U.S. DEPARTMENT OF ENERGY

PNNL-22033
WTP-RPT-226, Rev 0

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

Methods for Quantifying the Uncertainties of LSIT Test Parameters, Test Results, and Full-Scale Mixing Performance Using Models Developed from Scaled Test Data

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May 2015

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UNITED STATES DEPARTMENT OF ENERGY
under Contract DE-AC05-76RL01830

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(8/2010)

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Test Specification:	N/A
Work Authorization:	WA# 039
Test Plan:	TP-WTPSP-027
Test Exceptions:	N/A
PETD Focus Area:	Pretreatment
Test Scoping Statement(s):	N/A
QA Technology Level:	Basic Research

Prepared for
the U.S. Department of Energy
under Contract DE-AC05-76RL01830

Pacific Northwest National Laboratory
Richland, Washington 99352

Completeness of Testing

This report describes the results of work and testing specified by Test Plan TP-WTPSP-027 "Test Plan for PNNL Support of Large Scale Testing". The work and any associated testing followed the quality assurance requirements outlined in the test plan. The descriptions provided in this test report are an accurate account of both the conduct of the work and the data collected. Test plan results are reported. Also reported are any unusual or anomalous occurrences that are different from expected results. The test results and this report have been reviewed and verified.

Approved:

Reid A. Peterson, Manager
WTP R&T Support Project

5/8/15
Date

Executive Summary

Hanford's Waste Treatment and Immobilization Plant (WTP) project may predict the mixing performance of full-scale vessels based on tests that are planned to be conducted in the Large Scale Integrated Testing (LSIT) program using reduced-scale vessels, equipment, and facilities. This report discusses the statistical methods for quantifying uncertainties in

A) test responses and other parameters that would be measured or calculated in the LSIT

B) estimates of coefficients and predictions of mixing performance from models developed to relate test responses to test parameters.

Current plans for the LSIT involve testing pulse jet mixer (PJM) technology in three scaled vessels with nominal diameters of 43 in., 8 ft, and 14 ft. It is anticipated that LSIT testing would use several test responses to quantify mixing performance, including effective clearing radius (*ECR*), bottom-clearing velocity (U_{BC})[(1)], blending criteria, no solids accumulation during pump-out, and sampling requirements.

There may be practical restrictions on the order of performing LSIT tests over the three scales, including:

1. performing all tests for a given test vessel size (scale) before switching to a different test vessel size.

2. performing all tests with a given simulant for a given test vessel size before switching to a different simulant.

3. performing all tests with a given solids concentration for a given test vessel size and a given simulant before switching to a different solids concentration.

4. performing all tests with varying nozzle-jet velocities for a given combination of test vessel size, simulant, and solids concentration before switching to a different combination.

For example, restrictions 1–4 are expected to apply to *ECR* data and restrictions 1–3 are expected to apply to U_{BC} data from LSIT. Such restrictions on the order of performing tests complicate the error structure of the resulting test data. Specifically, there are $k + 1$ uncertainty components when there are k restrictions. Also, the restrictions cause subgroups of the test response values to be correlated. The complicated error structure must be accounted for in developing the (i) LSIT

(1) The minimum PJM nozzle-jet velocity required to achieve bottom motion of solids.

experimental design and (ii) models to predict mixing performance as a function of scale and other LSIT test parameters.

The LSIT experimental design (i.e., the test matrix, replicates, order of performing the tests) should be developed to support quantifying the uncertainties in A) and B) and reducing the uncertainties in B). Statistical experimental design methods guided by subject-matter knowledge provide for (i) distributing test parameter combinations (tests) over the test parameter space to provide optimal support for the model forms fitted to the test data, and (ii) determining the amount of replication needed at each level of restriction to estimate the $k + 1$ uncertainty components.

Section 3 discusses methods for quantifying the uncertainties in test responses and associated calculated parameters that account for the complicated data structure resulting from restrictions on the order of performing LSIT tests. Error propagation methods for calculating the uncertainty in a parameter expressed as a known function of other uncertain parameters are also presented.

Section 4 discusses the following methods for developing, and quantifying uncertainties in, models for mixing performance metrics expressed as functions of dimensional and/or dimensionless parameters.

- Methods to avoid models with spurious correlation, which can result in a model appearing to fit experimental data better than it actually does, are presented.

- The feasible generalized least squares (FGLS) methodology for fitting models to data with error structures resulting from restrictions on the order of performing tests is presented. FGLS formulas are presented for quantifying uncertainties in model coefficients and the uncertainty in model predictions of mixing performance.

- Methods are presented for evaluating how well a model fits the associated data and whether the uncertainties in model predictions are within the uncertainty of the data.

Section 5 presents example applications and discussions of the methods for quantifying uncertainties discussed in Sections 3 and 4. For the examples in Section 5, it is assumed that the $k + 1$ uncertainty components for a given mixing performance metric have a multiplicative structure, which is converted to an additive structure by taking natural logarithms (ln). This yields the formulas for the uncertainties (standard deviations, SD) in the ECR and U_{BC} test

responses:

$$SD_{Total}^{\ln(ECR)} = [(SD_{Scale}^{\ln(ECR)})^2 + (SD_{Simulant}^{\ln(ECR)})^2 + (SD_{SolidsConc}^{\ln(ECR)}) + (SD_{NozzleVel}^{\ln(ECR)})^2 + (SD_{Error}^{\ln(ECR)})^2]^{0.5} \quad \text{(S.1)}$$

$$SD_{Total}^{\ln(U_{BC})} = [(SD_{Scale}^{\ln(U_{BC})})^2 + (SD_{Simulant}^{\ln(U_{BC})})^2 + (SD_{SolidsConc}^{\ln(U_{BC})}) + (SD_{Error}^{\ln(U_{BC})})^2]^{0.5}, \quad \text{(S.2)}$$

where the *Scale*, *Simulant*, *SolidsConc* and *NozzleVel* subscripts correspond to the uncertainty components associated with the restrictions 1–4 (for *ECR*) and 1–3 (for U_{BC}). The *Error* subscript refers to the uncertainties within test combinations of all other test parameters. If the original data structure is additive rather than multiplicative, the formulas in Equations (S.1) and (S.2) are the same, except that the natural logarithms of *ECR* and U_{BC} would not be taken. Example calculations with Equations (S.1) and (S.2) are provided in Section 5. Section 5 also contains an example of applying the error propagation methods from Section 3 to calculate the uncertainty in the estimated PJM nozzle velocity based on uncertainties of the input parameters in the calculation equation.

Section 5 also includes discussion and examples of the methods for quantifying uncertainties in model coefficients and predictions for mixing performance metrics (presented in Section 4). An example model for U_{BC} (developed to avoid spurious correlation, see Appendix B) used in Section 5 is

$$U_{BC} = c_{WTP} D^{c_D} \phi_S^{c_\phi} u_S^{c_u} (u_* \phi_0)^{c_*} \quad \text{(S.3)}$$

where D = diameter of the scaled test vessel, ϕ_S = volume fraction of solids in the vessel, u_S = nominal settling velocity of the particles as they settle on to the floor of the vessel, u_* and ϕ_0 = material properties of the layer of settled solids, and c_{WTP}, c_D, c_ϕ, c_u, and c_* are coefficients to be estimated by fitting the model to experimental data. Assuming a multiplicative data structure for Equation (S.3) and taking the natural logarithm of both sides yields

$$\ln(U_{BC}) = ln(c_{WTP}) + c_D \ln(D) + c_\phi \ln(\phi_S) + c_u \ln(u_S) + c_* \ln(u_* \phi_0) \quad \text{(S.4)}$$

where all notation is as previously defined. Assuming that the experimental design would be subject to restrictions 1–3 on the order of performing tests, the model term(s) in Equation (S.4) associated with the three uncertainty components are: Scale [ln(*D*)], Simulant [$\ln(u_S)$, $\ln(u_* \phi)$], and Solids Concentration [$\ln(\phi_S)$]. Section 5.2.4 contains discussion and examples of the methods in Section 4.3.4 for quantifying uncertainties in model predictions of mixing performance.

In summary, LSIT testing is currently planned to be performed in three scaled test vessels, with the order of performing the tests expected to be subject to several restrictions. Such restrictions result in a complicated uncertainty structure for the data. The experimental design for LSIT must be constructed to adequately "cover" the test parameter space (in dimensional and/or nondimensional parameter space) so as to provide support for fitting the model forms hypothesized. The experimental design must also include sufficient replication at each level of restriction to provide for quantifying the associated variance components. Then, statistical methods can be applied to fit the physically based models to the experimental data, and to evaluate the data for outliers and the models for adequate fits. Initially hypothesized model forms may be revised based on model evaluation methods. When final fitted versions of physically based models are obtained that fit the data within its uncertainty, they can then be used to predict mixing performance for full-scale vessels. Statistical methods for quantifying uncertainties of model predictions can be applied to attach uncertainties to predicted values of the mixing performance metrics.

Quality Requirements

The quality requirements for this report, as established in Test Plan TP-WTPSP-027[(1)], are described in this section.

The Pacific Northwest National Laboratory (PNNL) Quality Assurance Program is based on the requirements as defined in the U.S. Department of Energy Order 414.1D, Quality Assurance (DOE 2011), and 10 CFR 830, Energy/Nuclear Safety Management, Subpart A – Quality Assurance Requirements (10 CFR 830, 2011), a.k.a., the "Quality Rule." PNNL has chosen to implement the following consensus standards in a graded approach:

- American Society of Mechanical Engineers (ASME) NQA-1-2000, Quality Assurance Requirements for Nuclear Facility Applications, Part 1, Requirements for Quality Assurance Programs for Nuclear Facilities
- ASME NQA-1-2000, Part II, Subpart 2.7, Quality Assurance Requirements for Computer Software for Nuclear Facility Applications
- ASME NQA-1-2000, Part IV, Subpart 4.2, Graded Approach Application of Quality Assurance Requirements for Research and Development.

The quality assurance plan for the Waste Treatment Plant Support Project (WTPSP) implements the requirements of ASME NQA-1-2000, Part 1: Requirements for Quality Assurance Programs for Nuclear Facilities, presented in two parts. Part 1 of the Quality

(1) Minette M. 2011. *Test Plan for PNNL Support of Large Scale Testing*. TP-WTPSP-027 Rev. 0, WTP Support Program at Pacific Northwest National Laboratory, Richland, Washington.

Assurance Manual describes the graded approach developed by applying ASME NQA-1-2000, Subpart 4.2, Guidance on Graded Application of Quality Assurance (QA) for Nuclear-Related Research and Development to the requirements based on the type of work scope the WTPSP is facing. Part 2 of the QA Manual lists all of the ASME NQA-1-2000 requirements that the project is implementing for the different technology levels of research and development (R&D) work. Requirements are clearly listed for the technology level to which they apply.

The *Waste Treatment Plant Support Project Quality Assurance Manual* (QA-WTPSP-0002) describes the technology life cycle stages under the *Waste Treatment Plant Support Program Quality Assurance Plan* (QA-WTPSP-0001). The technology life cycle includes the progression of technology development, commercialization, and retirement in process phases of basic and applied R&D, engineering and production, and operation until process completion. The life cycle is characterized by flexible and informal quality assurance activities in basic research, which becomes more structured and formalized through the applied R&D stages:

- BASIC RESEARCH – Basic research consists of research tasks that are conducted to acquire and disseminate new scientific knowledge. During basic research, maximum flexibility is desired in order to allow the researcher the necessary latitude to conduct the research.

- APPLIED RESEARCH – Applied research consists of research tasks that acquire data and documentation necessary to provide satisfactory reproducibility of results. The emphasis during this stage of a research task is on achieving adequate documentation and controls necessary to be able to reproduce results.

- DEVELOPMENT WORK – Development work consists of research tasks moving toward technology commercialization. These tasks still require a degree of flexibility, and there is still a degree of uncertainty that exists in many cases. The role of quality in development work is to make sure that adequate controls to support movement into commercialization exist.

- RESEARCH AND DEVELOPMENT SUPPORT ACTIVITIES – Support activities are those that are conventional and secondary in nature to the advancement of knowledge or development of technology, but allow the primary purpose of the work to be accomplished in a credible manner. An example of a support activity is controlling and maintaining documents and records. The level of quality for these activities is the same as for development work.

This work was performed at the Basic Research technology level, though many of the recommendations in this report are likely to require further research to establish specific approaches for quantifying uncertainties as the LSIT work is further planned.

Acronyms and Abbreviations

APV	application prediction variance
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
CFR	Code of Federal Regulations
DF	degrees of freedom
DOE	U.S. Department of Energy
ECR	effective clearing radius
FGLS	feasible generalized least squares
FPV	fitting prediction variance
GLS	generalized least squares
ln	natural logarithm
LOF	lack of fit
LSIT	Large Scale Integrated Testing
NLS	nonlinear least squares
OED	optimal experimental design
OLS	ordinary least squares
%RSD	percent relative standard deviation
PJM	pulse jet mixer
PNNL	Pacific Northwest National Laboratory
QA	Quality Assurance

R&D	research and development
REML	restricted maximum likelihood
RSD	relative standard deviation
SD	standard deviation
TPSD	total prediction standard deviation
WP	whole plot
WTP	Hanford Waste Treatment and Immobilization Plant
WTPSP	Waste Treatment Plant Support Project

Symbols

APV	application prediction variance
B	constant bias regardless of the k^{th} replicate of the j^{th} test in the i^{th} performance of the complete test matrix (or a subset thereof)
c_0, c_r, c_H, c_S, c_θ	coefficients to be estimated by fitting an example model for $\sqrt{K_{BC}}$ to data
c_D, c_ϕ, c_*, c_u, c_{WTP}	coefficients of example U_{BC} model
COV_{ij}, COV_{ji}	covariance of the ith and jth values of a given test response
D	diameter of the scaled test vessel
D_n	nozzle diameter of a PJM tube
D_{PI}	inner diameter of a PJM tube
D_{PR}	diameter of a Drexelbrook probe rod
d_J	diameter of the PJM nozzle
d_S	nominal diameter of the particles forming the settled solids
ECR	effective clearing radius
$ECR_{ha,ib,jc,kd,e}$	e^{th} replicate measurement of ECR for the d^{th} replicate of the k^{th} nozzle velocity for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale
$E(y_{ij})$	statistical expectation of y_{ij}
$E(\bar{y}_i)$	statistical expectation of $\bar{y}_i$
$\mathrm{E}[R(X_1,\cdots,X_n)\big\|_{x_1,\cdots,x_n}]$	statistical expectation of a function R of input parameters $X_1, X_2, \cdots, X_n$ evaluated at the values $x_1, x_2, \cdots, x_n$

$FPV_{Individual}$	fitting prediction variance when the model prediction is considered as an individual value from one test at a given set of test conditions
FPV_{Mean}	fitting prediction variance when the model prediction is considered as the mean value over a conceptually large number of tests at a given set of test conditions
H	distance from the PJM nozzle to the vessel floor
h_s	PJM stroke length
$\mathbf{I}_n$	$n \times n$ identity matrix with 1's on the diagonal and 0's elsewhere
K	constant to convert inches to meters (1/39.37 m/inch)
K_{BC}	minimum kinematic momentum flow from the PJM that clears the settled solids (termed the "bottom clearing" condition)
M	number of sets of test conditions in a test matrix
n	number of test response values
n_i	number of replicate measurements of a test response at the i^{th} set of test conditions and during the specific data collection period
N_J	number of PJMs in a vessel
NozzleVel_k^{ECR}	effect of the k^{th} nozzle velocity on *ECR*
%RSD	percent relative standard deviation
$\%RSD_{LT}$	long-term percent relative standard deviation
$\%RSD_{ST}$	short-term percent relative standard deviation
$\%RSD_{ST+LT}$	total (long-term and short-term) percent relative standard deviation
$\%RSD_{Error}^{ECR}$	percent relative standard deviation of the distribution of multiplicative random errors $\varepsilon_{ha,ib,jc,kd,e}^{ECR}$ associated with determinations of *ECR* at given settings of all other test parameters

$\%RSD^{ECR}_{NozzleVel}$	percent relative standard deviation of the distribution of multiplicative random errors $\tau^{ECR}_{ha,ib,jc,kd}$ in *ECR*, corresponding to the restriction (on the order of performing tests) associated with nozzle velocity
$\%RSD^{ECR}_{Scale}$	percent relative standard deviation of the distribution of multiplicative random errors δ^{ECR}_{ha} in *ECR*, corresponding to the restriction (on the order of performing tests) associated with scale
$\%RSD^{ECR}_{Simulant}$	percent relative standard deviation of the distribution of multiplicative random errors $\gamma^{ECR}_{ha,ib}$ in *ECR*, corresponding to the restriction (on the order of performing tests) associated with simulant
$\%RSD^{ECR}_{SolidsConc}$	percent relative standard deviation of the distribution of multiplicative random errors $\lambda^{ECR}_{ha,ib,ic}$ in *ECR*, corresponding to the restriction (on the order of performing tests) associated with solids concentration
$\%RSD^{ECR}_{Total}$	percent relative standard deviation of total uncertainty in *ECR*, calculated using the root mean squared error of the percent relative standard deviations $\%RSD^{ECR}_{Scale}$, $\%RSD^{ECR}_{Simulant}$, $\%RSD^{ECR}_{SolidsConc}$, $\%RSD^{ECR}_{NozzleVel}$, and $\%RSD^{ECR}_{Error}$ corresponding to the multiplicative random errors in *ECR*
$\%RSD^{U_{BC}}_{Error}$	percent relative standard deviation of the distribution of multiplicative random errors $\varepsilon^{U_{BC}}_{ha,ib,jc,e}$, associated with determinations of U_{BC} at given settings of all other test parameters
$\%RSD^{U_{BC}}_{Scale}$	percent relative standard deviation of the distribution of multiplicative random errors $\delta^{U_{BC}}_{ha}$ in U_{BC}, corresponding to the restriction (on the order of performing tests) associated with scale

