \frac{1}{rm}\sum_{j=1}^{m}\sum_{k=1}^{r}\sigma_m^2(\boldsymbol{x}_{ijk})$.

H.1 Derivation of the Formula for an X%/Y% UTI with Adjustment for Nuisance Uncertainties

Let G denote a random variable having the distribution of true PCT or VHT releases (or their mathematical transformations) from IHLW or ILAW produced from a given HLW or LAW waste type. For this derivation, G is assumed to be normally distributed with mean μ_g and variance σ_g^2, denoted $G \sim N(\mu_g,\ \sigma_g^2)$.

Defining $\tilde{\mu}$ as in Equation (3.7) of Section 3.3, we have $\tilde{\mu} \sim N\left(\mu_{\tilde{\mu}}, \sigma_{\tilde{\mu}}^2\right)$. Assuming that samples, chemical analyses, and property-composition model predictions are unbiased, $\mu_{\tilde{\mu}} = \mu_g$. Also, we have $\sigma_{\tilde{\mu}}^2 = \sigma_2^2 / n$. Then, $\tilde{\mu} \sim N\left(\mu_g, \dfrac{\sigma_2^2}{n}\right)$. This implies that $\dfrac{\tilde{\mu} - \mu_g}{\sqrt{\dfrac{\sigma_2^2}{n}}} \sim N(0,\ 1)$ and thus that $Z = \dfrac{\mu_g - \tilde{\mu}}{\dfrac{\sigma_2}{\sqrt{n}}} \sim N(0,1)$. That is, Z follows the standard normal distribution. Furthermore, if U is a random variable so that $U \sim \chi_\nu^2$, where ν is the degrees of freedom associated with U, then $T = \dfrac{Z + \delta}{\sqrt{U/\nu}}$ has a noncentral-t distribution with ν degrees of freedom and noncentrality parameter δ, provided Z and U are independent (Graybill 1976). That is, $T \sim t\ (\nu,\ \delta)$. Note that when $\delta = 0$, T follows the central-t distribution with ν degrees of freedom. Because the distribution of T is known, a tolerance interval formula can be constructed using the pivotal approach and pivoting on T.

The assumption that random variable G (in this report, a true PCT or VHT release or a mathematical transformation thereof) follows a normal distribution is very important in constructing an X%/Y% UTI. If $G \sim N(\mu_g,\ \sigma_g^2)$, then $\beta = \mathrm{P}(G \le \mu_g + z_{1-\beta}\sigma_g)$, so the content level prescribed in the tolerance interval is Y = $\beta \cdot 100\%$. If the content level is Y = 95 (i.e., $\beta = 0.95$), then $z_{1-\beta} \approx 1.6449$. Attaining a tolerance interval confidence level of X = $\gamma \cdot 100\%$ requires that $\gamma = \mathrm{P}[\ \mathrm{P}\{G \le \tilde{\mu} + k\tilde{\sigma}\ \} \ge \beta]$, or equivalently that $\gamma = \mathrm{P}[\ \mu_g + z_{1-\beta}\,\sigma_g\ \le\ \tilde{\mu} + k\tilde{\sigma}\ ]$. For example, if the confidence level is X = 95%, then $\gamma = 0.95$.

Let $\tilde{\mu}$ denote the estimate of μ and $\tilde{\sigma} = \sqrt{\hat{\sigma}_2^2 - \hat{\sigma}_0^2}$ denote the estimate of σ. Here $\hat{\sigma}_0^2$ denotes the combined nuisance uncertainty estimates to be subtracted. When nuisance uncertainties are not subtracted, $\hat{\sigma}_0^2 = 0$. The σ of which $\tilde{\sigma}$ is an estimate is the standard deviation of the distribution of G inflated by any nuisance uncertainties not subtracted.

The pivotal approach to deriving the formula for an X%/Y% UTI with adjustment for nuisance uncertainties proceeds as follows:

$$\gamma = \mathrm{P}[\mu_g + z_{1-\beta}\sigma_g \ \le\ \tilde{\mu} + k\tilde{\sigma}\,] \tag{H.2}$$

$$= \mathrm{P}\left[\frac{\mu_g - \tilde{\mu} + z_{1-\beta}\sigma_g}{\sigma_{\tilde{\mu}}} \ \le\ \frac{k\tilde{\sigma}}{\sigma_{\tilde{\mu}}}\right]$$

$$= \mathrm{P}\left[\frac{\mu_g - \tilde{\mu} + z_{1-\beta}\sigma_g}{\frac{\sigma_2}{\sqrt{n}}} \ \le\ \frac{k\tilde{\sigma}}{\frac{\sigma_2}{\sqrt{n}}}\right]$$

$$= \mathrm{P}\left[\frac{\mu_g - \tilde{\mu}}{\frac{\sigma_2}{\sqrt{n}}} \ +\ z_{1-\beta}\sqrt{n}\,\frac{\sigma_g}{\sigma_2} \ \le\ k\sqrt{n}\,\frac{\tilde{\sigma}}{\sigma_2}\right]$$

$$= \mathrm{P}\left[\frac{\frac{\mu_g - \tilde{\mu}}{\frac{\sigma_2}{\sqrt{n}}} \ +\ z_{1-\beta}\sqrt{n}\,\frac{\sigma_g}{\sigma_2}}{\frac{\tilde{\sigma}}{\sigma}} \ \le\ \frac{k\sqrt{n}\,\frac{\tilde{\sigma}}{\sigma_2}}{\frac{\tilde{\sigma}}{\sigma}}\right]$$

$$= \mathrm{P}\left[\frac{\frac{\mu_g - \tilde{\mu}}{\frac{\sigma_2}{\sqrt{n}}} \ +\ \delta}{\frac{\tilde{\sigma}}{\sigma}} \ \le\ k\sqrt{n}\,\frac{\sigma}{\sigma_2}\right]$$

$$= \mathrm{P}[T \le k\sqrt{n}\,\frac{\sigma}{\sigma_2}] \ \text{ where } T = \frac{\frac{\mu_g - \tilde{\mu}}{\frac{\sigma_2}{\sqrt{n}}} \ +\ \delta}{\frac{\tilde{\sigma}}{\sigma}}.$$

We denote the degrees of freedom associated with $\tilde{\sigma}$ as f, and let

$$\delta = z_{1-\beta}\sqrt{n}\,\frac{\sigma_g}{\sigma_2}. \tag{H.3}$$

Then, T follows a noncentral-t distribution with f degrees of freedom and noncentrality parameter δ. This result follows provided that: $\tilde{\mu} \sim N\left(\mu_g, \frac{\sigma_2^2}{n}\right)$ so that $Z = \frac{\mu_g - \tilde{\mu}}{\frac{\sigma_2}{\sqrt{n}}} \sim N(0, 1)$, $U = \frac{f \cdot \tilde{\sigma}^2}{\sigma^2} \sim \chi_f^2$, and Z and U are independent. Quantile values for T based on f and δ can be found in Owen (1963) or using software packages such as SAS® (SAS 2001).

Because $\gamma = P[T \le k\sqrt{n}\frac{\sigma}{\sigma_2}]$, the factor k in the tolerance interval formula is obtained by: (i) finding the $t(\gamma, \beta, f, \delta) = k\sqrt{n}\frac{\sigma}{\sigma_2}$ statistic associated with confidence level X = 100γ, degrees of freedom f, and noncentrality parameter $\delta = z_{1-\beta}\sqrt{n}\frac{\sigma_g}{\sigma_2}$, and (ii) dividing $t(\gamma, \beta, f, \delta)$ by $\sqrt{n}\frac{\sigma}{\sigma_2}$, so that

$$k = \frac{t(\gamma, \beta, f, \delta)}{\sqrt{n}} \frac{\sigma_2}{\sigma} = \frac{t(\gamma, \beta, f, \delta)}{\sqrt{n}} \frac{\sigma_2}{\sqrt{\sigma_2^2 - \sigma_0^2}} \quad . \tag{H.4a}$$

When nuisance uncertainties are not subtracted $\hat{\sigma}_0^2 = 0$, so $\sigma = \sigma_2$. Then, (H.4a) reduces to

$$k = \frac{t(\gamma, \beta, f, \delta)}{\sqrt{n}} . \tag{H.4b}$$

Note that (H.4b) depends on unknown parameters only through the non-centrality parameter δ used to determine $t(\gamma, \beta, f, \delta)$. Regardless of whether (H.4a) or (H.4b) applies, notice k depends not only on n that appears directly in those equations, but also on m and r that appear indirectly through σ and σ_2.

To calculate X%/Y% UTIs, the ratios $\frac{\sigma_g}{\sigma_2}$ and $\frac{\sigma}{\sigma_2}$ of true standard deviations must be known when nuisance uncertainties are subtracted, while only $\frac{\sigma_g}{\sigma_2}$ must be known when nuisance uncertainties are not subtracted. Having known values for these ratios causes no problem for the UTIHW calculations in Section 4, because σ_g, σ_2, and σ can be calculated from the input parameters that take various "known" values summarized in Table 4.1. However, a problem exists for practical application of the X%/Y% UTI formula during IHLW or ILAW production operations, when $\frac{\sigma_g}{\sigma_2}$ and $\frac{\sigma}{\sigma_2}$ will not be known. It may be that the ratios $\frac{\sigma_g}{\sigma_2}$ and

$\frac{\sigma}{\sigma_2}$ will be estimated well enough for each HLW and LAW waste type based on qualification activities to be treated as known. Certainly, the sampling, analytical, and model-prediction nuisance uncertainties should be very well estimated during qualification activities. Simulations of IHLW or ILAW production for a given waste type should be able to provide reasonable prior estimates of σ_g. Hence, it may be possible to estimate the ratios well enough during qualification activities for a given waste type to treat the ratios as known per the theoretical development earlier in this appendix.

If the ratios $\frac{\sigma_g}{\sigma_1}$ and $\frac{\sigma}{\sigma_1}$ cannot be treated as known prior to IHLW or ILAW production, they will have to be estimated from production data to calculate X%/Y% UTIs. However, this creates two potential problems.

1. For some situations, it may not be possible to estimate σ_g free of other uncertainty components. For example, when m = 1 and r > 1 with the no-subtraction and ANOVA-subtraction approaches, σ_g cannot be estimated free of σ_s. Similarly, when m = 1 and r = 1 with the no-subtraction and ANOVA-subtraction approaches, σ_g cannot be estimated free of σ_s and σ_a. Using an inflated estimate of σ_g in obtaining the non-centrality parameter δ violates the theoretical development of X%/Y% UTIs presented earlier in this appendix. The consequence of this violation is that the X%/Y% UTI will not be a statement about the true distribution of transformed PCT or VHT releases [e.g., ln(PCT)], but rather a statement about that distribution inflated by the uncertainty source(s) confounded in the estimate of σ_g. Thus, in such cases an X%/Y% UTI will be larger (and theoretically correct) for the inflated distribution.

2. Using estimates of the ratios $\frac{\sigma_g}{\sigma_2}$ and $\frac{\sigma}{\sigma_2}$ may affect the tolerance interval confidence (X) and content (Y) values that can be achieved. The extent of such effects should be investigated in future work after more details of the IHLW and ILAW reporting compliance strategies are determined. If needed, methods to account for the uncertainties in estimates of these ratios similar to those discussed by Mee (1984) for his Cases 2 and 3 could be developed in the future for this more complicated situation.

H.2 Derivation of the Formula for an X%/Y% UTI without Adjustment for Nuisance Uncertainties

Let H denote a random variable having the distribution of predicted PCT or VHT releases (or their mathematical transformations) from IHLW or ILAW produced from a given HLW or LAW waste type. Note that G in Section H.1 has a distribution of true PCT or VHT release values for glass made from a waste type. In this section, H has a distribution of predicted values that are subject to sampling, analytical, and model-prediction nuisance uncertainties. For this derivation, H is assumed normally distributed with mean μ and variance σ^2, denoted $H \sim N(\mu,\ \sigma^2)$. Assuming samples, chemical analyses, and property-composition model predictions are unbiased, $\mu = \mu_g$, where μ_g is the same as defined in Section H.1.

Defining $\tilde{\mu}$ as in Equation (3.7) of Section 3.3, we have $\tilde{\mu} \sim N\left(\mu_{\tilde{\mu}}, \sigma^2_{\tilde{\mu}}\right)$. Assuming samples, chemical analyses, and property-composition model predictions are unbiased, $\mu_{\tilde{\mu}} = \mu_g$. Also, we have $\sigma^2_{\tilde{\mu}} = \sigma^2_2 / n$, where σ^2_2 is defined in (H.1).

Using the same notation as in Section H.1, the goal here is to develop an X%/Y% UTI for the distribution of H where X = $\gamma \cdot 100\%$ and Y = $\beta \cdot 100\%$. Thus, the goal may be written as $\gamma = \mathrm{P}[\ \mathrm{P}\{H \le \tilde{\mu} + k\tilde{\sigma}\} \ge \beta]$, which is equivalent to

$$\gamma = \mathrm{P}[\ \mu_g + z_{1-\beta}\sigma \le \tilde{\mu} + k\tilde{\sigma}\ ]. \tag{H.5}$$

Equation (H.5) is the same as equation (H.2) in Section H.1, except for the presence of σ instead of σ_g on the left side of the inequality. Hence, the theoretical development of an X%/Y% UTI (without adjusting for nuisance uncertainties) proceeds in the same fashion as in Section H.1, except with σ replacing σ_g. Hence, (H.3) becomes

$$\delta = z_{1-\beta}\sqrt{n}\,\frac{\sigma}{\sigma_2}\,. \tag{H.6a}$$

When nuisance uncertainties are not subtracted, $\sigma = \sigma_2$, and (H.6a) reduces to

$$\delta = z_{1-\beta}\sqrt{n}\,, \tag{H.6b}$$

The formulas for k in (H.4a) and (H.4b) do not depend on σ_g, so they are the same for the "no adjustment for nuisance uncertainties" case in this section. However, for completeness the formulas are given here again, when subtracting nuisance uncertainties (σ_0^2)

$$k = \frac{t(\gamma,\beta,f,\delta)}{\sqrt{n}}\frac{\sigma_2}{\sigma} = \frac{t(\gamma,\beta,f,\delta)}{\sqrt{n}}\frac{\sigma_2}{\sqrt{\sigma_2^2 - \sigma_0^2}}\ . \tag{H.7a}$$

and when not subtracting nuisance uncertainties

$$k = \frac{t(\gamma,\beta,f,\delta)}{\sqrt{n}}\,. \tag{H.7b}$$

Note, when not subtracting nuisance uncertainties, that (H.6b) and (H.7b) are free of unknown parameters. Hence, no prior knowledge of relative magnitudes of variance components is required to compute an unadjusted X%/Y% UTI = $\tilde{\mu} + k\tilde{\sigma}$. Also, although k in (H.7b) only depends on n, $\tilde{\sigma}^2 = \tilde{\sigma}_2^2 = \bar{\hat{\sigma}}_m^2 + \hat{\sigma}_g^2 + \hat{\sigma}_s^2 / m + \hat{\sigma}_a^2 / rm$ depends on m and r as well. Hence, n, m, and r all influence the magnitude of an unadjusted X%/Y% UTI just as is the case for an adjusted X%/Y% UTI.

H.3 Subtracting Nuisance Uncertainties Always Increases the Magnitudes of Adjusted X%/Y% UTIs

Recall that the general formula for an X%/Y% UTI is given by $\tilde{\mu} + k\tilde{\sigma}$. Intuitively, subtracting nuisance uncertainties yields a smaller $\tilde{\sigma}$, suggesting that the resulting X%/Y% UTI should be smaller. However, subtracting nuisance uncertainties increases k, so that a UTI might be larger with subtraction of nuisance uncertainties than without. In fact, for adjusted X%/Y% UTIs (as developed in Section H.1), the value of k increases by a larger ratio than the value of $\tilde{\sigma}$ decreases. Hence, adjusted X%/Y% UTIs are smaller (which is desirable) when nuisance uncertainties are not subtracted. The proof of this result follows.

Consider the expectation of an adjusted X%/Y% UTI and expand the general formula by substituting the formula for k from (H.4a)

$$\begin{aligned}
\text{E[X\%/Y\% UTI]} &= E[\tilde{\mu} + k\tilde{\sigma}] = \tilde{\mu} + k\sigma \\
&= \tilde{\mu} + \left(\frac{t_1(X, Y, f, \delta_1)}{\sqrt{n}} \frac{\sigma_2}{\sigma} \right) \sigma \\
&= \tilde{\mu} + \frac{t_1(X, Y, f, \delta_1)\sigma_2}{\sqrt{n}} . \qquad \text{(H.8)}
\end{aligned}$$

Note that t_1 has been written in the form $t_1(\mathrm{X,Y}, f, \delta_1)$ to emphasize its dependence on X, Y, the degrees of freedom f, and the non-centrality parameter $\delta_1 = z_{1-\beta} \sqrt{n} \dfrac{\sigma_g}{\sigma_2}$ from (H.3). Neither σ_g nor σ_2 is affected by subtracting nuisance uncertainties, so the value of δ_1 is not affected by subtracting nuisance uncertainties. Hence, the only quantity in (H.8) that is affected by subtracting nuisance uncertainties is f. It is clear from the equations for f in Appendices D to G that f decreases when nuisance uncertainties are subtracted. Further, the decrease is larger using the ANOVA subtraction method than the independent-estimates subtraction method. A decrease in the value of f results in a larger value of t_1. Hence, in expectation, an adjusted X/%Y% UTI will always be larger when subtracting nuisance uncertainties than when not subtracting nuisance uncertainties. Intuitively, this makes sense in that there is no additional value to subtracting nuisance uncertainties given that they are adjusted for, per the development in Section H.1.

It is not possible to determine in the same manner whether subtracting nuisance uncertainties always increases or can possibly decrease unadjusted X%/Y% UTIs. The expectation of an unadjusted X%/Y% UTI still takes the form of (H.8). Hence, whether subtracting nuisance uncertainties increases or decreases $t_0(X,Y, f, \delta_0)$ determines whether an unadjusted X%/Y% UTI increases or decreases. For unadjusted X%/Y% UTIs, $\delta_0 = z_{1-\beta}\sqrt{n}\,\dfrac{\sigma}{\sigma_2}$ from (H.6a). In this case, σ decreases when nuisance uncertainties are subtracted, so that δ_0 decreases. Decreasing δ_0 decreases $t_0(X,Y, f, \delta_0)$. However, subtracting nuisance uncertainties decreases f, which increases $t_0(X,Y, f, \delta_0)$ as noted previously. Thus, subtracting nuisance uncertainties has conflicting effects on δ_0 and f, so it is not clear whether unadjusted X%/Y% UTIs become smaller or larger. While this issue could be addressed via additional work, from a practical standpoint there is no need to do so as discussed in the following section.

H.4 Adjusted X%/Y% UTIs without Subtracting Nuisance Uncertainties are Always Smaller than Unadjusted X%/Y% UTIs with Subtracting Nuisance Uncertainties

Adjusted X%/Y% UTIs without subtracting nuisance uncertainties will always be smaller than unadjusted X%/Y% UTIs with subtracting nuisance uncertainties. To see this, note for both cases that an X%/Y% UTI has the general form given in (H.8). Only $t(X, Y, f, \delta)$ in (H.8) changes for the two cases. The δ_1 given by (H.3) for an adjusted X%/Y% UTI without subtracting nuisance uncertainties is always less than the δ_0 given by (H.6a) for an unadjusted X%/Y% UTI with subtracting nuisance uncertainties. Also, the degrees of freedom f are always larger without subtraction, as noted previously. Thus, in expectation, adjusted X%/Y% UTIs without subtracting nuisance uncertainties will always be smaller than unadjusted X%/Y% UTIs with subtracting nuisance uncertainties.

Appendix I: X%/Y% Upper Tolerance Interval Half-Width Results for Various Combinations of Input Parameters

Appendix I

X%/Y% Upper Tolerance Interval Half-Width Results for Various Combinations of Input Parameters

This appendix contains tables of X%/Y% UTIHWs and other related quantities such as δ, $\tilde{\sigma}$, *f*, and *k* calculated for various combinations of input parameters as discussed in Section 4. Table I.1 contains results for unadjusted and adjusted 95%/95% UTIs, as discussed in Section 3.7. Similar results for unadjusted and adjusted 99%/99% UTIs were also obtained, but are not included here because of the number of additional pages required.

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
1	10	1	1	20	0.1	0.05	0.05	0.2	5.2015	0.2345	28.8095	2.3923	0.5610	2.2179	0.2345	28.8095	1.3023	0.3054
2	10	1	1	20	0.1	0.05	0.05	0.4	5.2015	0.4183	23.4674	2.4440	1.0224	1.2434	0.4183	23.4674	0.9721	0.4067
3	10	1	1	40	0.1	0.05	0.05	0.2	5.2015	0.2345	46.5385	2.3060	0.5408	2.2179	0.2345	46.5385	1.2708	0.2980
4	10	1	1	40	0.1	0.05	0.05	0.4	5.2015	0.4183	46.0526	2.3075	0.9653	1.2434	0.4183	46.0526	0.9426	0.3943
5	10	1	1	20	0.1	0.05	0.2	0.2	5.2015	0.3041	22.1521	2.4606	0.7484	1.7102	0.3041	22.1521	1.1431	0.3477
6	10	1	1	20	0.1	0.05	0.2	0.4	5.2015	0.4610	28.4673	2.3950	1.1040	1.1284	0.4610	28.4673	0.9215	0.4248
7	10	1	1	40	0.1	0.05	0.2	0.2	5.2015	0.3041	24.7112	2.4299	0.7390	1.7102	0.3041	24.7112	1.1342	0.3450
8	10	1	1	40	0.1	0.05	0.2	0.4	5.2015	0.4610	47.7213	2.3025	1.0614	1.1284	0.4610	47.7213	0.9031	0.4163
9	10	1	1	20	0.1	0.05	0.5	0.2	5.2015	0.5500	11.8282	2.7247	1.4986	0.9457	0.5500	11.8282	0.9195	0.5057
10	10	1	1	20	0.1	0.05	0.5	0.4	5.2015	0.6500	19.9755	2.4930	1.6204	0.8002	0.6500	19.9755	0.8246	0.5360
11	10	1	1	40	0.1	0.05	0.5	0.2	5.2015	0.5500	11.8897	2.7217	1.4969	0.9457	0.5500	11.8897	0.9190	0.5054
12	10	1	1	40	0.1	0.05	0.5	0.4	5.2015	0.6500	21.5165	2.4694	1.6051	0.8002	0.6500	21.5165	0.8207	0.5335
13	10	1	3	20	0.1	0.05	0.05	0.2	5.2015	0.2309	28.5149	2.3946	0.5530	2.2523	0.2309	28.5149	1.3154	0.3038
14	10	1	3	20	0.1	0.05	0.05	0.4	5.2015	0.4163	23.1155	2.4482	1.0193	1.2494	0.4163	23.1155	0.9751	0.4060
15	10	1	3	40	0.1	0.05	0.05	0.2	5.2015	0.2309	47.6033	2.3029	0.5318	2.2523	0.2309	47.6033	1.2814	0.2959
16	10	1	3	40	0.1	0.05	0.05	0.4	5.2015	0.4163	45.5389	2.3091	0.9613	1.2494	0.4163	45.5389	0.9449	0.3934
17	10	1	3	20	0.1	0.05	0.2	0.2	5.2015	0.2566	28.1154	2.3979	0.6152	2.0272	0.2566	28.1154	1.2367	0.3173
18	10	1	3	20	0.1	0.05	0.2	0.4	5.2015	0.4311	25.5023	2.4217	1.0440	1.2066	0.4311	25.5023	0.9543	0.4114
19	10	1	3	40	0.1	0.05	0.2	0.2	5.2015	0.2566	37.9674	2.3376	0.5998	2.0272	0.2566	37.9674	1.2166	0.3122
20	10	1	3	40	0.1	0.05	0.2	0.4	5.2015	0.4311	48.3567	2.3007	0.9918	1.2066	0.4311	48.3567	0.9289	0.4004
21	10	1	3	20	0.1	0.05	0.5	0.2	5.2015	0.3686	16.7665	2.5565	0.9422	1.4113	0.3686	16.7665	1.0594	0.3905
22	10	1	3	20	0.1	0.05	0.5	0.4	5.2015	0.5058	28.4513	2.3951	1.2115	1.0284	0.5058	28.4513	0.8871	0.4487
23	10	1	3	40	0.1	0.05	0.5	0.2	5.2015	0.3686	17.3990	2.5420	0.9369	1.4113	0.3686	17.3990	1.0558	0.3891
24	10	1	3	40	0.1	0.05	0.5	0.4	5.2015	0.5058	39.4175	2.3313	1.1792	1.0284	0.5058	39.4175	0.8751	0.4426
25	10	1	1	20	0.1	0.1	0.05	0.2	5.2015	0.2500	28.6697	2.3934	0.5983	2.0806	0.2500	28.6697	1.2541	0.3135
26	10	1	1	20	0.1	0.1	0.05	0.4	5.2015	0.4272	24.9252	2.4276	1.0371	1.2176	0.4272	24.9252	0.9594	0.4099
27	10	1	1	40	0.1	0.1	0.05	0.2	5.2015	0.2500	40.5844	2.3266	0.5816	2.0806	0.2500	40.5844	1.2312	0.3078
28	10	1	1	40	0.1	0.1	0.05	0.4	5.2015	0.4272	47.8366	2.3022	0.9835	1.2176	0.4272	47.8366	0.9328	0.3985
29	10	1	1	20	0.1	0.1	0.2	0.2	5.2015	0.3162	20.8333	2.4794	0.7841	1.6449	0.3162	20.8333	1.1248	0.3557
30	10	1	1	20	0.1	0.1	0.2	0.4	5.2015	0.4690	28.8095	2.3923	1.1221	1.1090	0.4690	28.8095	0.9143	0.4288
31	10	1	1	40	0.1	0.1	0.2	0.2	5.2015	0.3162	22.7273	2.4531	0.7757	1.6449	0.3162	22.7273	1.1174	0.3534
32	10	1	1	40	0.1	0.1	0.2	0.4	5.2015	0.4690	46.5385	2.3060	1.0816	1.1090	0.4690	46.5385	0.8973	0.4209
33	10	1	1	20	0.1	0.1	0.5	0.2	5.2015	0.5568	11.7482	2.7287	1.5193	0.9342	0.5568	11.7482	0.9158	0.5099
34	10	1	1	20	0.1	0.1	0.5	0.4	5.2015	0.6557	19.7122	2.4974	1.6377	0.7932	0.6557	19.7122	0.8228	0.5396