$\%RSD^{U_{BC}}_{Simulant}$	percent relative standard deviation of the distribution of multiplicative random errors $\gamma^{U_{BC}}_{ha,ib}$ in U_{BC}, corresponding to the restriction (on the order of performing tests) associated with simulant
$\%RSD^{U_{BC}}_{SolidsConc}$	percent relative standard deviation of the distribution of multiplicative random errors $\lambda^{U_{BC}}_{ha,ib,ic}$ in U_{BC}, corresponding to the restriction (on the order of performing tests) associated with solids concentration
$\%RSD^{U_{BC}}_{Total}$	percent relative standard deviation of total uncertainty in U_{BC}, calculated using the root mean squared error of the percent relative standard deviations $\%RSD^{U_{BC}}_{Scale}$, $\%RSD^{U_{BC}}_{Simulant}$, $\%RSD^{U_{BC}}_{SolidsConc}$, and $\%RSD^{U_{BC}}_{Error}$ corresponding to the multiplicative random errors in U_{BC}
$\%RSD^{Y}_{Error}$	percent relative standard deviation of the distribution of additive random errors in test response Y (e.g., ECR or U_{BC}), associated with determinations of Y at given settings of all other test parameters
$\%RSD^{\mathrm{Y}}_{\mathrm{NozzleVel}}$	percent relative standard deviation of the distribution of additive random errors $\tau^{Y}_{ha,ib,jc,kd}$ in test response Y (e.g., ECR), corresponding to the restriction (on the order of performing tests) associated with nozzle velocity
$\%RSD^{Y}_{Scale}$	percent relative standard deviation of the distribution of additive random errors δ^{Y}_{ha} in test response Y (e.g., ECR or U_{BC}), corresponding to the restriction (on the order of performing tests) associated with scale
$\%RSD^{Y}_{Simulant}$	percent relative standard deviation of the distribution of additive random errors $\gamma^{Y}_{ha,ib}$ in test response Y (e.g., ECR or U_{BC}), corresponding to the restriction (on the order of performing tests) associated with simulant

$\%RSD^{Y}_{SolidsConc}$	percent relative standard deviation of the distribution of additive random errors $\lambda^{Y}_{ha,ib,ic}$ in test response Y (e.g., ECR or U_{BC}), corresponding to the restriction (on the order of performing tests) associated with solids concentration
$\%RSD^{Y}_{Total}$	total percent relative standard deviation that accounts for all of the variance components associated with the structure of the data set for test response Y (e.g., $Y = ECR$ or U_{BC})
P	$n \times c$ matrix with i^{th} row equal to $\mathbf{p_i}$, where $\mathbf{p}_i$ is an indicator vector with a 1 in the k^{th} position if the i^{th} run involves the k^{th} simulant (within a scale) or a 0 otherwise. Also, n is the number of test runs in the test matrix and c is the number of distinct simulants.
Q	$n \times d$ matrix with ith row equal to $\mathbf{q_i}$, where $\mathbf{q}_i$ is an indicator vector with a 1 in the k^{th} position if the i^{th} run involves the k^{th} solids concentration (within a scale and simulant) or a 0 otherwise. Also, n is the number of test runs in the test matrix and c is the number of distinct solids concentrations.
R	$n \times e$ matrix with i^{th} row equal to $\mathbf{r_i}$, where $\mathbf{r}_i$ is an indicator vector with a 1 in the k^{th} position if the i^{th} run involves the k^{th} nozzle velocity (within a scale, simulant, and solids concentration) or a 0 otherwise. Also, n is the number of test runs in the test matrix and e is the number of distinct nozzle velocities.
R	output parameter that is expressed as a function of input parameters $X_1, X_2, \cdots, X_n$; that is, $R = R(X_1, X_2, \cdots, X_n)$
r	radius from the centerline of the PJM out to the collision of the radial wall jet with those from surrounding PJMs
$RSD(y)$	relative standard deviation of y
s_i^2	sample variance of n replicate measurements y_{ij}, $j = 1, 2, \ldots, n$
s^2	pooled sample variance to estimate $\sigma_Y^2 = \sigma_{Y_1}^2 = \sigma_{Y_2}^2 = \ldots = \sigma_{Y_K}^2$

$Scale_h^{ECR}$	effect of the h^{th} scale on ECR
$Scale_h^{U_{BC}}$	effect of the h^{th} scale on U_{BC}
$SD[\ln(y)]$	standard deviation of the natural logarithm of y
SD_{LT}	long-term standard deviation
SD_{ST}	short-term standard deviation
SD_{ST+LT}	total (long-term and short-term) standard deviation
SD_{Error}^{ECR}	standard deviation of the distribution of additive random errors $\varepsilon_{ha,ib,jc,kd,e}^{ECR}$ associated with determinations of ECR at given settings of all other test parameters
$SD_{NozzleVel}^{ECR}$	standard deviation of the distribution of additive random errors $\tau_{ha,ib,jc,kd}^{ECR}$ in ECR, corresponding to the restriction (on the order of performing tests) associated with nozzle velocity
SD_{Scale}^{ECR}	standard deviation of the distribution of additive random errors δ_{ha}^{ECR} in ECR, corresponding to the restriction (on the order of performing tests) associated with scale
$SD_{Simulant}^{ECR}$	standard deviation of the distribution of additive random errors $\gamma_{ha,ib}^{ECR}$ in ECR, corresponding to the restriction (on the order of performing tests) associated with simulant
$SD_{Simulant}^{\ln(ECR)}$	standard deviation of the distribution of additive random errors $\gamma_{ha,ib}^{ln(ECR)}$ in $\ln(ECR)$, corresponding to the restriction (on the order of performing tests) associated with simulant
$SD_{SolidsConc}^{ECR}$	standard deviation of the distribution of additive random errors $\lambda_{ha,ib,ic}^{ECR}$ in ECR, corresponding to the restriction (on the order of performing tests) associated with solids concentration

SD_{Total}^{ECR} standard deviation of total uncertainty in *ECR*, calculated using the root mean squared error of the standard deviations SD_{Scale}^{ECR}, $SD_{Simulant}^{ECR}$, $SD_{SolidsConc}^{ECR}$, $SD_{NozzleVel}^{ECR}$, and SD_{Error}^{ECR} corresponding to the additive random errors in *ECR*

$SD_{Error}^{\ln(ECR)}$ standard deviation of the distribution of additive random errors $\varepsilon_{ha,ib,jc,kd,e}^{ln(ECR)}$ associated with determinations of ln(*ECR*) at given settings of all other test parameters

$SD_{NozzleVel}^{\ln(ECR)}$ standard deviation of the distribution of additive random errors $\tau_{ha,ib,jc,kd}^{ln(ECR)}$ in ln(*ECR*), corresponding to the restriction (on the order of performing tests) associated with nozzle velocity

$SD_{Scale}^{\ln(ECR)}$ standard deviation of the distribution of additive random errors $\delta_{ha}^{ln(ECR)}$ in ln(*ECR*), corresponding to the restriction (on the order of performing tests) associated with scale

$SD_{SolidsConc}^{\ln(ECR)}$ standard deviation of the distribution of additive random errors $\lambda_{ha,ib,ic}^{ln(ECR)}$ in ln(*ECR*), corresponding to the restriction (on the order of performing tests) associated with solids concentration

$SD_{Total}^{ln(ECR)}$ standard deviation of total uncertainty in ln(*ECR*), calculated using the root mean squared error of the standard deviations $SD_{Scale}^{ln(ECR)}$, $SD_{Simulant}^{ln(ECR)}$, $SD_{SolidsConc}^{ln(ECR)}$, $SD_{NozzleVel}^{ln(ECR)}$, and $SD_{Error}^{ln(ECR)}$ corresponding to the additive random errors in ln(*ECR*)

$SD_{Error}^{U_{BC}}$ standard deviation of the distribution of additive random errors $\varepsilon_{ha,ib,jc,e}^{U_{BC}}$ in U_{BC}, associated with determinations of U_{BC} at given settings of all other test parameters

$SD_{Scale}^{U_{BC}}$ standard deviation of the distribution of additive random errors $\delta_{ha}^{U_{BC}}$ in U_{BC}, corresponding to the restriction (on the order of performing tests) associated with scale

$SD^{U_{BC}}_{Simulant}$ standard deviation of the distribution of additive random errors $\gamma^{U_{BC}}_{ha,ib}$ in U_{BC}, corresponding to the restriction (on the order of performing tests) associated with simulant

$SD^{U_{BC}}_{SolidsConc}$ standard deviation of the distribution of additive random errors $\lambda^{U_{BC}}_{ha,ib,ic}$ in U_{BC}, corresponding to the restriction (on the order of performing tests) associated with solids concentration

$SD^{\ln(U_{BC})}_{SolidsConc}$ standard deviation of the distribution of additive random errors $\lambda^{ln(U_{BC})}_{ha,ib,ic}$ in $\ln(U_{BC})$, corresponding to the restriction (on the order of performing tests) associated with solids concentration

$SD^{U_{BC}}_{Total}$ standard deviation of total uncertainty in U_{BC}, calculated using the root mean squared error of the standard deviations $SD^{U_{BC}}_{Scale}$, $SD^{U_{BC}}_{Simulant}$, $SD^{U_{BC}}_{SolidsConc}$, and $SD^{U_{BC}}_{Error}$ corresponding to the additive random errors in U_{BC}

$SD^{\ln(U_{BC})}_{Error}$ standard deviation of the distribution of additive random errors $\varepsilon^{ln(U_{BC})}_{ha,ib,jc,e}$ in $\ln(U_{BC})$, associated with determinations of U_{BC} at given settings of all other test parameters

$SD^{\ln(U_{BC})}_{Scale}$ standard deviation of the distribution of additive random errors $\delta^{ln(U_{BC})}_{ha}$ in $\ln(U_{BC})$, corresponding to the restriction (on the order of performing tests) associated with scale

$SD^{\ln(U_{BC})}_{Simulant}$ standard deviation of the distribution of additive random errors $\gamma^{ln(U_{BC})}_{ha,ib}$ in $\ln(U_{BC})$, corresponding to the restriction (on the order of performing tests) associated with simulant

$SD^{ln(U_{BC})}_{Total}$ standard deviation of total uncertainty in U_{BC}, calculated using the root mean squared error of the standard deviations $SD^{ln(U_{BC})}_{Scale}$, $SD^{ln(U_{BC})}_{Simulant}$, $SD^{ln(U_{BC})}_{SolidsConc}$, and $SD^{ln(U_{BC})}_{Error}$ corresponding to the additive random errors in $\ln(U_{BC})$

$SD_{Error}^{\ln(Y)}$ standard deviation of the distribution of additive random errors in the natural logarithm of test response Y (e.g., ECR or U_{BC}), associated with determinations of Y at given settings of all other test parameters

$SD_{\text{NozzleVel}}^{\ln(Y)}$ standard deviation of the distribution of additive random errors in the natural logarithm of test response Y (e.g., ECR), corresponding to the restriction (on the order of performing tests) associated with nozzle velocity

$SD_{Scale}^{\ln(Y)}$ standard deviation of the distribution of additive random errors in the natural logarithm of test response Y (e.g., ECR or U_{BC}), corresponding to the restriction (on the order of performing tests) associated with scale

$SD_{Simulant}^{\ln(Y)}$ standard deviation of the distribution of additive random errors in the natural logarithm of test response Y (e.g., ECR or U_{BC}), corresponding to the restriction (on the order of performing tests) associated with simulant

$SD_{SolidsConc}^{\ln(Y)}$ standard deviation of the distribution of additive random errors $\lambda_{ha,ib,ic}^{Y}$ in test response Y (e.g., ECR or U_{BC}), corresponding to the restriction (on the order of performing tests) associated with solids concentration

SD_{Error}^{Y} standard deviation of the distribution of additive random errors in test response Y (e.g., ECR), associated with determinations of Y at given settings of all other test parameters

$SD_{\text{NozzleVel}}^{\text{Y}}$ standard deviation of the distribution of additive random errors $\tau_{ha,ib,jc,kd}^{Y}$ in test response Y (e.g., ECR), corresponding to the restriction (on the order of performing tests) associated with nozzle velocity

SD_{Scale}^{Y} standard deviation of the distribution of additive random errors δ_{ha}^{Y} in test response Y (e.g., ECR or U_{BC}), corresponding to the restriction (on the order of performing tests) associated with scale

$SD^{Y}_{Simulant}$	standard deviation of the distribution of additive random errors $\gamma^{Y}_{ha,ib}$ in test response Y (e.g., ECR or U_{BC}), corresponding to the restriction (on the order of performing tests) associated with simulant
$SD^{Y}_{SolidsConc}$	standard deviation of the distribution of additive random errors $\lambda^{Y}_{ha,ib,ic}$ in test response Y (e.g., ECR or U_{BC}), corresponding to the restriction (on the order of performing tests) associated with solids concentration
SD^{Y}_{Total}	total standard deviation that accounts for all of the variance components associated with the structure of the data set for test response Y (e.g., $Y = ECR$ or U_{BC})
$Simulant_i^{ECR}$	effect of the i^{th} simulant on ECR
$Simulant_i^{U_{BC}}$	effect of the i^{th} simulant on U_{BC}
$SolidsConc_j^{ECR}$	effect of the j^{th} solids concentration on ECR
$SolidsConc_j^{U_{BC}}$	effect of the j^{th} solids concentration on U_{BC}
t_C	cycle time
T_d	drive time of the duty cycle for a pulse
t_D	time available for the PJM momentum to clear the settled solids
t_S	time during which particles settle
$TPSD_{Individual}$	total prediction standard deviation, formed as the square root of the sum of $FPV_{Individual}$ and APV
$TPSD_{Mean}$	total prediction standard deviation, formed as the square root of the sum of FPV_{Mean} and APV
u_S	nominal settling velocity of the particles as they settle on to the floor of the vessel

u_*	material property of the layer of settled solids in a vessel
U	PJM nozzle velocity
U_{BC}	minimum PJM nozzle-jet velocity required to achieve bottom clearing
$(U_{BC})_{ha,ib,jc,e}$	e^{th} replicate measurement of U_{BC} for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale
V_1	estimated PJM nozzle velocity
$V(y_{ij})$	variance of y_{ij}
$V(\bar{y}_i)$	variance of $\bar{y}_i$
$\hat{V}(\bar{y}_i)$	estimate of the variance of $\bar{y}_i$
$\text{Var}(\hat{\boldsymbol{\beta}}_{\text{FGLS}})$	variance-covariance matrix of the coefficient vector estimated by feasible generalized least squares
$\mathbf{V}$	true, unknown $n \times n$ variance-covariance matrix for data from LSIT for a given test response
$\mathbf{V}_{\text{ECR}}$	true, unknown $n \times n$ variance-covariance matrix for ECR data from LSIT assuming the data structure discussed in Section 2.3
$\hat{\mathbf{V}}$	estimated $n \times n$ variance-covariance matrix for data from LSIT for a given test response
$\mathbf{W}$	$p \times p$ variance-covariance matrix of the vector $\mathbf{x}$, expanded in the form of the model
$\bar{x}_i$	estimate of the long-term mean of the test response for the i^{th} row of a test matrix
$X_1, X_2, \cdots, X_n$	input parameters that are related to a different parameter through a known functional relationship

$x_1, x_2, \cdots, x_n$	specific values of $X_1, X_2, \cdots, X_n$
$\mathbf{x}$	$p \times 1$ vector formed by expanding the model parameters in the form of the terms in the model
$\mathbf{x}'$	$1 \times p$ vector (the vector transpose of $\mathbf{x}$) formed by expanding the model parameters in the form of the terms in the model
$\mathbf{X}$	$n \times p$ matrix formed by expanding the test matrix so that the columns of $\mathbf{X}$ correspond to the p terms in the model
Y	test response
Y_i	test response for the i^{th} combination of experimental conditions during a specific data collection period
$y_{i1}, y_{i2}, \cdots, y_{in}$	a set of n replicate measurements of Y_i obtained under the i^{th} set of test conditions and during the specific data collection period
$\mathbf{Z}$	$n \times b$ matrix with i^{th} row equal to $\mathbf{z_i}$, where $\mathbf{z}_i$ is an indicator vector with a 1 in the k^{th} position if the i^{th} run belongs to the k^{th} scale and zero otherwise. Also, n is the number of test runs in the test matrix and b is the number of distinct scaled test vessels.
y_{ij}	the j^{th} replicate measured value of a test response Y_i for the i^{th} combination of experimental conditions during a specific data collection period
y_{ijk}	measured test response for the k^{th} replicate of the j^{th} test in the i^{th} performance of the complete test matrix (or a subset thereof)
$\bar{y}_i$	sample mean of n replicate measurements y_{ij}, $j = 1, 2, \ldots, n$
$\mathbf{y}$	$n \times 1$ vector of test response values
$\hat{y}(\mathbf{x})$	model-predicted value of the mixing performance metric y at the expanded vector of model parameters $\mathbf{x}$

Greek Symbols

$\boldsymbol{\beta}$	$p \times 1$ vector of true, unknown model coefficients
$\hat{\boldsymbol{\beta}}_{\text{FGLS}}$	$p \times 1$ vector of model coefficients estimated using feasible generalized least squares
$\gamma_{ha,ib}^{ECR}$	random error in *ECR* for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale
$\gamma_{ha,ib}^{U_{BC}}$	random error in U_{BC} for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale
δ_t	longer-term random error, which is constant for all tests j and replicates k in the i^{th} performance of the complete test matrix (or a subset thereof), but varies randomly over different performances i
δ_{ha}^{ECR}	random error in *ECR* for the a^{th} replicate of the h^{th} scale
$\delta_{ha}^{U_{BC}}$	random error in U_{BC} for the a^{th} replicate of the h^{th} scale
$\boldsymbol{\varepsilon}$	$n \times 1$ vector of random experimental/testing errors with variance-covariance matrix $\mathbf{V}$
ε_{ijk}	random error for the k^{th} replicate of the j^{th} test in the i^{th} performance of the complete test matrix (or a subset thereof)
$\varepsilon_{ha,ib,jc,kd,e}^{ECR}$	random error for the e^{th} replicate measurement of *ECR* for d^{th} replicate of the k^{th} nozzle velocity for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale
$\varepsilon_{ha,ib,jc,e}^{U_{BC}}$	random error for the e^{th} replicate measurement of U_{BC} for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale