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
35	10	1	1	40	0.1	0.1	0.5	0.2	5.2015	0.5568	11.8059	2.7258	1.5177	0.9342	0.5568	11.8059	0.9153	0.5096
36	10	1	1	40	0.1	0.1	0.5	0.4	5.2015	0.6557	21.1556	2.4746	1.6227	0.7932	0.6557	21.1556	0.8191	0.5371
37	10	1	3	20	0.1	0.1	0.05	0.2	5.2015	0.2466	28.8609	2.3919	0.5899	2.1089	0.2466	28.8609	1.2636	0.3117
38	10	1	3	20	0.1	0.1	0.05	0.4	5.2015	0.4253	24.6198	2.4309	1.0337	1.2232	0.4253	24.6198	0.9621	0.4091
39	10	1	3	40	0.1	0.1	0.05	0.2	5.2015	0.2466	41.9460	2.3213	0.5725	2.1089	0.2466	41.9460	1.2391	0.3056
40	10	1	3	40	0.1	0.1	0.05	0.4	5.2015	0.4253	47.5145	2.3031	0.9794	1.2232	0.4253	47.5145	0.9349	0.3976
41	10	1	3	20	0.1	0.1	0.2	0.2	5.2015	0.2708	26.4320	2.4127	0.6534	1.9208	0.2708	26.4320	1.2038	0.3260
42	10	1	3	20	0.1	0.1	0.2	0.4	5.2015	0.4397	26.6327	2.4108	1.0600	1.1830	0.4397	26.6327	0.9437	0.4150
43	10	1	3	40	0.1	0.1	0.2	0.2	5.2015	0.2708	32.9003	2.3641	0.6402	1.9208	0.2708	32.9003	1.1883	0.3218
44	10	1	3	40	0.1	0.1	0.2	0.4	5.2015	0.4397	48.9586	2.2991	1.0109	1.1830	0.4397	48.9586	0.9206	0.4048
45	10	1	3	20	0.1	0.1	0.5	0.2	5.2015	0.3786	16.2225	2.5698	0.9729	1.3739	0.3786	16.2225	1.0488	0.3971
46	10	1	3	20	0.1	0.1	0.5	0.4	5.2015	0.5132	28.1154	2.3979	1.2305	1.0136	0.5132	28.1154	0.8825	0.4529
47	10	1	3	40	0.1	0.1	0.5	0.2	5.2015	0.3786	16.7516	2.5568	0.9680	1.3739	0.3786	16.7516	1.0456	0.3959
48	10	1	3	40	0.1	0.1	0.5	0.4	5.2015	0.5132	37.9674	2.3376	1.1996	1.0136	0.5132	37.9674	0.8713	0.4471
49	10	3	1	20	0.1	0.05	0.05	0.2	5.2015	0.2273	28.0629	2.3983	0.5451	2.2883	0.2273	28.0629	1.3296	0.3022
50	10	3	1	20	0.1	0.05	0.05	0.4	5.2015	0.4143	22.7542	2.4528	1.0162	1.2554	0.4143	22.7542	0.9783	0.4053
51	10	3	1	40	0.1	0.05	0.05	0.2	5.2015	0.2273	48.4267	2.3005	0.5229	2.2883	0.2273	48.4267	1.2928	0.2939
52	10	3	1	40	0.1	0.05	0.05	0.4	5.2015	0.4143	44.9830	2.3108	0.9574	1.2554	0.4143	44.9830	0.9473	0.3925
53	10	3	1	20	0.1	0.05	0.2	0.2	5.2015	0.2533	28.4168	2.3954	0.6068	2.0534	0.2533	28.4168	1.2452	0.3154
54	10	3	1	20	0.1	0.05	0.2	0.4	5.2015	0.4292	25.2194	2.4246	1.0405	1.2121	0.4292	25.2194	0.9568	0.4106
55	10	3	1	40	0.1	0.05	0.2	0.2	5.2015	0.2533	39.2533	2.3320	0.5907	2.0534	0.2533	39.2533	1.2237	0.3100
56	10	3	1	40	0.1	0.05	0.2	0.4	5.2015	0.4292	48.1171	2.3014	0.9876	1.2121	0.4292	48.1171	0.9308	0.3995
57	10	3	1	20	0.1	0.05	0.5	0.2	5.2015	0.3663	16.8979	2.5534	0.9353	1.4201	0.3663	16.8979	1.0619	0.3890
58	10	3	1	20	0.1	0.05	0.5	0.4	5.2015	0.5042	28.5180	2.3946	1.2072	1.0317	0.5042	28.5180	0.8881	0.4477
59	10	3	1	40	0.1	0.05	0.5	0.2	5.2015	0.3663	17.5572	2.5386	0.9299	1.4201	0.3663	17.5572	1.0582	0.3876
60	10	3	1	40	0.1	0.05	0.5	0.4	5.2015	0.5042	39.7479	2.3299	1.1746	1.0317	0.5042	39.7479	0.8760	0.4416
61	10	3	3	20	0.1	0.05	0.05	0.2	5.2015	0.2261	27.8747	2.3999	0.5426	2.3008	0.2261	27.8747	1.3346	0.3017
62	10	3	3	20	0.1	0.05	0.05	0.4	5.2015	0.4137	22.6317	2.4543	1.0152	1.2574	0.4137	22.6317	0.9794	0.4051
63	10	3	3	40	0.1	0.05	0.05	0.2	5.2015	0.2261	48.6313	2.3000	0.5200	2.3008	0.2261	48.6313	1.2968	0.2932
64	10	3	3	40	0.1	0.05	0.05	0.4	5.2015	0.4137	44.7885	2.3115	0.9562	1.2574	0.4137	44.7885	0.9481	0.3922
65	10	3	3	20	0.1	0.05	0.2	0.2	5.2015	0.2351	28.8445	2.3920	0.5624	2.2123	0.2351	28.8445	1.3002	0.3057
66	10	3	3	20	0.1	0.05	0.2	0.4	5.2015	0.4187	23.5251	2.4433	1.0229	1.2424	0.4187	23.5251	0.9716	0.4068
67	10	3	3	40	0.1	0.05	0.2	0.2	5.2015	0.2351	46.3435	2.3066	0.5423	2.2123	0.2351	46.3435	1.2692	0.2984

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
68	10	3	3	40	0.1	0.05	0.2	0.4	5.2015	0.4187	46.1341	2.3072	0.9659	1.2424	0.4187	46.1341	0.9422	0.3945
69	10	3	3	20	0.1	0.05	0.5	0.2	5.2015	0.2804	25.1569	2.4252	0.6800	1.8552	0.2804	25.1569	1.1845	0.3321
70	10	3	3	20	0.1	0.05	0.5	0.4	5.2015	0.4457	27.2863	2.4049	1.0718	1.1671	0.4457	27.2863	0.9370	0.4176
71	10	3	3	40	0.1	0.05	0.5	0.2	5.2015	0.2804	30.0502	2.3829	0.6681	1.8552	0.2804	30.0502	1.1713	0.3284
72	10	3	3	40	0.1	0.05	0.5	0.4	5.2015	0.4457	48.9624	2.2991	1.0246	1.1671	0.4457	48.9624	0.9154	0.4079
73	10	3	1	20	0.1	0.1	0.05	0.2	5.2015	0.2327	28.6808	2.3933	0.5570	2.2349	0.2327	28.6808	1.3087	0.3046
74	10	3	1	20	0.1	0.1	0.05	0.4	5.2015	0.4173	23.2927	2.4461	1.0208	1.2464	0.4173	23.2927	0.9736	0.4063
75	10	3	1	40	0.1	0.1	0.05	0.2	5.2015	0.2327	47.0956	2.3043	0.5363	2.2349	0.2327	47.0956	1.2760	0.2970
76	10	3	1	40	0.1	0.1	0.05	0.4	5.2015	0.4173	45.8011	2.3083	0.9633	1.2464	0.4173	45.8011	0.9437	0.3939
77	10	3	1	20	0.1	0.1	0.2	0.2	5.2015	0.2582	27.9503	2.3992	0.6195	2.0145	0.2582	27.9503	1.2327	0.3183
78	10	3	1	20	0.1	0.1	0.2	0.4	5.2015	0.4321	25.6395	2.4203	1.0457	1.2039	0.4321	25.6395	0.9531	0.4118
79	10	3	1	40	0.1	0.1	0.2	0.2	5.2015	0.2582	37.3444	2.3405	0.6043	2.0145	0.2582	37.3444	1.2132	0.3132
80	10	3	1	40	0.1	0.1	0.2	0.4	5.2015	0.4321	48.4615	2.3004	0.9939	1.2039	0.4321	48.4615	0.9279	0.4009
81	10	3	1	20	0.1	0.1	0.5	0.2	5.2015	0.3697	16.7024	2.5580	0.9457	1.4070	0.3697	16.7024	1.0582	0.3912
82	10	3	1	20	0.1	0.1	0.5	0.4	5.2015	0.5066	28.4168	2.3954	1.2136	1.0267	0.5066	28.4168	0.8865	0.4491
83	10	3	1	40	0.1	0.1	0.5	0.2	5.2015	0.3697	17.3220	2.5437	0.9404	1.4070	0.3697	17.3220	1.0547	0.3899
84	10	3	1	40	0.1	0.1	0.5	0.4	5.2015	0.5066	39.2533	2.3320	1.1814	1.0267	0.5066	39.2533	0.8747	0.4431
85	10	3	3	20	0.1	0.1	0.05	0.2	5.2015	0.2315	28.5744	2.3941	0.5543	2.2465	0.2315	28.5744	1.3131	0.3040
86	10	3	3	20	0.1	0.1	0.05	0.4	5.2015	0.4167	23.1748	2.4475	1.0198	1.2484	0.4167	23.1748	0.9746	0.4061
87	10	3	3	40	0.1	0.1	0.05	0.2	5.2015	0.2315	47.4402	2.3033	0.5333	2.2465	0.2315	47.4402	1.2796	0.2963
88	10	3	3	40	0.1	0.1	0.05	0.4	5.2015	0.4167	45.6275	2.3088	0.9620	1.2484	0.4167	45.6275	0.9445	0.3935
89	10	3	3	20	0.1	0.1	0.2	0.2	5.2015	0.2404	28.9990	2.3908	0.5747	2.1639	0.2404	28.9990	1.2827	0.3083
90	10	3	3	20	0.1	0.1	0.2	0.4	5.2015	0.4216	24.0320	2.4374	1.0277	1.2336	0.4216	24.0320	0.9672	0.4078
91	10	3	3	40	0.1	0.1	0.2	0.2	5.2015	0.2404	44.4412	2.3126	0.5559	2.1639	0.2404	44.4412	1.2548	0.3016
92	10	3	3	40	0.1	0.1	0.2	0.4	5.2015	0.4216	46.8140	2.3052	0.9719	1.2336	0.4216	46.8140	0.9388	0.3958
93	10	3	3	20	0.1	0.1	0.5	0.2	5.2015	0.2848	24.5677	2.4315	0.6925	1.8264	0.2848	24.5677	1.1761	0.3350
94	10	3	3	20	0.1	0.1	0.5	0.4	5.2015	0.4485	27.5555	2.4026	1.0775	1.1599	0.4485	27.5555	0.9340	0.4189
95	10	3	3	40	0.1	0.1	0.5	0.2	5.2015	0.2848	28.8817	2.3917	0.6812	1.8264	0.2848	28.8817	1.1639	0.3315
96	10	3	3	40	0.1	0.1	0.5	0.4	5.2015	0.4485	48.8597	2.2993	1.0312	1.1599	0.4485	48.8597	0.9130	0.4094
97	10	1	1	20	0.25	0.05	0.05	0.2	5.2015	0.3279	19.7122	2.4974	0.8188	3.9661	0.3279	19.7122	2.0096	0.6589
98	10	1	1	20	0.25	0.05	0.05	0.4	5.2015	0.4770	28.9748	2.3910	1.1404	2.7263	0.4770	28.9748	1.4830	0.7074
99	10	1	1	40	0.25	0.05	0.05	0.2	5.2015	0.3279	21.1556	2.4746	0.8113	3.9661	0.3279	21.1556	1.9931	0.6535
100	10	1	1	40	0.25	0.05	0.05	0.4	5.2015	0.4770	45.1527	2.3103	1.1019	2.7263	0.4770	45.1527	1.4462	0.6898
101	10	1	1	20	0.25	0.05	0.2	0.2	5.2015	0.3808	16.1111	2.5726	0.9796	3.4149	0.3808	16.1111	1.8418	0.7013

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
102	10	1	1	20	0.25	0.05	0.2	0.4	5.2015	0.5148	28.0339	2.3985	1.2347	2.5261	0.5148	28.0339	1.4146	0.7282
103	10	1	1	40	0.25	0.05	0.2	0.2	5.2015	0.3808	16.6206	2.5599	0.9748	3.4149	0.3808	16.6206	1.8340	0.6984
104	10	1	1	40	0.25	0.05	0.2	0.4	5.2015	0.5148	37.6542	2.3391	1.2041	2.5261	0.5148	37.6542	1.3896	0.7153
105	10	1	1	20	0.25	0.05	0.5	0.2	5.2015	0.5958	11.3485	2.7493	1.6381	2.1825	0.5958	11.3485	1.4242	0.8486
106	10	1	1	20	0.25	0.05	0.5	0.4	5.2015	0.6892	18.3360	2.5226	1.7386	1.8868	0.6892	18.3360	1.2269	0.8456
107	10	1	1	40	0.25	0.05	0.5	0.2	5.2015	0.5958	11.3895	2.7471	1.6368	2.1825	0.5958	11.3895	1.4234	0.8481
108	10	1	1	40	0.25	0.05	0.5	0.4	5.2015	0.6892	19.3420	2.5038	1.7256	1.8868	0.6892	19.3420	1.2209	0.8414
109	10	1	3	20	0.25	0.05	0.05	0.2	5.2015	0.3253	19.9457	2.4935	0.8112	3.9972	0.3253	19.9457	2.0189	0.6568
110	10	1	3	20	0.25	0.05	0.05	0.4	5.2015	0.4752	28.9520	2.3911	1.1363	2.7364	0.4752	28.9520	1.4867	0.7065
111	10	1	3	40	0.25	0.05	0.05	0.2	5.2015	0.3253	21.4754	2.4700	0.8035	3.9972	0.3253	21.4754	2.0017	0.6512
112	10	1	3	40	0.25	0.05	0.05	0.4	5.2015	0.4752	45.4731	2.3093	1.0974	2.7364	0.4752	45.4731	1.4492	0.6887
113	10	1	3	20	0.25	0.05	0.2	0.2	5.2015	0.3440	18.3814	2.5217	0.8674	3.7802	0.3440	18.3814	1.9538	0.6721
114	10	1	3	20	0.25	0.05	0.2	0.4	5.2015	0.4882	28.9546	2.3911	1.1673	2.6636	0.4882	28.9546	1.4607	0.7131
115	10	1	3	40	0.25	0.05	0.2	0.2	5.2015	0.3440	19.4001	2.5028	0.8610	3.7802	0.3440	19.4001	1.9409	0.6677
116	10	1	3	40	0.25	0.05	0.2	0.4	5.2015	0.4882	42.9741	2.3176	1.1314	2.6636	0.4882	42.9741	1.4279	0.6971
117	10	1	3	20	0.25	0.05	0.5	0.2	5.2015	0.4340	14.0487	2.6338	1.1430	2.9964	0.4340	14.0487	1.7075	0.7410
118	10	1	3	20	0.25	0.05	0.5	0.4	5.2015	0.5553	25.5237	2.4215	1.3446	2.3418	0.5553	25.5237	1.3578	0.7540
119	10	1	3	40	0.25	0.05	0.5	0.2	5.2015	0.4340	14.2748	2.6262	1.1397	2.9964	0.4340	14.2748	1.7034	0.7393
120	10	1	3	40	0.25	0.05	0.5	0.4	5.2015	0.5553	30.8191	2.3775	1.3202	2.3418	0.5553	30.8191	1.3406	0.7444
121	10	1	1	20	0.25	0.1	0.05	0.2	5.2015	0.3391	18.7589	2.5144	0.8527	3.8346	0.3391	18.7589	1.9702	0.6681
122	10	1	1	20	0.25	0.1	0.05	0.4	5.2015	0.4848	28.9895	2.3909	1.1590	2.6825	0.4848	28.9895	1.4673	0.7113
123	10	1	1	40	0.25	0.1	0.05	0.2	5.2015	0.3391	19.8872	2.4944	0.8459	3.8346	0.3391	19.8872	1.9563	0.6634
124	10	1	1	40	0.25	0.1	0.05	0.4	5.2015	0.4848	43.6561	2.3152	1.1224	2.6825	0.4848	43.6561	1.4334	0.6948
125	10	1	1	20	0.25	0.1	0.2	0.2	5.2015	0.3905	15.6476	2.5849	1.0094	3.3299	0.3905	15.6476	1.8151	0.7088
126	10	1	1	20	0.25	0.1	0.2	0.4	5.2015	0.5220	27.6431	2.4018	1.2538	2.4911	0.5220	27.6431	1.4035	0.7326
127	10	1	1	40	0.25	0.1	0.2	0.2	5.2015	0.3905	16.0804	2.5734	1.0050	3.3299	0.3905	16.0804	1.8082	0.7061
128	10	1	1	40	0.25	0.1	0.2	0.4	5.2015	0.5220	36.2889	2.3456	1.2244	2.4911	0.5220	36.2889	1.3801	0.7204
129	10	1	1	20	0.25	0.1	0.5	0.2	5.2015	0.6021	11.2928	2.7523	1.6571	2.1598	0.6021	11.2928	1.4159	0.8525
130	10	1	1	20	0.25	0.1	0.5	0.4	5.2015	0.6946	18.1366	2.5265	1.7550	1.8721	0.6946	18.1366	1.2227	0.8493
131	10	1	1	40	0.25	0.1	0.5	0.2	5.2015	0.6021	11.3318	2.7502	1.6558	2.1598	0.6021	11.3318	1.4151	0.8520
132	10	1	1	40	0.25	0.1	0.5	0.4	5.2015	0.6946	19.0883	2.5083	1.7424	1.8721	0.6946	19.0883	1.2169	0.8453
133	10	1	3	20	0.25	0.1	0.05	0.2	5.2015	0.3367	18.9577	2.5107	0.8452	3.8627	0.3367	18.9577	1.9786	0.6661
134	10	1	3	20	0.25	0.1	0.05	0.4	5.2015	0.4831	28.9979	2.3908	1.1549	2.6920	0.4831	28.9979	1.4707	0.7104
135	10	1	3	40	0.25	0.1	0.05	0.2	5.2015	0.3367	20.1472	2.4902	0.8383	3.8627	0.3367	20.1472	1.9642	0.6613

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
136	10	1	3	40	0.25	0.1	0.05	0.4	5.2015	0.4831	43.9944	2.3141	1.1178	2.6920	0.4831	43.9944	1.4361	0.6937
137	10	1	3	20	0.25	0.1	0.2	0.2	5.2015	0.3547	17.6209	2.5372	0.9000	3.6658	0.3547	17.6209	1.9192	0.6808
138	10	1	3	20	0.25	0.1	0.2	0.4	5.2015	0.4958	28.7974	2.3924	1.1862	2.6227	0.4958	28.7974	1.4466	0.7172
139	10	1	3	40	0.25	0.1	0.2	0.2	5.2015	0.3547	18.4418	2.5205	0.8941	3.6658	0.3547	18.4418	1.9081	0.6769
140	10	1	3	40	0.25	0.1	0.2	0.4	5.2015	0.4958	41.4330	2.3233	1.1519	2.6227	0.4958	41.4330	1.4163	0.7022
141	10	1	3	20	0.25	0.1	0.5	0.2	5.2015	0.4425	13.8040	2.6423	1.1693	2.9385	0.4425	13.8040	1.6883	0.7471
142	10	1	3	20	0.25	0.1	0.5	0.4	5.2015	0.5620	25.0742	2.4261	1.3634	2.3139	0.5620	25.0742	1.3495	0.7584
143	10	1	3	40	0.25	0.1	0.5	0.2	5.2015	0.4425	14.0057	2.6352	1.1662	2.9385	0.4425	14.0057	1.6846	0.7455
144	10	1	3	40	0.25	0.1	0.5	0.4	5.2015	0.5620	29.8814	2.3841	1.3399	2.3139	0.5620	29.8814	1.3332	0.7493
145	10	3	1	20	0.25	0.05	0.05	0.2	5.2015	0.3228	20.1879	2.4895	0.8035	4.0291	0.3228	20.1879	2.0284	0.6547
146	10	3	1	20	0.25	0.05	0.05	0.4	5.2015	0.4735	28.9215	2.3914	1.1322	2.7465	0.4735	28.9215	1.4905	0.7057
147	10	3	1	40	0.25	0.05	0.05	0.2	5.2015	0.3228	21.8111	2.4652	0.7957	4.0291	0.3228	21.8111	2.0105	0.6489
148	10	3	1	40	0.25	0.05	0.05	0.4	5.2015	0.4735	45.7872	2.3083	1.0929	2.7465	0.4735	45.7872	1.4522	0.6876
149	10	3	1	20	0.25	0.05	0.2	0.2	5.2015	0.3416	18.5669	2.5181	0.8601	3.8071	0.3416	18.5669	1.9619	0.6701
150	10	3	1	20	0.25	0.05	0.2	0.4	5.2015	0.4865	28.9750	2.3910	1.1632	2.6730	0.4865	28.9750	1.4639	0.7122
151	10	3	1	40	0.25	0.05	0.2	0.2	5.2015	0.3416	19.6384	2.4987	0.8535	3.8071	0.3416	19.6384	1.9485	0.6655
152	10	3	1	40	0.25	0.05	0.2	0.4	5.2015	0.4865	43.3158	2.3164	1.1269	2.6730	0.4865	43.3158	1.4306	0.6960
153	10	3	1	20	0.25	0.05	0.5	0.2	5.2015	0.4321	14.1064	2.6318	1.1371	3.0098	0.4321	14.1064	1.7119	0.7396
154	10	3	1	20	0.25	0.05	0.5	0.4	5.2015	0.5538	25.6243	2.4205	1.3404	2.3482	0.5538	25.6243	1.3597	0.7530
155	10	3	1	40	0.25	0.05	0.5	0.2	5.2015	0.4321	14.3385	2.6241	1.1337	3.0098	0.4321	14.3385	1.7078	0.7378
156	10	3	1	40	0.25	0.05	0.5	0.4	5.2015	0.5538	31.0365	2.3760	1.3158	2.3482	0.5538	31.0365	1.3422	0.7433
157	10	3	3	20	0.25	0.05	0.05	0.2	5.2015	0.3219	20.2706	2.4882	0.8009	4.0398	0.3219	20.2706	2.0316	0.6539
158	10	3	3	20	0.25	0.05	0.05	0.4	5.2015	0.4729	28.9096	2.3915	1.1309	2.7499	0.4729	28.9096	1.4917	0.7054
159	10	3	3	40	0.25	0.05	0.05	0.2	5.2015	0.3219	21.9267	2.4636	0.7930	4.0398	0.3219	21.9267	2.0135	0.6481
160	10	3	3	40	0.25	0.05	0.05	0.4	5.2015	0.4729	45.8903	2.3080	1.0914	2.7499	0.4729	45.8903	1.4533	0.6872
161	10	3	3	20	0.25	0.05	0.2	0.2	5.2015	0.3283	19.6740	2.4980	0.8201	3.9610	0.3283	19.6740	2.0081	0.6592
162	10	3	3	20	0.25	0.05	0.2	0.4	5.2015	0.4773	28.9779	2.3909	1.1411	2.7247	0.4773	28.9779	1.4824	0.7075
163	10	3	3	40	0.25	0.05	0.2	0.2	5.2015	0.3283	21.1038	2.4753	0.8126	3.9610	0.3283	21.1038	1.9917	0.6539
164	10	3	3	40	0.25	0.05	0.2	0.4	5.2015	0.4773	45.0987	2.3105	1.1027	2.7247	0.4773	45.0987	1.4457	0.6900
165	10	3	3	20	0.25	0.05	0.5	0.2	5.2015	0.3621	17.1497	2.5476	0.9225	3.5913	0.3621	17.1497	1.8964	0.6867
166	10	3	3	20	0.25	0.05	0.5	0.4	5.2015	0.5011	28.6315	2.3937	1.1995	2.5950	0.5011	28.6315	1.4372	0.7202
167	10	3	3	40	0.25	0.05	0.5	0.2	5.2015	0.3621	17.8625	2.5321	0.9169	3.5913	0.3621	17.8625	1.8864	0.6830
168	10	3	3	40	0.25	0.05	0.5	0.4	5.2015	0.5011	40.3600	2.3274	1.1663	2.5950	0.5011	40.3600	1.4085	0.7058
169	10	3	1	20	0.25	0.1	0.05	0.2	5.2015	0.3266	19.8279	2.4954	0.8150	3.9816	0.3266	19.8279	2.0142	0.6578

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
170	10	3	1	20	0.25	0.1	0.05	0.4	5.2015	0.4761	28.9644	2.3910	1.1384	2.7313	0.4761	28.9644	1.4849	0.7069
171	10	3	1	40	0.25	0.1	0.05	0.2	5.2015	0.3266	21.3136	2.4723	0.8074	3.9816	0.3266	21.3136	1.9974	0.6523
172	10	3	1	40	0.25	0.1	0.05	0.4	5.2015	0.4761	45.3136	2.3098	1.0997	2.7313	0.4761	45.3136	1.4477	0.6892
173	10	3	1	20	0.25	0.1	0.2	0.2	5.2015	0.3452	18.2911	2.5235	0.8711	3.7670	0.3452	18.2911	1.9498	0.6731
174	10	3	1	20	0.25	0.1	0.2	0.4	5.2015	0.4891	28.9422	2.3912	1.1694	2.6590	0.4891	28.9422	1.4590	0.7135
175	10	3	1	40	0.25	0.1	0.2	0.2	5.2015	0.3452	19.2846	2.5048	0.8647	3.7670	0.3452	19.2846	1.9371	0.6687
176	10	3	1	40	0.25	0.1	0.2	0.4	5.2015	0.4891	42.8029	2.3182	1.1337	2.6590	0.4891	42.8029	1.4266	0.6977
177	10	3	1	20	0.25	0.1	0.5	0.2	5.2015	0.4349	14.0203	2.6347	1.1459	2.9898	0.4349	14.0203	1.7053	0.7417
178	10	3	1	20	0.25	0.1	0.5	0.4	5.2015	0.5560	25.4735	2.4220	1.3467	2.3387	0.5560	25.4735	1.3569	0.7545
179	10	3	1	40	0.25	0.1	0.5	0.2	5.2015	0.4349	14.2435	2.6272	1.1427	2.9898	0.4349	14.2435	1.7013	0.7400
180	10	3	1	40	0.25	0.1	0.5	0.4	5.2015	0.5560	30.7117	2.3782	1.3224	2.3387	0.5560	30.7117	1.3397	0.7449
181	10	3	3	20	0.25	0.1	0.05	0.2	5.2015	0.3258	19.9062	2.4941	0.8125	3.9920	0.3258	19.9062	2.0173	0.6571
182	10	3	3	20	0.25	0.1	0.05	0.4	5.2015	0.4755	28.9564	2.3911	1.1370	2.7347	0.4755	28.9564	1.4861	0.7067
183	10	3	3	40	0.25	0.1	0.05	0.2	5.2015	0.3258	21.4210	2.4707	0.8048	3.9920	0.3258	21.4210	2.0003	0.6516
184	10	3	3	40	0.25	0.1	0.05	0.4	5.2015	0.4755	45.4201	2.3094	1.0982	2.7347	0.4755	45.4201	1.4487	0.6889
185	10	3	3	20	0.25	0.1	0.2	0.2	5.2015	0.3321	19.3411	2.5038	0.8315	3.9158	0.3321	19.3411	1.9946	0.6624
186	10	3	3	20	0.25	0.1	0.2	0.4	5.2015	0.4799	28.9964	2.3908	1.1473	2.7098	0.4799	28.9964	1.4771	0.7088
187	10	3	3	40	0.25	0.1	0.2	0.2	5.2015	0.3321	20.6551	2.4821	0.8243	3.9158	0.3321	20.6551	1.9791	0.6572
188	10	3	3	40	0.25	0.1	0.2	0.4	5.2015	0.4799	44.6072	2.3121	1.1095	2.7098	0.4799	44.6072	1.4413	0.6917
189	10	3	3	20	0.25	0.1	0.5	0.2	5.2015	0.3655	16.9426	2.5523	0.9330	3.5575	0.3655	16.9426	1.8860	0.6894
190	10	3	3	20	0.25	0.1	0.5	0.4	5.2015	0.5036	28.5395	2.3944	1.2058	2.5822	0.5036	28.5395	1.4330	0.7216
191	10	3	3	40	0.25	0.1	0.5	0.2	5.2015	0.3655	17.6112	2.5374	0.9275	3.5575	0.3655	17.6112	1.8765	0.6859
192	10	3	3	40	0.25	0.1	0.5	0.4	5.2015	0.5036	39.8586	2.3295	1.1731	2.5822	0.5036	39.8586	1.4050	0.7075
193	10	1	1	20	0.5	0.05	0.05	0.2	5.2015	0.5431	11.9131	2.7206	1.4776	4.7884	0.5431	11.9131	2.5358	1.3773
194	10	1	1	20	0.5	0.05	0.05	0.4	5.2015	0.6442	20.2499	2.4885	1.6031	4.0371	0.6442	20.2499	2.0308	1.3082
195	10	1	1	40	0.5	0.05	0.05	0.2	5.2015	0.5431	11.9787	2.7174	1.4759	4.7884	0.5431	11.9787	2.5329	1.3757
196	10	1	1	40	0.5	0.05	0.05	0.4	5.2015	0.6442	21.8976	2.4640	1.5874	4.0371	0.6442	21.8976	2.0127	1.2966
197	10	1	1	20	0.5	0.05	0.2	0.2	5.2015	0.5766	11.5328	2.7396	1.5797	4.5103	0.5766	11.5328	2.4284	1.4003
198	10	1	1	20	0.5	0.05	0.2	0.4	5.2015	0.6727	18.9831	2.5103	1.6886	3.8662	0.6727	18.9831	1.9797	1.3317
199	10	1	1	40	0.5	0.05	0.2	0.2	5.2015	0.5766	11.5811	2.7371	1.5783	4.5103	0.5766	11.5811	2.4263	1.3991
200	10	1	1	40	0.5	0.05	0.2	0.4	5.2015	0.6727	20.1805	2.4896	1.6747	3.8662	0.6727	20.1805	1.9652	1.3220
201	10	1	1	20	0.5	0.05	0.5	0.2	5.2015	0.7366	10.4600	2.8013	2.0633	3.5310	0.7366	10.4600	2.0356	1.4993
202	10	1	1	20	0.5	0.05	0.5	0.4	5.2015	0.8139	14.9612	2.6046	2.1200	3.1952	0.8139	14.9612	1.7722	1.4425
203	10	1	1	40	0.5	0.05	0.5	0.2	5.2015	0.7366	10.4749	2.8003	2.0626	3.5310	0.7366	10.4749	2.0350	1.4989

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
204	10	1	1	40	0.5	0.05	0.5	0.4	5.2015	0.8139	15.2949	2.5948	2.1120	3.1952	0.8139	15.2949	1.7666	1.4379
205	10	1	3	20	0.5	0.05	0.05	0.2	5.2015	0.5416	11.9326	2.7196	1.4730	4.8019	0.5416	11.9326	2.5410	1.3762
206	10	1	3	20	0.5	0.05	0.05	0.4	5.2015	0.6429	20.3124	2.4875	1.5992	4.0453	0.6429	20.3124	2.0332	1.3072
207	10	1	3	40	0.5	0.05	0.05	0.2	5.2015	0.5416	11.9992	2.7164	1.4712	4.8019	0.5416	11.9992	2.5381	1.3746
208	10	1	3	40	0.5	0.05	0.05	0.4	5.2015	0.6429	21.9853	2.4628	1.5834	4.0453	0.6429	21.9853	2.0149	1.2954
209	10	1	3	20	0.5	0.05	0.2	0.2	5.2015	0.5530	11.7921	2.7265	1.5078	4.7028	0.5530	11.7921	2.5030	1.3842
210	10	1	3	20	0.5	0.05	0.2	0.4	5.2015	0.6526	19.8571	2.4950	1.6281	3.9855	0.6526	19.8571	2.0154	1.3151
211	10	1	3	40	0.5	0.05	0.2	0.2	5.2015	0.5530	11.8519	2.7235	1.5062	4.7028	0.5530	11.8519	2.5004	1.3828
212	10	1	3	40	0.5	0.05	0.2	0.4	5.2015	0.6526	21.3537	2.4717	1.6129	3.9855	0.6526	21.3537	1.9984	1.3041
213	10	1	3	20	0.5	0.05	0.5	0.2	5.2015	0.6131	11.2001	2.7574	1.6904	4.2423	0.6131	11.2001	2.3231	1.4242
214	10	1	3	20	0.5	0.05	0.5	0.4	5.2015	0.7042	17.8004	2.5334	1.7839	3.6934	0.7042	17.8004	1.9276	1.3573
215	10	1	3	40	0.5	0.05	0.5	0.2	5.2015	0.6131	11.2357	2.7554	1.6892	4.2423	0.6131	11.2357	2.3216	1.4232
216	10	1	3	40	0.5	0.05	0.5	0.4	5.2015	0.7042	18.6653	2.5162	1.7718	3.6934	0.7042	18.6653	1.9160	1.3492
217	10	1	1	20	0.5	0.1	0.05	0.2	5.2015	0.5500	11.8282	2.7247	1.4986	4.7286	0.5500	11.8282	2.5129	1.3821
218	10	1	1	20	0.5	0.1	0.05	0.4	5.2015	0.6500	19.9755	2.4930	1.6204	4.0011	0.6500	19.9755	2.0200	1.3130
219	10	1	1	40	0.5	0.1	0.05	0.2	5.2015	0.5500	11.8897	2.7217	1.4969	4.7286	0.5500	11.8897	2.5102	1.3806
220	10	1	1	40	0.5	0.1	0.05	0.4	5.2015	0.6500	21.5165	2.4694	1.6051	4.0011	0.6500	21.5165	2.0028	1.3018
221	10	1	1	20	0.5	0.1	0.2	0.2	5.2015	0.5831	11.4683	2.7430	1.5994	4.4602	0.5831	11.4683	2.4089	1.4046
222	10	1	1	20	0.5	0.1	0.2	0.4	5.2015	0.6782	18.7589	2.5144	1.7054	3.8346	0.6782	18.7589	1.9702	1.3363
223	10	1	1	40	0.5	0.1	0.2	0.2	5.2015	0.5831	11.5139	2.7406	1.5980	4.4602	0.5831	11.5139	2.4069	1.4035
224	10	1	1	40	0.5	0.1	0.2	0.4	5.2015	0.6782	19.8872	2.4944	1.6918	3.8346	0.6782	19.8872	1.9563	1.3268
225	10	1	1	20	0.5	0.1	0.5	0.2	5.2015	0.7416	10.4382	2.8027	2.0785	3.5068	0.7416	10.4382	2.0257	1.5023
226	10	1	1	20	0.5	0.1	0.5	0.4	5.2015	0.8185	14.8741	2.6072	2.1341	3.1773	0.8185	14.8741	1.7664	1.4459
227	10	1	1	40	0.5	0.1	0.5	0.2	5.2015	0.7416	10.4527	2.8017	2.0778	3.5068	0.7416	10.4527	2.0251	1.5018
228	10	1	1	40	0.5	0.1	0.5	0.4	5.2015	0.8185	15.1963	2.5976	2.1262	3.1773	0.8185	15.1963	1.7610	1.4414
229	10	1	3	20	0.5	0.1	0.05	0.2	5.2015	0.5485	11.8467	2.7238	1.4940	4.7417	0.5485	11.8467	2.5179	1.3810
230	10	1	3	20	0.5	0.1	0.05	0.4	5.2015	0.6487	20.0355	2.4920	1.6166	4.0091	0.6487	20.0355	2.0224	1.3120
231	10	1	3	40	0.5	0.1	0.05	0.2	5.2015	0.5485	11.9090	2.7208	1.4923	4.7417	0.5485	11.9090	2.5152	1.3795
232	10	1	3	40	0.5	0.1	0.05	0.4	5.2015	0.6487	21.5994	2.4682	1.6012	4.0091	0.6487	21.5994	2.0050	1.3007
233	10	1	3	20	0.5	0.1	0.2	0.2	5.2015	0.5598	11.7140	2.7304	1.5284	4.6462	0.5598	11.7140	2.4812	1.3889
234	10	1	3	20	0.5	0.1	0.2	0.4	5.2015	0.6583	19.5985	2.4993	1.6453	3.9508	0.6583	19.5985	2.0050	1.3199
235	10	1	3	40	0.5	0.1	0.2	0.2	5.2015	0.5598	11.7702	2.7276	1.5268	4.6462	0.5598	11.7702	2.4787	1.3875
236	10	1	3	40	0.5	0.1	0.2	0.4	5.2015	0.6583	21.0013	2.4769	1.6305	3.9508	0.6583	21.0013	1.9888	1.3092
237	10	1	3	20	0.5	0.1	0.5	0.2	5.2015	0.6191	11.1511	2.7601	1.7089	4.2006	0.6191	11.1511	2.3066	1.4281

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
238	10	1	3	20	0.5	0.1	0.5	0.4	5.2015	0.7095	17.6209	2.5372	1.8001	3.6658	0.7095	17.6209	1.9192	1.3616
239	10	1	3	40	0.5	0.1	0.5	0.2	5.2015	0.6191	11.1851	2.7582	1.7077	4.2006	0.6191	11.1851	2.3051	1.4272
240	10	1	3	40	0.5	0.1	0.5	0.4	5.2015	0.7095	18.4418	2.5205	1.7882	3.6658	0.7095	18.4418	1.9081	1.3537
241	10	3	1	20	0.5	0.05	0.05	0.2	5.2015	0.5401	11.9524	2.7187	1.4682	4.8156	0.5401	11.9524	2.5462	1.3751
242	10	3	1	20	0.5	0.05	0.05	0.4	5.2015	0.6416	20.3754	2.4865	1.5954	4.0534	0.6416	20.3754	2.0356	1.3061
243	10	3	1	40	0.5	0.05	0.05	0.2	5.2015	0.5401	12.0200	2.7154	1.4665	4.8156	0.5401	12.0200	2.5433	1.3735
244	10	3	1	40	0.5	0.05	0.05	0.4	5.2015	0.6416	22.0740	2.4616	1.5794	4.0534	0.6416	22.0740	2.0172	1.2943
245	10	3	1	20	0.5	0.05	0.2	0.2	5.2015	0.5515	11.8101	2.7256	1.5032	4.7156	0.5515	11.8101	2.5079	1.3832
246	10	3	1	20	0.5	0.05	0.2	0.4	5.2015	0.6513	19.9161	2.4940	1.6243	3.9933	0.6513	19.9161	2.0177	1.3141
247	10	3	1	40	0.5	0.05	0.2	0.2	5.2015	0.5515	11.8707	2.7226	1.5016	4.7156	0.5515	11.8707	2.5053	1.3817
248	10	3	1	40	0.5	0.05	0.2	0.4	5.2015	0.6513	21.4346	2.4705	1.6090	3.9933	0.6513	21.4346	2.0006	1.3030
249	10	3	1	20	0.5	0.05	0.5	0.2	5.2015	0.6117	11.2113	2.7568	1.6863	4.2517	0.6117	11.2113	2.3269	1.4233
250	10	3	1	20	0.5	0.05	0.5	0.4	5.2015	0.7030	17.8412	2.5326	1.7803	3.6996	0.7030	17.8412	1.9295	1.3563
251	10	3	1	40	0.5	0.05	0.5	0.2	5.2015	0.6117	11.2473	2.7548	1.6851	4.2517	0.6117	11.2473	2.3253	1.4224
252	10	3	1	40	0.5	0.05	0.5	0.4	5.2015	0.7030	18.7163	2.5152	1.7681	3.6996	0.7030	18.7163	1.9178	1.3482
253	10	3	3	20	0.5	0.05	0.05	0.2	5.2015	0.5396	11.9591	2.7183	1.4667	4.8202	0.5396	11.9591	2.5480	1.3748
254	10	3	3	20	0.5	0.05	0.05	0.4	5.2015	0.6412	20.3966	2.4862	1.5941	4.0562	0.6412	20.3966	2.0364	1.3057
255	10	3	3	40	0.5	0.05	0.05	0.2	5.2015	0.5396	12.0270	2.7151	1.4649	4.8202	0.5396	12.0270	2.5450	1.3732
256	10	3	3	40	0.5	0.05	0.05	0.4	5.2015	0.6412	22.1038	2.4612	1.5781	4.0562	0.6412	22.1038	2.0179	1.2939
257	10	3	3	20	0.5	0.05	0.2	0.2	5.2015	0.5434	11.9098	2.7207	1.4784	4.7861	0.5434	11.9098	2.5349	1.3775
258	10	3	3	20	0.5	0.05	0.2	0.4	5.2015	0.6444	20.2395	2.4887	1.6038	4.0358	0.6444	20.2395	2.0304	1.3084
259	10	3	3	40	0.5	0.05	0.2	0.2	5.2015	0.5434	11.9753	2.7176	1.4767	4.7861	0.5434	11.9753	2.5321	1.3759
260	10	3	3	40	0.5	0.05	0.2	0.4	5.2015	0.6444	21.8832	2.4642	1.5880	4.0358	0.6444	21.8832	2.0123	1.2968
261	10	3	3	20	0.5	0.05	0.5	0.2	5.2015	0.5645	11.6616	2.7330	1.5427	4.6075	0.5645	11.6616	2.4662	1.3921
262	10	3	3	20	0.5	0.05	0.5	0.4	5.2015	0.6623	19.4227	2.5024	1.6573	3.9270	0.6623	19.4227	1.9979	1.3232
263	10	3	3	40	0.5	0.05	0.5	0.2	5.2015	0.5645	11.7154	2.7303	1.5411	4.6075	0.5645	11.7154	2.4639	1.3907
264	10	3	3	40	0.5	0.05	0.5	0.4	5.2015	0.6623	20.7643	2.4804	1.6427	3.9270	0.6623	20.7643	1.9822	1.3128
265	10	3	1	20	0.5	0.1	0.05	0.2	5.2015	0.5424	11.9228	2.7201	1.4753	4.7951	0.5424	11.9228	2.5384	1.3768
266	10	3	1	20	0.5	0.1	0.05	0.4	5.2015	0.6436	20.2810	2.4880	1.6012	4.0412	0.6436	20.2810	2.0320	1.3077
267	10	3	1	40	0.5	0.1	0.05	0.2	5.2015	0.5424	11.9889	2.7169	1.4736	4.7951	0.5424	11.9889	2.5355	1.3752
268	10	3	1	40	0.5	0.1	0.05	0.4	5.2015	0.6436	21.9413	2.4634	1.5854	4.0412	0.6436	21.9413	2.0138	1.2960
269	10	3	1	20	0.5	0.1	0.2	0.2	5.2015	0.5538	11.7832	2.7269	1.5101	4.6964	0.5538	11.7832	2.5005	1.3847
270	10	3	1	20	0.5	0.1	0.2	0.4	5.2015	0.6532	19.8279	2.4954	1.6300	3.9816	0.6532	19.8279	2.0142	1.3157
271	10	3	1	40	0.5	0.1	0.2	0.2	5.2015	0.5538	11.8425	2.7240	1.5085	4.6964	0.5538	11.8425	2.4979	1.3833

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
272	10	3	1	40	0.5	0.1	0.2	0.4	5.2015	0.6532	21.3136	2.4723	1.6149	3.9816	0.6532	21.3136	1.9974	1.3047
273	10	3	1	20	0.5	0.1	0.5	0.2	5.2015	0.6137	11.1945	2.7577	1.6925	4.2376	0.6137	11.1945	2.3212	1.4246
274	10	3	1	20	0.5	0.1	0.5	0.4	5.2015	0.7048	17.7801	2.5339	1.7857	3.6903	0.7048	17.7801	1.9266	1.3578
275	10	3	1	40	0.5	0.1	0.5	0.2	5.2015	0.6137	11.2300	2.7557	1.6913	4.2376	0.6137	11.2300	2.3197	1.4237
276	10	3	1	40	0.5	0.1	0.5	0.4	5.2015	0.7048	18.6399	2.5167	1.7736	3.6903	0.7048	18.6399	1.9151	1.3497
277	10	3	3	20	0.5	0.1	0.05	0.2	5.2015	0.5419	11.9293	2.7198	1.4737	4.7997	0.5419	11.9293	2.5401	1.3764
278	10	3	3	20	0.5	0.1	0.05	0.4	5.2015	0.6431	20.3019	2.4877	1.5999	4.0439	0.6431	20.3019	2.0328	1.3073
279	10	3	3	40	0.5	0.1	0.05	0.2	5.2015	0.5419	11.9957	2.7166	1.4720	4.7997	0.5419	11.9957	2.5372	1.3748
280	10	3	3	40	0.5	0.1	0.05	0.4	5.2015	0.6431	21.9706	2.4630	1.5841	4.0439	0.6431	21.9706	2.0146	1.2956
281	10	3	3	20	0.5	0.1	0.2	0.2	5.2015	0.5457	11.8811	2.7221	1.4854	4.7660	0.5457	11.8811	2.5272	1.3791
282	10	3	3	20	0.5	0.1	0.2	0.4	5.2015	0.6464	20.1469	2.4902	1.6095	4.0237	0.6464	20.1469	2.0268	1.3100
283	10	3	3	40	0.5	0.1	0.2	0.2	5.2015	0.5457	11.9451	2.7190	1.4837	4.7660	0.5457	11.9451	2.5244	1.3776
284	10	3	3	40	0.5	0.1	0.2	0.4	5.2015	0.6464	21.7540	2.4660	1.5939	4.0237	0.6464	21.7540	2.0090	1.2985
285	10	3	3	20	0.5	0.1	0.5	0.2	5.2015	0.5667	11.6375	2.7342	1.5494	4.5895	0.5667	11.6375	2.4593	1.3936
286	10	3	3	20	0.5	0.1	0.5	0.4	5.2015	0.6642	19.3411	2.5038	1.6629	3.9158	0.6642	19.3411	1.9946	1.3247
287	10	3	3	40	0.5	0.1	0.5	0.2	5.2015	0.5667	11.6902	2.7316	1.5479	4.5895	0.5667	11.6902	2.4569	1.3923
288	10	3	3	40	0.5	0.1	0.5	0.4	5.2015	0.6642	20.6551	2.4821	1.6485	3.9158	0.6642	20.6551	1.9791	1.3144
289	30	1	1	20	0.1	0.05	0.05	0.2	9.0092	0.2345	34.4695	2.1790	0.5110	3.8416	0.2345	34.4695	1.0754	0.2522
290	30	1	1	20	0.1	0.05	0.05	0.4	9.0092	0.4183	23.7816	2.2756	0.9520	2.1536	0.4183	23.7816	0.7487	0.3132
291	30	1	1	40	0.1	0.05	0.05	0.2	9.0092	0.2345	63.3394	2.0772	0.4872	3.8416	0.2345	63.3394	1.0415	0.2443
292	30	1	1	40	0.1	0.05	0.05	0.4	9.0092	0.4183	47.2784	2.1191	0.8865	2.1536	0.4183	47.2784	0.7207	0.3015
293	30	1	1	20	0.1	0.05	0.2	0.2	9.0092	0.3041	48.8808	2.1138	0.6429	2.9622	0.3041	48.8808	0.8786	0.2672
294	30	1	1	20	0.1	0.05	0.2	0.4	9.0092	0.4610	32.8399	2.1898	1.0094	1.9544	0.4610	32.8399	0.6929	0.3194
295	30	1	1	40	0.1	0.05	0.2	0.2	9.0092	0.3041	63.3594	2.0772	0.6318	2.9622	0.3041	63.3594	0.8700	0.2646
296	30	1	1	40	0.1	0.05	0.2	0.4	9.0092	0.4610	61.4335	2.0811	0.9593	1.9544	0.4610	61.4335	0.6760	0.3116
297	30	1	1	20	0.1	0.05	0.5	0.2	9.0092	0.5500	37.2571	2.1626	1.1894	1.6380	0.5500	37.2571	0.6259	0.3442
298	30	1	1	20	0.1	0.05	0.5	0.4	9.0092	0.6500	48.8245	2.1140	1.3741	1.3860	0.6500	48.8245	0.5707	0.3710
299	30	1	1	40	0.1	0.05	0.5	0.2	9.0092	0.5500	37.8739	2.1593	1.1876	1.6380	0.5500	37.8739	0.6255	0.3440
300	30	1	1	40	0.1	0.05	0.5	0.4	9.0092	0.6500	59.1849	2.0860	1.3559	1.3860	0.6500	59.1849	0.5676	0.3690
301	30	1	3	20	0.1	0.05	0.05	0.2	9.0092	0.2309	33.0249	2.1885	0.5054	3.9011	0.2309	33.0249	1.0911	0.2520
302	30	1	3	20	0.1	0.05	0.05	0.4	9.0092	0.4163	23.3603	2.2812	0.9497	2.1639	0.4163	23.3603	0.7519	0.3131
303	30	1	3	40	0.1	0.05	0.05	0.2	9.0092	0.2309	61.6611	2.0806	0.4805	3.9011	0.2309	61.6611	1.0543	0.2435
304	30	1	3	40	0.1	0.05	0.05	0.4	9.0092	0.4163	46.4991	2.1219	0.8834	2.1639	0.4163	46.4991	0.7232	0.3011
305	30	1	3	20	0.1	0.05	0.2	0.2	9.0092	0.2566	42.0729	2.1392	0.5489	3.5113	0.2566	42.0729	0.9951	0.2553

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
306	30	1	3	20	0.1	0.05	0.2	0.4	9.0092	0.4311	26.5032	2.2439	0.9673	2.0899	0.4311	26.5032	0.7297	0.3146
307	30	1	3	40	0.1	0.05	0.2	0.2	9.0092	0.2566	68.7805	2.0673	0.5304	3.5113	0.2566	68.7805	0.9741	0.2499
308	30	1	3	40	0.1	0.05	0.2	0.4	9.0092	0.4311	52.0865	2.1040	0.9070	2.0899	0.4311	52.0865	0.7057	0.3042
309	30	1	3	20	0.1	0.05	0.5	0.2	9.0092	0.3686	46.5115	2.1218	0.7820	2.4445	0.3686	46.5115	0.7783	0.2868
310	30	1	3	20	0.1	0.05	0.5	0.4	9.0092	0.5058	40.9915	2.1440	1.0844	1.7812	0.5058	40.9915	0.6515	0.3295
311	30	1	3	40	0.1	0.05	0.5	0.2	9.0092	0.3686	51.7274	2.1050	0.7758	2.4445	0.3686	51.7274	0.7750	0.2856
312	30	1	3	40	0.1	0.05	0.5	0.4	9.0092	0.5058	68.4136	2.0680	1.0460	1.7812	0.5058	68.4136	0.6409	0.3242
313	30	1	1	20	0.1	0.1	0.05	0.2	9.0092	0.2500	40.0818	2.1482	0.5371	3.6037	0.2500	40.0818	1.0166	0.2541
314	30	1	1	20	0.1	0.1	0.05	0.4	9.0092	0.4272	25.6704	2.2529	0.9624	2.1089	0.4272	25.6704	0.7352	0.3141
315	30	1	1	40	0.1	0.1	0.05	0.2	9.0092	0.2500	67.9857	2.0687	0.5172	3.6037	0.2500	67.9857	0.9924	0.2481
316	30	1	1	40	0.1	0.1	0.05	0.4	9.0092	0.4272	50.6592	2.1082	0.9006	2.1089	0.4272	50.6592	0.7101	0.3034
317	30	1	1	20	0.1	0.1	0.2	0.2	9.0092	0.3162	48.9865	2.1134	0.6683	2.8490	0.3162	48.9865	0.8562	0.2708
318	30	1	1	20	0.1	0.1	0.2	0.4	9.0092	0.4690	34.4695	2.1790	1.0220	1.9208	0.4690	34.4695	0.6844	0.3210
319	30	1	1	40	0.1	0.1	0.2	0.2	9.0092	0.3162	60.9244	2.0822	0.6584	2.8490	0.3162	60.9244	0.8491	0.2685
320	30	1	1	40	0.1	0.1	0.2	0.4	9.0092	0.4690	63.3394	2.0772	0.9743	1.9208	0.4690	63.3394	0.6689	0.3138
321	30	1	1	20	0.1	0.1	0.5	0.2	9.0092	0.5568	37.0500	2.1637	1.2047	1.6181	0.5568	37.0500	0.6221	0.3464
322	30	1	1	20	0.1	0.1	0.5	0.4	9.0092	0.6557	48.7375	2.1142	1.3864	1.3739	0.6557	48.7375	0.5684	0.3727
323	30	1	1	40	0.1	0.1	0.5	0.2	9.0092	0.5568	37.6303	2.1606	1.2030	1.6181	0.5568	37.6303	0.6217	0.3461
324	30	1	1	40	0.1	0.1	0.5	0.4	9.0092	0.6557	58.6278	2.0872	1.3687	1.3739	0.6557	58.6278	0.5654	0.3708
325	30	1	3	20	0.1	0.1	0.05	0.2	9.0092	0.2466	38.9684	2.1537	0.5312	3.6527	0.2466	38.9684	1.0283	0.2536
326	30	1	3	20	0.1	0.1	0.05	0.4	9.0092	0.4253	25.2522	2.2577	0.9601	2.1186	0.4253	25.2522	0.7381	0.3139
327	30	1	3	40	0.1	0.1	0.05	0.2	9.0092	0.2466	67.3264	2.0698	0.5105	3.6527	0.2466	67.3264	1.0023	0.2472
328	30	1	3	40	0.1	0.1	0.05	0.4	9.0092	0.4253	49.9273	2.1104	0.8975	2.1186	0.4253	49.9273	0.7124	0.3029
329	30	1	3	20	0.1	0.1	0.2	0.2	9.0092	0.2708	45.4534	2.1257	0.5756	3.3269	0.2708	45.4534	0.9542	0.2584
330	30	1	3	20	0.1	0.1	0.2	0.4	9.0092	0.4397	28.3527	2.2257	0.9786	2.0490	0.4397	28.3527	0.7181	0.3157
331	30	1	3	40	0.1	0.1	0.2	0.2	9.0092	0.2708	68.6693	2.0675	0.5599	3.3269	0.2708	68.6693	0.9383	0.2541
332	30	1	3	40	0.1	0.1	0.2	0.4	9.0092	0.4397	55.1039	2.0958	0.9215	2.0490	0.4397	55.1039	0.6965	0.3062
333	30	1	3	20	0.1	0.1	0.5	0.2	9.0092	0.3786	45.8378	2.1243	0.8042	2.3797	0.3786	45.8378	0.7660	0.2900
334	30	1	3	20	0.1	0.1	0.5	0.4	9.0092	0.5132	42.0729	2.1392	1.0978	1.7556	0.5132	42.0729	0.6458	0.3314
335	30	1	3	40	0.1	0.1	0.5	0.2	9.0092	0.3786	50.3295	2.1092	0.7985	2.3797	0.3786	50.3295	0.7631	0.2889
336	30	1	3	40	0.1	0.1	0.5	0.4	9.0092	0.5132	68.7805	2.0673	1.0609	1.7556	0.5132	68.7805	0.6360	0.3264
337	30	3	1	20	0.1	0.05	0.05	0.2	9.0092	0.2273	31.5189	2.1993	0.4999	3.9635	0.2273	31.5189	1.1079	0.2518
338	30	3	1	20	0.1	0.05	0.05	0.4	9.0092	0.4143	22.9389	2.2870	0.9476	2.1744	0.4143	22.9389	0.7552	0.3129
339	30	3	1	40	0.1	0.05	0.05	0.2	9.0092	0.2273	59.7278	2.0848	0.4739	3.9635	0.2273	59.7278	1.0680	0.2428