$\lambda^{ECR}_{ha,ib,jc}$	random error in *ECR* for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale
$\lambda^{U_{BC}}_{ha,ib,jc}$	random error in U_{BC} for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale
μ_j	unknown long-term mean of a test response for the j^{th} test in a test matrix, which is assumed not to depend on the i^{th} performance of a complete test matrix (or a subset thereof) or on the k^{th} replicate of the j^{th} test
$\mu^{ECR}_{h,i,j,k}$	unknown mean *ECR* for the k^{th} nozzle velocity at the j^{th} solids concentration of the i^{th} simulant at the h^{th} scale
$\mu^{U_{BC}}_{h,i,j}$	true mean U_{BC} for the j^{th} solids concentration of the i^{th} simulant at the h^{th} scale
μ_{Y_i}	true mean of the distribution of y_{ij} values for the j^{th} replicate measured value of a test response Y_i for the i^{th} combination of experimental conditions during a specific data-collection period
μ_R	true, unknown mean of a function R of random variables
$\mu_{X_1}, \mu_{X_2}, \cdots, \mu_{X_n}$	means of input parameters $X_1, X_2, \cdots, X_n$
ϕ_0	solids volume fraction in vortices after entraining solids from vessel floor
ϕ_S	volume fraction of solids in the vessel
σ^2_{Error}	variance component associated with the random errors in the test response for a given set of values of all other test parameters
$\sigma^2_{NozzleVel}$	variance component of the test response corresponding to the restriction (on the order of performing tests) associated with nozzle velocity
σ^2_{Scale}	variance component of the test response corresponding to the restriction (on the order of performing tests) associated with the size of the scaled test vessel

$\sigma^2_{Simulant}$	variance component of the test response corresponding to the restriction (on the order of performing tests) associated with the simulant
$\sigma^2_{SolidsConc}$	variance component of the test response corresponding to the restriction (on the order of performing tests) associated with the solids concentration
$\hat{\sigma}^2_R$	estimate of the variance of a function R of input parameters $X_1, X_2, \cdots, X_n$
$\sigma^2_{X_1}, \sigma^2_{X_2}, \cdots, \sigma^2_{X_n}$	true variances of the input parameters $X_1, X_2, \cdots, X_n$
$\hat{\sigma}^2_{X_i}$	estimate of the variance for input parameter X_i
σ^2_Y	true variance of the test response Y
σ_{Y_i}, $\sigma^2_{Y_i}$	true standard deviation and variance of the distribution of y_{ij} values for the j^{th} replicate measured value of a test response Y_i for the i^{th} combination of experimental conditions during a specific data-collection period
$\tau^{ECR}_{ha,ib,jc,kd}$	random error in *ECR* for the d^{th} replicate of the k^{th} nozzle velocity for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale
θ_{X_i}	sensitivity coefficient for the input parameter X_i in for a function R of input parameters $X_1, X_2, \cdots, X_n$
θ_S	dimensionless group as defined in Eq. (B.2)

Contents

Tables

1.0 Introduction

This report discusses the statistical methods for quantifying uncertainties in 1) test responses and other parameters in the Large Scale Integrated Testing (LSIT), and 2) estimates of coefficients and predictions of mixing performance from models that relate test responses to test parameters. Testing at a larger scale has been committed to by Bechtel National Inc. and the U.S. Department of Energy (DOE) to "address uncertainties and increase confidence in the projected, full-scale mixing performance and operations"[(1)] in the Waste Treatment and Immobilization Plant (WTP).

1.1 Background and Organization of This Document

Current plans for the LSIT involve testing pulse jet mixer (PJM) technology in three scaled vessels, namely 43 in., 8 ft, and 14 ft. It is envisioned that LSIT would use several metrics to quantify mixing performance, including the effective clearing radius (*ECR*), the minimum PJM nozzle-jet velocity required to achieve bottom motion of solids (U_{BC}), blending criteria, no solids accumulation during pump-out, and sampling requirements. In this report, the discussion focuses on *ECR* and U_{BC}, but the methods can be applied or adapted to other metrics of mixing performance.

In LSIT work, it will be important to quantify the uncertainties of test responses and other parameters of interest. Test data could be used to develop models relating test responses (of mixing performance) to test parameters. Such models would enable predicting the mixing performance of parameter combinations not tested in LSIT, including extrapolations to full-scale WTP vessels. In such work, it is very important to reduce (to the extent possible) and quantify the 1) uncertainties of model coefficient estimates (which may be interpretable in physical models), and 2) predictions of mixing performance, including extrapolations to full scale.

Section 2 discusses the important role of the error structure in experimental data when quantifying uncertainties in the data and in models developed from the data. Possible error structures for two mixing performance test responses are presented and discussed. Section 3 discusses and illustrates the statistical methods that could be used to quantify uncertainties in test responses and other parameters associated with LSIT to assess mixing performance in the WTP. Section 4 discusses and illustrates the approach and methods that could be used to reduce and quantify uncertainties for predictions of full-scale mixing performance using models developed from scaled test data collected during LSIT. Section 5 presents and discusses applications of the

(1) Hazen H. September 2011. *Contract No. DE-AC27-01RV14136, Hanford Tank Waste Treatment and Immobilization Plant, Memorandum of agreement (MOA) 24590-QL-WA49-00001, - Directive subcontractor change notice No. 119 for WA39LSIT testing*, CCN237865, Bechtel National Inc., Richland, Washington.

methods from Sections 3 and 4 to an example LSIT situation. Section 6 summarizes the content of the report, while Section 7 lists the references cited in the report.

1.2 Quality Requirements

The quality requirements for this report were established in Test Plan TP-WTPSP-027[(1)]. The test plan requirements related to this report are described below.

The Pacific Northwest National Laboratory (PNNL) Quality Assurance Program is based on the requirements as defined in DOE Order 414.1D, Quality Assurance, and 10 CFR 830, Energy/Nuclear Safety Management, Subpart A - Quality Assurance Requirements (a.k.a., the "Quality Rule"). PNNL has chosen to implement the following consensus standards in a graded approach:

- American Society of Mechanical Engineers (ASME) NQA-1-2000, Quality Assurance Requirements for Nuclear Facility Applications, Part 1, Requirements for Quality Assurance Programs for Nuclear Facilities

- ASME NQA-1-2000, Part II, Subpart 2.7, Quality Assurance Requirements for Computer Software for Nuclear Facility Applications

- ASME NQA-1-2000, Part IV, Subpart 4.2, Graded Approach Application of Quality Assurance Requirements for Research and Development.

The quality assurance plan for the Waste Treatment Plant Support Project (WTPSP) implements the requirements of ASME NQA-1-2000, Part 1: Requirements for Quality Assurance Programs for Nuclear Facilities, presented in two parts. Part 1 of the Quality Assurance (QA) Manual describes the graded approach developed by applying ASME NQA-1-2000, Subpart 4.2, Guidance on Graded Application of Quality Assurance for Nuclear-Related Research and Development to the requirements based on the type of work scope the WTPSP is facing. Part 2 of the QA Manual lists all of the ASME NQA-1-2000 requirements that the project is implementing for the different technology levels of research and development (R&D) work. Requirements are clearly listed for the technology level to which they apply.

The *Waste Treatment Plant Support Project Quality Assurance Manual* (QA-WTPSP-0002) describes the technology life cycle stages under the *Waste Treatment Plant Support Program Quality Assurance Plan* (QA-WTPSP-0001). The technology life cycle includes the progression of technology development, commercialization, and retirement in process phases of basic and applied R&D, engineering and production, and operation until process completion. The life

(1) Minette M. 2011. *Test Plan for PNNL Support of Large Scale Testing*. TP-WTPSP-027, Rev 0, WTP Support Program at Pacific Northwest National Laboratory, Richland, Washington.

cycle is characterized by flexible and informal quality assurance activities in basic research, which becomes more structured and formalized through the applied R&D stages.

- BASIC RESEARCH – Basic research consists of research tasks that are conducted to acquire and disseminate new scientific knowledge. During basic research, maximum flexibility is desired to allow the researcher the necessary latitude to conduct the research.

- APPLIED RESEARCH – Applied research consists of research tasks that acquire data and documentation necessary to provide satisfactory reproducibility of results. The emphasis during this stage of a research task is on achieving adequate documentation and controls necessary to be able to reproduce results.

- DEVELOPMENT WORK – Development work consists of research tasks moving toward technology commercialization. These tasks still require a degree of flexibility, and there is still a degree of uncertainty that exists in many cases. The role of quality in development work is to make sure that adequate controls to support movement into commercialization exist.

- RESEARCH AND DEVELOPMENT SUPPORT ACTIVITIES – Support activities are conventional and secondary in nature to the advancement of knowledge or development of technology, but allow the primary purpose of the work to be accomplished in a credible manner. An example of a support activity is controlling and maintaining documents and records. The level of quality for these activities is the same as for development work.

The work undertaken in developing the report was performed at the Basic Research technology level, although many of the recommendations are likely to require further research to establish specific approaches for quantifying uncertainties as the LSIT work is further planned.

2.0 The Important Role of Error Structure in Experimental Data when Quantifying Uncertainties in Data and Models Developed from Data

Before discussing methods for quantifying uncertainties in

- test responses and other parameters from LSIT
- estimates of coefficients and predictions of mixing performance from models that relate test responses to test parameters

it is important to first discuss how the error structure of experimental data impacts quantifying these two kinds of uncertainties.

In this report, "test response" refers to a measured parameter, or a parameter calculated from one or more measured quantities, which represents mixing results from an LSIT test. Other parameters associated with LSIT testing may also be subject to uncertainty, such as parameters varied during testing whose values can only be measured or calculated with uncertainty. During LSIT, it is assumed there will be a test matrix (maybe more than one) that specifies the test runs to be performed. Test runs are the combinations of test parameters at which scaled mixing tests are to be performed and test response (e.g., mixing performance) data obtained.

Section 2.1 discusses the error structure that results when test runs of a test matrix are performed in a completely random order. Section 2.2 discusses the error structure that results when the test runs of a test matrix must be performed with restrictions on the order of testing. Restrictions of this kind are expected in the LSIT. The error structure when there are restrictions on the order of performing test matrix runs is much more complicated, and must be accounted for in 1) developing the test matrix, 2) quantifying the uncertainties of test responses, and 3) modeling the data and quantifying uncertainties of the model predictions. Sections 2.3 and 2.4 discuss possible error structures for two mixing performance metrics and provide the equations for the uncertainty [standard deviation (SD) or percent relative standard deviation (%RSD)] in test responses based on possible restrictions on the order of performing test matrix runs in the LSIT.

2.1 Error Structure of Test Response Data When the Test Runs are Performed in a Completely Randomized Order

Conducting the test runs comprising a test matrix in a completely randomized order generally provides the simplest error structure for the resulting test response data. Performing test runs in a completely randomized order protects against trend effects and the effects of uncontrolled

parameters being confounded with the effects of the test parameters of interest (Draper and Smith 1998; Montgomery et al. 2001).

Consider the following two statistical models for test data, where it is assumed that the test responses are directly measured

$$y_{ijk} = \mu_j + B + \delta_i + \varepsilon_{ijk} \tag{2.1}$$

$$y_{ijk} = \mu_j \times B \times \delta_i \times \varepsilon_{ijk} \tag{2.2}$$

where
- y_{ijk} = measured test response for the k^{th} replicate of the j^{th} test in the i^{th} performance of the complete test matrix (or a subset thereof)
- μ_j = unknown long-term mean of a test response for the j^{th} test in a test matrix (assumed not to depend on i or k)
- B = constant bias regardless of the values of i, j, or k
- δ_i = longer-term random error, which is constant for all tests j and replicates k in the i^{th} performance of the complete test matrix (or a subset thereof), but varies randomly over different performances i
- ε_{ijk} = random error for the k^{th} replicate of the j^{th} test in the i^{th} performance of the complete test matrix (or a subset thereof).

The difference between Equations (2.1) and (2.2) is whether the errors combine additively or multiplicatively. In general, additive errors are appropriate when the magnitudes of the errors do not depend on the magnitudes of test response values. On the other hand, multiplicative errors generally depend on the magnitudes of test response values. When values of a test response at different test conditions span more than a factor of 10, it is more likely that the magnitudes of errors are dependent on the magnitude of the test response. In such cases, multiplicative errors would be more likely to be appropriate. Performing a logarithmic transformation of both sides of Equation (2.2) converts the multiplicative structure to an additive structure.

When the test runs comprising the test matrix are performed in a completely randomized order, it is often reasonable to make the assumptions in Table 2.1. In that table, the SD_{LT}, SD_{ST}, $\%RSD_{LT}$, and $\%RSD_{ST}$ quantities are true, unknown values that must be estimated using data. Because the subsequent interest in this document is for estimates of those quantities, for simplicity the same notation is used to represent the estimates of the true, unknown quantities. Finally, the topic of bias estimation, assessment, and correction is not discussed further in this report, since it is presumed that materials with representative and certified mixing results do not exist.

Table 2.1. Assumptions for Test Runs Performed in Completely Randomized Order

Equation(s)	Assumption
(2.1)	The δ_i are independently and identically distributed with a normal (Gaussian) distribution having mean 0 and standard deviation SD_{LT} and that the ε_{ijk} are independently and identically distributed with a normal (Gaussian) distribution having mean zero and standard deviation SD_{ST}.[(a)]
(2.2)	The δ_i are independently and identically distributed with a normal (Gaussian) distribution having mean 1 and a percent relative standard deviation $\%RSD_{LT}$, and that the ε_{ijk} are independently and identically distributed with a normal (Gaussian) distribution having mean 1 and percent relative standard deviation $\%RSD_{ST}$.[(b)]
(2.1), (2.2)	In many cases the bias B may be negligible. However, if possible, certified standards should be measured along with tests to provide a basis for estimating the bias [e.g., B in Equations (2.1) and (2.2)], determining whether the estimate is statistically different from zero given the uncertainty of the estimate, and correcting for bias if it exists.

(a) LT = long-term and ST = short-term.
(b) %RSD = percent relative standard deviation = 100 (standard deviation)/mean.

The assumptions in Table 2.1 associated with performing test matrix runs in a completely randomized order provide for simple quantification of the random uncertainties in the test responses, as well as simple statistical data analyses. For example, the estimated combined SD and combined %RSD are given by

$$SD_{ST+LT} = (SD_{LT}^2 + SD_{ST}^2)^{0.5} \tag{2.3}$$

and

$$\%RSD_{ST+LT} = (\%RSD_{LT}^2 + \%RSD_{ST}^2)^{0.5} \tag{2.4}$$

for the cases of Equations (2.1) and (2.2), respectively.

In addition to the variances of the test response values, it is important to quantify the covariances of the i^{th} and jth test response values (COV_{ij}). The variances and covariances for a set of test response values $i = 1, 2, \ldots, n$ can be summarized as a variance-covariance matrix, denoted **V** (which is of dimension $n \times n$). The i^{th} diagonal element of **V** is the variance of the i^{th} test response value, while the entry in the i^{th} row and j^{th} column is the covariance of the i^{th} and j^{th} test response values. Note that a covariance matrix is always symmetric, since $COV_{ij} = COV_{ji}$.

Under the assumptions in Table 2.1, the variance-covariance matrix for the test response data resulting from a test matrix performed in a completely randomized order is diagonal (i.e., all off-diagonal entries are zero). For Equation (2.1), the estimated variance-covariance matrix is denoted by

$$\mathbf{V} = \begin{bmatrix} SD_{LT+ST}^2 & 0 & \ldots & 0 \\ 0 & SD_{LT+ST}^2 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & SD_{LT+ST}^2 \end{bmatrix} \tag{2.5}$$

For Equation (2.2), the estimated variance-covariance matrix is given by

$$\mathbf{V} = \begin{bmatrix} (\bar{x}_1 \%RSD_{LT+ST})^2 & 0 & \ldots & 0 \\ 0 & (\bar{x}_2 \%RSD_{LT+ST})^2 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & (\bar{x}_n \%RSD_{LT+ST})^2 \end{bmatrix} \tag{2.6}$$

where $\bar{x}_i$ denotes an estimate of the long-term mean of the test response for the i^{th} row of the test matrix (which contains n tests), and the other notation is as previously defined.

Variance-covariance matrices and statistical methods for analyzing experimental data are more complicated when errors are not independent and/or identically distributed. One more complicated method is discussed in Section 3, while others are discussed by Draper and Smith (1998), Myers and Montgomery (1995), and Montgomery et al. (2001). The more complicated methods should be applied as appropriate during uncertainty and data analyses of experimental results from LSIT.

The subscript "i" in Equations (2.1) and (2.2) assumes it is possible to perform a whole test matrix over one period of time, and then re-perform the test matrix (or a subset of the test runs in the test matrix) at one or more subsequent periods of time. Performing a whole test matrix (or a subset thereof) during subsequent periods of time is what provides data for quantifying SD_{LT} or $\%RSD_{LT}$. However, even if a test matrix is performed only once, the error structure given by Equations (2.1) or (2.2) still applies. In such cases, it is necessary to quantify the longer-term random uncertainty (i.e., SD_{LT} or $\%RSD_{LT}$) using data or information external to the testing results from performing the test matrix only once (e.g., previous testing results).

2.2 Experiments When There are Restrictions on the Order of Performing Test Matrix Runs

There are often cost, time, or other reasons why the test runs in a test matrix cannot be performed in a completely randomized order. Restrictions on randomization (i.e., restrictions on the order of performing tests) in a test matrix must be accounted for as part of developing the experimental design, as well as in analyzing and modeling the data from testing. The order of performing LSIT tests could have practical restrictions, which may include those listed in Table 2.2. There may be still other, or different, restrictions on the order of performing LSIT tests. For example, the PJM array in a scale vessel, the duty cycle, or other test parameters may also be varied with associated restrictions on the order of performing tests. However, the restrictions listed in Table 2.2 are sufficient to illustrate the concepts in this report.

Table 2.2. Possible Practical Restrictions on the Order of Performing LSIT Tests

Restriction Number	Restriction on the Order of Performing Tests
1	Performing all tests for a given test vessel size (scale) before switching to a different test vessel size
2	Performing all tests with a given simulant for a given test vessel size before switching to a different simulant
3	Performing all tests with a given solids concentration for a given test vessel size and a given simulant before switching to a different solids concentration
4	Performing all tests with varying nozzle-jet velocities for a given combination of test vessel size, simulant, and solids concentration before switching to a different combination

Each restriction on the order of performing tests creates an additional component of uncertainty (i.e., variance), and causes values of test responses within groups and subgroups of tests to be correlated (i.e., have nonzero covariances). Hence, data collected from experiments with restrictions on the order of performing tests have a more complicated variance-covariance matrix than when tests can be performed in a completely randomized order.