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
340	30	3	1	40	0.1	0.05	0.05	0.4	9.0092	0.4143	45.7108	2.1247	0.8803	2.1744	0.4143	45.7108	0.7257	0.3007
341	30	3	1	20	0.1	0.05	0.2	0.2	9.0092	0.2533	41.1165	2.1435	0.5430	3.5566	0.2533	41.1165	1.0056	0.2547
342	30	3	1	20	0.1	0.05	0.2	0.4	9.0092	0.4292	26.0875	2.2483	0.9649	2.0993	0.4292	26.0875	0.7324	0.3143
343	30	3	1	40	0.1	0.05	0.2	0.2	9.0092	0.2533	68.4642	2.0679	0.5238	3.5566	0.2533	68.4642	0.9830	0.2490
344	30	3	1	40	0.1	0.05	0.2	0.4	9.0092	0.4292	51.3791	2.1061	0.9038	2.0993	0.4292	51.3791	0.7079	0.3038
345	30	3	1	20	0.1	0.05	0.5	0.2	9.0092	0.3663	46.6616	2.1213	0.7770	2.4596	0.3663	46.6616	0.7811	0.2861
346	30	3	1	20	0.1	0.05	0.5	0.4	9.0092	0.5042	40.7377	2.1452	1.0815	1.7870	0.5042	40.7377	0.6528	0.3291
347	30	3	1	40	0.1	0.05	0.5	0.2	9.0092	0.3663	52.0596	2.1041	0.7707	2.4596	0.3663	52.0596	0.7778	0.2849
348	30	3	1	40	0.1	0.05	0.5	0.4	9.0092	0.5042	68.3048	2.0681	1.0427	1.7870	0.5042	68.3048	0.6421	0.3237
349	30	3	3	20	0.1	0.05	0.05	0.2	9.0092	0.2261	31.0044	2.2033	0.4981	3.9850	0.2261	31.0044	1.1139	0.2518
350	30	3	3	20	0.1	0.05	0.05	0.4	9.0092	0.4137	22.7984	2.2889	0.9468	2.1780	0.4137	22.7984	0.7564	0.3129
351	30	3	3	40	0.1	0.05	0.05	0.2	9.0092	0.2261	59.0265	2.0863	0.4717	3.9850	0.2261	59.0265	1.0728	0.2425
352	30	3	3	40	0.1	0.05	0.05	0.4	9.0092	0.4137	45.4462	2.1257	0.8793	2.1780	0.4137	45.4462	0.7266	0.3006
353	30	3	3	20	0.1	0.05	0.2	0.2	9.0092	0.2351	34.7039	2.1775	0.5120	3.8319	0.2351	34.7039	1.0729	0.2523
354	30	3	3	20	0.1	0.05	0.2	0.4	9.0092	0.4187	23.8518	2.2747	0.9523	2.1519	0.4187	23.8518	0.7482	0.3133
355	30	3	3	40	0.1	0.05	0.2	0.2	9.0092	0.2351	63.5946	2.0767	0.4883	3.8319	0.2351	63.5946	1.0395	0.2444
356	30	3	3	40	0.1	0.05	0.2	0.4	9.0092	0.4187	47.4074	2.1187	0.8870	2.1519	0.4187	47.4074	0.7203	0.3016
357	30	3	3	20	0.1	0.05	0.5	0.2	9.0092	0.2804	47.0270	2.1200	0.5944	3.2133	0.2804	47.0270	0.9300	0.2608
358	30	3	3	20	0.1	0.05	0.5	0.4	9.0092	0.4457	29.6276	2.2144	0.9869	2.0216	0.4457	29.6276	0.7106	0.3167
359	30	3	3	40	0.1	0.05	0.5	0.2	9.0092	0.2804	67.6061	2.0693	0.5802	3.2133	0.2804	67.6061	0.9168	0.2570
360	30	3	3	40	0.1	0.05	0.5	0.4	9.0092	0.4457	57.0523	2.0909	0.9319	2.0216	0.4457	57.0523	0.6904	0.3077
361	30	3	1	20	0.1	0.1	0.05	0.2	9.0092	0.2327	33.7553	2.1836	0.5082	3.8710	0.2327	33.7553	1.0831	0.2521
362	30	3	1	20	0.1	0.1	0.05	0.4	9.0092	0.4173	23.5710	2.2784	0.9509	2.1588	0.4173	23.5710	0.7503	0.3131
363	30	3	1	40	0.1	0.1	0.05	0.2	9.0092	0.2327	62.5319	2.0789	0.4838	3.8710	0.2327	62.5319	1.0478	0.2439
364	30	3	1	40	0.1	0.1	0.05	0.4	9.0092	0.4173	46.8899	2.1205	0.8850	2.1588	0.4173	46.8899	0.7219	0.3013
365	30	3	1	20	0.1	0.1	0.2	0.2	9.0092	0.2582	42.5220	2.1373	0.5519	3.4893	0.2582	42.5220	0.9901	0.2557
366	30	3	1	20	0.1	0.1	0.2	0.4	9.0092	0.4321	26.7105	2.2417	0.9685	2.0852	0.4321	26.7105	0.7283	0.3147
367	30	3	1	40	0.1	0.1	0.2	0.2	9.0092	0.2582	68.8836	2.0672	0.5337	3.4893	0.2582	68.8836	0.9697	0.2504
368	30	3	1	40	0.1	0.1	0.2	0.4	9.0092	0.4321	52.4354	2.1030	0.9086	2.0852	0.4321	52.4354	0.7047	0.3045
369	30	3	1	20	0.1	0.1	0.5	0.2	9.0092	0.3697	46.4365	2.1221	0.7845	2.4370	0.3697	46.4365	0.7768	0.2872
370	30	3	1	20	0.1	0.1	0.5	0.4	9.0092	0.5066	41.1165	2.1435	1.0859	1.7783	0.5066	41.1165	0.6509	0.3297
371	30	3	1	40	0.1	0.1	0.5	0.2	9.0092	0.3697	51.5644	2.1055	0.7784	2.4370	0.3697	51.5644	0.7736	0.2860
372	30	3	1	40	0.1	0.1	0.5	0.4	9.0092	0.5066	68.4642	2.0679	1.0476	1.7783	0.5066	68.4642	0.6404	0.3244
373	30	3	3	20	0.1	0.1	0.05	0.2	9.0092	0.2315	33.2701	2.1868	0.5063	3.8910	0.2315	33.2701	1.0884	0.2520

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
374	30	3	3	20	0.1	0.1	0.05	0.4	9.0092	0.4167	23.4306	2.2803	0.9501	2.1622	0.4167	23.4306	0.7514	0.3131
375	30	3	3	40	0.1	0.1	0.05	0.2	9.0092	0.2315	61.9585	2.0800	0.4816	3.8910	0.2315	61.9585	1.0521	0.2436
376	30	3	3	40	0.1	0.1	0.05	0.4	9.0092	0.4167	46.6296	2.1214	0.8839	2.1622	0.4167	46.6296	0.7227	0.3011
377	30	3	3	20	0.1	0.1	0.2	0.2	9.0092	0.2404	36.7254	2.1655	0.5205	3.7481	0.2404	36.7254	1.0516	0.2528
378	30	3	3	20	0.1	0.1	0.2	0.4	9.0092	0.4216	24.4829	2.2668	0.9558	2.1367	0.4216	24.4829	0.7436	0.3135
379	30	3	3	40	0.1	0.1	0.2	0.2	9.0092	0.2404	65.5872	2.0730	0.4983	3.7481	0.2404	65.5872	1.0219	0.2456
380	30	3	3	40	0.1	0.1	0.2	0.4	9.0092	0.4216	48.5559	2.1148	0.8917	2.1367	0.4216	48.5559	0.7166	0.3022
381	30	3	3	20	0.1	0.1	0.5	0.2	9.0092	0.2848	47.5774	2.1181	0.6032	3.1634	0.2848	47.5774	0.9196	0.2619
382	30	3	3	20	0.1	0.1	0.5	0.4	9.0092	0.4485	30.2221	2.2095	0.9909	2.0090	0.4485	30.2221	0.7072	0.3171
383	30	3	3	40	0.1	0.1	0.5	0.2	9.0092	0.2848	66.9414	2.0705	0.5897	3.1634	0.2848	66.9414	0.9074	0.2584
384	30	3	3	40	0.1	0.1	0.5	0.4	9.0092	0.4485	57.9219	2.0889	0.9368	2.0090	0.4485	57.9219	0.6877	0.3084
385	30	1	1	20	0.25	0.05	0.05	0.2	9.0092	0.3279	48.7375	2.1142	0.6932	6.8695	0.3279	48.7375	1.6693	0.5473
386	30	1	1	20	0.25	0.05	0.05	0.4	9.0092	0.4770	36.0141	2.1696	1.0348	4.7221	0.4770	36.0141	1.2547	0.5985
387	30	1	1	40	0.25	0.05	0.05	0.2	9.0092	0.3279	58.6278	2.0872	0.6844	6.8695	0.3279	58.6278	1.6504	0.5411
388	30	1	1	40	0.25	0.05	0.05	0.4	9.0092	0.4770	64.9297	2.0742	0.9893	4.7221	0.4770	64.9297	1.2136	0.5789
389	30	1	1	20	0.25	0.05	0.2	0.2	9.0092	0.3808	45.6894	2.1248	0.8091	5.9149	0.3808	45.6894	1.4792	0.5633
390	30	1	1	20	0.25	0.05	0.2	0.4	9.0092	0.5148	42.2998	2.1383	1.1007	4.3753	0.5148	42.2998	1.1701	0.6023
391	30	1	1	40	0.25	0.05	0.2	0.2	9.0092	0.3808	50.0390	2.1101	0.8035	5.9149	0.3808	50.0390	1.4708	0.5601
392	30	1	1	40	0.25	0.05	0.2	0.4	9.0092	0.5148	68.8364	2.0672	1.0642	4.3753	0.5148	68.8364	1.1427	0.5882
393	30	1	1	20	0.25	0.05	0.5	0.2	9.0092	0.5958	35.9912	2.1697	1.2928	3.7802	0.5958	35.9912	1.0596	0.6313
394	30	1	1	20	0.25	0.05	0.5	0.4	9.0092	0.6892	47.9895	2.1167	1.4588	3.2680	0.6892	47.9895	0.9400	0.6478
395	30	1	1	40	0.25	0.05	0.5	0.2	9.0092	0.5958	36.4071	2.1673	1.2913	3.7802	0.5958	36.4071	1.0588	0.6308
396	30	1	1	40	0.25	0.05	0.5	0.4	9.0092	0.6892	55.5514	2.0947	1.4436	3.2680	0.6892	55.5514	0.9341	0.6438
397	30	1	3	20	0.25	0.05	0.05	0.2	9.0092	0.3253	48.8156	2.1140	0.6877	6.9234	0.3253	48.8156	1.6802	0.5466
398	30	1	3	20	0.25	0.05	0.05	0.4	9.0092	0.4752	35.6786	2.1716	1.0320	4.7395	0.4752	35.6786	1.2592	0.5984
399	30	1	3	40	0.25	0.05	0.05	0.2	9.0092	0.3253	59.1224	2.0861	0.6787	6.9234	0.3253	59.1224	1.6605	0.5402
400	30	1	3	40	0.25	0.05	0.05	0.4	9.0092	0.4752	64.6029	2.0748	0.9860	4.7395	0.4752	64.6029	1.2173	0.5785
401	30	1	3	20	0.25	0.05	0.2	0.2	9.0092	0.3440	48.0221	2.1166	0.7281	6.5475	0.3440	48.0221	1.6045	0.5519
402	30	1	3	20	0.25	0.05	0.2	0.4	9.0092	0.4882	38.0820	2.1582	1.0536	4.6136	0.4882	38.0820	1.2272	0.5991
403	30	1	3	40	0.25	0.05	0.2	0.2	9.0092	0.3440	55.6571	2.0944	0.7205	6.5475	0.3440	55.6571	1.5899	0.5469
404	30	1	3	40	0.25	0.05	0.2	0.4	9.0092	0.4882	66.7020	2.0709	1.0110	4.6136	0.4882	66.7020	1.1909	0.5814
405	30	1	3	20	0.25	0.05	0.5	0.2	9.0092	0.4340	42.2901	2.1383	0.9280	5.1900	0.4340	42.2901	1.3371	0.5803
406	30	1	3	20	0.25	0.05	0.5	0.4	9.0092	0.5553	46.6320	2.1214	1.1780	4.0562	0.5553	46.6320	1.0991	0.6103
407	30	1	3	40	0.25	0.05	0.5	0.2	9.0092	0.4340	44.4081	2.1297	0.9242	5.1900	0.4340	44.4081	1.3329	0.5784

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
408	30	1	3	40	0.25	0.05	0.5	0.4	9.0092	0.5553	67.9691	2.0687	1.1487	4.0562	0.5553	67.9691	1.0807	0.6001
409	30	1	1	20	0.25	0.1	0.05	0.2	9.0092	0.3391	48.2725	2.1158	0.7175	6.6417	0.3391	48.2725	1.6233	0.5505
410	30	1	1	20	0.25	0.1	0.05	0.4	9.0092	0.4848	37.4670	2.1615	1.0478	4.6462	0.4848	37.4670	1.2354	0.5989
411	30	1	1	40	0.25	0.1	0.05	0.2	9.0092	0.3391	56.5254	2.0922	0.7095	6.6417	0.3391	56.5254	1.6076	0.5452
412	30	1	1	40	0.25	0.1	0.05	0.4	9.0092	0.4848	66.2198	2.0718	1.0043	4.6462	0.4848	66.2198	1.1977	0.5806
413	30	1	1	20	0.25	0.1	0.2	0.2	9.0092	0.3905	45.0334	2.1273	0.8307	5.7676	0.3905	45.0334	1.4503	0.5664
414	30	1	1	20	0.25	0.1	0.2	0.4	9.0092	0.5220	43.2622	2.1342	1.1141	4.3146	0.5220	43.2622	1.1561	0.6035
415	30	1	1	40	0.25	0.1	0.2	0.2	9.0092	0.3905	48.8143	2.1140	0.8255	5.7676	0.3905	48.8143	1.4429	0.5635
416	30	1	1	40	0.25	0.1	0.2	0.4	9.0092	0.5220	68.9843	2.0670	1.0790	4.3146	0.5220	68.9843	1.1307	0.5902
417	30	1	1	20	0.25	0.1	0.5	0.2	9.0092	0.6021	35.8405	2.1706	1.3069	3.7409	0.6021	35.8405	1.0518	0.6333
418	30	1	1	20	0.25	0.1	0.5	0.4	9.0092	0.6946	47.8393	2.1172	1.4707	3.2425	0.6946	47.8393	0.9351	0.6495
419	30	1	1	40	0.25	0.1	0.5	0.2	9.0092	0.6021	36.2358	2.1683	1.3055	3.7409	0.6021	36.2358	1.0510	0.6328
420	30	1	1	40	0.25	0.1	0.5	0.4	9.0092	0.6946	55.0835	2.0959	1.4558	3.2425	0.6946	55.0835	0.9294	0.6456
421	30	1	3	20	0.25	0.1	0.05	0.2	9.0092	0.3367	48.3891	2.1154	0.7121	6.6904	0.3367	48.3891	1.6331	0.5498
422	30	1	3	20	0.25	0.1	0.05	0.4	9.0092	0.4831	37.1523	2.1632	1.0449	4.6627	0.4831	37.1523	1.2395	0.5988
423	30	1	3	40	0.25	0.1	0.05	0.2	9.0092	0.3367	56.9748	2.0911	0.7040	6.6904	0.3367	56.9748	1.6167	0.5443
424	30	1	3	40	0.25	0.1	0.05	0.4	9.0092	0.4831	65.9580	2.0723	1.0010	4.6627	0.4831	65.9580	1.2011	0.5802
425	30	1	3	20	0.25	0.1	0.2	0.2	9.0092	0.3547	47.4006	2.1187	0.7516	6.3494	0.3547	47.4006	1.5650	0.5552
426	30	1	3	20	0.25	0.1	0.2	0.4	9.0092	0.4958	39.3952	2.1515	1.0668	4.5426	0.4958	39.3952	1.2098	0.5998
427	30	1	3	40	0.25	0.1	0.2	0.2	9.0092	0.3547	53.8486	2.0991	0.7446	6.3494	0.3547	53.8486	1.5527	0.5508
428	30	1	3	40	0.25	0.1	0.2	0.4	9.0092	0.4958	67.5960	2.0694	1.0260	4.5426	0.4958	67.5960	1.1763	0.5832
429	30	1	3	20	0.25	0.1	0.5	0.2	9.0092	0.4425	41.8046	2.1404	0.9472	5.0896	0.4425	41.8046	1.3175	0.5830
430	30	1	3	20	0.25	0.1	0.5	0.4	9.0092	0.5620	47.1104	2.1197	1.1913	4.0077	0.5620	47.1104	1.0888	0.6119
431	30	1	3	40	0.25	0.1	0.5	0.2	9.0092	0.4425	43.7105	2.1324	0.9437	5.0896	0.4425	43.7105	1.3136	0.5813
432	30	1	3	40	0.25	0.1	0.5	0.4	9.0092	0.5620	67.5186	2.0695	1.1630	4.0077	0.5620	67.5186	1.0715	0.6022
433	30	3	1	20	0.25	0.05	0.05	0.2	9.0092	0.3228	48.8819	2.1138	0.6822	6.9785	0.3228	48.8819	1.6914	0.5459
434	30	3	1	20	0.25	0.05	0.05	0.4	9.0092	0.4735	35.3386	2.1736	1.0291	4.7571	0.4735	35.3386	1.2638	0.5984
435	30	3	1	40	0.25	0.05	0.05	0.2	9.0092	0.3228	59.6264	2.0850	0.6729	6.9785	0.3228	59.6264	1.6709	0.5393
436	30	3	1	40	0.25	0.05	0.05	0.4	9.0092	0.4735	64.2610	2.0755	0.9827	4.7571	0.4735	64.2610	1.2211	0.5781
437	30	3	1	20	0.25	0.05	0.2	0.2	9.0092	0.3416	48.1499	2.1162	0.7228	6.5941	0.3416	48.1499	1.6138	0.5512
438	30	3	1	20	0.25	0.05	0.2	0.4	9.0092	0.4865	37.7769	2.1598	1.0507	4.6298	0.4865	37.7769	1.2313	0.5990
439	30	3	1	40	0.25	0.05	0.2	0.2	9.0092	0.3416	56.0862	2.0933	0.7150	6.5941	0.3416	56.0862	1.5987	0.5460
440	30	3	1	40	0.25	0.05	0.2	0.4	9.0092	0.4865	66.4677	2.0714	1.0077	4.6298	0.4865	66.4677	1.1943	0.5810
441	30	3	1	20	0.25	0.05	0.5	0.2	9.0092	0.4321	42.4021	2.1378	0.9236	5.2131	0.4321	42.4021	1.3417	0.5797

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
442	30	3	1	20	0.25	0.05	0.5	0.4	9.0092	0.5538	46.5161	2.1218	1.1750	4.0672	0.5538	46.5161	1.1015	0.6100
443	30	3	1	40	0.25	0.05	0.5	0.2	9.0092	0.4321	44.5717	2.1290	0.9198	5.2131	0.4321	44.5717	1.3373	0.5778
444	30	3	1	40	0.25	0.05	0.5	0.4	9.0092	0.5538	68.0612	2.0686	1.1455	4.0672	0.5538	68.0612	1.0828	0.5996
445	30	3	3	20	0.25	0.05	0.05	0.2	9.0092	0.3219	48.9011	2.1137	0.6804	6.9972	0.3219	48.9011	1.6953	0.5457
446	30	3	3	20	0.25	0.05	0.05	0.4	9.0092	0.4729	35.2243	2.1743	1.0282	4.7630	0.4729	35.2243	1.2653	0.5983
447	30	3	3	40	0.25	0.05	0.05	0.2	9.0092	0.3219	59.7964	2.0846	0.6710	6.9972	0.3219	59.7964	1.6744	0.5390
448	30	3	3	40	0.25	0.05	0.05	0.4	9.0092	0.4729	64.1437	2.0757	0.9815	4.7630	0.4729	64.1437	1.2223	0.5780
449	30	3	3	20	0.25	0.05	0.2	0.2	9.0092	0.3283	48.7234	2.1143	0.6941	6.8606	0.3283	48.7234	1.6675	0.5474
450	30	3	3	20	0.25	0.05	0.2	0.4	9.0092	0.4773	36.0695	2.1693	1.0353	4.7192	0.4773	36.0695	1.2540	0.5985
451	30	3	3	40	0.25	0.05	0.2	0.2	9.0092	0.3283	58.5463	2.0874	0.6853	6.8606	0.3283	58.5463	1.6487	0.5413
452	30	3	3	40	0.25	0.05	0.2	0.4	9.0092	0.4773	64.9827	2.0741	0.9899	4.7192	0.4773	64.9827	1.2130	0.5789
453	30	3	3	20	0.25	0.05	0.5	0.2	9.0092	0.3621	46.9356	2.1203	0.7678	6.2203	0.3621	46.9356	1.5395	0.5574
454	30	3	3	20	0.25	0.05	0.5	0.4	9.0092	0.5011	40.2597	2.1474	1.0761	4.4946	0.5011	40.2597	1.1982	0.6004
455	30	3	3	40	0.25	0.05	0.5	0.2	9.0092	0.3621	52.6901	2.1023	0.7612	6.2203	0.3621	52.6901	1.5284	0.5534
456	30	3	3	40	0.25	0.05	0.5	0.4	9.0092	0.5011	68.0775	2.0685	1.0366	4.4946	0.5011	68.0775	1.1666	0.5846
457	30	3	1	20	0.25	0.1	0.05	0.2	9.0092	0.3266	48.7779	2.1141	0.6905	6.8963	0.3266	48.7779	1.6747	0.5470
458	30	3	1	20	0.25	0.1	0.05	0.4	9.0092	0.4761	35.8469	2.1706	1.0334	4.7308	0.4761	35.8469	1.2570	0.5984
459	30	3	1	40	0.25	0.1	0.05	0.2	9.0092	0.3266	58.8739	2.0867	0.6815	6.8963	0.3266	58.8739	1.6554	0.5407
460	30	3	1	40	0.25	0.1	0.05	0.4	9.0092	0.4761	64.7682	2.0745	0.9877	4.7308	0.4761	64.7682	1.2155	0.5787
461	30	3	1	20	0.25	0.1	0.2	0.2	9.0092	0.3452	47.9565	2.1168	0.7307	6.5245	0.3452	47.9565	1.5999	0.5523
462	30	3	1	20	0.25	0.1	0.2	0.4	9.0092	0.4891	38.2328	2.1574	1.0551	4.6055	0.4891	38.2328	1.2252	0.5992
463	30	3	1	40	0.25	0.1	0.2	0.2	9.0092	0.3452	55.4464	2.0949	0.7232	6.5245	0.3452	55.4464	1.5856	0.5474
464	30	3	1	40	0.25	0.1	0.2	0.4	9.0092	0.4891	66.8142	2.0707	1.0127	4.6055	0.4891	66.8142	1.1892	0.5816
465	30	3	1	20	0.25	0.1	0.5	0.2	9.0092	0.4349	42.2347	2.1385	0.9301	5.1785	0.4349	42.2347	1.3349	0.5806
466	30	3	1	20	0.25	0.1	0.5	0.4	9.0092	0.5560	46.6886	2.1212	1.1794	4.0507	0.5560	46.6886	1.0979	0.6105
467	30	3	1	40	0.25	0.1	0.5	0.2	9.0092	0.4349	44.3275	2.1300	0.9264	5.1785	0.4349	44.3275	1.3307	0.5788
468	30	3	1	40	0.25	0.1	0.5	0.4	9.0092	0.5560	67.9218	2.0688	1.1503	4.0507	0.5560	67.9218	1.0797	0.6003
469	30	3	3	20	0.25	0.1	0.05	0.2	9.0092	0.3258	48.8033	2.1140	0.6886	6.9143	0.3258	48.8033	1.6784	0.5467
470	30	3	3	20	0.25	0.1	0.05	0.4	9.0092	0.4755	35.7348	2.1712	1.0324	4.7366	0.4755	35.7348	1.2585	0.5984
471	30	3	3	40	0.25	0.1	0.05	0.2	9.0092	0.3258	59.0393	2.0863	0.6796	6.9143	0.3258	59.0393	1.6588	0.5404
472	30	3	3	40	0.25	0.1	0.05	0.4	9.0092	0.4755	64.6584	2.0747	0.9865	4.7366	0.4755	64.6584	1.2167	0.5786
473	30	3	3	20	0.25	0.1	0.2	0.2	9.0092	0.3321	48.5847	2.1147	0.7023	6.7824	0.3321	48.5847	1.6517	0.5485
474	30	3	3	20	0.25	0.1	0.2	0.4	9.0092	0.4799	36.5631	2.1664	1.0396	4.6936	0.4799	36.5631	1.2474	0.5986
475	30	3	3	40	0.25	0.1	0.2	0.2	9.0092	0.3321	57.8253	2.0891	0.6938	6.7824	0.3321	57.8253	1.6340	0.5426

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
476	30	3	3	40	0.25	0.1	0.2	0.4	9.0092	0.4799	65.4415	2.0732	0.9949	4.6936	0.4799	65.4415	1.2076	0.5795
477	30	3	3	20	0.25	0.1	0.5	0.2	9.0092	0.3655	46.7115	2.1211	0.7753	6.1618	0.3655	46.7115	1.5279	0.5585
478	30	3	3	20	0.25	0.1	0.5	0.4	9.0092	0.5036	40.6520	2.1456	1.0805	4.4724	0.5036	40.6520	1.1929	0.6007
479	30	3	3	40	0.25	0.1	0.5	0.2	9.0092	0.3655	52.1721	2.1038	0.7690	6.1618	0.3655	52.1721	1.5174	0.5546
480	30	3	3	40	0.25	0.1	0.5	0.4	9.0092	0.5036	68.2662	2.0682	1.0415	4.4724	0.5036	68.2662	1.1621	0.5852
481	30	1	1	20	0.5	0.05	0.05	0.2	9.0092	0.5431	37.4746	2.1614	1.1740	8.2937	0.5431	37.4746	2.0072	1.0902
482	30	1	1	20	0.5	0.05	0.05	0.4	9.0092	0.6442	48.8964	2.1137	1.3617	6.9925	0.6442	48.8964	1.6943	1.0915
483	30	1	1	40	0.5	0.05	0.05	0.2	9.0092	0.5431	38.1314	2.1579	1.1721	8.2937	0.5431	38.1314	2.0040	1.0885
484	30	1	1	40	0.5	0.05	0.05	0.4	9.0092	0.6442	59.7538	2.0847	1.3430	6.9925	0.6442	59.7538	1.6736	1.0781
485	30	1	1	20	0.5	0.05	0.2	0.2	9.0092	0.5766	36.4846	2.1669	1.2495	7.8120	0.5766	36.4846	1.9083	1.1004
486	30	1	1	20	0.5	0.05	0.2	0.4	9.0092	0.6727	48.4033	2.1153	1.4229	6.6965	0.6727	48.4033	1.6344	1.0994
487	30	1	1	40	0.5	0.05	0.2	0.2	9.0092	0.5766	36.9727	2.1642	1.2479	7.8120	0.5766	36.9727	1.9061	1.0991
488	30	1	1	40	0.5	0.05	0.2	0.4	9.0092	0.6727	57.0317	2.0910	1.4066	6.6965	0.6727	57.0317	1.6179	1.0883
489	30	1	1	20	0.5	0.05	0.5	0.2	9.0092	0.7366	33.4929	2.1853	1.6096	6.1159	0.7366	33.4929	1.5576	1.1473
490	30	1	1	20	0.5	0.05	0.5	0.4	9.0092	0.8139	43.9473	2.1315	1.7349	5.5343	0.8139	43.9473	1.4046	1.1432
491	30	1	1	40	0.5	0.05	0.5	0.2	9.0092	0.7366	33.6461	2.1843	1.6088	6.1159	0.7366	33.6461	1.5570	1.1468
492	30	1	1	40	0.5	0.05	0.5	0.4	9.0092	0.8139	46.9563	2.1203	1.7258	5.5343	0.8139	46.9563	1.3986	1.1384
493	30	1	3	20	0.5	0.05	0.05	0.2	9.0092	0.5416	37.5244	2.1611	1.1705	8.3172	0.5416	37.5244	2.0120	1.0897
494	30	1	3	20	0.5	0.05	0.05	0.4	9.0092	0.6429	48.9101	2.1137	1.3589	7.0066	0.6429	48.9101	1.6972	1.0911
495	30	1	3	40	0.5	0.05	0.05	0.2	9.0092	0.5416	38.1906	2.1576	1.1686	8.3172	0.5416	38.1906	2.0088	1.0880
496	30	1	3	40	0.5	0.05	0.05	0.4	9.0092	0.6429	59.8818	2.0844	1.3401	7.0066	0.6429	59.8818	1.6762	1.0777
497	30	1	3	20	0.5	0.05	0.2	0.2	9.0092	0.5530	37.1638	2.1631	1.1962	8.1455	0.5530	37.1638	1.9768	1.0932
498	30	1	3	20	0.5	0.05	0.2	0.4	9.0092	0.6526	48.7876	2.1141	1.3796	6.9030	0.6526	48.7876	1.6761	1.0937
499	30	1	3	40	0.5	0.05	0.2	0.2	9.0092	0.5530	37.7640	2.1599	1.1945	8.1455	0.5530	37.7640	1.9739	1.0916
500	30	1	3	40	0.5	0.05	0.2	0.4	9.0092	0.6526	58.9358	2.0865	1.3616	6.9030	0.6526	58.9358	1.6567	1.0811
501	30	1	3	20	0.5	0.05	0.5	0.2	9.0092	0.6131	35.5875	2.1721	1.3316	7.3478	0.6131	35.5875	1.8128	1.1113
502	30	1	3	20	0.5	0.05	0.5	0.4	9.0092	0.7042	47.5616	2.1182	1.4915	6.3972	0.7042	47.5616	1.5745	1.1087
503	30	1	3	40	0.5	0.05	0.5	0.2	9.0092	0.6131	35.9498	2.1700	1.3303	7.3478	0.6131	35.9498	1.8111	1.1103
504	30	1	3	40	0.5	0.05	0.5	0.4	9.0092	0.7042	54.2824	2.0979	1.4773	6.3972	0.7042	54.2824	1.5617	1.0996
505	30	1	1	20	0.5	0.1	0.05	0.2	9.0092	0.5500	37.2571	2.1626	1.1894	8.1902	0.5500	37.2571	1.9860	1.0923
506	30	1	1	20	0.5	0.1	0.05	0.4	9.0092	0.6500	48.8245	2.1140	1.3741	6.9302	0.6500	48.8245	1.6816	1.0930
507	30	1	1	40	0.5	0.1	0.05	0.2	9.0092	0.5500	37.8739	2.1593	1.1876	8.1902	0.5500	37.8739	1.9830	1.0907
508	30	1	1	40	0.5	0.1	0.05	0.4	9.0092	0.6500	59.1849	2.0860	1.3559	6.9302	0.6500	59.1849	1.6618	1.0802
509	30	1	1	20	0.5	0.1	0.2	0.2	9.0092	0.5831	36.3128	2.1679	1.2641	7.7254	0.5831	36.3128	1.8905	1.1024

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
510	30	1	1	20	0.5	0.1	0.2	0.4	9.0092	0.6782	48.2725	2.1158	1.4350	6.6417	0.6782	48.2725	1.6233	1.1010
511	30	1	1	40	0.5	0.1	0.2	0.2	9.0092	0.5831	36.7749	2.1653	1.2626	7.7254	0.5831	36.7749	1.8884	1.1011
512	30	1	1	40	0.5	0.1	0.2	0.4	9.0092	0.6782	56.5254	2.0922	1.4190	6.6417	0.6782	56.5254	1.6076	1.0903
513	30	1	1	20	0.5	0.1	0.5	0.2	9.0092	0.7416	33.4292	2.1857	1.6210	6.0740	0.7416	33.4292	1.5489	1.1487
514	30	1	1	20	0.5	0.1	0.5	0.4	9.0092	0.8185	43.7995	2.1321	1.7452	5.5033	0.8185	43.7995	1.3985	1.1447
515	30	1	1	40	0.5	0.1	0.5	0.2	9.0092	0.7416	33.5777	2.1848	1.6203	6.0740	0.7416	33.5777	1.5483	1.1483
516	30	1	1	40	0.5	0.1	0.5	0.4	9.0092	0.8185	46.7168	2.1211	1.7362	5.5033	0.8185	46.7168	1.3927	1.1400
517	30	1	3	20	0.5	0.1	0.05	0.2	9.0092	0.5485	37.3045	2.1623	1.1860	8.2129	0.5485	37.3045	1.9906	1.0918
518	30	1	3	20	0.5	0.1	0.05	0.4	9.0092	0.6487	48.8419	2.1139	1.3713	6.9439	0.6487	48.8419	1.6844	1.0927
519	30	1	3	40	0.5	0.1	0.05	0.2	9.0092	0.5485	37.9299	2.1590	1.1842	8.2129	0.5485	37.9299	1.9876	1.0902
520	30	1	3	40	0.5	0.1	0.05	0.4	9.0092	0.6487	59.3103	2.0857	1.3530	6.9439	0.6487	59.3103	1.6644	1.0797
521	30	1	3	20	0.5	0.1	0.2	0.2	9.0092	0.5598	36.9611	2.1642	1.2114	8.0474	0.5598	36.9611	1.9567	1.0953
522	30	1	3	20	0.5	0.1	0.2	0.4	9.0092	0.6583	48.6945	2.1144	1.3919	6.8430	0.6583	48.6945	1.6639	1.0953
523	30	1	3	40	0.5	0.1	0.2	0.2	9.0092	0.5598	37.5262	2.1611	1.2097	8.0474	0.5598	37.5262	1.9540	1.0938
524	30	1	3	40	0.5	0.1	0.2	0.4	9.0092	0.6583	58.3842	2.0878	1.3744	6.8430	0.6583	58.3842	1.6454	1.0832
525	30	1	3	20	0.5	0.1	0.5	0.2	9.0092	0.6191	35.4531	2.1729	1.3453	7.2756	0.6191	35.4531	1.7979	1.1131
526	30	1	3	20	0.5	0.1	0.5	0.4	9.0092	0.7095	47.4006	2.1187	1.5031	6.3494	0.7095	47.4006	1.5650	1.1103
527	30	1	3	40	0.5	0.1	0.5	0.2	9.0092	0.6191	35.7986	2.1709	1.3441	7.2756	0.6191	35.7986	1.7963	1.1122
528	30	1	3	40	0.5	0.1	0.5	0.4	9.0092	0.7095	53.8486	2.0991	1.4892	6.3494	0.7095	53.8486	1.5527	1.1016
529	30	3	1	20	0.5	0.05	0.05	0.2	9.0092	0.5401	37.5748	2.1609	1.1670	8.3409	0.5401	37.5748	2.0168	1.0892
530	30	3	1	20	0.5	0.05	0.05	0.4	9.0092	0.6416	48.9230	2.1136	1.3561	7.0208	0.6416	48.9230	1.7001	1.0908
531	30	3	1	40	0.5	0.05	0.05	0.2	9.0092	0.5401	38.2506	2.1573	1.1651	8.3409	0.5401	38.2506	2.0136	1.0875
532	30	3	1	40	0.5	0.05	0.05	0.4	9.0092	0.6416	60.0103	2.0842	1.3372	7.0208	0.6416	60.0103	1.6789	1.0772
533	30	3	1	20	0.5	0.05	0.2	0.2	9.0092	0.5515	37.2102	2.1628	1.1928	8.1677	0.5515	37.2102	1.9814	1.0928
534	30	3	1	20	0.5	0.05	0.2	0.4	9.0092	0.6513	48.8064	2.1140	1.3768	6.9166	0.6513	48.8064	1.6788	1.0934
535	30	3	1	40	0.5	0.05	0.2	0.2	9.0092	0.5515	37.8186	2.1596	1.1910	8.1677	0.5515	37.8186	1.9785	1.0912
536	30	3	1	40	0.5	0.05	0.2	0.4	9.0092	0.6513	59.0601	2.0863	1.3587	6.9166	0.6513	59.0601	1.6593	1.0806
537	30	3	1	20	0.5	0.05	0.5	0.2	9.0092	0.6117	35.6182	2.1719	1.3285	7.3642	0.6117	35.6182	1.8161	1.1109
538	30	3	1	20	0.5	0.05	0.5	0.4	9.0092	0.7030	47.5969	2.1180	1.4889	6.4080	0.7030	47.5969	1.5767	1.1084
539	30	3	1	40	0.5	0.05	0.5	0.2	9.0092	0.6117	35.9844	2.1698	1.3272	7.3642	0.6117	35.9844	1.8145	1.1099
540	30	3	1	40	0.5	0.05	0.5	0.4	9.0092	0.7030	54.3804	2.0977	1.4746	6.4080	0.7030	54.3804	1.5637	1.0992
541	30	3	3	20	0.5	0.05	0.05	0.2	9.0092	0.5396	37.5917	2.1608	1.1658	8.3489	0.5396	37.5917	2.0185	1.0891
542	30	3	3	20	0.5	0.05	0.05	0.4	9.0092	0.6412	48.9271	2.1136	1.3552	7.0255	0.6412	48.9271	1.7010	1.0907
543	30	3	3	40	0.5	0.05	0.05	0.2	9.0092	0.5396	38.2707	2.1572	1.1639	8.3489	0.5396	38.2707	2.0152	1.0873

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
544	30	3	3	40	0.5	0.05	0.05	0.4	9.0092	0.6412	60.0533	2.0841	1.3363	7.0255	0.6412	60.0533	1.6798	1.0770
545	30	3	3	20	0.5	0.05	0.2	0.2	9.0092	0.5434	37.4663	2.1615	1.1745	8.2898	0.5434	37.4663	2.0064	1.0902
546	30	3	3	20	0.5	0.05	0.2	0.4	9.0092	0.6444	48.8941	2.1137	1.3621	6.9902	0.6444	48.8941	1.6938	1.0915
547	30	3	3	40	0.5	0.05	0.2	0.2	9.0092	0.5434	38.1216	2.1580	1.1726	8.2898	0.5434	38.1216	2.0032	1.0885
548	30	3	3	40	0.5	0.05	0.2	0.4	9.0092	0.6444	59.7326	2.0848	1.3435	6.9902	0.6444	59.7326	1.6731	1.0782
549	30	3	3	20	0.5	0.05	0.5	0.2	9.0092	0.5645	36.8242	2.1650	1.2220	7.9805	0.5645	36.8242	1.9429	1.0967
550	30	3	3	20	0.5	0.05	0.5	0.4	9.0092	0.6623	48.6213	2.1146	1.4005	6.8017	0.6623	48.6213	1.6556	1.0964
551	30	3	3	40	0.5	0.05	0.5	0.2	9.0092	0.5645	37.3664	2.1620	1.2204	7.9805	0.5645	37.3664	1.9404	1.0953
552	30	3	3	40	0.5	0.05	0.5	0.4	9.0092	0.6623	58.0034	2.0887	1.3833	6.8017	0.6623	58.0034	1.6377	1.0846
553	30	3	1	20	0.5	0.1	0.05	0.2	9.0092	0.5424	37.4994	2.1613	1.1722	8.3054	0.5424	37.4994	2.0096	1.0899
554	30	3	1	20	0.5	0.1	0.05	0.4	9.0092	0.6436	48.9034	2.1137	1.3603	6.9996	0.6436	48.9034	1.6957	1.0913
555	30	3	1	40	0.5	0.1	0.05	0.2	9.0092	0.5424	38.1609	2.1578	1.1703	8.3054	0.5424	38.1609	2.0064	1.0882
556	30	3	1	40	0.5	0.1	0.05	0.4	9.0092	0.6436	59.8178	2.0846	1.3416	6.9996	0.6436	59.8178	1.6749	1.0779
557	30	3	1	20	0.5	0.1	0.2	0.2	9.0092	0.5538	37.1408	2.1632	1.1979	8.1344	0.5538	37.1408	1.9745	1.0934
558	30	3	1	20	0.5	0.1	0.2	0.4	9.0092	0.6532	48.7779	2.1141	1.3809	6.8963	0.6532	48.7779	1.6747	1.0939
559	30	3	1	40	0.5	0.1	0.2	0.2	9.0092	0.5538	37.7369	2.1600	1.1962	8.1344	0.5538	37.7369	1.9717	1.0919
560	30	3	1	40	0.5	0.1	0.2	0.4	9.0092	0.6532	58.8739	2.0867	1.3630	6.8963	0.6532	58.8739	1.6554	1.0813
561	30	3	1	20	0.5	0.1	0.5	0.2	9.0092	0.6137	35.5723	2.1722	1.3331	7.3397	0.6137	35.5723	1.8111	1.1115
562	30	3	1	20	0.5	0.1	0.5	0.4	9.0092	0.7048	47.5438	2.1182	1.4928	6.3918	0.7048	47.5438	1.5735	1.1089
563	30	3	1	40	0.5	0.1	0.5	0.2	9.0092	0.6137	35.9327	2.1701	1.3318	7.3397	0.6137	35.9327	1.8094	1.1105
564	30	3	1	40	0.5	0.1	0.5	0.4	9.0092	0.7048	54.2336	2.0981	1.4786	6.3918	0.7048	54.2336	1.5606	1.0999
565	30	3	3	20	0.5	0.1	0.05	0.2	9.0092	0.5419	37.5161	2.1612	1.1711	8.3133	0.5419	37.5161	2.0112	1.0898
566	30	3	3	20	0.5	0.1	0.05	0.4	9.0092	0.6431	48.9079	2.1137	1.3594	7.0043	0.6431	48.9079	1.6967	1.0912
567	30	3	3	40	0.5	0.1	0.05	0.2	9.0092	0.5419	38.1807	2.1577	1.1692	8.3133	0.5419	38.1807	2.0080	1.0881
568	30	3	3	40	0.5	0.1	0.05	0.4	9.0092	0.6431	59.8605	2.0845	1.3406	7.0043	0.6431	59.8605	1.6758	1.0777
569	30	3	3	20	0.5	0.1	0.2	0.2	9.0092	0.5457	37.3928	2.1619	1.1797	8.2549	0.5457	37.3928	1.9992	1.0910
570	30	3	3	20	0.5	0.1	0.2	0.4	9.0092	0.6464	48.8717	2.1138	1.3663	6.9692	0.6464	48.8717	1.6895	1.0921
571	30	3	3	40	0.5	0.1	0.2	0.2	9.0092	0.5457	38.0343	2.1584	1.1778	8.2549	0.5457	38.0343	1.9962	1.0893
572	30	3	3	40	0.5	0.1	0.2	0.4	9.0092	0.6464	59.5418	2.0852	1.3478	6.9692	0.6464	59.5418	1.6692	1.0789
573	30	3	3	20	0.5	0.1	0.5	0.2	9.0092	0.5667	36.7609	2.1653	1.2270	7.9493	0.5667	36.7609	1.9366	1.0974
574	30	3	3	20	0.5	0.1	0.5	0.4	9.0092	0.6642	48.5847	2.1147	1.4045	6.7824	0.6642	48.5847	1.6517	1.0970
575	30	3	3	40	0.5	0.1	0.5	0.2	9.0092	0.5667	37.2927	2.1624	1.2254	7.9493	0.5667	37.2927	1.9340	1.0960
576	30	3	3	40	0.5	0.1	0.5	0.4	9.0092	0.6642	57.8253	2.0891	1.3875	6.7824	0.6642	57.8253	1.6340	1.0853
577	50	1	1	20	0.1	0.05	0.05	0.2	11.6309	0.2345	35.7600	2.1263	0.4987	4.9594	0.2345	35.7600	1.0108	0.2371

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
578	50	1	1	20	0.1	0.05	0.05	0.4	11.6309	0.4183	23.8403	2.2350	0.9350	2.7803	0.4183	23.8403	0.6822	0.2854
579	50	1	1	40	0.1	0.05	0.05	0.2	11.6309	0.2345	67.8375	2.0171	0.4730	4.9594	0.2345	67.8375	0.9746	0.2286
580	50	1	1	40	0.1	0.05	0.05	0.4	11.6309	0.4183	47.5107	2.0703	0.8661	2.7803	0.4183	47.5107	0.6536	0.2734
581	50	1	1	20	0.1	0.05	0.2	0.2	11.6309	0.3041	62.7982	2.0272	0.6166	3.8242	0.3041	62.7982	0.8044	0.2447
582	50	1	1	20	0.1	0.05	0.2	0.4	11.6309	0.4610	33.7933	2.1392	0.9861	2.5231	0.4610	33.7933	0.6247	0.2880
583	50	1	1	40	0.1	0.05	0.2	0.2	11.6309	0.3041	88.8961	1.9864	0.6041	3.8242	0.3041	88.8961	0.7953	0.2419
584	50	1	1	40	0.1	0.05	0.2	0.4	11.6309	0.4610	64.8564	2.0229	0.9325	2.5231	0.4610	64.8564	0.6076	0.2801
585	50	1	1	20	0.1	0.05	0.5	0.2	11.6309	0.5500	61.5685	2.0300	1.1165	2.1147	0.5500	61.5685	0.5475	0.3011
586	50	1	1	20	0.1	0.05	0.5	0.4	11.6309	0.6500	66.4518	2.0197	1.3128	1.7894	0.6500	66.4518	0.4980	0.3237
587	50	1	1	40	0.1	0.05	0.5	0.2	11.6309	0.5500	63.2714	2.0262	1.1144	2.1147	0.5500	63.2714	0.5470	0.3009
588	50	1	1	40	0.1	0.05	0.5	0.4	11.6309	0.6500	87.2358	1.9883	1.2924	1.7894	0.6500	87.2358	0.4950	0.3218
589	50	1	3	20	0.1	0.05	0.05	0.2	11.6309	0.2309	34.0130	2.1377	0.4937	5.0363	0.2309	34.0130	1.0273	0.2373
590	50	1	3	20	0.1	0.05	0.05	0.4	11.6309	0.4163	23.4059	2.2409	0.9330	2.7936	0.4163	23.4059	0.6855	0.2854
591	50	1	3	40	0.1	0.05	0.05	0.2	11.6309	0.2309	65.1975	2.0222	0.4670	5.0363	0.2309	65.1975	0.9880	0.2282
592	50	1	3	40	0.1	0.05	0.05	0.4	11.6309	0.4163	46.6798	2.0734	0.8632	2.7936	0.4163	46.6798	0.6561	0.2732
593	50	1	3	20	0.1	0.05	0.2	0.2	11.6309	0.2566	46.2940	2.0749	0.5324	4.5330	0.2566	46.2940	0.9263	0.2377
594	50	1	3	20	0.1	0.05	0.2	0.4	11.6309	0.4311	26.6957	2.2006	0.9487	2.6981	0.4311	26.6957	0.6626	0.2857
595	50	1	3	40	0.1	0.05	0.2	0.2	11.6309	0.2566	80.8291	1.9963	0.5122	4.5330	0.2566	80.8291	0.9038	0.2319
596	50	1	3	40	0.1	0.05	0.2	0.4	11.6309	0.4311	52.8351	2.0527	0.8849	2.6981	0.4311	52.8351	0.6383	0.2751
597	50	1	3	20	0.1	0.05	0.5	0.2	11.6309	0.3686	68.9928	2.0149	0.7426	3.1558	0.3686	68.9928	0.7010	0.2584
598	50	1	3	20	0.1	0.05	0.5	0.4	11.6309	0.5058	44.6023	2.0816	1.0529	2.2995	0.5058	44.6023	0.5818	0.2943
599	50	1	3	40	0.1	0.05	0.5	0.2	11.6309	0.3686	81.1272	1.9959	0.7356	3.1558	0.3686	81.1272	0.6977	0.2571
600	50	1	3	40	0.1	0.05	0.5	0.4	11.6309	0.5058	79.1013	1.9987	1.0110	2.2995	0.5058	79.1013	0.5712	0.2889
601	50	1	1	20	0.1	0.1	0.05	0.2	11.6309	0.2500	43.2434	2.0873	0.5218	4.6523	0.2500	43.2434	0.9489	0.2372
602	50	1	1	20	0.1	0.1	0.05	0.4	11.6309	0.4272	25.8122	2.2105	0.9443	2.7226	0.4272	25.8122	0.6684	0.2855
603	50	1	1	40	0.1	0.1	0.05	0.2	11.6309	0.2500	77.6102	2.0009	0.5002	4.6523	0.2500	77.6102	0.9231	0.2308
604	50	1	1	40	0.1	0.1	0.05	0.4	11.6309	0.4272	51.2143	2.0577	0.8790	2.7226	0.4272	51.2143	0.6428	0.2746
605	50	1	1	20	0.1	0.1	0.2	0.2	11.6309	0.3162	65.1596	2.0223	0.6395	3.6780	0.3162	65.1596	0.7811	0.2470
606	50	1	1	20	0.1	0.1	0.2	0.4	11.6309	0.4690	35.7600	2.1263	0.9973	2.4797	0.4690	35.7600	0.6159	0.2889
607	50	1	1	40	0.1	0.1	0.2	0.2	11.6309	0.3162	88.1295	1.9872	0.6284	3.6780	0.3162	88.1295	0.7737	0.2447
608	50	1	1	40	0.1	0.1	0.2	0.4	11.6309	0.4690	67.8375	2.0171	0.9461	2.4797	0.4690	67.8375	0.6003	0.2816
609	50	1	1	20	0.1	0.1	0.5	0.2	11.6309	0.5568	61.2978	2.0306	1.1306	2.0890	0.5568	61.2978	0.5437	0.3027
610	50	1	1	20	0.1	0.1	0.5	0.4	11.6309	0.6557	66.8050	2.0190	1.3240	1.7737	0.6557	66.8050	0.4956	0.3250
611	50	1	1	40	0.1	0.1	0.5	0.2	11.6309	0.5568	62.9028	2.0270	1.1286	2.0890	0.5568	62.9028	0.5433	0.3025