Experiments with restrictions on the order of performing tests (such as discussed previously) are called split-plot experiments because they were initially developed for agricultural experiments where plots of land were subdivided (split) with restrictions on the ways in which test matrix runs were conducted. However, split-plot experiments are now widely used in many areas of industrial and scientific experimentation (Steel and Torrie 1960; Montgomery et al.

2001; Goos et al. 2006; Kowalski et al. 2007). Instead of fields of land that are subdivided, split-plot experiments often involve investigating the effects of test parameters on test responses in iteratively subdivided periods of time corresponding to certain settings of test parameters. In such applications of split-plot experiments, it is not the restrictions on the order of performing tests and subdivided periods of time that are directly the issue. Rather, by not "starting over" and resetting values of test parameters for each test run in a test matrix, subgroups of data are affected systematically by random uncertainties, which causes subgroups of results to be correlated. In addition, restrictions on the order of performing tests increase the number of variance components. The number of variance components is one more than the number of restrictions (i.e., $k + 1$ if there are k restrictions).

The following Sections 2.3 and 2.4 present the statistical models and the structures of the variance-covariance matrices for split-plot experiments associated with two of the test responses to be investigated in LSIT:

- *ECR*: The effective clearing radius of a pulse jet for a given nozzle velocity. We assume that at least two nozzle velocities would be investigated. The split-plot experiment to measure *ECR* for each test matrix run and nozzle velocity value involves all four of the restrictions on the order of performing tests listed in Table 2.2.

- U_{BC}: The minimum nozzle velocity at which all particles are cleared from the bottom of the test vessel (U_{BC}), referred to as bottom-clearing velocity. This velocity could be determined experimentally for each test run by increasing nozzle velocity incrementally until 'bottom clearing' occurs. The split-plot experiment to measure U_{BC} for each test run involves only the first three of the restrictions on the order of performing tests listed in Table 2.2. The nozzle-jet velocities are not counted as a restriction because the test response (U_{BC}) is only a single velocity determined from the progression of nozzle velocities considered.

Hence, because *ECR* has four restrictions on the order of performing tests, there are five variance components that affect the total variance. Because U_{BC} has three restrictions on the order of performing tests, there are four variance components that affect the total variance. These are discussed in the following subsection.

2.3 *ECR* Error Structure and Uncertainties for the Anticipated Restrictions on the Order of Performing LSIT Tests

The statistical models for *ECR* corresponding to the anticipated structure of the LSIT experiments are given in the following equations, for the situations of additive and multiplicative structures of test parameter effects and errors.

ECR, Additive Structure

$$\begin{aligned} ECR_{ha,ib,jc,kd,e} = \mu^{ECR}_{h,i,j,k} &+ (Scale^{ECR}_{h} + \delta^{ECR}_{ha}) + (Simulant^{ECR}_{i} + \gamma^{ECR}_{ha,ib}) \\ &+ (SolidsConc^{ECR}_{j} + \lambda^{ECR}_{ha,ib,jc}) \\ &+ (NozzleVeloc^{ECR}_{k} + \tau^{ECR}_{ha,ib,jc,kd}) + \varepsilon^{ECR}_{ha,ib,jc,kd,e} \end{aligned} \tag{2.7}$$

ECR, Multiplicative Structure

$$\begin{aligned} ECR_{ha,ib,jc,kd,e} = \mu^{ECR}_{h,i,j,k} &\times (Scale^{ECR}_{h} \times \delta^{ECR}_{ha}) \times (Simulant^{ECR}_{i} \times \gamma^{ECR}_{ha,ib}) \\ &\times (SolidsConc^{ECR}_{j} \times \lambda^{ECR}_{ha,ib,jc}) \\ &\times (NozzleVel^{ECR}_{k} \times \tau^{ECR}_{ha,ib,jc,kd}) \times \varepsilon^{ECR}_{ha,ib,jc,kd,e} \end{aligned} \tag{2.8}$$

where $ECR_{ha,ib,jc,kd,e}$ = e^{th} replicate measurement of *ECR* for the d^{th} replicate of the k^{th} nozzle velocity for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale

$\mu^{ECR}_{h,i,j,k}$ = unknown mean *ECR* for the k^{th} nozzle velocity at the j^{th} solids concentration of the i^{th} simulant at the h^{th} scale

$Scale^{ECR}_{h}$ = effect of the h^{th} scale on *ECR*

δ^{ECR}_{ha} = random error in *ECR* for the a^{th} replicate of the h^{th} scale

$Simulant^{ECR}_{i}$ = effect of the i^{th} simulant on *ECR*

$\gamma^{ECR}_{ha,ib}$ = random error in *ECR* for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale

$SolidsConc^{ECR}_{j}$ = effect of the j^{th} solids concentration on *ECR*

$\lambda^{ECR}_{ha,ib,jc}$ = random error in *ECR* for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale

$\text{NozzleVel}^{ECR}_{k}$ = effect of the k^{th} nozzle velocity on *ECR*

$\tau^{ECR}_{ha,ib,jc,kd}$ = random error in *ECR* for the d^{th} replicate of the k^{th} nozzle velocity for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale

$\varepsilon^{ECR}_{ha,ib,jc,kd,e}$ = random error for the e^{th} replicate measurement of *ECR* for d^{th} replicate of the k^{th} nozzle velocity for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale.

The terms $Scale_h^{ECR}$, $Simulant_i^{ECR}$, $SolidsConc_j^{ECR}$, and $NozzleVel_k^{ECR}$ are general representations of the effects of those test parameters on *ECR*. Each one can be replaced with any applicable model term or terms. If a model is to include two-parameter interaction terms (to represent the effect of one parameter depending on the value of another parameter), then any such interaction term has as its error term the rightmost of the error terms [in Equation (2.7) or (2.8)] for the two parameters. For example, if a model for *ECR* were to include an interaction term between *SolidsConc* and *NozzleVel*, then that interaction would have the error term associated with *NozzleVel*.

Because the statistical models [Equations (2.7) and (2.8)] are already complicated enough, it was assumed that there is no possibility of a constant bias, so such a model term was not included in these *ECR* models as it was in Equations (2.1) and (2.2). Depending on the situation, performing a logarithmic transformation of both sides of Equation (2.8) may convert a multiplicative structure to an additive structure as in Equation (2.7). That approach is used for a U_{BC} example in Section 5.

For *ECR* data collected with the previous experimental structures, the assumptions in Table 2.3 are typically made to provide for statistical analyses of the experimental data. The assumptions in Table 2.3 lead to the following expressions for total SD (SD^{ECR}_{Total}) and the total %RSD ($\%RSD^{ECR}_{Total}$) of *ECR* for Equations (2.7) and (2.8), respectively:

$$SD^{ECR}_{Total} = [(SD^{ECR}_{Scale})^2 + (SD^{ECR}_{Simulant})^2 + (SD^{ECR}_{SolidsConc})^2 + (SD^{ECR}_{NozzleVel})^2 + (SD^{ECR}_{Error})^2]^{0.5} \quad (2.9)$$

$$\%RSD^{ECR}_{Total} = [(\%RSD^{ECR}_{Scale})^2 + (\%RSD^{ECR}_{Simulant})^2 + (\%RSD^{ECR}_{SolidsConc})^2 + (\%RSD^{ECR}_{NozzleVel})^2 + (\%RSD^{ECR}_{Error})^2]^{0.5} \quad (2.10)$$

As noted previously, these expressions account only for random uncertainties under the assumption that the data are not biased.

Table 2.3. Assumptions Associated with Equations (2.7) and (2.8)

Equation	Assumptions
(2.7)	The δ_{ha}^{ECR}, $\gamma_{ha,ib}^{ECR}$, $\lambda_{ha,ib,jc}^{ECR}$, and $\tau_{ha,ib,jc,kd}^{ECR}$ are each independently and identically distributed with a normal (Gaussian) distribution having mean 0 and standard deviations SD_{Scale}^{ECR}, $SD_{Simulant}^{ECR}$, $SD_{SolidsConc}^{ECR}$, and $SD_{NozzleVel}^{ECR}$. The $\varepsilon_{ha,ib,jc,kd,e}^{ECR}$ are independently and identically distributed with a normal (Gaussian) distribution having mean 0 and standard deviation SD_{Error}^{ECR}. Further, the $\varepsilon_{ha,ib,jc,kd,e}^{ECR}$ terms are independent of the δ_{ha}^{ECR}, $\gamma_{ha,ib}^{ECR}$, $\lambda_{ha,ib,jc}^{ECR}$, and $\tau_{ha,ib,jc,kd}^{ECR}$ terms.
(2.8)	The δ_{ha}^{ECR}, $\gamma_{ha,ib}^{ECR}$, $\lambda_{ha,ib,jc}^{ECR}$, and $\tau_{ha,ib,jc,kd}^{ECR}$ are each independently and identically distributed with a normal (Gaussian) distribution having mean 1 and percent relative standard deviations $\%RSD_{Scale}^{ECR}$, $\%RSD_{Simulant}^{ECR}$, $\%RSD_{SolidsConc}^{ECR}$, and $\%RSD_{NozzleVel}^{ECR}$. The $\varepsilon_{ha,ib,jc,kd,e}^{ECR}$ terms are independently and identically distributed with a normal (Gaussian) distribution having mean 1 and percent relative standard deviation $\%RSD_{Error}^{ECR}$. Further, the $\varepsilon_{ha,ib,jc,kd,e}^{ECR}$ terms are independent of the δ_{ha}^{ECR}, $\gamma_{ha,ib}^{ECR}$, $\lambda_{ha,ib,jc}^{ECR}$, and $\tau_{ha,ib,jc,kd}^{ECR}$ terms.

Although the random errors within each of Equations (2.7) and (2.8) are assumed to be independently and identically distributed, the *ECR* values for a test matrix have a complicated covariance structure because of the multiple restrictions on the order of performing tests. The variance-covariance matrices corresponding to Equations (2.7) and (2.8) are given in Section A.1 of Appendix A. Note that the covariances in Section A.1 are all functions of the variances. Hence, the problem of estimating the variance-covariance matrix for *ECR* data reduces to the problem of estimating the variance components in Equations (2.9) or (2.10). The methods for estimating variance components using data from split-plot experiments are discussed in Section 2.2 and subsequently in Section 3.1.3.

2.4 U_{BC} Error Structure and Uncertainties for the Anticipated Restrictions on the Order of Performing LSIT Tests

The statistical models for U_{BC} corresponding to the anticipated structure of the LSIT experiments are given in the following equations, for the situations of additive and multiplicative structures of test parameter effects and errors.

U_{BC}, Additive Structure

$$(U_{BC})_{ha,ib,jc,e} = \mu_{h,i,j}^{U_{BC}} + (Scale_{h}^{U_{BC}} + \delta_{ha}^{U_{BC}}) + (Simulant_{i}^{U_{BC}} + \gamma_{ha,ib}^{U_{BC}}) + (SolidsConc_{j}^{U_{BC}} + \lambda_{ha,ib,jc}^{U_{BC}}) + \varepsilon_{ha,ib,jc,e}^{U_{BC}} \quad (2.11)$$

U_{BC}, Multiplicative Structure

$$(U_{BC})_{ha,ib,jc,e} = \mu_{h,i,j}^{U_{BC}} \times (Scale_{h}^{U_{BC}} \times \delta_{ha}^{U_{BC}}) \times (Simulant_{i}^{U_{BC}} \times \gamma_{ha,ib}^{U_{BC}}) \times (SolidsConc_{j}^{U_{BC}} \times \lambda_{ha,ib,jc}^{U_{BC}}) \times \varepsilon_{ha,ib,jc,e}^{U_{BC}} \quad (2.12)$$

where $(U_{BC})_{ha,ib,jc,e}$ = e^{th} replicate measurement of U_{BC} for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale

$\mu_{h,i,j}^{U_{BC}}$ = true mean U_{BC} for the j^{th} solids concentration of the i^{th} simulant at the h^{th} scale

$Scale_{h}^{U_{BC}}$ = effect of the h^{th} scale on U_{BC}

$\delta_{ha}^{U_{BC}}$ = random error in U_{BC} for the a^{th} replicate of the h^{th} scale

$Simulant_{i}^{U_{BC}}$ = effect of the i^{th} simulant on U_{BC}

$\gamma_{ha,ib}^{U_{BC}}$ = random error in U_{BC} for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale

$SolidsConc_{j}^{U_{BC}}$ = effect of the j^{th} solids concentration on U_{BC}

$\lambda_{ha,ib,jc}^{U_{BC}}$ = random error in U_{BC} for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale

$\varepsilon_{ha,ib,jc,e}^{U_{BC}}$ = random error for the e^{th} replicate measurement of U_{BC} for the c^{th} replicate of the j^{th} solids concentration for the b^{th} replicate of the i^{th} simulant for the a^{th} replicate of the h^{th} scale.

The terms $Scale_{h}^{U_{BC}}$, $Simulant_{i}^{U_{BC}}$, and $SolidsConc_{j}^{U_{BC}}$ are general representations of the effects of those test parameters on U_{BC}. Each one can be replaced with any applicable model term or terms. If a model is to include two-parameter interaction terms (to represent the effect of one parameter depending on the value of another parameter), then any such interaction term has as its error term the rightmost of the error terms [in Equation (2.11) or (2.12)] for the two

parameters. For example, if a model for U_{BC} were to include an interaction term between *Simulant* and *SolidsConc*, that interaction would have the error term associated with *SolidsConc*.

Because Equations (2.11) and (2.12) are already complicated enough, it was assumed that there is no possibility of a constant bias, so such a model term was not included in these U_{BC} models as it was in Equations (2.1) and (2.2). Depending on the situation, performing a logarithmic transformation of both sides of Equation (2.12) may convert a multiplicative structure to an additive structure as in Equation (2.11). That approach is used for an U_{BC} example in Section 5.

For U_{BC} data collected with the previous experimental structures, the assumptions in Table 2.4 are typically made to provide for statistical analyses of the experimental data.

Table 2.4. Assumptions Associated with Equations (2.11) and (2.12)

Equation	Assumption
(2.11)	The $\delta_{ha}^{U_{BC}}$, $\gamma_{ha,ib}^{U_{BC}}$, and $\lambda_{ha,ib,jc}^{U_{BC}}$ terms are each independently and identically distributed with a normal (Gaussian) distribution having mean 0 and standard deviations $SD_{Scale}^{U_{BC}}$, $SD_{Simulant}^{U_{BC}}$, and $SD_{SolidsConc}^{U_{BC}}$. The $\varepsilon_{ha,ib,jc,e}^{U_{BC}}$ terms are independently and identically distributed with a normal (Gaussian) distribution having mean 0 and standard deviation $SD_{Error}^{U_{BC}}$. Further, the $\varepsilon_{ha,ib,jc,e}^{U_{BC}}$ terms are independent of the $\delta_{ha}^{U_{BC}}$, $\gamma_{ha,ib}^{U_{BC}}$, and $\lambda_{ha,ib,jc}^{U_{BC}}$.
(2.12)	The $\delta_{ha}^{U_{BC}}$, $\gamma_{ha,ib}^{U_{BC}}$, and $\lambda_{ha,ib,jc}^{U_{BC}}$ terms are each independently and identically distributed with a normal (Gaussian) distribution having mean 1 and percent relative standard deviations $\%RSD_{Scale}^{U_{BC}}$, $\%RSD_{Simulant}^{U_{BC}}$, and $\%RSD_{SolidsConc}^{U_{BC}}$. The $\varepsilon_{ha,ib,jc,e}^{U_{BC}}$ terms are independently and identically distributed with a normal (Gaussian) distribution having mean 1 and percent relative standard deviation $\%RSD_{Error}^{U_{BC}}$. Further, the $\varepsilon_{ha,ib,jc,e}^{U_{BC}}$ terms are independent of the $\delta_{ha}^{U_{BC}}$, $\gamma_{ha,ib}^{U_{BC}}$, and $\lambda_{ha,ib,jc}^{U_{BC}}$ terms.

The assumptions in Table 2.4 lead to the following expressions for the total SD ($SD_{Total}^{U_{BC}}$) and the total %RSD ($\%RSD_{Total}^{U_{BC}}$) of U_{BC} for Equations (2.11) and (2.12), respectively.

$$SD_{Total}^{U_{BC}} = [(SD_{Scale}^{U_{BC}})^2 + (SD_{Simulant}^{U_{BC}})^2 + (SD_{SolidsConc}^{U_{BC}})^2 + (SD_{Error}^{U_{BC}})^2]^{0.5} \quad (2.13)$$

$$\%RSD_{Total}^{U_{BC}} = [(\%RSD_{Scale}^{U_{BC}})^2 + (\%RSD_{Simulant}^{U_{BC}})^2 + (\%RSD_{SolidsConc}^{U_{BC}})^2 + (\%RSD_{Error}^{U_{BC}})^2]^{0.5} \quad (2.14)$$

Equations (2.13) and (2.14) for U_{BC} are similar to Equations (2.9) and (2.10) for *ECR*, except that the former do not include the SD or %RSD associated with nozzle velocity because of the way U_{BC} is determined. As noted previously, these expressions account only for random uncertainties under the assumption that the data are not biased.

Although the random errors within each of Equations (2.11) and (2.12) are assumed to be independently and identically distributed, the U_{BC} values for a test matrix have a complicated covariance structure because of the multiple restrictions on the order of performing tests. The variance-covariance matrices corresponding to Equations (2.11) and (2.12) are given in Section A.2 of Appendix A. Note that the covariances in Section A.2 are all functions of the variances. Hence, the problem of estimating the variance-covariance matrix for U_{BC} data reduces to the problem of estimating the variance components in Equations (2.13) or (2.14). The methods for estimating variance components using data from split-plot experiments are discussed in Section 3.2.

3.0 Methods for Quantifying Uncertainties of LSIT Test Responses and Other Parameters

This section describes and illustrates the methods that could be used to quantify the uncertainties in test responses and other parameters resulting from the LSIT. For test responses that are directly measured, uncertainties could be quantified using appropriate statistical methods that consider the error structure of the test data resulting from the number, nature, and order of tests in the experimental design (test matrix) and the testing/measurement method(s) and the contributing uncertainties. For test responses or other parameters associated with LSIT testing that are obtained by calculation rather than direct measurement, the methods for quantifying uncertainties can account for the specific form of the equation used to perform the calculations, as well as the uncertainties of parameters appearing in the equation.