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
612	50	1	1	40	0.1	0.1	0.5	0.4	11.6309	0.6557	86.8991	1.9887	1.3041	1.7737	0.6557	86.8991	0.4928	0.3231
613	50	1	3	20	0.1	0.1	0.05	0.2	11.6309	0.2466	41.6474	2.0945	0.5166	4.7156	0.2466	41.6474	0.9612	0.2371
614	50	1	3	20	0.1	0.1	0.05	0.4	11.6309	0.4253	25.3718	2.2156	0.9422	2.7351	0.4253	25.3718	0.6713	0.2855
615	50	1	3	40	0.1	0.1	0.05	0.2	11.6309	0.2466	75.7443	2.0037	0.4942	4.7156	0.2466	75.7443	0.9334	0.2302
616	50	1	3	40	0.1	0.1	0.05	0.4	11.6309	0.4253	50.3973	2.0603	0.8761	2.7351	0.4253	50.3973	0.6451	0.2743
617	50	1	3	20	0.1	0.1	0.2	0.2	11.6309	0.2708	52.3763	2.0540	0.5562	4.2950	0.2708	52.3763	0.8833	0.2392
618	50	1	3	20	0.1	0.1	0.2	0.4	11.6309	0.4397	28.6931	2.1805	0.9587	2.6452	0.4397	28.6931	0.6507	0.2861
619	50	1	3	40	0.1	0.1	0.2	0.2	11.6309	0.2708	85.8032	1.9900	0.5389	4.2950	0.2708	85.8032	0.8664	0.2346
620	50	1	3	40	0.1	0.1	0.2	0.4	11.6309	0.4397	56.4043	2.0426	0.8981	2.6452	0.4397	56.4043	0.6287	0.2765
621	50	1	3	20	0.1	0.1	0.5	0.2	11.6309	0.3786	68.9610	2.0150	0.7629	3.0721	0.3786	68.9610	0.6885	0.2607
622	50	1	3	20	0.1	0.1	0.5	0.4	11.6309	0.5132	46.2940	2.0749	1.0647	2.2665	0.5132	46.2940	0.5759	0.2955
623	50	1	3	40	0.1	0.1	0.5	0.2	11.6309	0.3786	79.6562	1.9980	0.7564	3.0721	0.3786	79.6562	0.6856	0.2596
624	50	1	3	40	0.1	0.1	0.5	0.4	11.6309	0.5132	80.8291	1.9963	1.0244	2.2665	0.5132	80.8291	0.5660	0.2905
625	50	3	1	20	0.1	0.05	0.05	0.2	11.6309	0.2273	32.2483	2.1504	0.4888	5.1169	0.2273	32.2483	1.0451	0.2376
626	50	3	1	20	0.1	0.05	0.05	0.4	11.6309	0.4143	22.9731	2.2470	0.9310	2.8072	0.4143	22.9731	0.6889	0.2854
627	50	3	1	40	0.1	0.05	0.05	0.2	11.6309	0.2273	62.4026	2.0281	0.4610	5.1169	0.2273	62.4026	1.0023	0.2278
628	50	3	1	40	0.1	0.05	0.05	0.4	11.6309	0.4143	45.8470	2.0766	0.8604	2.8072	0.4143	45.8470	0.6587	0.2729
629	50	3	1	20	0.1	0.05	0.2	0.2	11.6309	0.2533	44.7934	2.0808	0.5271	4.5915	0.2533	44.7934	0.9373	0.2374
630	50	3	1	20	0.1	0.05	0.2	0.4	11.6309	0.4292	26.2535	2.2055	0.9465	2.7102	0.4292	26.2535	0.6655	0.2856
631	50	3	1	40	0.1	0.05	0.2	0.2	11.6309	0.2533	79.3037	1.9985	0.5062	4.5915	0.2533	79.3037	0.9132	0.2313
632	50	3	1	40	0.1	0.05	0.2	0.4	11.6309	0.4292	52.0270	2.0551	0.8819	2.7102	0.4292	52.0270	0.6405	0.2749
633	50	3	1	20	0.1	0.05	0.5	0.2	11.6309	0.3663	68.9770	2.0150	0.7381	3.1753	0.3663	68.9770	0.7040	0.2579
634	50	3	1	20	0.1	0.05	0.5	0.4	11.6309	0.5042	44.2178	2.0832	1.0502	2.3070	0.5042	44.2178	0.5831	0.2940
635	50	3	1	40	0.1	0.05	0.5	0.2	11.6309	0.3663	81.4634	1.9955	0.7309	3.1753	0.3663	81.4634	0.7005	0.2566
636	50	3	1	40	0.1	0.05	0.5	0.4	11.6309	0.5042	78.6886	1.9993	1.0080	2.3070	0.5042	78.6886	0.5724	0.2886
637	50	3	3	20	0.1	0.05	0.05	0.2	11.6309	0.2261	31.6573	2.1550	0.4872	5.1446	0.2261	31.6573	1.0513	0.2377
638	50	3	3	20	0.1	0.05	0.05	0.4	11.6309	0.4137	22.8293	2.2491	0.9304	2.8117	0.4137	22.8293	0.6900	0.2854
639	50	3	3	40	0.1	0.05	0.05	0.2	11.6309	0.2261	61.4387	2.0303	0.4590	5.1446	0.2261	61.4387	1.0073	0.2277
640	50	3	3	40	0.1	0.05	0.05	0.4	11.6309	0.4137	45.5691	2.0777	0.8594	2.8117	0.4137	45.5691	0.6596	0.2729
641	50	3	3	20	0.1	0.05	0.2	0.2	11.6309	0.2351	36.0489	2.1245	0.4995	4.9469	0.2351	36.0489	1.0082	0.2370
642	50	3	3	20	0.1	0.05	0.2	0.4	11.6309	0.4187	23.9128	2.2340	0.9353	2.7781	0.4187	23.9128	0.6817	0.2854
643	50	3	3	40	0.1	0.05	0.2	0.2	11.6309	0.2351	68.2617	2.0163	0.4741	4.9469	0.2351	68.2617	0.9724	0.2286
644	50	3	3	40	0.1	0.05	0.2	0.4	11.6309	0.4187	47.6489	2.0698	0.8665	2.7781	0.4187	47.6489	0.6532	0.2735
645	50	3	3	20	0.1	0.05	0.5	0.2	11.6309	0.2804	55.9630	2.0438	0.5730	4.1483	0.2804	55.9630	0.8579	0.2406

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
646	50	3	3	20	0.1	0.05	0.5	0.4	11.6309	0.4457	30.1020	2.1678	0.9661	2.6098	0.4457	30.1020	0.6429	0.2865
647	50	3	3	40	0.1	0.05	0.5	0.2	11.6309	0.2804	87.7489	1.9877	0.5573	4.1483	0.2804	87.7489	0.8439	0.2366
648	50	3	3	40	0.1	0.05	0.5	0.4	11.6309	0.4457	58.8379	2.0364	0.9075	2.6098	0.4457	58.8379	0.6225	0.2774
649	50	3	1	20	0.1	0.1	0.05	0.2	11.6309	0.2327	34.8891	2.1319	0.4962	4.9974	0.2327	34.8891	1.0189	0.2371
650	50	3	1	20	0.1	0.1	0.05	0.4	11.6309	0.4173	23.6229	2.2379	0.9340	2.7870	0.4173	23.6229	0.6839	0.2854
651	50	3	1	40	0.1	0.1	0.05	0.2	11.6309	0.2327	66.5376	2.0195	0.4700	4.9974	0.2327	66.5376	0.9812	0.2284
652	50	3	1	40	0.1	0.1	0.05	0.4	11.6309	0.4173	47.0955	2.0718	0.8646	2.7870	0.4173	47.0955	0.6548	0.2733
653	50	3	1	20	0.1	0.1	0.2	0.2	11.6309	0.2582	47.0250	2.0721	0.5350	4.5046	0.2582	47.0250	0.9210	0.2378
654	50	3	1	20	0.1	0.1	0.2	0.4	11.6309	0.4321	26.9170	2.1982	0.9498	2.6920	0.4321	26.9170	0.6613	0.2857
655	50	3	1	40	0.1	0.1	0.2	0.2	11.6309	0.2582	81.5308	1.9954	0.5152	4.5046	0.2582	81.5308	0.8993	0.2322
656	50	3	1	40	0.1	0.1	0.2	0.4	11.6309	0.4321	53.2373	2.0515	0.8863	2.6920	0.4321	53.2373	0.6372	0.2753
657	50	3	1	20	0.1	0.1	0.5	0.2	11.6309	0.3697	68.9973	2.0149	0.7449	3.1462	0.3697	68.9973	0.6996	0.2586
658	50	3	1	20	0.1	0.1	0.5	0.4	11.6309	0.5066	44.7934	2.0808	1.0542	2.2958	0.5066	44.7934	0.5811	0.2944
659	50	3	1	40	0.1	0.1	0.5	0.2	11.6309	0.3697	80.9603	1.9962	0.7380	3.1462	0.3697	80.9603	0.6963	0.2574
660	50	3	1	40	0.1	0.1	0.5	0.4	11.6309	0.5066	79.3037	1.9985	1.0125	2.2958	0.5066	79.3037	0.5706	0.2891
661	50	3	3	20	0.1	0.1	0.05	0.2	11.6309	0.2315	34.3056	2.1357	0.4945	5.0233	0.2315	34.3056	1.0245	0.2372
662	50	3	3	20	0.1	0.1	0.05	0.4	11.6309	0.4167	23.4782	2.2399	0.9333	2.7914	0.4167	23.4782	0.6850	0.2854
663	50	3	3	40	0.1	0.1	0.05	0.2	11.6309	0.2315	65.6486	2.0213	0.4680	5.0233	0.2315	65.6486	0.9857	0.2282
664	50	3	3	40	0.1	0.1	0.05	0.4	11.6309	0.4167	46.8184	2.0729	0.8637	2.7914	0.4167	46.8184	0.6557	0.2732
665	50	3	3	20	0.1	0.1	0.2	0.2	11.6309	0.2404	38.6151	2.1098	0.5071	4.8387	0.2404	38.6151	0.9858	0.2370
666	50	3	3	20	0.1	0.1	0.2	0.4	11.6309	0.4216	24.5676	2.2255	0.9384	2.7585	0.4216	24.5676	0.6769	0.2854
667	50	3	3	40	0.1	0.1	0.2	0.2	11.6309	0.2404	71.8681	2.0099	0.4831	4.8387	0.2404	71.8681	0.9540	0.2293
668	50	3	3	40	0.1	0.1	0.2	0.4	11.6309	0.4216	48.8900	2.0654	0.8708	2.7585	0.4216	48.8900	0.6495	0.2738
669	50	3	3	20	0.1	0.1	0.5	0.2	11.6309	0.2848	57.4625	2.0398	0.5809	4.0839	0.2848	57.4625	0.8470	0.2412
670	50	3	3	20	0.1	0.1	0.5	0.4	11.6309	0.4485	30.7690	2.1621	0.9696	2.5935	0.4485	30.7690	0.6394	0.2868
671	50	3	3	40	0.1	0.1	0.5	0.2	11.6309	0.2848	88.3180	1.9870	0.5659	4.0839	0.2848	88.3180	0.8341	0.2376
672	50	3	3	40	0.1	0.1	0.5	0.4	11.6309	0.4485	59.9646	2.0337	0.9120	2.5935	0.4485	59.9646	0.6196	0.2779
673	50	1	1	20	0.25	0.05	0.05	0.2	11.6309	0.3279	66.8050	2.0190	0.6620	8.8685	0.3279	66.8050	1.5819	0.5187
674	50	1	1	20	0.25	0.05	0.05	0.4	11.6309	0.4770	37.6962	2.1149	1.0087	6.0962	0.4770	37.6962	1.1914	0.5683
675	50	1	1	40	0.25	0.05	0.05	0.2	11.6309	0.3279	86.8991	1.9887	0.6520	8.8685	0.3279	86.8991	1.5608	0.5117
676	50	1	1	40	0.25	0.05	0.05	0.4	11.6309	0.4770	70.6103	2.0120	0.9597	6.0962	0.4770	70.6103	1.1469	0.5470
677	50	1	1	20	0.25	0.05	0.2	0.2	11.6309	0.3808	68.9344	2.0150	0.7673	7.6360	0.3808	68.9344	1.3866	0.5280
678	50	1	1	20	0.25	0.05	0.2	0.4	11.6309	0.5148	46.6611	2.0735	1.0674	5.6485	0.5148	46.6611	1.1019	0.5672
679	50	1	1	40	0.25	0.05	0.2	0.2	11.6309	0.3808	79.3396	1.9984	0.7610	7.6360	0.3808	79.3396	1.3772	0.5244

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
680	50	1	1	40	0.25	0.05	0.2	0.4	11.6309	0.5148	81.1850	1.9959	1.0274	5.6485	0.5148	81.1850	1.0722	0.5519
681	50	1	1	20	0.25	0.05	0.5	0.2	11.6309	0.5958	59.8694	2.0339	1.2118	4.8802	0.5958	59.8694	0.9677	0.5766
682	50	1	1	20	0.25	0.05	0.5	0.4	11.6309	0.6892	68.2678	2.0163	1.3896	4.2190	0.6892	68.2678	0.8617	0.5939
683	50	1	1	40	0.25	0.05	0.5	0.2	11.6309	0.5958	61.0291	2.0312	1.2102	4.8802	0.5958	61.0291	0.9669	0.5761
684	50	1	1	40	0.25	0.05	0.5	0.4	11.6309	0.6892	84.6623	1.9914	1.3725	4.2190	0.6892	84.6623	0.8554	0.5895
685	50	1	3	20	0.25	0.05	0.05	0.2	11.6309	0.3253	66.4929	2.0196	0.6570	8.9380	0.3253	66.4929	1.5932	0.5183
686	50	1	3	20	0.25	0.05	0.05	0.4	11.6309	0.4752	37.2690	2.1173	1.0062	6.1187	0.4752	37.2690	1.1961	0.5684
687	50	1	3	40	0.25	0.05	0.05	0.2	11.6309	0.3253	87.1992	1.9883	0.6468	8.9380	0.3253	87.1992	1.5713	0.5112
688	50	1	3	40	0.25	0.05	0.05	0.4	11.6309	0.4752	70.0127	2.0131	0.9567	6.1187	0.4752	70.0127	1.1508	0.5469
689	50	1	3	20	0.25	0.05	0.2	0.2	11.6309	0.3440	68.2308	2.0163	0.6936	8.4528	0.3440	68.2308	1.5148	0.5211
690	50	1	3	20	0.25	0.05	0.2	0.4	11.6309	0.4882	40.4225	2.1004	1.0254	5.9561	0.4882	40.4225	1.1623	0.5674
691	50	1	3	40	0.25	0.05	0.2	0.2	11.6309	0.3440	84.7489	1.9913	0.6850	8.4528	0.3440	84.7489	1.4986	0.5155
692	50	1	3	40	0.25	0.05	0.2	0.4	11.6309	0.4882	74.2300	2.0060	0.9793	5.9561	0.4882	74.2300	1.1230	0.5482
693	50	1	3	20	0.25	0.05	0.5	0.2	11.6309	0.4340	67.0454	2.0186	0.8760	6.7002	0.4340	67.0454	1.2431	0.5395
694	50	1	3	20	0.25	0.05	0.5	0.4	11.6309	0.5553	54.9841	2.0464	1.1363	5.2365	0.5553	54.9841	1.0271	0.5703
695	50	1	3	40	0.25	0.05	0.5	0.2	11.6309	0.4340	72.5293	2.0088	0.8718	6.7002	0.4340	72.5293	1.2384	0.5374
696	50	1	3	40	0.25	0.05	0.5	0.4	11.6309	0.5553	87.2969	1.9882	1.1040	5.2365	0.5553	87.2969	1.0072	0.5593
697	50	1	1	20	0.25	0.1	0.05	0.2	11.6309	0.3391	67.8916	2.0170	0.6840	8.5744	0.3391	67.8916	1.5343	0.5203
698	50	1	1	20	0.25	0.1	0.05	0.4	11.6309	0.4848	39.5936	2.1046	1.0203	5.9982	0.4848	39.5936	1.1709	0.5676
699	50	1	1	40	0.25	0.1	0.05	0.2	11.6309	0.3391	85.4351	1.9904	0.6750	8.5744	0.3391	85.4351	1.5167	0.5144
700	50	1	1	40	0.25	0.1	0.05	0.4	11.6309	0.4848	73.1655	2.0077	0.9733	5.9982	0.4848	73.1655	1.1301	0.5478
701	50	1	1	20	0.25	0.1	0.2	0.2	11.6309	0.3905	68.7463	2.0154	0.7870	7.4459	0.3905	68.7463	1.3572	0.5300
702	50	1	1	20	0.25	0.1	0.2	0.4	11.6309	0.5220	48.2719	2.0675	1.0793	5.5702	0.5220	48.2719	1.0872	0.5675
703	50	1	1	40	0.25	0.1	0.2	0.2	11.6309	0.3905	77.9650	2.0004	0.7812	7.4459	0.3905	77.9650	1.3490	0.5268
704	50	1	1	40	0.25	0.1	0.2	0.4	11.6309	0.5220	82.6639	1.9939	1.0409	5.5702	0.5220	82.6639	1.0596	0.5531
705	50	1	1	20	0.25	0.1	0.5	0.2	11.6309	0.6021	59.6602	2.0344	1.2249	4.8295	0.6021	59.6602	0.9601	0.5781
706	50	1	1	20	0.25	0.1	0.5	0.4	11.6309	0.6946	68.4206	2.0160	1.4003	4.1860	0.6946	68.4206	0.8566	0.5950
707	50	1	1	40	0.25	0.1	0.5	0.2	11.6309	0.6021	60.7637	2.0318	1.2233	4.8295	0.6021	60.7637	0.9593	0.5776
708	50	1	1	40	0.25	0.1	0.5	0.4	11.6309	0.6946	84.2714	1.9919	1.3836	4.1860	0.6946	84.2714	0.8506	0.5908
709	50	1	3	20	0.25	0.1	0.05	0.2	11.6309	0.3367	67.6912	2.0173	0.6791	8.6372	0.3367	67.6912	1.5444	0.5199
710	50	1	3	20	0.25	0.1	0.05	0.4	11.6309	0.4831	39.1757	2.1068	1.0177	6.0195	0.4831	39.1757	1.1753	0.5677
711	50	1	3	40	0.25	0.1	0.05	0.2	11.6309	0.3367	85.7723	1.9900	0.6699	8.6372	0.3367	85.7723	1.5261	0.5138
712	50	1	3	40	0.25	0.1	0.05	0.4	11.6309	0.4831	72.6167	2.0086	0.9703	6.0195	0.4831	72.6167	1.1337	0.5477
713	50	1	3	20	0.25	0.1	0.2	0.2	11.6309	0.3547	68.7377	2.0154	0.7149	8.1970	0.3547	68.7377	1.4742	0.5230

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
714	50	1	3	20	0.25	0.1	0.2	0.4	11.6309	0.4958	42.2511	2.0918	1.0371	5.8645	0.4958	42.2511	1.1439	0.5671
715	50	1	3	40	0.25	0.1	0.2	0.2	11.6309	0.3547	83.1819	1.9933	0.7071	8.1970	0.3547	83.1819	1.4604	0.5181
716	50	1	3	40	0.25	0.1	0.2	0.4	11.6309	0.4958	76.4645	2.0026	0.9929	5.8645	0.4958	76.4645	1.1076	0.5492
717	50	1	3	20	0.25	0.1	0.5	0.2	11.6309	0.4425	66.6282	2.0194	0.8936	6.5707	0.4425	66.6282	1.2234	0.5414
718	50	1	3	20	0.25	0.1	0.5	0.4	11.6309	0.5620	56.1788	2.0432	1.1483	5.1740	0.5620	56.1788	1.0162	0.5711
719	50	1	3	40	0.25	0.1	0.5	0.2	11.6309	0.4425	71.6043	2.0103	0.8896	6.5707	0.4425	71.6043	1.2192	0.5395
720	50	1	3	40	0.25	0.1	0.5	0.4	11.6309	0.5620	87.8402	1.9876	1.1170	5.1740	0.5620	87.8402	0.9976	0.5607
721	50	3	1	20	0.25	0.05	0.05	0.2	11.6309	0.3228	66.1516	2.0203	0.6521	9.0092	0.3228	66.1516	1.6049	0.5180
722	50	3	1	20	0.25	0.05	0.05	0.4	11.6309	0.4735	36.8399	2.1198	1.0036	6.1414	0.4735	36.8399	1.2010	0.5686
723	50	3	1	40	0.25	0.05	0.05	0.2	11.6309	0.3228	87.4860	1.9880	0.6416	9.0092	0.3228	87.4860	1.5820	0.5106
724	50	3	1	40	0.25	0.05	0.05	0.4	11.6309	0.4735	69.4044	2.0142	0.9536	6.1414	0.4735	69.4044	1.1548	0.5467
725	50	3	1	20	0.25	0.05	0.2	0.2	11.6309	0.3416	68.0710	2.0166	0.6888	8.5129	0.3416	68.0710	1.5244	0.5207
726	50	3	1	20	0.25	0.05	0.2	0.4	11.6309	0.4865	40.0092	2.1025	1.0228	5.9770	0.4865	40.0092	1.1666	0.5675
727	50	3	1	40	0.25	0.05	0.2	0.2	11.6309	0.3416	85.0936	1.9909	0.6800	8.5129	0.3416	85.0936	1.5075	0.5149
728	50	3	1	40	0.25	0.05	0.2	0.4	11.6309	0.4865	73.7032	2.0069	0.9763	5.9770	0.4865	73.7032	1.1265	0.5480
729	50	3	1	20	0.25	0.05	0.5	0.2	11.6309	0.4321	67.1374	2.0184	0.8720	6.7301	0.4321	67.1374	1.2476	0.5390
730	50	3	1	20	0.25	0.05	0.5	0.4	11.6309	0.5538	54.7087	2.0472	1.1337	5.2507	0.5538	54.7087	1.0296	0.5702
731	50	3	1	40	0.25	0.05	0.5	0.2	11.6309	0.4321	72.7438	2.0084	0.8677	6.7301	0.4321	72.7438	1.2428	0.5370
732	50	3	1	40	0.25	0.05	0.5	0.4	11.6309	0.5538	87.1587	1.9884	1.1011	5.2507	0.5538	87.1587	1.0094	0.5590
733	50	3	3	20	0.25	0.05	0.05	0.2	11.6309	0.3219	66.0310	2.0205	0.6504	9.0334	0.3219	66.0310	1.6089	0.5179
734	50	3	3	20	0.25	0.05	0.05	0.4	11.6309	0.4729	36.6965	2.1206	1.0028	6.1490	0.4729	36.6965	1.2026	0.5687
735	50	3	3	40	0.25	0.05	0.05	0.2	11.6309	0.3219	87.5783	1.9879	0.6399	9.0334	0.3219	87.5783	1.5856	0.5104
736	50	3	3	40	0.25	0.05	0.05	0.4	11.6309	0.4729	69.1993	2.0145	0.9526	6.1490	0.4729	69.1993	1.1561	0.5467
737	50	3	3	20	0.25	0.05	0.2	0.2	11.6309	0.3283	66.8544	2.0189	0.6628	8.8570	0.3283	66.8544	1.5800	0.5187
738	50	3	3	20	0.25	0.05	0.2	0.4	11.6309	0.4773	37.7672	2.1145	1.0091	6.0925	0.4773	37.7672	1.1906	0.5682
739	50	3	3	40	0.25	0.05	0.2	0.2	11.6309	0.3283	86.8479	1.9887	0.6529	8.8570	0.3283	86.8479	1.5591	0.5118
740	50	3	3	40	0.25	0.05	0.2	0.4	11.6309	0.4773	70.7088	2.0119	0.9602	6.0925	0.4773	70.7088	1.1463	0.5471
741	50	3	3	20	0.25	0.05	0.5	0.2	11.6309	0.3621	68.9223	2.0151	0.7296	8.0303	0.3621	68.9223	1.4480	0.5243
742	50	3	3	20	0.25	0.05	0.5	0.4	11.6309	0.5011	43.5051	2.0862	1.0454	5.8026	0.5011	43.5051	1.1316	0.5671
743	50	3	3	40	0.25	0.05	0.5	0.2	11.6309	0.3621	82.0872	1.9947	0.7223	8.0303	0.3621	82.0872	1.4357	0.5198
744	50	3	3	40	0.25	0.05	0.5	0.4	11.6309	0.5011	77.9044	2.0004	1.0024	5.8026	0.5011	77.9044	1.0973	0.5499
745	50	3	1	20	0.25	0.1	0.05	0.2	11.6309	0.3266	66.6525	2.0193	0.6595	8.9030	0.3266	66.6525	1.5875	0.5185
746	50	3	1	20	0.25	0.1	0.05	0.4	11.6309	0.4761	37.4828	2.1161	1.0074	6.1074	0.4761	37.4828	1.1938	0.5683
747	50	3	1	40	0.25	0.1	0.05	0.2	11.6309	0.3266	87.0507	1.9885	0.6494	8.9030	0.3266	87.0507	1.5660	0.5115

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
748	50	3	1	40	0.25	0.1	0.05	0.4	11.6309	0.4761	70.3128	2.0126	0.9582	6.1074	0.4761	70.3128	1.1489	0.5470
749	50	3	1	20	0.25	0.1	0.2	0.2	11.6309	0.3452	68.3037	2.0162	0.6960	8.4232	0.3452	68.3037	1.5101	0.5213
750	50	3	1	20	0.25	0.1	0.2	0.4	11.6309	0.4891	40.6282	2.0994	1.0267	5.9457	0.4891	40.6282	1.1602	0.5674
751	50	3	1	40	0.25	0.1	0.2	0.2	11.6309	0.3452	84.5756	1.9915	0.6875	8.4232	0.3452	84.5756	1.4941	0.5158
752	50	3	1	40	0.25	0.1	0.2	0.4	11.6309	0.4891	74.4893	2.0056	0.9808	5.9457	0.4891	74.4893	1.1212	0.5483
753	50	3	1	20	0.25	0.1	0.5	0.2	11.6309	0.4349	66.9993	2.0187	0.8780	6.6854	0.4349	66.9993	1.2408	0.5397
754	50	3	1	20	0.25	0.1	0.5	0.4	11.6309	0.5560	55.1204	2.0461	1.1377	5.2294	0.5560	55.1204	1.0259	0.5704
755	50	3	1	40	0.25	0.1	0.5	0.2	11.6309	0.4349	72.4233	2.0090	0.8738	6.6854	0.4349	72.4233	1.2362	0.5377
756	50	3	1	40	0.25	0.1	0.5	0.4	11.6309	0.5560	87.3635	1.9881	1.1055	5.2294	0.5560	87.3635	1.0062	0.5595
757	50	3	3	20	0.25	0.1	0.05	0.2	11.6309	0.3258	66.5469	2.0195	0.6579	8.9263	0.3258	66.5469	1.5913	0.5184
758	50	3	3	20	0.25	0.1	0.05	0.4	11.6309	0.4755	37.3403	2.1169	1.0066	6.1149	0.4755	37.3403	1.1953	0.5684
759	50	3	3	40	0.25	0.1	0.05	0.2	11.6309	0.3258	87.1500	1.9884	0.6477	8.9263	0.3258	87.1500	1.5695	0.5113
760	50	3	3	40	0.25	0.1	0.05	0.4	11.6309	0.4755	70.1130	2.0129	0.9572	6.1149	0.4755	70.1130	1.1502	0.5469
761	50	3	3	20	0.25	0.1	0.2	0.2	11.6309	0.3321	67.2650	2.0181	0.6702	8.7561	0.3321	67.2650	1.5636	0.5192
762	50	3	3	20	0.25	0.1	0.2	0.4	11.6309	0.4799	38.4039	2.1109	1.0130	6.0594	0.4799	38.4039	1.1836	0.5680
763	50	3	3	40	0.25	0.1	0.2	0.2	11.6309	0.3321	86.3750	1.9893	0.6606	8.7561	0.3321	86.3750	1.5439	0.5127
764	50	3	3	40	0.25	0.1	0.2	0.4	11.6309	0.4799	71.5823	2.0104	0.9647	6.0594	0.4799	71.5823	1.1406	0.5473
765	50	3	3	20	0.25	0.1	0.5	0.2	11.6309	0.3655	68.9696	2.0150	0.7365	7.9548	0.3655	68.9696	1.4362	0.5250
766	50	3	3	20	0.25	0.1	0.5	0.4	11.6309	0.5036	44.0889	2.0837	1.0494	5.7739	0.5036	44.0889	1.1260	0.5671
767	50	3	3	40	0.25	0.1	0.5	0.2	11.6309	0.3655	81.5762	1.9953	0.7294	7.9548	0.3655	81.5762	1.4245	0.5207
768	50	3	3	40	0.25	0.1	0.5	0.4	11.6309	0.5036	78.5487	1.9995	1.0070	5.7739	0.5036	78.5487	1.0926	0.5502
769	50	1	1	20	0.5	0.05	0.05	0.2	11.6309	0.5431	61.8497	2.0293	1.1022	10.7071	0.5431	61.8497	1.8815	1.0219
770	50	1	1	20	0.5	0.05	0.05	0.4	11.6309	0.6442	66.0615	2.0205	1.3016	9.0273	0.6442	66.0615	1.6079	1.0358
771	50	1	1	40	0.5	0.05	0.05	0.2	11.6309	0.5431	63.6594	2.0254	1.1001	10.7071	0.5431	63.6594	1.8779	1.0200
772	50	1	1	40	0.5	0.05	0.05	0.4	11.6309	0.6442	87.5554	1.9879	1.2806	9.0273	0.6442	87.5554	1.5847	1.0209
773	50	1	1	20	0.5	0.05	0.2	0.2	11.6309	0.5766	60.5441	2.0323	1.1719	10.0852	0.5766	60.5441	1.7848	1.0291
774	50	1	1	20	0.5	0.05	0.2	0.4	11.6309	0.6727	67.6646	2.0174	1.3571	8.6452	0.6727	67.6646	1.5457	1.0398
775	50	1	1	40	0.5	0.05	0.2	0.2	11.6309	0.5766	61.9000	2.0292	1.1701	10.0852	0.5766	61.9000	1.7822	1.0277
776	50	1	1	40	0.5	0.05	0.2	0.4	11.6309	0.6727	85.8140	1.9900	1.3386	8.6452	0.6727	85.8140	1.5273	1.0274
777	50	1	1	20	0.5	0.05	0.5	0.2	11.6309	0.7366	56.2384	2.0430	1.5048	7.8956	0.7366	56.2384	1.4438	1.0634
778	50	1	1	20	0.5	0.05	0.5	0.4	11.6309	0.8139	68.2253	2.0163	1.6412	7.1448	0.8139	68.2253	1.3109	1.0670
779	50	1	1	40	0.5	0.05	0.5	0.2	11.6309	0.7366	56.6716	2.0419	1.5039	7.8956	0.7366	56.6716	1.4431	1.0629
780	50	1	1	40	0.5	0.05	0.5	0.4	11.6309	0.8139	75.7625	2.0036	1.6308	7.1448	0.8139	75.7625	1.3043	1.0617
781	50	1	3	20	0.5	0.05	0.05	0.2	11.6309	0.5416	61.9136	2.0292	1.0990	10.7375	0.5416	61.9136	1.8862	1.0216

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
782	50	1	3	20	0.5	0.05	0.05	0.4	11.6309	0.6429	65.9695	2.0207	1.2991	9.0455	0.6429	65.9695	1.6109	1.0357
783	50	1	3	40	0.5	0.05	0.05	0.2	11.6309	0.5416	63.7484	2.0252	1.0969	10.7375	0.5416	63.7484	1.8826	1.0196
784	50	1	3	40	0.5	0.05	0.05	0.4	11.6309	0.6429	87.6237	1.9878	1.2780	9.0455	0.6429	87.6237	1.5875	1.0206
785	50	1	3	20	0.5	0.05	0.2	0.2	11.6309	0.5530	61.4470	2.0302	1.1228	10.5157	0.5530	61.4470	1.8517	1.0240
786	50	1	3	20	0.5	0.05	0.2	0.4	11.6309	0.6526	66.6133	2.0194	1.3178	8.9117	0.6526	66.6133	1.5889	1.0369
787	50	1	3	40	0.5	0.05	0.2	0.2	11.6309	0.5530	63.1052	2.0266	1.1207	10.5157	0.5530	63.1052	1.8485	1.0223
788	50	1	3	40	0.5	0.05	0.2	0.4	11.6309	0.6526	87.0881	1.9885	1.2976	8.9117	0.6526	87.0881	1.5673	1.0228
789	50	1	3	20	0.5	0.05	0.5	0.2	11.6309	0.6131	59.3063	2.0352	1.2477	9.4860	0.6131	59.3063	1.6915	1.0370
790	50	1	3	20	0.5	0.05	0.5	0.4	11.6309	0.7042	68.6405	2.0156	1.4193	8.2588	0.7042	68.6405	1.4840	1.0450
791	50	1	3	40	0.5	0.05	0.5	0.2	11.6309	0.6131	60.3193	2.0328	1.2462	9.4860	0.6131	60.3193	1.6897	1.0359
792	50	1	3	40	0.5	0.05	0.5	0.4	11.6309	0.7042	83.5739	1.9928	1.4032	8.2588	0.7042	83.5739	1.4696	1.0349
793	50	1	1	20	0.5	0.1	0.05	0.2	11.6309	0.5500	61.5685	2.0300	1.1165	10.5735	0.5500	61.5685	1.8607	1.0234
794	50	1	1	20	0.5	0.1	0.05	0.4	11.6309	0.6500	66.4518	2.0197	1.3128	8.9468	0.6500	66.4518	1.5947	1.0365
795	50	1	1	40	0.5	0.1	0.05	0.2	11.6309	0.5500	63.2714	2.0262	1.1144	10.5735	0.5500	63.2714	1.8574	1.0216
796	50	1	1	40	0.5	0.1	0.05	0.4	11.6309	0.6500	87.2358	1.9883	1.2924	8.9468	0.6500	87.2358	1.5726	1.0222
797	50	1	1	20	0.5	0.1	0.2	0.2	11.6309	0.5831	60.3109	2.0328	1.1853	9.9734	0.5831	60.3109	1.7674	1.0305
798	50	1	1	20	0.5	0.1	0.2	0.4	11.6309	0.6782	67.8916	2.0170	1.3680	8.5744	0.6782	67.8916	1.5343	1.0406
799	50	1	1	40	0.5	0.1	0.2	0.2	11.6309	0.5831	61.5963	2.0299	1.1836	9.9734	0.5831	61.5963	1.7649	1.0291
800	50	1	1	40	0.5	0.1	0.2	0.4	11.6309	0.6782	85.4351	1.9904	1.3500	8.5744	0.6782	85.4351	1.5167	1.0287
801	50	1	1	20	0.5	0.1	0.5	0.2	11.6309	0.7416	56.1416	2.0433	1.5153	7.8415	0.7416	56.1416	1.4353	1.0645
802	50	1	1	20	0.5	0.1	0.5	0.4	11.6309	0.8185	68.1374	2.0165	1.6506	7.1047	0.8185	68.1374	1.3048	1.0680
803	50	1	1	40	0.5	0.1	0.5	0.2	11.6309	0.7416	56.5615	2.0422	1.5145	7.8415	0.7416	56.5615	1.4347	1.0640
804	50	1	1	40	0.5	0.1	0.5	0.4	11.6309	0.8185	75.4687	2.0041	1.6404	7.1047	0.8185	75.4687	1.2984	1.0628
805	50	1	3	20	0.5	0.1	0.05	0.2	11.6309	0.5485	61.6301	2.0298	1.1133	10.6028	0.5485	61.6301	1.8653	1.0231
806	50	1	3	20	0.5	0.1	0.05	0.4	11.6309	0.6487	66.3684	2.0199	1.3103	8.9645	0.6487	66.3684	1.5976	1.0364
807	50	1	3	40	0.5	0.1	0.05	0.2	11.6309	0.5485	63.3559	2.0260	1.1112	10.6028	0.5485	63.3559	1.8619	1.0212
808	50	1	3	40	0.5	0.1	0.05	0.4	11.6309	0.6487	87.3084	1.9882	1.2898	8.9645	0.6487	87.3084	1.5753	1.0219
809	50	1	3	20	0.5	0.1	0.2	0.2	11.6309	0.5598	61.1808	2.0308	1.1368	10.3891	0.5598	61.1808	1.8320	1.0255
810	50	1	3	20	0.5	0.1	0.2	0.4	11.6309	0.6583	66.9507	2.0187	1.3289	8.8343	0.6583	66.9507	1.5763	1.0376
811	50	1	3	40	0.5	0.1	0.2	0.2	11.6309	0.5598	62.7448	2.0274	1.1348	10.3891	0.5598	62.7448	1.8290	1.0238
812	50	1	3	40	0.5	0.1	0.2	0.4	11.6309	0.6583	86.7447	1.9889	1.3092	8.8343	0.6583	86.7447	1.5557	1.0241
813	50	1	3	20	0.5	0.1	0.5	0.2	11.6309	0.6191	59.1167	2.0357	1.2604	9.3928	0.6191	59.1167	1.6770	1.0383
814	50	1	3	20	0.5	0.1	0.5	0.4	11.6309	0.7095	68.7377	2.0154	1.4298	8.1970	0.7095	68.7377	1.4742	1.0459
815	50	1	3	40	0.5	0.1	0.5	0.2	11.6309	0.6191	60.0835	2.0334	1.2589	9.3928	0.6191	60.0835	1.6752	1.0372

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs
Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
816	50	1	3	40	0.5	0.1	0.5	0.4	11.6309	0.7095	83.1819	1.9933	1.4141	8.1970	0.7095	83.1819	1.4604	1.0361
817	50	3	1	20	0.5	0.05	0.05	0.2	11.6309	0.5401	61.9781	2.0290	1.0958	10.7681	0.5401	61.9781	1.8910	1.0212
818	50	3	1	20	0.5	0.05	0.05	0.4	11.6309	0.6416	65.8754	2.0208	1.2966	9.0638	0.6416	65.8754	1.6139	1.0355
819	50	3	1	40	0.5	0.05	0.05	0.2	11.6309	0.5401	63.8385	2.0250	1.0936	10.7681	0.5401	63.8385	1.8873	1.0193
820	50	3	1	40	0.5	0.05	0.05	0.4	11.6309	0.6416	87.6911	1.9877	1.2754	9.0638	0.6416	87.6911	1.5902	1.0203
821	50	3	1	20	0.5	0.05	0.2	0.2	11.6309	0.5515	61.5075	2.0301	1.1196	10.5445	0.5515	61.5075	1.8562	1.0237
822	50	3	1	20	0.5	0.05	0.2	0.4	11.6309	0.6513	66.5335	2.0196	1.3153	8.9292	0.6513	66.5335	1.5918	1.0367
823	50	3	1	40	0.5	0.05	0.2	0.2	11.6309	0.5515	63.1878	2.0264	1.1176	10.5445	0.5515	63.1878	1.8529	1.0219
824	50	3	1	40	0.5	0.05	0.2	0.4	11.6309	0.6513	87.1623	1.9884	1.2950	8.9292	0.6513	87.1623	1.5700	1.0225
825	50	3	1	20	0.5	0.05	0.5	0.2	11.6309	0.6117	59.3493	2.0351	1.2449	9.5071	0.6117	59.3493	1.6948	1.0367
826	50	3	1	20	0.5	0.05	0.5	0.4	11.6309	0.7030	68.6164	2.0156	1.4169	8.2727	0.7030	68.6164	1.4862	1.0448
827	50	3	1	40	0.5	0.05	0.5	0.2	11.6309	0.6117	60.3731	2.0327	1.2434	9.5071	0.6117	60.3731	1.6929	1.0356
828	50	3	1	40	0.5	0.05	0.5	0.4	11.6309	0.7030	83.6612	1.9926	1.4008	8.2727	0.7030	83.6612	1.4717	1.0346
829	50	3	3	20	0.5	0.05	0.05	0.2	11.6309	0.5396	61.9997	2.0290	1.0947	10.7784	0.5396	61.9997	1.8926	1.0211
830	50	3	3	20	0.5	0.05	0.05	0.4	11.6309	0.6412	65.8437	2.0209	1.2958	9.0699	0.6412	65.8437	1.6149	1.0354
831	50	3	3	40	0.5	0.05	0.05	0.2	11.6309	0.5396	63.8687	2.0250	1.0926	10.7784	0.5396	63.8687	1.8889	1.0192
832	50	3	3	40	0.5	0.05	0.05	0.4	11.6309	0.6412	87.7133	1.9877	1.2745	9.0699	0.6412	87.7133	1.5912	1.0202
833	50	3	3	20	0.5	0.05	0.2	0.2	11.6309	0.5434	61.8391	2.0294	1.1027	10.7020	0.5434	61.8391	1.8807	1.0220
834	50	3	3	20	0.5	0.05	0.2	0.4	11.6309	0.6444	66.0766	2.0205	1.3020	9.0243	0.6444	66.0766	1.6074	1.0358
835	50	3	3	40	0.5	0.05	0.2	0.2	11.6309	0.5434	63.6447	2.0254	1.1006	10.7020	0.5434	63.6447	1.8772	1.0200
836	50	3	3	40	0.5	0.05	0.2	0.4	11.6309	0.6444	87.5439	1.9879	1.2811	9.0243	0.6444	87.5439	1.5843	1.0209
837	50	3	3	20	0.5	0.05	0.5	0.2	11.6309	0.5645	60.9993	2.0313	1.1466	10.3027	0.5645	60.9993	1.8186	1.0265
838	50	3	3	20	0.5	0.05	0.5	0.4	11.6309	0.6623	67.1678	2.0183	1.3367	8.7810	0.6623	67.1678	1.5676	1.0382
839	50	3	3	40	0.5	0.05	0.5	0.2	11.6309	0.5645	62.5016	2.0279	1.1447	10.3027	0.5645	62.5016	1.8157	1.0249
840	50	3	3	40	0.5	0.05	0.5	0.4	11.6309	0.6623	86.4952	1.9892	1.3174	8.7810	0.6623	86.4952	1.5477	1.0250
841	50	3	1	20	0.5	0.1	0.05	0.2	11.6309	0.5424	61.8816	2.0293	1.1006	10.7222	0.5424	61.8816	1.8838	1.0217
842	50	3	1	20	0.5	0.1	0.05	0.4	11.6309	0.6436	66.0157	2.0206	1.3004	9.0364	0.6436	66.0157	1.6094	1.0357
843	50	3	1	40	0.5	0.1	0.05	0.2	11.6309	0.5424	63.7038	2.0253	1.0985	10.7222	0.5424	63.7038	1.8803	1.0198
844	50	3	1	40	0.5	0.1	0.05	0.4	11.6309	0.6436	87.5897	1.9879	1.2793	9.0364	0.6436	87.5897	1.5861	1.0207
845	50	3	1	20	0.5	0.1	0.2	0.2	11.6309	0.5538	61.4169	2.0303	1.1243	10.5014	0.5538	61.4169	1.8495	1.0242
846	50	3	1	20	0.5	0.1	0.2	0.4	11.6309	0.6532	66.6525	2.0193	1.3190	8.9030	0.6532	66.6525	1.5875	1.0370
847	50	3	1	40	0.5	0.1	0.2	0.2	11.6309	0.5538	63.0643	2.0267	1.1223	10.5014	0.5538	63.0643	1.8463	1.0224
848	50	3	1	40	0.5	0.1	0.2	0.4	11.6309	0.6532	87.0507	1.9885	1.2989	8.9030	0.6532	87.0507	1.5660	1.0229
849	50	3	1	20	0.5	0.1	0.5	0.2	11.6309	0.6137	59.2849	2.0353	1.2491	9.4755	0.6137	59.2849	1.6899	1.0371

Table I.1. Values of δ, $\tilde{\sigma}$, *f*, *k*, and UTIHW Associated with 95%/95% UTIs Without and With Adjustments for Nuisance Uncertainties (cont'd)

Obs	n	m	r	df_m	$\hat{\sigma}_g$	$\hat{\sigma}_s$	$\hat{\sigma}_a$	$\hat{\sigma}_m$	Without Adjustment					With Adjustment				
									δ	$\tilde{\sigma}$	*f*	*k*	UTIHW	δ	$\tilde{\sigma}$	*f*	*k*	UTIHW
850	50	3	1	20	0.5	0.1	0.5	0.4	11.6309	0.7048	68.6522	2.0155	1.4204	8.2518	0.7048	68.6522	1.4829	1.0451
851	50	3	1	40	0.5	0.1	0.5	0.2	11.6309	0.6137	60.2927	2.0329	1.2477	9.4755	0.6137	60.2927	1.6880	1.0360
852	50	3	1	40	0.5	0.1	0.5	0.4	11.6309	0.7048	83.5303	1.9928	1.4044	8.2518	0.7048	83.5303	1.4686	1.0350
853	50	3	3	20	0.5	0.1	0.05	0.2	11.6309	0.5419	61.9029	2.0292	1.0995	10.7324	0.5419	61.9029	1.8854	1.0216
854	50	3	3	20	0.5	0.1	0.05	0.4	11.6309	0.6431	65.9849	2.0206	1.2995	9.0425	0.6431	65.9849	1.6104	1.0357
855	50	3	3	40	0.5	0.1	0.05	0.2	11.6309	0.5419	63.7335	2.0252	1.0974	10.7324	0.5419	63.7335	1.8818	1.0197
856	50	3	3	40	0.5	0.1	0.05	0.4	11.6309	0.6431	87.6124	1.9878	1.2784	9.0425	0.6431	87.6124	1.5870	1.0207
857	50	3	3	20	0.5	0.1	0.2	0.2	11.6309	0.5457	61.7443	2.0296	1.1075	10.6570	0.5457	61.7443	1.8737	1.0225
858	50	3	3	20	0.5	0.1	0.2	0.4	11.6309	0.6464	66.2105	2.0202	1.3058	8.9972	0.6464	66.2105	1.6029	1.0361
859	50	3	3	40	0.5	0.1	0.2	0.2	11.6309	0.5457	63.5133	2.0257	1.1054	10.6570	0.5457	63.5133	1.8702	1.0206
860	50	3	3	40	0.5	0.1	0.2	0.4	11.6309	0.6464	87.4392	1.9880	1.2850	8.9972	0.6464	87.4392	1.5802	1.0214
861	50	3	3	20	0.5	0.1	0.5	0.2	11.6309	0.5667	60.9151	2.0314	1.1512	10.2625	0.5667	60.9151	1.8123	1.0270
862	50	3	3	20	0.5	0.1	0.5	0.4	11.6309	0.6642	67.2650	2.0181	1.3404	8.7561	0.6642	67.2650	1.5636	1.0385
863	50	3	3	40	0.5	0.1	0.5	0.2	11.6309	0.5667	62.3893	2.0281	1.1493	10.2625	0.5667	62.3893	1.8095	1.0254
864	50	3	3	40	0.5	0.1	0.5	0.4	11.6309	0.6642	86.3750	1.9893	1.3212	8.7561	0.6642	86.3750	1.5439	1.0254

Appendix J: SAS® Programs for Calculating X%/Y% Upper Tolerance Intervals and Half-Widths

Appendix J

SAS® Programs for Calculating X%/Y% Upper Tolerance Intervals and Half-Widths

This appendix contains the listings for two sets of SAS (SAS 2001) programs. The first program, listed in Section J.1, was used to compute the X%/Y% UTI half-widths presented in Section 4 and Appendix I. The second set of programs, listed in Section J.2, was used to calculate the X%/Y% UTIs and values of X and Y for the simulated example problem discussed in Section 5 (see Table 5.3).

Advanced notation used in the main body of the report (e.g., subscripts, superscripts, tildes, and hats) is not possible in SAS programs. Hence, the alternate notations used in the SAS programs, compared to the notations used in the report, are summarized in Table J.1.

Table J.1. Notation Used in SAS Programs versus Notation Used in the Report

Notation in Report	Notation in SAS Program
$\hat{\sigma}_g$	g, sigma_g
$\hat{\sigma}_s$	s
$\hat{\sigma}_a$	a
$\bar{\hat{\sigma}}_m$	mod
$\hat{\sigma}_2$	sigma_2
n	n
m	m
r	r
df_m	dfm
f (for the no-subtraction cases)[a]	f0, f1
f (for the anovasub case)	f2
f (for the indepsub case)	f3
k (for the no-adjustment, no-subtraction case)	k0
k (for the adjustment, no-subtraction case)	k1
k (for the anovasub case)	k2
k (for the indepsub case)	k3
$\tilde{\sigma}$ (for the no-subtraction cases)[a]	sig_til0, sig_til1
$\tilde{\sigma}$ (for the anovasub case)	sig_til2

(a) The f and $\tilde{\sigma}$ parameters are the same for the unadjusted and adjusted X%/Y% UTI approaches when not subtracting nuisance uncertainties. However, it was convenient in the SAS code to use different names.

Table J.1. Notation Used in SAS Programs versus Notation Used in the Report (cont'd)

$\tilde{\sigma}$ (for the indepsub case)	sig_til3
UTIHW (for the no-adjustment, no-subtraction case)	noadjust
UTIHW (for the adjustment, no-subtraction case)	adjust
UTIHW (for the anovasub case)	anovasub
UTIHW (for the indepsub case)	indepsub
β	beta
γ	gamma
$z_{1-\beta}$	z1mb
δ_0 (for the no-adjustment, no-subtraction case)	delta0
δ_1 (for the adjustment, no-subtraction case)	delta1
δ (for the anovasub case)	delta2
δ (for the indepsub case)	delta3
MS_g	msg
df_g	dfg
MS_s	mss
df_s	dfs
MS_a	msa
df_a	dfa
$\hat{\sigma}_s^2$	anova_s2
$\hat{\sigma}_a^2$	anova_a2
$\tilde{\sigma}_s^2$	indep_s2
$\tilde{\sigma}_a^2$	indep_a2
$\tilde{\mu}$	mutilde
$\tilde{\sigma}$	sigtilde
$t_0(X,Y,f,\delta_0)$	t0
$t_1(X,Y,f,\delta_1)$	t1
UTI	uti
MS_p (for the anovasub case)	msp2
MS_p (for the indepsub case)	msp3
MS_n (for the anovasub case)	msn2
MS_n (for the indepsub case)	msn3
f_p (for the anovasub case)	fp2
f_p (for the indepsub case)	fp3
f_n (for the anovasub case)	fn2
f_n (for the indepsub case)	fn3