3.1 Methods for Estimating Uncertainties in Test Responses

This section discusses methods for estimating uncertainties in test responses from experiments performed during LSIT. Section 3.1.1 introduces terminology and some key references for the methods. Section 3.1.2 discusses the role of the experimental design (i.e., the test matrix and the order in which the tests are performed). Section 3.1.3 discusses the methods for estimating the uncertainties of LSIT test responses.

3.1.1 Terminology and References for Methods to Estimate Uncertainties in Test Responses

ASME PTC 19.1-2005, *Test Uncertainty,* (ASME 2006) discusses many useful methods for quantifying test uncertainties that could be applied to test responses and parameters associated with LSIT. For example, it discusses methods for 1) quantifying the standard uncertainty of measured test responses, and 2) error propagation methods for quantifying the standard uncertainty in a parameter of interest that is calculated using a specified function of one or more other parameters. However, uncertainties resulting from restrictions on the order of performing tests in a test matrix are not directly addressed by ASME (2006), although such restrictions do result in systematic error as defined by ASME (2006). Because ASME does not directly address quantifying standard uncertainties when there are restrictions on the order of performing tests in a test matrix, statistical methods from other references (e.g., Montgomery et al. 2001; Goos et al. 2006; Kowalski et al. 2007) are likely to be needed.

A more complete set of terminology than used in ASME (2006) is used in this report to refer to uncertainties of LSIT results. One reason is the restrictions on the order of performing LSIT tests, as discussed in Section 2.2. Second, in ASME (2006) all uncertainties are categorized as resulting from either

- Random Error: The portion of total error that varies randomly in repeated measurements of the true value throughout a test process.

- Systematic Error: The portion of total error that remains constant in repeated measurements of the true value throughout a test process.

While the definitions of these terms are typical, ASME (2006) departs from standard statistical practice by using SDs to quantify uncertainties resulting from systematic errors as well as random errors. That practice is appropriate if the magnitude of an error is constant throughout a test process, but the magnitude varies randomly over different applications of the test process. In such cases, what ASME (2006) refers to as a systematic error is actually just a random error that changes systematically over a longer period of time. Because the term "systematic error" is often equated to the term "bias" in the measurement uncertainty literature (e.g., ISO 1993; Ellison and Williams 2012; ASTM 2007; ASTM 2010), "systematic error" is best reserved for situations when the magnitude of the difference (or relative difference) in a test result from the true value remains the same over different applications of a test process. Statistical methods for estimating bias, quantifying the uncertainty in the estimate of bias, and bias-correcting data appear in the literature (Bowen and Bennett 1988; ASTM 2007) and can be applied in situations where 1) standards with certified values of test responses and uncertainties of the certified values have been developed, and 2) the standards can be included as a part of testing. However, there are no standard simulants with certified response values for various mixing test conditions that can be included in the LSIT. Hence, it probably will not be possible to quantify and correct for bias in LSIT test results.

Because the LSIT is expected to have the error structure discussed in Section 2.2, the variance components discussed in Section 2.3 (for *ECR*) and Section 2.4 (for U_{BC}) are referred to in this report as having resulted from random errors associated with different restrictions on the order of performing tests. Hence, the "systematic error" terminology of ASME (2006) is not used, although in fact the sources of error associated with the restrictions on the order of performing tests are "systematic errors" which are applicable to (and vary randomly over) different subsets of the data. The calculations of the total uncertainty in this report do account for several categories of systematic error and one category of random error in the sense of ASME (2006). However, ultimately all of the categories of error are random errors with different periods of time over which they are constant or vary.

3.1.2 Experimental Design and Replicates

Statistical experimental design methods should be used to select the test matrix for LSIT to support the planned data analyses and modeling of data. The number of tests, distribution of test combinations over the test-parameter space, and order of performing the tests must be addressed in specifying the experimental design. Statistical experimental design methods enable reducing (to the extent possible given the test budget and limitations) the uncertainties of model coefficients and predictions obtained by fitting the model to test data. See Section 4.2 for further discussion of this topic.

A sufficient number of tests should be replicated to provide a basis for quantifying the testing and measurement uncertainties that affect the test responses. In an experiment with restrictions on the order of performing tests, there is a different uncertainty (variance) component associated with each restriction. Replicates at the level of each restriction provide for estimating the uncertainty component associated with that restriction. For example, to estimate the uncertainty component associated with the effect of test vessel size, replicate tests are needed for each vessel size. More specifically, after the full set of tests with all vessel sizes are completed, some tests at some vessel sizes must be replicated. Similarly, for a given vessel size, after the full set of tests with all simulants is completed, some tests with some simulants must be replicated. The same is true for different 1) solids concentrations of a given simulant with a given test vessel size, and 2) nozzle velocities for a given solids concentration of a given simulant with a given vessel size.

There has been some discussion of 'replicates' and 'duplicates' in other documents for planning LSIT testing. However, those concepts and terms are insufficient for the structure of data that will occur if there are restrictions on the order of performing tests (see Sections 2.2, 2.3, and 2.4). Hence, the term "replicate" is used in this report in a more general sense to refer to tests that must be performed more than once at each level of restriction, with the level of restriction determining the sources of uncertainty included in replicates at that level.

3.1.3 Methods for Estimating Variance Components when There are Restrictions on the Order of Performing Tests in an Experiment

This section discusses the method for estimating the variance components associated with the restrictions on the order of performing test matrix runs, as discussed in Sections 2.2 to 2.4. It is assumed that data are available from an experimental design with appropriate replication at each level of restriction (see Section 3.1.2 and additional discussion in Section 4.2.4).

Restricted maximum likelihood (REML) is the standard method used to estimate variance components when replicate data are available from each level of restriction in a split-plot data structure. REML works with balanced and unbalanced data structures, as well as data structures resulting from restrictions on the order of performing tests. The REML methodology ensures that the variance component estimates are non-negative. The REML methodology is discussed by West et al. (2006, Section 2.4.2) and is available in full-featured statistical software packages.

3.1.4 Averaging Over Replicate Measurements to Effectively Reduce Uncertainty

Consider cases where replicate measurements are available at the "lowest" level of the data structure, that is, associated with the ε error term in Equations (2.7), (2.8), (2.11), and (2.12). In such cases, the replicate measurements can be averaged to obtain an estimate of the quantity of interest. This averaging offers the benefit of effectively reducing the uncertainty in the estimated quantity of interest. For such cases, the averaging must be conducted using replicate measurements obtained for a particular combination of experimental conditions during a specific data-collection period (the "lowest" level of the data structure). The following discussion presents the relevant formulas.

Let y_{ij} represent the j^{th} replicate measured value of a test response Y_i for the i^{th} combination of experimental conditions during a specific data-collection period. Also, let μ_{Y_i} and σ_{Y_i} denote the true mean and true SD of the distribution of y_{ij} values for the i^{th} combination of experimental conditions and during the specified data-collection period. If a single measured value y_{ij} is used to estimate μ_{Y_i}, and y_{ij} is assumed to be a randomly selected measurement of Y_i, then the expectation and variance of y_{ij} are

$$E(y_{ij}) = \mu_{Y_i} \quad \text{and} \quad V(y_{ij}) = \sigma_{Y_i}^2 . \tag{3.1}$$

Suppose instead that replicate measurements of Y_i are available to estimate μ_{Y_i}. Let $y_{i1}, y_{i2}, \cdots, y_{in}$ denote a set of n replicate measurements of Y_i obtained under the i^{th} set of test conditions and during the specific data-collection period. Further, assume these values represent a random sample of Y_i values. Then the *sample mean* of the n replicate measurements, calculated as

$$\bar{y}_i = \frac{\sum_{j=1}^{n} y_{ij}}{n} \tag{3.2}$$

has the properties

$$E(\bar{y}_i) = \mu_{Y_i} \quad \text{and} \quad V(\bar{y}_i) = \frac{\sigma_{Y_i}^2}{n} . \tag{3.3}$$

Thus, $\bar{y}_i$ is an unbiased estimator of μ_{Y_i} and has reduced uncertainty [i.e., the variance in Equation (3.3)] compared to that of a single measured value of Y_i [i.e., the variance in Equation (3.1)]. The variance is reduced by a divisor of n, while the SD is reduced by a divisor of $\sqrt{n}$.

Just as $\bar{y}_i$ was selected as an estimator for μ_{Y_i}, an estimator for $\sigma^2_{Y_i}$ must also be selected. Regardless of whether the experimental runs were conducted using 1) a completely randomized structure (as discussed in Section 2.1), or 2) a more complicated data structure involving restrictions on the order of performing tests (as discussed in Sections 2.2 to 2.4), the sample variance

$$s_i^2 = \frac{\sum_{j=1}^{n}\left(y_{ij} - \bar{y}_i\right)^2}{n-1} \tag{3.4}$$

is an appropriate estimator for $\sigma^2_{Y_i}$. Then, if $\sigma^2_{Y_1} = \sigma^2_{Y_2} = \ldots = \sigma^2_{Y_M} = \sigma^2_Y$ for all M sets of test conditions in the test matrix, the pooled sample variance

$$s^2 = \frac{1}{M}\sum_{i=1}^{M}\left(\frac{\sum_{j=1}^{n}\left(y_{ij} - \bar{y}_i\right)^2}{n-1}\right) \tag{3.5}$$

can be used as an estimator for σ^2_Y. In this case, the estimated variance of $\bar{y}_i$ is

$$\hat{V}(\bar{y}_i) = \frac{s^2}{n} \tag{3.6}$$

and the estimated SD would be the square root of the above.

Note that Equation (3.5) assumes there are exactly n replicate measurements y_{ij} for every $i = 1, 2, \ldots, M$. A more complicated formula for the pooled sample variance applies when there are different numbers (n_i) of replicate measurements for at least some of $i = 1, 2, \ldots, M$:

$$s^2 = \frac{\sum_{i=1}^{M}\sum_{j=1}^{n_i}\left(y_{ij} - \bar{y}_i\right)^2}{\sum_{i=1}^{M}(n_i - 1)} \tag{3.7}$$

However, averaging over different numbers of replicate measurements would require that subsequent data analyses be more complicated, because the sample means ($\bar{y}_i$) for the different test conditions would have different estimated variances

$$\hat{V}(\bar{y}_i) = \frac{s^2}{n_i} \tag{3.8}$$

rather than the same estimated variance (s^2/n) as in Equation (3.6).

If the assumption $\sigma^2_{Y1} = \sigma^2_{Y2} = \ldots = \sigma^2_{YM} = \sigma^2_Y$ for all M sets of test conditions in the test matrix is not appropriate, then the pooled sample variance formulas [Equations (3.5) and (3.7)] are not appropriate. In that situation, the individual sample variance estimates s_i^2 in Equation (3.4) would need to be used, so that

$$\hat{V}(\bar{y}_i) = \frac{s_i^2}{n} \quad or \quad \frac{s_i^2}{n_i} \tag{3.9}$$

depending on whether the number of replicate measurements y_{ij} of Y_i is the same (n) or different (n_i) for $i = 1, 2, \ldots, M$.

It is important to note that the discussion in this subsection applies only to the last error term and its variance component (or SD) when there are multiple variance components because of restrictions on the order of performing tests, as discussed in Sections 2.2 to 2.4. The variance components "earlier" in the structure would still be estimated using the methods discussed in Section 3.1.4, using the averages of replicate measurements at the "lowest" level of the structure.

Finally, note that the reduction in uncertainty associated with an estimate obtained by averaging over replicate measurements only applies to the random error components; averaging does not reduce bias or systematic error.

3.1.5 Methods for Estimating Uncertainties in Test Response Values

Ultimately, the goal is to estimate the uncertainties in test response values obtained from conducting the experimental test runs. These uncertainties must be the total uncertainties, accounting for all of the variance components associated with the structure of the data set (see Sections 2.2 to 2.4). The formulas for the total SD (SD^Y_{Total}) and the total %RSD ($\%RSD^Y_{Total}$) depend on whether the model and error structure is multiplicative or additive for the test response Y (e.g., ECR or U_{BC}). These formulas are given in Section 2.3 for the ECR performance metric and in Section 2.4 for the U_{BC} performance metric. Specifically, the formula for

SD^{Y}_{Total} when the model and error structure are additive is given by Equation (2.9) for *ECR* and by Equation (2.13) for U_{BC}. The formula for $\%RSD^{Y}_{Total}$ when the model and error structure are multiplicative is given by Equation (2.10) for *ECR* and by Equation (2.14) for U_{BC}.

The formulas referred to in the previous paragraph are for the true, unknown values of SD^{Y}_{Total} and $\%RSD^{Y}_{Total}$. Hence, it is necessary to substitute estimates of the variance components (in the form of SD or %RSD) into the right-hand sides of those equations. However, as noted in Section 2, this report uses the same notation for the true, unknown values of SD and %RSD for convenience. Hence the equations for the estimated SD or %RSD are the same, and are listed here again for convenience.

ECR, Additive Structure

$$SD^{ECR}_{Total} = [(SD^{ECR}_{Scale})^2 + (SD^{ECR}_{Simulant})^2 + (SD^{ECR}_{SolidsConc}) + (SD^{ECR}_{NozzleVel})^2 + (SD^{ECR}_{Error})^2]^{0.5} \quad (3.10)$$

ECR, Multiplicative Structure

$$\%RSD^{ECR}_{Total} = \begin{array}{l}[(\%RSD^{ECR}_{Scale})^2 + (\%RSD^{ECR}_{Simulant})^2 + (\%RSD^{ECR}_{SolidsConc}) \\ + (\%RSD^{ECR}_{NozzleVel})^2 + (\%RSD^{ECR}_{Error})^2]^{0.5}\end{array} \quad (3.11)$$

U_{BC}, Additive Structure

$$SD^{U_{BC}}_{Total} = [(SD^{U_{BC}}_{Scale})^2 + (SD^{U_{BC}}_{Simulant})^2 + (SD^{U_{BC}}_{SolidsConc}) + (SD^{U_{BC}}_{Error})^2]^{0.5} \quad (3.12)$$

U_{BC}, Multiplicative Structure

$$\%RSD^{U_{BC}}_{Total} = [(\%RSD^{U_{BC}}_{Scale})^2 + (\%RSD^{U_{BC}}_{Simulant})^2 + (\%RSD^{U_{BC}}_{SolidsConc})^2 + (\%RSD^{U_{BC}}_{Error})^2]^{0.5} \quad (3.13)$$

In the above equations SD^{ECR}_{Total} and $SD^{U_{BC}}_{Total}$ denote the estimated total SDs, while $\%RSD^{ECR}_{Total}$ and $\%RSD^{U_{BC}}_{Total}$ denote the estimated total %RSDs, for *ECR* and U_{BC}, as indicated in the superscripts. The SD^{Y}_{Scale}, $SD^{Y}_{Simulant}$, $SD^{Y}_{SolidsConc}$, and SD^{Y}_{Error} quantities (with Y either *ECR* or U_{BC}) denote the estimated SDs corresponding to the sources of uncertainty in the *ECR* or U_{BC} additive data structure. Those estimates are obtained using the methodology discussed in Section 3.1.3 (and Section 3.1.4 if applicable). The $\%RSD^{Y}_{Scale}$, $\%RSD^{Y}_{Simulant}$, $\%RSD^{Y}_{SolidsConc}$, and $\%RSD^{Y}_{Error}$ (with Y = either *ECR* or U_{BC}) denote the estimated %RSDs corresponding to the sources of uncertainty in the Y = *ECR* or U_{BC} multiplicative data structure. The estimated %RSD values are calculated in general as

$$\%RSD = \frac{100(SD)}{Mean} \tag{3.14}$$

where *SD* = one of the estimated SDs listed above, and *Mean* = estimated mean of *ECR* or U_{BC} over the whole data set.

3.2 Quantifying the Uncertainty in a Parameter that is a Function of Uncertain Parameters Using Error Propagation Methods

In some cases, one parameter (the output parameter) may be expressed as a known function of other parameters (the input parameters), where the input parameters are subject to uncertainty. The methodology referred to as error propagation can be applied to propagate the uncertainties of the input parameters through the function to approximate the uncertainty in the output parameter. The following describes first-order error propagation methods.

Let *R* denote the output parameter that is expressed as a function of the input parameters $X_1, X_2, \cdots, X_n$. That is, $R = R(X_1, X_2, \cdots, X_n)$. Assume the input parameters are subject to random uncertainty, and hence are random variables in statistical terminology.

Assume that $X_1, X_2, \cdots, X_n$ have means $\mu_{X_1}, \mu_{X_2}, \cdots, \mu_{X_n}$ and variances $\sigma^2_{X_1}, \sigma^2_{X_2}, \cdots, \sigma^2_{X_n}$, respectively. Now, consider expanding *R* using a Taylor series in a neighborhood of the point $(x_1, x_2, \cdots, x_n)$ where it is assumed that higher-order terms in the expansion are negligible compared to the first-order terms. Then, if the random variables $X_1, X_2, \cdots, X_n$ are all statistically independent, the true, unknown mean of *R* is

$$\mu_R = R(\mu_{X_1}, \mu_{X_2}, \cdots, \mu_{X_n}) \tag{3.15}$$

and the expected value of *R* evaluated at the point $(x_1, x_2, \cdots, x_n)$ is

$$\mathrm{E}[R(X_1, X_2, \cdots, X_n)|_{x_1, x_2, \cdots, x_n}] = R(x_1, x_2, \cdots, x_n) . \tag{3.16}$$

Then, the variance of *R* when $X_1 = x_1,\ X_2 = x_2,\ \cdots,\ X_n = x_n$ can be approximated using first-order error propagation as

$$\hat{\sigma}^2_R \approx \sum_{i=1}^{n} \left(\left. \frac{\partial R}{\partial X_i} \right|_{x_1, x_2, \cdots, x_n} \right)^2 \hat{\sigma}^2_{X_i} \tag{3.17}$$

where $\theta_{X_i} = \left.\frac{\partial R}{\partial X_i}\right|_{x_1, x_2, \cdots, x_n}$ is often referred to as the sensitivity coefficient for X_i (ASME 2006). Because the random variables $X_1, X_2, \cdots, X_n$ are considered statistically independent, no covariance terms appear in Equation (3.17). Other error propagation formulas are available that make use of higher-order terms from the Taylor-series expansion, or that do not assume independence among the random variables involved in the function of interest (Colman and Steele 1999; Hahn and Shapiro 1967). However, Equation (3.17) is commonly used and is considered adequate for the purposes of many applications. Note that Equation (3.17) only accounts for random uncertainty in *R* due to the random variables $X_1, X_2, \cdots, X_n$; it does not account for bias.

An example illustrating the application of this methodology is discussed in Section 5.1.2.

3.3 Combined and Expanded Uncertainties

A fundamental aspect of the uncertainty analyses outlined in ASME (2006) is to determine what is called the combined standard uncertainty associated with some quantity of interest. This combined uncertainty accounts for uncertainties (quantified as SDs or %RSDs) from all applicable error sources. Combined standard uncertainties for *ECR* are given by Equations (3.10) and (3.11) in Section 3.1.5, while combined standard uncertainties for U_{BC} are given by Equations (3.12) and (3.13) in Section 3.1.5.

An additional step that may be included in uncertainty analyses is to determine an expanded uncertainty associated with a particular quantity of interest. The expanded uncertainty includes an additional multiplying factor applied to the combined standard uncertainty. The multiplying factor is chosen to yield a desired confidence level, and generally depends on the structure of the data and replicates used to estimate the combined standard uncertainty. The expanded uncertainty hence establishes a confidence interval for estimating the quantity of interest.

4.0 Methods for Reducing and Quantifying the Uncertainties of Full-Scale Mixing Performance Using Models Developed from LSIT Data

This section discusses the methods for reducing and quantifying the uncertainties in model predictions of mixing performance for full-scale WTP vessels.

4.1 General Plans to Quantify Performance and Performance Uncertainty of WTP Mixing Systems

A general plan for quantifying the performance of the mixing systems in the WTP vessels is to

1. Select the mixing systems that have the least performance margin.

2. Conduct mixing performance tests of those systems in three successively larger geometrically scaled test vessels.

3. Develop mixing performance models and fit any adjustable coefficients to the experimental data.

4. Extrapolate the models for mixing performance to the full-scale systems. Mixing tests are planned to be conducted using vessels with diameters of 43 in., 8 ft, and 14 ft[(1)] having Newtonian designs.

There are two approaches that could be used to implement this general plan.

- Approach 1: Steps 2), 3), and 4) could be performed separately for each of the WTP vessels with lower performance margins. Separate sets of tests, mixing performance models, and extrapolations to full-scale mixing performance would be performed for each WTP vessel identified.

- Approach 2: Steps 2), 3), and 4) would be performed once with tests conducted over ranges of parameters corresponding to all the WTP vessels with lower performance margins.

[(1)] The technical basis for vessel sizing and array choices are provided in R. Hanson and J. Meehan, April 2012, *Vessel Configuration for Large Scale Integrated Testing*, 24590-WTP-RPT-ENG-12-017, Rev. 0, Bechtel National, Inc., Richland, Washington.

For each WTP vessel, Approach 1 would involve fewer tests in the test matrix and simpler models for mixing performance because some parameters would be constant for each WTP vessel. However, the total number of tests with Approach 1 could be substantively larger than with Approach 2, especially if there are more than a few WTP vessels of interest. In this case, the other advantage to Approach 2 is that the mixing performance models obtained under that approach would be applicable over the whole region of test parameters investigated in testing. Thus, the models could be used to predict mixing performance (and the uncertainties of predicted mixing performance) over combinations of test parameters not specifically tested. Approach 1 may not support that capability, or may support it to a lesser extent. The choice of an approach for testing in LSIT will be made in the future. Regardless of the approach chosen, the methods for reducing and quantifying uncertainties of extrapolated mixing performance discussed in this section are applicable.

A general plan to reduce and quantify the uncertainty in performance of WTP mixing systems would be to 1) select model forms for mixing performance metrics (e.g., *ECR* and U_{BC})[(1)] that would defensibly support extrapolation to full scale and represent the experimental data within their uncertainties, and 2) develop an experimental design for testing at the three scales that would minimize (to the extent possible) the uncertainties and provide for quantifying those uncertainties. Here, "uncertainties" refers to uncertainties in the 1) estimates of model coefficients, and 2) predictions of mixing performance metrics (e.g., *ECR* and U_{BC}) made with the models. The term "experimental design" refers to the number of test runs, the distribution of test combinations over the feasible space of test conditions, the order of performing the tests, any other restrictions on the tests, and appropriate replication of tests. Replicate tests provide for quantifying the uncertainties in test results (see Section 3.1.2) and for statistically assessing whether the models for mixing performance metrics (e.g., *ECR* and U_{BC}) adequately fit the experimental data.

4.2 Experimental Design for Large Scale Integrated Testing

The experimental design (i.e., the test matrix and specifics of testing) for the LSIT plays an important role in 1) developing models for quantifying the mixing performance in full-scale WTP vessels, and 2) reducing and quantifying uncertainties in model coefficients (which may be interpretable in physical models) and predictions of mixing performance.

4.2.1 Matched-Condition Tests

The experimental design for LSIT should be developed as part of future scope to prepare a test plan that includes the three scales of testing. The experimental design should be generated to

(1) While *ECR* and U_{BC} are discussed in this report, it is envisioned that the LSIT also examine other metrics of mixing performance, including blending, no solids accumulation during pump-out, and sampling. The concepts described for *ECR* and U_{BC} can be applied or adapted to these other metrics of mixing performance.

support developing models for key mixing-performance metrics (e.g., *ECR* and U_{BC}) that accurately 1) estimate model coefficients, and 2) predict mixing performance metrics for full-scale vessels, with uncertainties that are as low as possible for the number of tests performed. One option for the test matrix would be for it to consist of matched-condition tests performed at corresponding operating conditions and geometries, and with the same simulants, in the 43 in., 8 ft, and 14 ft vessels. For practical reasons, the simulated waste would not be scaled with the size of the test. For each size vessel, the matched-condition tests could exercise the following parameters:

- PJM configuration (number and configuration of jets operating)
- PJM operations (pulse volume fraction, dimensionless cycle time = $t_C(U/D)$, where t_C is the cycle time, U is nozzle velocity, and D is vessel diameter)
- slurry level in vessel relative to vessel size
- solids concentration
- particle settling velocity (by changing the particle densities or sizes)
- fluid rheological properties.

Matched-condition tests, when completed at all three scales, would provide for assessing the scaling relationships for the *ECR* and U_{BC} mixing performance criteria at each set of test conditions. If the scaling relationships differ for different sets of test conditions, the data from the matched-condition tests would provide for evaluating the differences and/or developing models for *ECR* and U_{BC} that account for the effects of the parameters varied in the testing. After the models are developed using the LSIT experimental data, they could be applied to predict mixing performance for various configurations and conditions in full-scale vessels. Uncertainties in the test data and other relevant uncertainties can then be accounted for in quantifying the uncertainties in model coefficients and predictions of mixing performance metrics (e.g., *ECR* and U_{BC}) in full-scale vessels.

4.2.2 Statistical Experimental Design Methods Guided by Subject-Matter Knowledge

The test conditions investigated should be selected using statistical experimental design methods, guided by subject-matter knowledge, to adequately cover the multidimensional parameter space relevant to WTP vessel/PJM configurations and waste properties. The parameter space of interest will depend on whether Approach 1 or Approach 2 (Section 4.1) to experimentation is chosen. Statistical experimental design methods, with subject-matter guidance, will enable reducing (to the extent possible given the test budget and limitations) the uncertainties of the *ECR* and U_{BC} model coefficients and predictions based on the resulting data. The coverage of the parameter space should be assessed in terms of the relevant dimensional parameters, as well as dimensionless parameters/groups relevant to modeling mixing performance metrics such as *ECR* and U_{BC}. Dimensionless parameters/groups may support interpolating over more of the parameter space of interest than when the space is expressed in

terms of dimensional parameters. Generally, interpolation is subject to less uncertainty than extrapolation. So, from this perspective, models expressed in terms of dimensionless parameters/groups may have an advantage over models expressed in terms of dimensional parameters. Designing the LSIT experiments to provide good coverage of the test condition spaces expressed in both dimensional parameters and dimensionless parameters/groups would provide robustness for developing predictive models that have acceptable accuracy and precision.

Statistical optimal experimental design (OED) methods (Atkinson et al. 2007) provide for selecting the test combinations in a test matrix to minimize the uncertainties of the model coefficients and/or predictions (e.g., of *ECR* and U_{BC}) from a prespecified model form. Hence, a test matrix developed using the OED approach is optimized for a specific model form. A test matrix developed for a model form expressed in terms of dimensionless parameters/groups may differ substantively from a test matrix developed for a model expressed in terms of dimensional parameters. Also, a model for a mixing performance metric ultimately developed from the LSIT data may be different from the model form hypothesized to develop the test matrix. Thus, it is recommended that model-robust experimental design methods be used, so that the data will provide good support for developing a range of model forms. For example, Albrecht et al. (2012) propose developing a test matrix that is relatively efficient for both a hypothesized model form (e.g., expressed in terms of dimensionless parameters/groups) and a second-order polynomial model in the dimensional test parameters. Second-order polynomial models (second-order, Taylor-series expansions) can well approximate many model forms. Hence, the experimental design method of Albrecht et al. (2012) would provide for generating a test matrix that is model-robust. That is, the experimental design will provide good support (i.e., reduce uncertainties of model coefficients and model predictions) regardless of the final forms of the mixing performance models to be fit to the data. Piepel (2010) provides a review of model-robust experimental design methods that have been proposed in the statistical literature.

4.2.3 Restrictions on the Order of Performing Test Matrix Runs

Tests in the LSIT must be sufficiently and appropriately replicated[(1)] (accounting for restrictions in the order of performing tests) to provide for quantifying the testing/measurement uncertainties of the test results, the model coefficients, and model predictions of *ECR* and U_{BC} in full-scale vessels. In a split-plot experiment, there is a different variance component associated with each restriction. Replicates at the level of each restriction provide for estimating the variance component associated with that restriction.

To estimate the variance component associated with the effect of test vessel size, replicate tests are needed using the different-size vessels. More specifically, after the set of tests with a given size vessel are completed in one period of time, at least some of those tests must be

[(1)] See Section 3.1.2 for a discussion of how the term "replicates" is used in this report.

replicated during one or more subsequent periods of time. Table 4.1 illustrates an example for LSIT with the three scaled vessels (43 in., 8 ft, and 14 ft) in which a complete test matrix is performed during the first three time periods, which are referred to as whole plots (WP) in the split-plot literature (Steel and Torrie 1960; Montgomery et al. 2001; Goos et al. 2006; Kowalski et al. 2007). Then, a smaller number of tests[(1)] are replicated in WPs 4 to 9. Note in Table 4.1 that WPs 4, 5, and 6 involve testing each of the three scaled vessels again, although in a different randomized order. Also, WPs 7, 8, and 9 involve testing in the 43 in. vessel twice and the 8 ft vessel once. The 14 ft vessel is not tested a third time, and instead the 43 in. vessel is tested again twice, because it saves time and money. Although desirable, it is not necessary to perform replicate tests with each scaled vessel size the same number of times, which the example in Table 4.1 illustrates.

Table 4.1. Example of Replicate Tests with Different-Size Vessels to Enable Quantifying the Variance Component Associated with the Scale Restriction on the Order of Performing Tests

Whole Plot (WP)	**1**	**2**	**3**	**4**	**5**	**6**	**7[(a)]**	**8**	**9[(a)]**
Test Vessel Scale	43 in.	8ft	14 ft	8 ft	43 in.	14 ft	43 in.	8 ft	43 in.
Other Test Parameters	Full test matrix			Small number of tests replicated			Small number of tests replicated		
(a) Rather than testing using all three sizes of vessel in WPs 7–9, the 43 in. vessel is tested in WPs 7 and 9, and the 8 ft vessel is tested in WP 8. While it would be ideal to replicate each vessel size the same number of times, it is possible to focus on smaller vessels in some WPs to save time and expense of testing in the 14 ft vessel.									

The amount of replicate testing of scaled vessel sizes in Table 4.1 provides eight degrees of freedom (DF) for WPs, because the DF is one less than the number of values (number of WPs in this case). Two of those DF are available to quantify the scale effect of the test response (since there are three scaled vessels tested), leaving six DF[(2)] for estimating SD^{Y}_{Scale} or $\%RSD^{Y}_{Scale}$ (this notation was introduced in Section 3.1.5). Performing only one set of replicates (WPs 4, 5, and 6) instead of two sets of replicates would require only six WPs rather than nine WPs. However, that would provide only three DF for estimating SD^{Y}_{Scale} or $\%RSD^{Y}_{Scale}$, which is considered too small. Variances (and %RSDs) are difficult to estimate precisely (Natrella 1966, Section 2-4), so even six DF is a very limited basis for estimating SD^{Y}_{Scale} or $\%RSD^{Y}_{Scale}$. Based on Figure 2-2 in Section 2-4 of Natrella (1966), 6 DF only provides for estimating a SD within about 47% of the

(1) The future work of developing the LSIT experimental design needs to determine the number of tests to perform with 'replicates' of test vessels.

(2) Statistical algorithms and software to fit models to split-plot data determine the applicable DF, which can be fractional values. Hence, the DF mentioned in the discussion are approximate and for conceptual understanding only.

true value with 90% confidence. However, from a practical standpoint, it was thought that nine sets (i.e., WPs) of tests with different-size test vessels may be the most that would be considered given time and budget constraints.

As a second example of replication at each level of restriction, consider replicate tests with simulants. Suppose there are three simulants (denoted A, B, C) that are to be tested at each of the three sizes of test vessels. Table 4.2 illustrates having two replicates of each of the three simulants within each of WPs 1, 2, and 3 (and hence for each test vessel size). The order of testing the two replicates of the three simulants was randomized for each of WPs 1, 2, and 3. The number of DF for estimating $SD^{Y}_{Simulant}$ or $\%RSD^{Y}_{Simulant}$ are calculated as follows. In WP 1, three simulants are each replicated twice, for a total of three DF. Because the three simulants are also replicated twice in WPs 2 and 3, there are a total of nine DF for estimating $SD^{Y}_{Simulant}$ or $\%RSD^{Y}_{Simulant}$.

Table 4.2. Example of Replicate Tests with Simulants at Three Test Vessel Sizes to Enable Quantifying the Simulant Variance Component

Whole Plot (WP)	**1**	**2**	**3**
Test Vessel Scale	43 in.	8 ft	14 ft
Simulants	A, B, C, B, C, A[(a)]	B, C, A, B, A, C	A, C, B, C, A, B
(a) This denotes that all 43 in. vessel tests with simulant A are completed first, then all tests with simulant B, then all tests with simulant C, then all tests with simulant B, then all tests with simulant C, and finally all tests with simulant A.			

Although no tables are provided to illustrate the concepts, the different solids concentrations must be replicated at combinations of test vessel size and simulant to enable quantifying the estimates $SD^{Y}_{SolidsConc}$ or $\%RSD^{Y}_{SolidsConc}$. For the U_{BC} test response, the nozzle velocity restriction on the order of performing tests does not apply. However, it does apply for the *ECR* test response, as discussed in Section 2.3. In that case, the nozzle velocities must be replicated at combinations of test vessel size, simulant, and solids concentration to enable quantifying the estimates $SD^{Y}_{NozzleVel}$ or $\%RSD^{Y}_{NozzleVel}$.

As one gets to the third and fourth restrictions on the order of performing tests, the DF accumulate very quickly. For example, consider Table 4.2, where in WPs 1, 2, and 3, there are a total of $3 \times 6 = 18$ combinations of test vessel size and simulant. If three solids concentrations were replicated twice at each of the 18 combinations, there would be $3 \times 18 = 54$ DF for estimating $SD^{Y}_{SolidsConc}$ or $\%RSD^{Y}_{SolidsConc}$. This accumulation of larger numbers of DF for subsequent restrictions is considered one of the advantages of split-plot experiments—namely, the effects of test parameters associated with such restrictions can be estimated very precisely.

However, this advantage comes with a significant consequence of larger numbers of tests. Fortunately, it is not necessary to replicate solids concentrations at every one of the 18 combinations. This aspect of designing split-plot experiments can be addressed by developing an experimental design using the OED methodology (see Section 4.2.2) and software specific to developing split-plot experimental designs. That methodology allows for partial replication, so that there are sufficient DF for estimating the variance component associated with each restriction, without there being too many DF and having too large a number of tests to perform.

In deciding on the number of replicate tests needed at each level of restriction in the experimental design, trade-offs generally have to be made between (i) wanting to estimate variance components with more precision, and (ii) practical limitations on the number of tests and replicates of different kinds that can be performed.

4.3 Model Development, Fitting, and Evaluation

Models for mixing performance metrics (e.g., *ECR* and U_{BC}) as functions of the parameters varied in LSIT can be developed, fitted to data, and evaluated using the experimental test data. These topics are discussed in the following subsections.

4.3.1 Models for Mixing Performance Responses and Spurious Correlation

Models of mixing performance metrics (e.g., *ECR* and U_{BC}) could be expressed as functions of dimensional test parameters or dimensionless parameters/groups. Typically, such models are written in terms of dimensionless parameters/groups, which can increase the appropriateness of extrapolating the model to full scale. However, models expressed in terms of dimensionless parameters/groups can be subject to spurious correlation, causing the model to appear to fit the test data better than it actually does (Pearson 1897; Kenney 1982; Jackson and Comers 1991; Brett 2004). Spurious correlation can result when a dependent dimensionless group contains 1) one or more dimensional parameters included in one or more independent dimensionless groups, and/or 2) one or more dimensional parameters that are highly correlated with dimensional parameters included in one or more independent dimensionless groups. The severity of spurious correlation depends on how the dependent and independent dimensionless groups are defined in terms of the dependent and independent dimensional parameters and the variations of the dimensional parameters in the experimental data (Brett 2004). Examples of spurious correlation in physical models for two mixing performance metrics, and how this was avoided, are discussed in Section 7.3.2 of Meyer et al. (2012).

Models for mixing performance metrics (e.g., *ECR* and U_{BC}) in LSIT may still be appropriately developed in terms of dimensionless groups, provided the models are fit and assessed using mathematically equivalent re-expressions of the models (which removes the possibility of spurious correlation).