J.1. SAS Program Used to Compute the X%/Y% UTI Half-Widths Discussed in Section 4

```
/* UTIHW_Rev0.sas, Dec. 12, 2001 */
/* SAS Program to Calculate Upper Tolerance Interval Half-widths (UTIHW) */

options nodate nonumber ls=80 ps=1000;
data halfwidt;
beta=0.99;           /* typically use either 0.95 or 0.99 */
gamma=0.99;          /* typically use either 0.95 or 0.99 */
z1mb=probit(beta);   /* z of one minus beta, the z-score associated   */
                     /* with the 100*beta-th percentile of a standard */
                     /* normal distribution                           */

/* input assumed sample sizes and variance/uncertainty components */
do n=10, 30, 50;
do g=0.10, 0.25, 0.50;
do m=1, 3;
do s=0.05, 0.10;
do r=1, 3;
do a=0.05, 0.20, 0.50;
do dfm=20, 40;
do mod=0.20, 0.40;

j=1;
do until ((j=2) or (k1=.) or (k2=.) or (k3=.));
/* form mean squares for glass, samples, and analyses */
msg=r*m*g**2+r*s**2+a**2;
mss=r*s**2+a**2;
msa=a**2;
/* determine degrees of freedom for glass, samples, and analyses   */
dfg=n-1;         /* degrees of freedom for glass mean squares      */
dfs=n*(m-1);     /* degrees of freedom for sample mean squares     */
dfa=n*m*(r-1);   /* degrees of freedom for analysis mean squares   */
fn3=1000000;     /* degrees of freedom for negative terms in sigma */
                 /* tilde under the indepsub strategy, large here  */
                 /* to simulate infinite degrees of freedom        */
/* other 'constants' needed for upcoming calculations */
sigma_2=sqrt(mod**2 + g**2 + s**2/m + a**2/(m*r));   /* see equation (H.1) */
sigma_g=g;




if m>1 and r>1 then do;  /***************************************************/
 /* Calculations related to the no adjustment case */
 delta0=z1mb*sqrt(n);                                       /* see (H.6b) */
 sig_til0=sqrt(mod**2 + msg/(r*m));                         /* see (D.2)  */
 f0=sig_til0**4/(mod**4/dfm + (msg/(r*m))**2/dfg);          /* see (D.3)  */
 if f0<1 then do;
 t0=.;  /* if degrees of freedom are less than one, return a missing value */
 end;
 else do;
 t0=tinv(gamma,f0,delta0);
 end;
 k0=t0/sqrt(n);                                             /* see (H.7b) */
```

```
k0star=k0*sig_til0/sigma_g;                                  /* see (3.17) */
noadjust=k0*sig_til0;       /* the UTIHW under the no adjustment strategy */
indicat0=1;  /* Indicates appropriateness of Satterthwaite's formula. A   */
             /* ‘1’ indicates the result for the UTIHW is reliable in the */
             /* sense that Satterthwaite's formula is appropriate when    */
             /* calculating the approximate degrees of freedom.  For the  */
             /* no subtraction cases, there are no negative terms in      */
             /* sigma tilde, so there is no potential for misusing        */
             /* Satterthwaite's formula.  In situations where nuisance    */
             /* uncertainties are subtracted, the applicability of        */
             /* Satterthwaite's formula must be verified.  A '0' will be  */
             /* used to indicate that the UTIHW may not be reliable       */
             /* because Satterthwaite's formula is not appropriate due to */
             /* the magnitude of the mean squares for the negative terms  */
             /* in sigma tilde and the corresponding degrees of freedom.  */
             /* See Appendix C for details.                               */

/* Calculations related to the adjustment case */
delta1=z1mb*sqrt(n)*sigma_g/sigma_2;                          /* see (H.3) */
sig_til1=sig_til0;           /* see (D.2) and footnote (a) to Table J.1 */
f1=f0;                       /* see (D.3) and footnote (a) to Table J.1 */
if f1<1 then do;
t1=.;
end;
else do;
t1=tinv(gamma, f1, delta1);
end;
k1=t1/sqrt(n);                                               /* see (H.4b) */
k1star=k1*sig_til1/sigma_g;                                  /* see (3.17) */
adjust=k1*sig_til1;          /* the UTIHW under the adjustment strategy */
indicat1=1;

/* Calculations related to the anovasub case */
delta2=delta1;                 /* see (H.8) and the comments thereafter */
sig_til2=sqrt(mod**2 + msg/(r*m) - mss/(r*m));                /* see (D.4) */
f2=sig_til2**4/(mod**4/dfm + (msg/(r*m))**2/dfg + (mss/(r*m))**2/dfs);
if f2<1 then do;                               /* for f2 above, see (D.5) */
t2=.;
end;
else do;
t2=tinv(gamma, f2, delta2);
end;
k2=t2*sigma_2/(sig_til2*sqrt(n));                            /* see (H.8)  */
k2star=k2*sig_til2/sigma_g;                                  /* see (3.17) */
anovasub=k2*sig_til2;          /* the UTIHW under the anovasub strategy */
/* Determine appropriateness of Satterthwaite's formula */
msp2=mod**2 + msg/(r*m);   /* mean squares for positive terms in sig_til2 */
msn2=mss/(r*m);            /* mean squares for negative terms in sig_til2 */
fp2=msp2**2/(mod**4/dfm + (msg/(r*m))**2/dfg);              /* df for msp2 */
fn2=msn2**2/((mss/(r*m))**2/dfs);        /* df for msn2, should equal dfs */
f2_check=(msp2-msn2)**2/(msp2**2/fp2 + msn2**2/fn2);        /* check on f2 */
 if (fp2<=100 and fn2>=fp2/2 and msp2/msn2>=finv(.975,fn2,fp2,0))
 or (fp2<=20 and msp2/msn2>=finv(.99,fn2,fp2,0))
 or (20<fp2<=100 and fn2>=fp2/5 and msp2/msn2>=finv(.99,fn2,fp2,0))
 then do;
 indicat2=1;
 end;
```

```
  else do;
  indicat2=0;       /* Indicates that the value of anovasub may not be     */
                    /* reliable because Satterthwaite's formula is not     */
                    /* appropriate for calculating the approximate degrees */
                    /* of freedom f2.                                      */
  end;

 /* Calculations related to the indepsub case. Note, it is assumed that    */
 /* the independent estimates of sampling and analysis uncertainty are     */
 /* equal to s-squared and a-squared, respectively.                        */
 delta3=delta1;                   /*see (H.8) and the comments thereafter */
 sig_til3=sqrt(mod**2 + msg/(r*m) - s**2/m - a**2/(r*m));     /* see (D.6) */
 f3=sig_til3**4/(mod**4/dfm + (msg/(r*m))**2/dfg);            /* see (D.8) */
 if f3<1 then do;
 t3=.;
 end;
 else do;
 t3=tinv(gamma, f3, delta3);
 end;
 k3=t3*sigma_2/(sig_til3*sqrt(n));                           /* see (H.8)  */
 k3star=k3*sig_til3/sigma_g;                                 /* see (3.17) */
 indepsub=k3*sig_til3;            /* the UTIHW under the indepsub strategy */
 /* Determine appropriateness of Satterthwaite's formula */
 msp3=mod**2 + msg/(r*m);   /* mean squares for positive terms in sig_til3 */
 msn3=(r*s**2+a**2)/(r*m);  /* mean squares for negative terms in sig_til3 */
 fp3=msp3**2/(mod**4/dfm + (msg/(r*m))**2/dfg);            /* df for msp3   */
 f3_check=(msp3-msn3)**2/(msp3**2/fp3 + 0);                /* a check on f3 */
  if fp3<=100 and msp3/msn3>=finv(.975,fn3,fp3,0) then do;
  indicat3=1;
  end;
  else do;
  indicat3=0;
  end;

end;



else if m=1 and r>1 then do;  /*********************************************/
 /* Calculations related to the no adjustment case */
 delta0=z1mb*sqrt(n);                                        /* see (H.6b) */
 sig_til0=sqrt(mod**2 + msg/r);                              /* see (E.2)  */
 f0=sig_til0**4/(mod**4/dfm + (msg/r)**2/dfg);               /* see (E.3)  */
 if f0<1 then do;
 t0=.;
 end;
 else do;
 t0=tinv(gamma,f0,delta0);
 end;
 k0=t0/sqrt(n);                                              /* see (H.7b) */
 k0star=k0*sig_til0/sigma_g;                                 /* see (3.17) */
 noadjust=k0*sig_til0;
 indicat0=1;

 /* Calculations related to the adjustment case */
 delta1=z1mb*sqrt(n)*sigma_g/sigma_2;                         /* see (H.3) */
```

```
 sig_til1=sig_til0;             /* see (E.2) and footnote (a) to Table J.1 */
 f1=f0;                         /* see (E.3) and footnote (a) to Table J.1 */
 if f1<1 then do;
 t1=.;
 end;
 else do;
 t1=tinv(gamma, f1, delta1);
 end;
 k1=t1/sqrt(n);                                              /* see (H.4b) */
 k1star=k1*sig_til1/sigma_g;                                 /* see (3.17) */
 adjust=k1*sig_til1;
 indicat1=1;

 /* Calculations related to the anovasub case */
 delta2=delta1;                   /* see (H.8) and the comments thereafter */
 sig_til2=sqrt(mod**2 + (msg-msa)/r);                         /* see (E.4) */
 f2=sig_til2**4/(mod**4/dfm + (msg/r)**2/dfg + (msa/r)**2/dfa);
 if f2<1 then do;                             /* for f2 above, see (E.5) */
 t2=.;
 end;
 else do;
 t2=tinv(gamma, f2, delta2);
 end;
 k2=t2*sigma_2/(sig_til2*sqrt(n));                           /* see (H.8)  */
 k2star=k2*sig_til2/sigma_g;                                 /* see (3.17) */
 anovasub=k2*sig_til2;
 /* Determine appropriateness of Satterthwaite's formula */
 msp2=mod**2 + msg/(r*m);
 msn2=msa/(r*m);
 fp2=msp2**2/(mod**4/dfm + (msg/(r*m))**2/dfg);
 fn2=msn2**2/((msa/(r*m))**2/dfa);   /* should equal dfa */
 f2_check=(msp2-msn2)**2/(msp2**2/fp2 + msn2**2/fn2);
  if (fp2<=100 and fn2>=fp2/2 and msp2/msn2>=finv(.975,fn2,fp2,0))
  or (fp2<=20 and msp2/msn2>=finv(.99,fn2,fp2,0))
  or (20<fp2<=100 and fn2>=fp2/5 and msp2/msn2>=finv(.99,fn2,fp2,0))
  then do;
  indicat2=1;
  end;
  else do;
  indicat2=0;
  end;

 /* Calculations related to the indepsub case.  Note, it is assumed that   */
 /* the sampling uncertainty that is actually confounded with glass        */
 /* variation can be separated from the glass variation and that the       */
 /* independent estimates of sampling and analysis uncertainty are equal   */
 /* to s-squared and a-squared, respectively.                              */
delta3=delta1;                    /* see (H.8) and the comments thereafter */
 sig_til3=sqrt(mod**2 + msg/r - s**2 - a**2/r);               /* see (E.6) */
 f3=sig_til3**4/(mod**4/dfm + (msg/r)**2/dfg);                /* see (E.8) */
 if f3<1 then do;
 t3=.;
 end;
 else do;
 t3=tinv(gamma, f3, delta3);
 end;
 k3=t3*sigma_2/(sig_til3*sqrt(n));                           /* see (H.8)  */
```

```
 k3star=k3*sig_til3/sigma_g;                                /* see (3.17) */
 indepsub=k3*sig_til3;
 /* Determine appropriateness of Satterthwaite's formula */
 msp3=mod**2 + msg/(r*m);
 msn3=(r*s**2 + a**2)/(r*m);
 fp3=msp3**2/(mod**4/dfm + (msg/(r*m))**2/dfg);
 f3_check=(msp3-msn3)**2/(msp3**2/fp3 + 0);
  if fp3<=100 and msp3/msn3>=finv(.975,fn3,fp3,0) then do;
  indicat3=1;
  end;
  else do;
  indicat3=0;
  end;

end;




else if m>1 and r=1 then do;  /********************************************/
 /* Calculations related to the no adjustment case */
 delta0=z1mb*sqrt(n);                                      /* see (H.6b) */
 sig_til0=sqrt(mod**2 + msg/m);                            /* see (F.2)  */
 f0=sig_til0**4/( mod**4/dfm + (msg/m)**2/dfg);            /* see (F.3)  */
 if f0<1 then do;
 t0=.;
 end;
 else do;
 t0=tinv(gamma,f0,delta0);
 end;
 k0=t0/sqrt(n);                                             /* see (H.7b) */
 k0star=k0*sig_til0/sigma_g;                                /* see (3.17) */
 noadjust=k0*sig_til0;
 indicat0=1;

 /* Calculations related to the adjustment case */
 delta1=z1mb*sqrt(n)*sigma_g/sigma_2;                        /* see (H.3) */
 sig_til1=sig_til0;            /* see (F.2) and footnote (a) to Table J.1 */
 f1=f0;                        /* see (F.3) and footnote (a) to Table J.1 */
 if f1<1 then do;
 t1=.;
 end;
 else do;
 t1=tinv(gamma, f1, delta1);
 end;
 k1=t1/sqrt(n);                                             /* see (H.4b) */
 k1star=k1*sig_til1/sigma_g;                                /* see (3.17) */
 adjust=k1*sig_til1;
 indicat1=1;

 /* Calculations related to the anovasub case.  Note, it is assumed that   */
 /* the sum s-squared plus a-squared equals the combined sampling and      */
 /* analysis uncertainty that results from the confounding of analysis     */
 /* uncertainty with sampling uncertainty, the combined uncertainty can    */
 /* then be subtracted when calculating sig_til2.                          */
delta2=delta1;                  /* see (H.8) and the comments thereafter */
 sig_til2=sqrt(mod**2 + (msg-mss)/m);                        /* see (F.4) */
```

```
 f2=sig_til2**4/(mod**4/dfm + (msg/m)**2/dfg + (mss/m)**2/dfs);
 if f2<1 then do;                               /* for f2 above, see (F.5) */
 t2=.;
 end;
 else do;
 t2=tinv(gamma, f2, delta2);
 end;
 k2=t2*sigma_2/(sig_til2*sqrt(n));                          /* see (H.8)  */
 k2star=k2*sig_til2/sigma_g;                                /* see (3.17) */
 anovasub=k2*sig_til2;
 /* Determine appropriateness of Satterthwaite's formula */
 msp2=mod**2 + msg/(r*m);
 msn2=mss/(r*m);
 fp2=msp2**2/(mod**4/dfm + (msg/(r*m))**2/dfg);
 fn2=msn2**2/((mss/(r*m))**2/dfs);                     /* should equal dfs */
 f2_check=(msp2-msn2)**2/(msp2**2/fp2 + msn2**2/fn2);
  if (fp2<=100 and fn2>=fp2/2 and msp2/msn2>=finv(.975,fn2,fp2,0))
  or (fp2<=20 and msp2/msn2>=finv(.99,fn2,fp2,0))
  or (20<fp2<=100 and fn2>=fp2/5 and msp2/msn2>=finv(.99,fn2,fp2,0))
  then do;
  indicat2=1;
  end;
  else do;
  indicat2=0;
  end;

 /* Calculations related to the indepsub case.  Note, it is assumed that   */
 /* the sum of the independent estimates of sampling and analysis          */
 /* uncertainty equals the combined sampling and analysis uncertainty that */
 /* results from the confounding of analysis uncertainty with sampling     */
 /* uncertainty. It is also assumed that the combined sampling and         */
 /* analysis uncertainty equals s-squared plus a-squared.                  */
delta3=delta1;                  /* see (H.8) and the comments thereafter */
 sig_til3=sqrt(mod**2 + msg/m - s**2/m - a**2/m);            /* see (F.6) */
 f3=sig_til3**4/(mod**4/dfm + (msg/m)**2/dfg);               /* see (F.8) */
 if f3<1 then do;
 t3=.;
 end;
 else do;
 t3=tinv(gamma, f3, delta3);
 end;
 k3=t3*sigma_2/(sig_til3*sqrt(n));                           /* see (H.8)  */
 k3star=k3*sig_til3/sigma_g;                                 /* see (3.17) */
 indepsub=k3*sig_til3;
 /* Determine appropriateness of Satterthwaite's formula */
 msp3=mod**2 + msg/(r*m);
 msn3=(r*s**2 + a**2)/(r*m);
 fp3=msp3**2/(mod**4/dfm + (msg/(r*m))**2/dfg);
 f3_check=(msp3-msn3)**2/(msp3**2/fp3 + 0);
  if fp3<=100 and msp3/msn3>=finv(.975,fn3,fp3,0) then do;
  indicat3=1;
  end;
  else do;
  indicat3=0;
  end;

end;
```

```
else do;  /*****************************************************************/
 /* Calculations related to the no adjustment case */
 delta0=z1mb*sqrt(n);                                           /* see (H.6b) */
 sig_til0=sqrt(mod**2 + msg);                                   /* see (G.2)  */
 f0=sig_til0**4/(mod**4/dfm + msg**2/dfg);                      /* see (G.3)  */
 if f0<1 then do;
 t0=.;
 end;
 else do;
 t0=tinv(gamma, f0, delta0);
 end;
 k0=t0/sqrt(n);                                                 /* see (H.7b) */
 k0star=k0*sig_til0/sigma_g;                                    /* see (3.17) */
 noadjust=k0*sig_til0;
 indicat0=1;

 /* Calculations related to the adjustment case */
 delta1=z1mb*sqrt(n)*sigma_g/sigma_2;                            /* see (H.3) */
 sig_til1=sig_til0;            /* see (G.2) and footnote (a) to Table J.1 */
 f1=f0;                        /* see (G.3) and footnote (a) to Table J.1 */
 if f1<1 then do;
 t1=.;
 end;
 else do;
 t1=tinv(gamma, f1, delta1);
 end;
 k1=t1/sqrt(n);                                                 /* see (H.4b) */
 k1star=k1*sig_til1/sigma_g;                                    /* see (3.17) */
 adjust=k1*sig_til1;
 indicat1=1;

 /* Calculations related to the anovasub case. Because neither sampling    */
 /* nor analysis uncertainties are estimable, no nuisance uncertainties    */
 /* can be subtracted under the anovasub strategy when m=r=1.              */
delta2=delta1;                   /* see (H.8) and the comments thereafter */
 sig_til2=sqrt(mod**2 + msg);   /* sig_til2 should equal sig_til1 in (G.2) */
 f2=sig_til2**4/(mod**4/dfm + msg**2/dfg); /* f2 should equal f1 in (G.3), */
 if f2<1 then do;                                  /* see Case 2 of App. G */
 t2=.;
 end;
 else do;
 t2=tinv(gamma, f2, delta2);
 end;
 k2=t2*sigma_2/(sig_til2*sqrt(n));                              /* see (H.8)  */
 k2star=k2*sig_til2/sigma_g;                                    /* see (3.17) */
 anovasub=k2*sig_til2;           /* anovasub should equal nosub when m=r=1 */
 /* Determine appropriateness of Satterthwaite's formula */
 f2_check=f2;       /* This is assumed because there is no msn2 when m=r=1 */
 indicat2=1;        /* Satterthwaite's formula should be appropriate here  */
                    /* because there are no negative terms in sig_til2.    */

 /* Calculations related to the indepsub case.  Note, it is assumed that   */
 /* the sum of the independent estimates of sampling and analysis          */
 /* uncertainty equals the combined sampling and analysis uncertainty, and */
```

```
 /* that the combined sampling and analysis uncertainty can be separated   */
 /* from the combined glass, sampling, and analysis uncertainty/variation  */
 /* that results from the confounding of sampling and analysis uncertainty */
 /* with glass variation. It is also assumed that the combined sampling    */
 /* and analysis uncertainty equals s-squared plus a-squared.              */
delta3=delta1;                    /* see (H.8) and the comments thereafter */
 sig_til3=sqrt(mod**2 + msg - s**2 - a**2);                  /* see (G.4) */
 f3=sig_til3**4/(mod**4/dfm + msg**2/dfg);                   /* see (G.6) */
 if f3<1 then do;
 t3=.;
 end;
 else do;
 t3=tinv(gamma, f3, delta3);
 end;
 k3=t3*sigma_2/(sig_til3*sqrt(n));                          /* see (H.8)  */
 k3star=k3*sig_til3/sigma_g;                                /* see (3.17) */
 indepsub=k3*sig_til3;
 /* Determine appropriateness of Satterthwaite's formula */
 msp3=mod**2 + msg/(r*m);
 msn3=(r*s**2 + a**2)/(r*m);
 fp3=msp3**2/(mod**4/dfm + (msg/(r*m))**2/dfg);
 f3_check=(msp3-msn3)**2/(msp3**2/fp3 + 0);
  if fp3<=100 and msp3/msn3>=finv(.975,fn3,fp3,0) then do;
  indicat3=1;
  end;
  else do;
  indicat3=0;
  end;

end;


j=j+1;
output;
end;
end;
end;
end;
end;
end;
end;
end;
end;
run;




proc print;  /*************************************************************/
var g n s m a r mod dfm;
run;

proc print noobs;
var delta0 sig_til0 f0 t0 k0 noadjust k0star indicat0;
run;
```

```
proc print noobs;
var delta1 sig_til1 f1 t1 k1 adjust k1star indicat1;
run;

proc print noobs;
var delta2 sig_til2 f2 t2 k2 anovasub k2star indicat2;
run;

proc print noobs;
var msp2 msn2 fp2 fn2;
run;

proc print noobs;
var delta3 sig_til3 f3 t3 k3 indepsub k3star indicat3;
run;

proc print noobs;
var msp3 msn3 fp3;
run;

proc print noobs;
var sigma_g sigma_2 f2_check f3_check;
run;




proc print;  /************************************************************/
var delta0 delta1 delta2 delta3;
run;

proc print;
var sig_til0 sig_til1 sig_til2 sig_til3;
run;

proc print;
var f0 f1 f2 f3;
run;

proc print;
var t0 t1 t2 t3;
run;

proc print;
var k0 k1 k2 k3;
run;

proc print;
var noadjust adjust anovasub indepsub;
run;

proc print;
var k0star k1star k2star k3star;
run;
```

```
quit;
```

J.2. SAS Programs Used to Compute X%/Y% UTIs for the Simulated Compliance Example Discussed in Section 5

This section contains the listings for four SAS (SAS 2001) programs. The first program computes the mean squares from the nested-structure data set of simulated, predicted ln(PCT release) values given in Table 5.1. The second program computes the X%/Y% UTIs without and with adjustments for nuisance uncertainties as described in Section 3.7 and Appendix H. Two separate programs are needed because the output of the first program cannot be loaded automatically into the second. Thus, the second program must be set up and run after running the first program. The third program calculates X given Y and other needed input. The fourth program calculates Y given X and other needed input.

Program 1

```
/* exprob_ms.sas, Nov. 21, 2001 */
/* SAS Program to Calculate Mean Squares */

options ls=80;
data ms_g_s_a;
infile 'C:\Documents and Settings\d3k269\My Documents\Projects\Vit_stuff
        \Wtp_01\TI_Report\early_stuff\des_mat_3.csv' DLM=',';
input glass $ samples $ analyses $ xhat mterm yhat;
run;

proc nested data=ms_g_s_a;
class glass samples;
var xhat;
run;

quit;
```

Program 2

```
/* exprob_ti.sas, Dec. 7, 2001 */
/* SAS Program to Calculate Upper Tolerance Intervals */

options ls=80 nodate nonumber;
data halfwdth;
/* The following variable values must be input to this program */
gamma=0.99;    /* try gamma=0.9999, beta=0.999963134 to check EA glass     */
beta=0.99;     /* uti of 2.12226 using adjust method results               */
               /* or try gamma=0.9999, beta=0.99930615 to check EA glass   */
               /* uti of 2.12226 using noadjust method results             */
               /* or try gamma=0.9993072178, beta=0.9999 to check EA glass */
```

```
               /* uti of 2.12226 using noadjust method results              */
               /* or try gamma=0.999956453, beta=0.9999 to check EA glass  */
               /* uti of 2.12226 using adjust method results               */

mutilde=-0.606955;        /* mutilde and the following mean square values  */
                          /* were obtained using the program exprob_ms.sas */
msg=0.355376;
mss=0.020090;
msa=0.027234;
mod=0.20;    /* mod**2 is the estimate for the regres. model uncert. comp. */
anova_s2=0;  /* for this dataset est.var.comp. was -0.0035723, so use 0.   */
anova_a2=0.027234;                                /* assumed equal to msa */
indep_s2=.0025;                                         /* assumed value */
indep_a2=.04;                                           /* assumed value */
n=10;
m=2;                            /* Note that m and r are greater than 1,   */
r=2;                            /* so Appendix D applies for this example. */
dfm=40;                                       /* this says that p-q=dfm=40 */
/* This concludes the input variables needed for this program */


dfg=n-1;
dfs=n*(m-1);
dfa=n*m*(r-1);
z1mb=probit(beta); /* z of one minus beta, z-score from a std. norm. dist. */
sigma_2=sqrt(mod**2 + msg/(r*m));                  /* see equation (H.1) */
sigma_g=sqrt((msg-mss)/(r*m));        /* This is an est. of the true SD of */
                                      /* interest, see (D.1) */

 delta0=z1mb*sqrt(n);                                      /* see (H.6b) */
 sig_til0=sqrt(mod**2 + msg/(r*m));                        /* see (D.2)  */
 f0=sig_til0**4/(mod**4/dfm + (msg/(r*m))**2/dfg);         /* see (D.3)  */
 t0=tinv(gamma, f0, delta0);
 k0=t0/sqrt(n);                                            /* see (H.7b) */
 noadjust=mutilde + k0*sig_til0;

 delta1=z1mb*sqrt(n)*sigma_g/sigma_2;                      /* see (H.3) */
 sig_til1=sqrt(mod**2 + msg/(r*m));                        /* see (D.2) */
 f1=sig_til1**4/(mod**4/dfm + (msg/(r*m))**2/dfg);         /* see (D.3) */
 t1=tinv(gamma, f1, delta1);
 k1=t1*sigma_2/(sig_til1*sqrt(n));                        /* see (H.4b) */
 adjust=mutilde + k1*sig_til1;

 delta2=delta1;                  /* see (H.8) and the comments thereafter */
 sig_til2=sqrt(mod**2+msg/(r*m)-anova_s2/m-anova_a2/(r*m));  /* see (D.4) */
 f2=sig_til2**4/(mod**4/dfm + (msg/(r*m))**2/dfg + (anova_s2/m)**2/dfs +
    (anova_a2/(r*m))**2/dfa);
 t2=tinv(gamma, f2, delta2);                   /* see (D.5) for sig_til2 */
 k2=t2*sigma_2/(sig_til2*sqrt(n));                         /* see (H.8) */
 anovasub=mutilde + k2*sig_til2;

 delta3=delta1;                 /* see (H.8) and the comments thereafter */
 sig_til3=sqrt(mod**2+msg/(r*m)-indep_s2/m-indep_a2/(r*m)); /* see (D.6) */
 f3=sig_til3**4/(mod**4/dfm + (msg/(r*m))**2/dfg);         /* see (D.7) */
 t3=tinv(gamma, f3, delta3);
 k3=t3*sigma_2/(sig_til3*sqrt(n));                         /* see (H.8) */
 indepsub=mutilde + k3*sig_til3;
```

```
run;

proc print noobs width=full double;
var delta0 sig_til0 f0 t0 k0 noadjust;
var delta1 sig_til1 f1 t1 k1 adjust;
var delta2 sig_til2 f2 t2 k2 anovasub;
var delta3 sig_til3 f3 t3 k3 indepsub;
var sigma_g sigma_2;
run;

quit;
```

Program 3

```
/* solve_gamma2.sas, Dec. 7, 2001 */
/* SAS Program to Solve for Gamma */

data solvgama;
method=1;     /* this must be set to either 1 for adjust or 0 for noadjust */
beta=0.9999;                                              /* content level */
uti=2.12226;             /* uti associated with EA glass, ln(8.35)=2.12226 */

n=10;
m=2;
r=2;
mutilde=-0.606955;        /* mutilde and the following mean square values  */
msg=0.355376;             /* were obtained using the program exprob_ms.sas */
mss=0.020090;
msa=0.027234;
mod=0.20;    /* mod**2 is the estimate for the regres. model uncert. comp. */
f=18.1028;                     /* obtained using the program exprob_ti.sas */
sigtilde=0.35895;              /* obtained using the program exprob_ti.sas */
sigma_2=sqrt(mod**2 + msg/(r*m));                     /* see equation (H.1) */
sigma_g=sqrt((msg-mss)/(r*m));        /* This is an est. of the true SD of */
                                      /* interest, see (D.1).              */

z1mb=probit(beta);
k=(uti-mutilde)/sigtilde;
if method=1 then do;
to=k*sigtilde*sqrt(n)/sigma_2;
delta=z1mb*sqrt(n)*sigma_g/sigma_2; /* the delta value under adjust method */
end;
else if method=0 then do;
to=k*sqrt(n);
delta=z1mb*sqrt(n);               /* the delta value under noadjust method */
end;

gamma=cdf('t',to,f,delta);                             /* confidence level */

run;

proc print noobs width=full;
```

```
var sigma_g sigma_2 z1mb delta to;
var f k gamma beta method;
run;

quit;
```

Program 4

```
/* solve_beta2.sas, Dec. 7, 2001 */
/* SAS Program to Solve for Beta */

data solvbeta;
method=1;     /* this must be set to either 1 for adjust or 0 for noadjust */
gamma=0.9999;                                          /* confidence level */
uti=2.12226;             /* uti associated with EA glass, ln(8.35)=2.12226 */

n=10;
m=2;
r=2;
mutilde=-0.606955;        /* mutilde and the following mean square values  */
msg=0.355376;             /* were obtained using the program exprob_ms.sas */
mss=0.020090;
msa=0.027234;
mod=0.20;    /* mod**2 is the estimate for the regres. model uncert. comp. */
f=18.1028;                     /* obtained using the program exprob_ti.sas */
sigtilde=0.35895;              /* obtained using the program exprob_ti.sas */
sigma_2=sqrt(mod**2 + msg/(r*m));                   /* see equation (H.1) */
sigma_g=sqrt((msg-mss)/(r*m));        /* This is an est. of the true SD of */
                                      /* interest, see (D.1).              */

beta=0.999999;              /* a starting value for beta, this will change */
z1mb=probit(beta);
z1=z1mb;                                             /* the initial z-value */
k=(uti-mutilde)/sigtilde;
if method=1 then do;
to=k*sigtilde*sqrt(n)/sigma_2;
delta=z1mb*sqrt(n)*sigma_g/sigma_2;       /* The initial delta value under */
end;                                      /* adjust method.                */
else if method=0 then do;
to=k*sqrt(n);
delta=z1mb*sqrt(n);       /* the initial delta value under noadjust method */
end;
delta1=delta;
tol=0.000001;
stepsize=.00001;
j=1;
p=cdf('t',to,f,delta);
p1=p;

do until ((abs(p-gamma)<tol) or (j=10000000));
delta=delta-stepsize;
p=cdf('t',to,f,delta);
j=j+1;
end;
```

```
if method=1 then do;
z1mb=(delta*sigma_2)/(sigma_g*sqrt(n));
end;
else if method=0 then do;
z1mb=delta/sqrt(n);
end;
beta=cdf('normal',z1mb);                                   /* content level */
run;

proc print noobs width=full;
var p1 p delta1 delta z1 z1mb;
var sigma_g sigma_2 f to k j;
var gamma beta method;
run;

quit
```

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