4.3.2 Fitting Mixing Performance Models to Data

Appropriate regression methods should be used to fit the models for mixing performance metrics (e.g., *ECR* and U_{BC}) to the experimental data. The most commonly used methods for fitting models to experimental data are 1) ordinary least squares (OLS) regression when the model is a linear function of the coefficients, and 2) nonlinear least squares (NLS) regression when the model is a nonlinear function of the coefficients. OLS and NLS regression assume (require) that the values of a test response for all test runs in the experiment have approximately equal uncertainty (variance) and are uncorrelated (i.e., all covariances equal to zero). The first of these assumptions (equal variance) may be violated if the variance increases with the magnitude of the test response. In that case, taking the natural logarithm of both sides of the model may provide for approximately equal variances for all test combinations. However, the second of these assumptions (zero covariances) is violated for split-plot experiments, as shown for *ECR* in Equation (A.1) of Section A.1 and for U_{BC} in Equation (A.2) of Section A.2, both in Appendix A. As seen by the equations in those locations, and as noted in Sections 2.3 and 2.4, the covariances are functions of the variance components. Hence, estimating the variance components provides for estimating all entries in the variance-covariance matrix of the test response values from the experiment.

If the testing and measurement uncertainties in test response values are additive (possibly after a natural-log transformation), generalized least squares (GLS) regression methods must be used to fit the model coefficients to the data, where the variance components are first estimated by the REML method (West et al. 2006, Section 2.4.2). These methods are applicable for fitting linear models[(1)] of the general form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon} \tag{4.1}$$

where
- $\mathbf{y}$ = $n \times 1$ vector of test response values
- $\mathbf{X}$ = $n \times p$ matrix formed by expanding the test matrix so that the columns of $\mathbf{X}$ correspond to the p terms in the model
- $\boldsymbol{\beta}$ = $p \times 1$ vector of true, unknown model coefficients
- $\boldsymbol{\varepsilon}$ = $n \times 1$ vector of random experimental/testing errors with variance-covariance matrix $\mathbf{V}$.

[(1)] Here, "linear model" refers to models that are linear in their coefficients.

In GLS theory, **V** is assumed to be known without uncertainty, so the formulas must be modified to account for the fact that the variance components are estimated. Using an estimate of **V** in the formulas is referred to as feasible generalized least squares (FGLS). Per the modified formula (Goos et al. 2006), the estimated coefficient vector is given by

$$\hat{\boldsymbol{\beta}}_{\text{FGLS}} = (\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}\mathbf{X}\hat{\mathbf{V}}^{-1}\mathbf{y} \tag{4.2}$$

and the variance-covariance matrix of the FGLS-estimated coefficient vector ($\hat{\boldsymbol{\beta}}_{\text{FGLS}}$) is given by

$$\text{Var}(\hat{\boldsymbol{\beta}}_{\text{FGLS}}) = (\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1} \tag{4.3}$$

where $\hat{\mathbf{V}}$ is the $n \times n$ estimated variance-covariance matrix of the data vector **y** and all other notation is as previously defined. The matrix $\hat{\mathbf{V}}$ is obtained by substituting in the estimates of the variance components [e.g., in Equations (3.10) or Eq. (3.12)]. Equation (4.3) is used in the formula for calculating uncertainties of mixing performance predictions, which is discussed in Section 4.3.4.

A statistical software package [e.g., SAS (2010) or R (R Development Core Team 2011)] with capabilities for fitting mixed models[(1)] (West et al. 2006; Jiang 2007) would provide for first estimating the variance components (and hence estimating **V**). Then, the coefficients of the mixing performance model (e.g., *ECR* or U_{BC}) would be estimated using FGLS. Estimates of the variance components coupled with knowledge of the data structure in the experiment would provide for quantifying the uncertainties of the test response values (see Sections 2.3 and 2.4). The statistical software also provides for quantifying the uncertainties of model coefficients and model predictions of the mixing performance test responses (discussed in Section 4.3.4).

If the model terms and testing/measurement uncertainties are multiplicative [as in Equation (2.8) or Equation (2.12)], it is often possible to transform the model (e.g., by taking the natural logarithm of both sides) to obtain model terms and uncertainties with an additive structure. Although the model-fitting capabilities in Microsoft Excel® (including using Solver) are often used to fit mixing performance models, those Excel capabilities are all based on OLS or NLS, which are only appropriate for data with an additive error structure with no nonzero entries in the variance-covariance matrix. Hence, the Excel model-fitting capabilities are not appropriate for the kinds of data structures envisioned for LSIT.

(1) A "mixed model" is one in which both model coefficients (fixed effects) and variance components of the data (random effects) must be estimated using the data.

4.3.3 Evaluating the Models for Mixing Performance

To reduce the uncertainty in predictions of mixing performance metrics (e.g., *ECR* and U_{BC}), the models developed from the test data should be evaluated for adequacy in three ways. First, subject-matter knowledge and statistical methods should be applied to assess whether there are any influential or outlying data points. Graphical and statistical methods for evaluating the goodness of a model should be applied (Draper and Smith 1998; Montgomery et al. 2001). If influential or outlying data points are found, appropriate resolutions should be made and the models refitted if necessary.

Second, statistical methods for model lack-of-fit (LOF) should be applied to ascertain whether the differences between model-predicted values and test values of mixing performance metrics (e.g., *ECR* and U_{BC}) are larger than can be accounted for by experimental/measurement uncertainty in the data. If the LOF for a particular model is not statistically (or practically) significant, then the model would be judged as adequately representing the true, unknown relationship between the dependent and independent variables (parameters). If a model LOF is statistically and practically significant, additional model forms would need to be assessed in an attempt to obtain a revised model without significant LOF. Almimi et al. (2009) and Goos and Gilmour (2013) discuss possible methods for assessing model LOF when the data structure involves restrictions on the order of performing tests.

Third, the models finally developed from the LSIT test data should be validated using test data not used to fit/develop the models. Statistical validation methods (Montgomery et al. 2001) should be used that account for model prediction uncertainties and the uncertainty in the validation data values of mixing performance metrics (e.g., *ECR* and U_{BC}). If there are no appropriate validation data (not used to fit/develop the models) available, then cross-validation methods (Montgomery et al. 2001) should be applied to the data used to develop the models.

Draper and Smith (1998), Montgomery et al. (2001), Myers and Montgomery (1995), and Seber and Wild (1989) discuss the methods for fitting, evaluating, and validating models that are linear or nonlinear in their coefficients. Although these references discuss these methods for linear and nonlinear models fitted to data using OLS or NLS, the methods can be extended for use with FGLS. FGLS, as noted previously, is used with the complicated data structure caused by restrictions on the order of performing the test matrix runs.

4.3.4 Quantifying Uncertainties in Model Coefficients and Predictions of Mixing Performance

Equally important to estimating model coefficients and predicting mixing performance metrics (e.g., *ECR* and U_{BC}) for various full-scale WTP situations is quantifying the uncertainties in the estimates of these quantities. Estimating the uncertainty in quantities derived from test data first requires quantifying the uncertainties in test responses obtained during LSIT. Methods for quantifying uncertainties of test responses or other test parameters are discussed in Section 3.

As discussed previously, it is envisioned that data analyses to assess the scaling relationships and develop models for mixing performance metrics (e.g., *ECR* and U_{BC}) would involve regression fitting of models to experimental data. There is considerable statistical theory on how to quantify uncertainties in estimated model coefficients and test response predictions made with fitted models (Draper and Smith 1998; Montgomery et al. 2001; Myers and Montgomery 1995; Seber and Wild 1989). This theory is more complicated as a result of restrictions on the order of performing test matrix runs (Steel and Torrie 1960; Montgomery et al. 2001; Goos et al. 2006; Kowalski et al. 2007). However, as noted previously, statistical software provides for implementing the statistical methods based on the appropriate theory.

4.3.4.1 Two Types of Uncertainty in Regression Models

There are two types of uncertainty that are commonly accounted for when working with model predictions of mixing performance metrics (e.g., *ECR* and U_{BC}).

- Uncertainty in Fitting a Model to Experimental Data. The model form fit to experimental data can be, at best, an adequate approximation of the true, unknown relationship between a test response (e.g., *ECR* or U_{BC}) and parameters varied as part of the experimental design. Also, the experimental data are subject to uncertainty from the testing and measurement processes. Hence, predictions of mixing performance metrics (e.g., *ECR* and U_{BC}) for full-scale mixing performance under various conditions are subject to uncertainty from fitting models to data. This is referred to as fitting prediction uncertainty.

- Uncertainty in Applying a Fitted Model to Make Response Predictions. Predictions of mixing performance metrics (e.g., *ECR* and U_{BC}) using models fitted to data are subject to a separate kind of uncertainty, which is referred to as application prediction uncertainty. This kind of uncertainty results from the uncertainties in the values of model parameters (e.g., solids concentration, particle size and density, PJM stroke length) used to make model predictions of the mixing performance metrics.

For known functions of uncertain parameters, error propagation methods can be used to approximate the total uncertainty of the parameter calculated by the equation for the known function. Section 3.2 discusses and provides references for error propagation methods.

A different situation occurs when a model for a mixing performance metric (e.g., *ECR* or U_{BC}) fitted to data is used to predict values of one of those test responses for a given set of values of the model parameters. The values of the model parameters can involve combinations different from those tested as part of the experimental design. For such applications of fitted *ECR* and U_{BC} models, the fitting uncertainty and application uncertainty are statistically independent. Hence, the total uncertainty of a model prediction (expressed as a SD) is the sum of the two uncertainties (variances or relative variances):

$$\text{Total Prediction Standard Deviation} = [\text{Fitting Prediction Variance} + \text{Application Prediction Variance}]^{0.5} \quad (4.4)$$

It is preferable to use this approach rather than first-order error propagation (Section 3.2) to quantify the total uncertainty in model predictions, because this approach utilizes the available statistical theory to quantify the fitting prediction variance. However, error propagation is typically used to quantify the application prediction variance, by propagating the uncertainties of the model parameters (not the coefficients) through the model form.

4.3.4.2 Matrix-Vector Notation for Model Predictions Conclusions

Using the matrix-vector notation introduced in Section 4.3.2, a model prediction at a vector **x** of parameter combinations (expanded in the form of terms in the model) is given by

$$\hat{y}(\mathbf{x}) = \mathbf{x}' \hat{\boldsymbol{\beta}}_{\text{FGLS}} \quad (4.5)$$

where $\hat{y}(\mathbf{x})$ = model-predicted value of the mixing performance metric y at the expanded vector of model parameters **x**

$\mathbf{x}'$ = $1 \times p$ vector (the vector transpose of **x**) formed by expanding the model parameters in the form of the terms in the model

$\hat{\boldsymbol{\beta}}_{\text{FGLS}}$ = $p \times 1$ vector of estimated model coefficients (from Equation (4.2)) obtained by FGLS regression.

Ideally the vector **x** of parameter combinations should be within the region of combinations explored experimentally, although it is realized that predicting the mixing performance of full-scale vessels will involve extrapolation on the length scale.

4.3.4.3 Formulas for Estimating the Fitting Prediction Variance

The fitting prediction variance of a model prediction at the vector **x** of parameter combinations (expanded in the form of the model terms) depends on whether the prediction is considered as 1) a mean value of the test response y over a conceptually large number of tests at **x**, or 2) an individual value of y at **x**. The matrix-vector formulas for the fitting prediction variance (FPV) in these two cases are given by:

Prediction Considered as the Mean

$$FPV_{Mean} = \text{Var}_{\text{Mean}}[\hat{y}(\mathbf{x})] \text{ w.r.t.} \hat{\boldsymbol{\beta}}_{FGLS} = \mathbf{x}'(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}\mathbf{x} \quad (4.6)$$

Prediction Considered as an Individual Value

$$FPV_{Individual} = \text{Var}_{\text{Individual}}[\hat{y}(\mathbf{x})] \text{ w.r.t. } \hat{\boldsymbol{\beta}}_{FGLS} = (SD_{Total}^{y})^2 + FPV_{Mean} = (SD_{Total}^{y})^2 + \mathbf{x}'(\mathbf{X}'\hat{\mathbf{V}}^{-1}\mathbf{X})^{-1}\mathbf{x} \quad (4.7)$$

where FPV_{Mean} and $FPV_{Individual}$ are the fitting prediction variances for the predicted value of the mixing performance metric considered as the mean or an individual value, respectively. The middle portions of Equations (4.6) and (4.7) clarify that the fitting prediction variances have to do with the variances in predicted $\hat{y}(\mathbf{x})$ values with respect to the estimated coefficient vector ($\hat{\boldsymbol{\beta}}_{\text{FGLS}}$). In Equation (4.7), SD_{Total}^{y} denotes the total SD of a test response value *y*, as discussed in Section 3.1.5. All other notation in Equations (4.6) and (4.7) is as previously defined.

4.3.4.4 Formulas for Estimating the Application Prediction Variance Conclusions

The application prediction variance (APV) of $\hat{y}(\mathbf{x})$ quantifies the uncertainty in *y* resulting from the uncertainties in the components of the **x** vector when making a prediction using a previously developed model. The matrix-vector formula for the *APV* is given by

$$APV = \text{Var}[\hat{y}(\mathbf{x})] \text{ where } \mathbf{x} = \begin{cases} 0 & \text{If } \mathbf{x} \text{ is not subject to uncertainty} \\ \hat{\boldsymbol{\beta}}'_{FGLS}\mathbf{W}\hat{\boldsymbol{\beta}}_{FGLS} & \text{If } \mathbf{x} \text{ is subject to uncertainty} \end{cases} \quad (4.8)$$

where $\mathbf{W}$ = $p \times p$ variance-covariance matrix of the vector **x**, expanded in the form of the model

$\hat{\boldsymbol{\beta}}_{\text{FGLS}}$ = $p \times 1$ vector of estimated model coefficients from previously fitting the model to experimental data

and all other notation is as defined previously. When **x** is not subject to uncertainty (e.g., nominal values are chosen and input to the model), then $APV = 0$. When **x** is subject to uncertainty (given by its variance-covariance matrix, **W**), then *APV* is calculated as shown in Equation (4.8). In this latter case, the difficulty of applying Equation (4.8) in practice is in obtaining an estimate of the variance-covariance matrix **W** for the **x** vector. Recall that the **x** vector contains all of the parameters used to develop the mixing performance model, and any transformations or extensions thereof in developing the model form. If the errors in measuring or determining the components of **x** are statistically independent, then covariances of all the components are zero. In that case, **W** is a diagonal matrix with the variance of each **x** component down the diagonal. If there is a basis for estimating the variance of each component of **x**, then Equation (4.8) may be directly applied to calculate *APV*. In this case, the results are equivalent to first-order error propagation, as discussed in Section 3.2.

4.3.4.5 Total Prediction Variance and Expanded Uncertainty

The total prediction standard deviation (*TPSD*) defined in Equation (4.4) can be rewritten as

$$TPSD_{Mean} = [FPV_{Mean} + APV]^{0.5} \tag{4.9}$$

$$TPSD_{Individual} = [FPV_{Individual} + APV]^{0.5} \tag{4.10}$$

where FPV_{Mean} and $FPV_{Individual}$ are calculated using Equations (4.6) and (4.7), respectively, and APV is calculated using Equation (4.8). The FPV and APV variance components can be added together because the uncertainties in the fitting and application processes for the model are statistically independent. Note that the $TPSD_{Mean}$ and $TPSD_{Individual}$ quantities are "standard uncertainties" in the terminology of ASTM (2006). Statistical methods for the sums of variances can be used to determine the proper multiplier if an expanded uncertainty (see Section 2.4) is desired. Examples of expanded uncertainties include 95% confidence intervals and 95% predictions interval (Hahn and Meeker 1991).

4.4 Quantifying Possible Uncertainties Not Observable from Testing Results

This section addresses two possible kinds of uncertainty that are not observable from testing results. Uncertainty associated with using an incorrect model form to represent the relationship between mixing performance responses and test parameters is discussed in Section 4.4.1. Uncertainties associated with differences in scaled test vessels and simulants compared to WTP vessels and actual waste feed materials are discussed in Section 4.4.2.

4.4.1 Uncertainty Associated with an Incorrect Model Form

The methods for quantifying the two types of uncertainty discussed in Section 4.3.4 (fitting prediction uncertainty and application prediction uncertainty) assume that the model forms for mixing performance metrics (e.g., *ECR* and U_{BC}) adequately represent the true, unknown relationships between these responses and the parameters varied during testing. This assumption can be assessed over the multivariate region of test parameters for which there are experimental data, using the model evaluation methods discussed in Section 4.3.3. Also, if the model form extrapolates accurately (i.e., without bias), then statistical methods for quantifying the uncertainty of model predictions will account for the increased random uncertainty associated with extrapolation (if applicable given the form of the model).

However, the methods for evaluating the mixing performance models and quantifying the uncertainties in their predictions do not address the accuracy (or possible bias) of extrapolating outside the multivariate experimental region of test parameters. The mixing performance models selected should have agreement of knowledgeable experts regarding the appropriateness of the

models for extrapolation to full scale. Assuming such agreement, it is advisable to determine whether predictions with such models should still include an uncertainty corresponding to some possibility of the model yielding biased predictions. The potential that the mixing performance at full scale is different from (biased compared to) what is predicted by mixing performance models would have to be assessed by experts based on beliefs about how accurate the utilized model forms may be when extrapolated. The greater the physical understanding of the observed behavior, the greater the ability to assess the validity of a scaling relationship at length scales beyond those tested, and hence the greater the ability to assess the uncertainty in extrapolating to larger scales. The usefulness of the test data is not just from regression to fit models to test data. Test data are equally important for validating a physical conceptual model, which then provides a basis for judging the range of length scales for which the model is valid.

The form of the model can be used to determine whether condition transitions are expected between the test vessel size and the plant vessel. Establishing accurate, physically based models can significantly reduce the uncertainty of projecting test results if key phenomenological thresholds are not crossed during scale-up. One example is describing the effect of PJM jets impinging on solids on the vessel floor using available models of impinging radial wall jets (see Sections 2.2.2 and 2.2.3 of Kuhn et al. 2012).

4.4.2 Uncertainties Associated with Differences Between Scaled Test Vessels and Actual WTP Vessels and Between Simulants and Actual Waste Materials

The two types of uncertainty discussed in Section 4.3.4 also assume that the experimental mixing-performance data from scaled vessels using simulants are unbiased estimates of what the mixing performance would be with actual waste slurries if WTP vessels were scaled down to the sizes of the scaled test vessels. It is unrealistic to believe that these assumptions are exactly met. The scaled test vessels would not be exact, scaled-down versions of real WTP vessels, and the simulants used in testing would not be as complex as actual waste materials. Unfortunately, the experimental results provide no information about the extent to which test responses may be biased or differ randomly compared to what the mixing performance responses would be for scaled versions of actual WTP vessels using actual waste materials. Hence, the experimental results provide no information about the representativeness uncertainty in model predictions of mixing performance metrics (e.g., *ECR* and U_{BC}) for full-scale WTP situations. Ultimately, any uncertainties (bias or random) associated with the representativeness of scaled test data using simulants must be based on expert knowledge.

Any expert-based estimates of random uncertainty in 1) estimates of model coefficients, or 2) model predictions of mixing performance metrics (e.g., *ECR* or U_{BC}) must be combined with the other estimates of random uncertainty (developed using statistical methods applied to test data) to yield the estimated total random uncertainty. Methods for combining estimates of representativeness uncertainty with estimates of the types of uncertainty discussed in Section 4.3.4 depend on whether the representativeness uncertainty is quantified as a bias or a

random uncertainty. If the representativeness uncertainty is quantified as a random uncertainty (variance), then that variance could be added to the total variance represented in Equation (4.9) or (4.10) for a new total variance. If the representativeness uncertainty is quantified as a bias, then methods for separately reporting or combining random and bias uncertainties discussed by (ASTM 2007, 2010; ISA 2000) could be applied.

5.0 Example Applications and Discussions of Methods for Quantifying Uncertainties

Example applications and discussion of the methods for quantifying uncertainties in mixing test results and models that were presented in Sections 3 and 4 are included in Sections 5.1 and 5.2, respectively.

5.1 Example Applications and Discussion of Methods for Quantifying Uncertainties in LSIT Test Responses and Other Parameters

Sections 5.1.1 and 5.1.2 present examples that illustrate applying the uncertainty quantification methods discussed in Sections 3.1.3 and 3.2, respectively.

5.1.1 Example of Methods for Estimating Uncertainties in Test Responses Using Replicate Data

There are no data sets from previous mixing test studies that have the proper replication structure to use as an example illustrating the REML method discussed in Section 3.1.3 for quantifying variance components associated with multiple restrictions on the order of performing tests. Also, it was beyond the scope of the work associated with this report to 1) develop a LSIT experimental design including replication at each level of restriction on the order of performing tests, and 2) simulate a data set with an assumed model to provide example data from which the REML method could be applied to estimate the applicable variance components. For *ECR* and U_{BC}, these estimated SDs or %RSDs (depending on whether the data have an additive or multiplicative structure) to be quantified are:

- ***ECR Additive***: SD^{ECR}_{Scale}, $SD^{ECR}_{Simulant}$, $SD^{ECR}_{SolidsConc}$, $SD^{ECR}_{NozzleVel}$, and SD^{ECR}_{Error}
- ***ECR Multiplicative***: $\%RSD^{ECR}_{Scale}$, $\%RSD^{ECR}_{Simulant}$, $\%RSD^{ECR}_{SolidsConc}$, $\%RSD^{ECR}_{NozzleVel}$, and $\%RSD^{ECR}_{Error}$
- ***U_{BC} Additive***: $SD^{U_{BC}}_{Scale}$, $SD^{U_{BC}}_{Simulant}$, $SD^{U_{BC}}_{SolidsConc}$, and $SD^{U_{BC}}_{Error}$
- ***U_{BC} Multiplicative***: $\%RSD^{U_{BC}}_{Scale}$, $\%RSD^{U_{BC}}_{Simulant}$, $\%RSD^{U_{BC}}_{SolidsConc}$, and $\%RSD^{U_{BC}}_{Error}$.

Instead, we consider two possible estimated values for each variance component applicable for *ECR* and U_{BC}, and then apply Equations (3.10) and (3.12) to calculate SD^{ECR}_{Total} and $SD^{U_{BC}}_{Total}$. For the purposes of this example, we assume that power-law models would be appropriate for *ECR* and U_{BC} and that the error structures (as well as the power-law model forms) are multiplicative (see Sections 2.3 and 2.4). Hence, taking the natural logarithm of both sides of each model would yield an additive model and error structure. This is the situation used for a

U_{BC} model example in Section 5.2, so it was appropriate to consider such a situation for this example as well. This situation required the following modifications of Equations (3.10) and (3.12):

$$SD_{Total}^{\ln(ECR)} = [(SD_{Scale}^{\ln(ECR)})^2 + (SD_{Simulant}^{\ln(ECR)})^2 + (SD_{SolidsConc}^{\ln(ECR)}) + (SD_{NozzleVel}^{\ln(ECR)})^2 + (SD_{Error}^{\ln(ECR)})^2]^{0.5} \quad (5.1)$$

$$SD_{Total}^{\ln(U_{BC})} = [(SD_{Scale}^{\ln(U_{BC})})^2 + (SD_{Simulant}^{\ln(U_{BC})})^2 + (SD_{SolidsConc}^{\ln(U_{BC})}) + (SD_{Error}^{\ln(U_{BC})})^2]^{0.5} \quad (5.2)$$

A useful relationship corresponding to the preceding equations is

$$SD[\ln(y)] \approx RSD(y) \quad (5.3)$$

where y represents a mixing performance metric (e.g., ECR or U_{BC}) and RSD denotes "relative standard deviation" (the SD divided by the mean). Based on this relationship, for the example we chose values of 0.05 and 0.10 for each of the SDs on the right-hand sides of Equations (5.1) and (5.2). That corresponds to choosing RSD values of 0.05 and 0.10 (or %RSD values of 5 and 10) for the test responses before logarithmic transformations. Any of these estimated SDs could be smaller than 0.05 or larger than 0.10 in practice, but for illustrative purposes here the values 0.05 and 0.10 suffice to demonstrate the range of total SD values that might result. Table 5.1 shows the combinations of values of the estimated SDs and the resulting values of $SD_{Total}^{\ln(ECR)}$ and $SD_{Total}^{\ln(U_{BC})}$ calculated using Equations (5.1) and (5.2), respectively. Note that the $SD_{Total}^{\ln(ECR)}$ values range from 0.112 to 0.224, while the $SD_{Total}^{\ln(U_{BC})}$ values range from 0.100 to 0.200. The $SD_{Total}^{\ln(U_{BC})}$ values are smaller than the $SD_{Total}^{\ln(ECR)}$ values because the latter have one extra estimated SD ($SD_{NozzleVel}^{\ln(ECR)}$) that contributes to the total SD.

Table 5.1. Example Calculations (for Information Only) of $SD_{Total}^{\ln(ECR)}$ and $SD_{Total}^{\ln(U_{BC})}$ for Various Combinations of the Input Variance Components

$SD_{Scale}^{\ln(Y)}$	$SD_{Simulant}^{\ln(Y)}$	$SD_{SolidsConc}^{\ln(Y)}$	$SD_{NozzleVel}^{\ln(Y)}$	$SD_{Error}^{\ln(Y)}$	$SD_{Total}^{\ln(ECR)}$	$SD_{Total}^{\ln(U_{BC})}$
0.05	0.05	0.05	0.05	0.05	0.112	0.100
0.05	0.05	0.05	0.05	0.10	0.141	0.132
0.05	0.05	0.05	0.10	0.05	0.141	0.100
0.05	0.05	0.05	0.10	0.10	0.166	0.132
0.05	0.05	0.10	0.05	0.05	0.141	0.132
0.05	0.05	0.10	0.05	0.10	0.166	0.158
0.05	0.05	0.10	0.10	0.05	0.166	0.132
0.05	0.05	0.10	0.10	0.10	0.187	0.158
0.05	0.10	0.05	0.05	0.05	0.141	0.132
0.05	0.10	0.05	0.05	0.10	0.166	0.158
0.05	0.10	0.05	0.10	0.05	0.166	0.132
0.05	0.10	0.05	0.10	0.10	0.187	0.158
0.05	0.10	0.10	0.05	0.05	0.166	0.158
0.05	0.10	0.10	0.05	0.10	0.187	0.180
0.05	0.10	0.10	0.10	0.05	0.187	0.158
0.05	0.10	0.10	0.10	0.10	0.206	0.180
0.10	0.05	0.05	0.05	0.05	0.141	0.132
0.10	0.05	0.05	0.05	0.10	0.166	0.158
0.10	0.05	0.05	0.10	0.05	0.166	0.132
0.10	0.05	0.05	0.10	0.10	0.187	0.158
0.10	0.05	0.10	0.05	0.05	0.166	0.158
0.10	0.05	0.10	0.05	0.10	0.187	0.180
0.10	0.05	0.10	0.10	0.05	0.187	0.158
0.10	0.05	0.10	0.10	0.10	0.206	0.180
0.10	0.10	0.05	0.05	0.05	0.166	0.158
0.10	0.10	0.05	0.05	0.10	0.187	0.180
0.10	0.10	0.05	0.10	0.05	0.187	0.158
0.10	0.10	0.05	0.10	0.10	0.206	0.180
0.10	0.10	0.10	0.05	0.05	0.187	0.180
0.10	0.10	0.10	0.05	0.10	0.206	0.200
0.10	0.10	0.10	0.10	0.05	0.206	0.180
0.10	0.10	0.10	0.10	0.10	0.224	0.200

(a) $y = ECR$ or U_{BC}

5.1.2 Example of Quantifying the Uncertainty in a Parameter that is a Function of Uncertain Parameters Using Error Propagation Methods

The following example illustrates using the error propagation methods discussed in Section 3.2. Consider the formula for calculating nozzle velocity based on the volume change within a single pulse jet tube that occurs over the duration of the duty cycle of a pulse. The calculation is given by

$$V_1 = \left[\frac{\pi\left(\frac{D_{PI}}{2}\right)^2 - \pi\left(\frac{D_{PR}}{2}\right)^2}{\pi\left(\frac{D_n}{2}\right)^2} \right] \left[\frac{K \cdot h_s}{T_d} \right] = \left[\frac{D_{PI}^2 - D_{PR}^2}{D_n^2} \right] \left[\frac{K \cdot h_s}{T_d} \right] \tag{5.4}$$

where
V_1 = estimated PJM nozzle velocity (m/sec)
D_{PI} = inner diameter of a PJM tube (in.)
D_{PR} = diameter of a Drexelbrook probe rod (in.)
D_n = nozzle diameter of a PJM tube (in.)
K = conversion constant to convert inches to meters (1/39.37 m/in.)
h_s = PJM stroke length (in.)
T_d = drive time of the duty cycle for a pulse (sec)
π = mathematical constant (approximately 3.1416).

Note that the function given in Equation (5.4) involves five measured quantities (random variables), D_{PI}, D_{PR}, D_n, h_S, and T_d. The function also involves two constants, k and π, although π cancels from the final expression in Equation (5.4). Nominal values are needed to represent a specified point, like $(x_1, x_2, \cdots, x_n)$ in the notation above, for the five measured quantities when applying Equations (3.15) and (3.16). Additionally, estimates or assumed values are needed for the $\sigma_{X_i}^2$ of the five measured (uncertain) quantities when applying Equation (3.17). Table 5.2 provides example values for the five measured quantities involved in Equation (5.4), thereby allowing the use of Equations (3.16) and (3.17) to calculate an expected nozzle velocity and associated uncertainty at this specified point.

Table 5.2. Example Inputs for Estimating Nozzle Velocity and Associated Uncertainty (for Information Only)

Input	Label Used in Equation (5.1)	Nominal Value	Assumed Standard Uncertainty (σ_{X_i})
Inner PJM Diameter	D_{PI}	5.72 in.	0.003 in.
Probe Rod Diameter	D_{PR}	0.56 in.	0.001 in.
Nozzle Diameter	D_n	0.655 in.	0.001 in.
PJM Stroke Length	h_s	24.784 in.	0.362 in.
PJM Drive Time	T_d	6.057 sec	0.001 sec
Conversion Constant	K	1/39.37 m/in	NA

Applying Equation (3.17) using the nominal values and assumed standard uncertainties in Table 5.2 yields the uncertainty estimates for the nozzle velocity listed in Table 5.3.

Table 5.3. Resulting Estimates of Nozzle Velocity and Associated Uncertainty (for Information Only)

Nozzle Velocity	Standard Uncertainty	Relative Standard Uncertainty
7.850 m/sec	0.117 m/sec	1.50%

5.2 Example Applications and Discussion of Methods for Quantifying Uncertainties of Full-Scale Mixing Performance Using Models Developed from LSIT Data

This section presents and discusses example applications of the methods from Section 4 for quantifying uncertainties of full-scale mixing performance using models developed from LSIT data.

5.2.1 Introduction of Example and a U_{BC} Model

We consider an example situation in which it is assumed that Approach 1 for LSIT is used. In particular, we consider the situation of the LSIT testing associated with a single WTP vessel. This choice was made because it simplifies the example, not because of judgments that Approach 1 is preferable to Approach 2 or that testing for only a single WTP vessel is adequate.

For this situation, an example model for the mixing performance metric U_{BC} is given by

$$U_{BC} = c_{WTP} D^{c_D} \phi_S^{c_\phi} u_S^{c_u} (u_* \phi_0)^{c_*} \tag{5.5}$$

where D = diameter of the scaled test vessel
ϕ_S = volume fraction of solids in the vessel
u_S = nominal settling velocity of the particles as they settle on to the floor of the vessel
u_*, ϕ_0 = material properties of the layer of settled solids

and c_{WTP}, c_D, c_ϕ, c_u, and c_* are coefficients to be estimated by fitting the model to experimental data. Equation (5.5) is the same as Equation (B.13) in Appendix B. This model was developed from a model presented by Kuhn et al. (2012), the details of which are shown in Appendix B. The model form in Equation (5.5) was developed to avoid the possibility of spurious correlation (Section 4.3.1), which results from having test parameters appear on both the right- and left-hand sides of the model equation. As shown in Appendix B, it is often possible to rewrite physically based models in mathematically equivalent forms so any input parameters on the left-hand side (e.g., in a dimensionless group) are transferred to the right-hand side of the model (thus avoiding the possibility of spurious correlation).

As discussed in Sections 2.1, 2.3, and 4.3.2, taking the natural logarithm of both sides of Equation (5.5) converts the model from having a multiplicative structure to having an additive structure. This assumes the error terms are also multiplicative (e.g., in Equations (2.8) and (2.12)), so that an additive structure is obtained for both model terms and error terms (e.g., in Equations (2.09) and (2.11)). Using natural logarithms instead of common logarithms is preferred because the SD of a natural-logarithm-transformed parameter is well approximated by the relative SD of the parameter without the transformation. This is a very useful approximation when quantifying uncertainties, so the natural logarithm transformation is preferred for that reason.

The model after taking the natural logarithms of both sides of Equation (5.5) is

$$\ln(U_{BC}) = ln(c_{WTP}) + c_D \ln(D) + c_\phi \ln(\phi_S) + c_u \ln(u_S) + c_* \ln(u_* \phi_0) \tag{5.6}$$

where all notation is as previously defined following Equation (5.5).

In this example, we assume that the experimental testing would be subject to restrictions 1–3 on the order of performing tests given in Table 2.2. Hence, the resulting data would have the

error structure discussed in Section 2.4, namely as given in Equation (2.11). The model term(s) in (5.6) associated with each error term identified in Equation (2.11) are

Scale: $\ln(D)$
Simulant: $\ln(u_S)$, $\ln(u_*\phi)$
Solids Concentration: $\ln(\phi_S)$

5.2.2 Discussion of Experimental Design for the Example

It was beyond the scope of this work to develop an experimental design (including a test matrix) for this U_{BC} example. However, we briefly discuss the steps of the process that would be used. The process would be somewhat different for Approach 1 versus Approach 2 as discussed in Section 4.1. The following discussion more directly addresses Approach 2, but some of the steps may still be applicable to Approach 1.

Several test parameters would be held fixed at specified levels indicated by Equations (B.7) to (B.10) in Appendix B. The test parameters that would be varied appear on the right-hand side of Equations (5.5) and (5.6), namely D, ϕ_S, u_S, and $u_*\phi_0$. It would be necessary for subject-matter experts working with a statistician to specify lower and upper bounds on these parameters and to determine the number of values and the values themselves of the parameters to be investigated experimentally. The spacing of the values must be decided, which for the example model in Equation (5.6) might be linear spacing in natural logarithm units of the parameters. In addition, if it is not possible or is undesirable for certain combinations of values of the test parameters to occur simultaneously, then the subject-matter experts and statistician would develop multiparameter constraints (i.e., inequality expressions) that specify the allowable combinations of test parameter values. The multidimensional space defined by the lower and upper bounds on the test parameters and the multiparameter constraints is referred to as the experimental region.

The experimental design would have to be constructed to contain a sufficient number of distinct test combinations to adequately "cover" the experimental region and provide for estimating the model coefficients (e.g., in Equation (5.6)) so as to provide acceptable uncertainties of model coefficients and model predictions of U_{BC}. If the matched-condition testing approach (Section 4.2.1) were chosen, then the distinct test combinations would be chosen independent of test scale, and run at all three test scales. Regardless, the statistical OED approach described in Section 4.2.2 could be used to provide for selecting test combinations adequately covering the experimental region to provide data robust to the assumed model form in Equation (5.6). That way, the experimental data will provide support for fitting other model forms if, after the data are collected, it is found that the model form in Equation (5.6) can be improved upon.

Also, sufficient replication would need to be planned into the text matrix to provide for estimating variance components associated with the restrictions on the order of performing tests (Section 4.2.4). As discussed in Section 4.2.4, partial replication must be used for some restrictions on the order of performing tests to avoid having a very large number of tests resulting from several kinds of replication. Determining appropriate numbers and patterns of replication requires significant effort, so that aspect of developing an experimental design is not illustrated in this example.

5.2.3 Discussion of Model Development, Fitting, and Evaluation for the Example

There are no existing data sets from previously conducted tank mixing studies that account for the restrictions on the order of performing tests and that included appropriate replication. Hence, there were no appropriate data to use for an example to illustrate model development, fitting, and evaluation as discussed in Section 4.3. We did consider using 1) the assumed model form in Equation (5.6), 2) some reasonable assumed coefficient values, and 3) the restricted error structure with assumed values of the multiple variance components to simulate a data set from an experimental design that could then have been used to illustrate model development, fitting, and evaluation. However, as noted previously, it was beyond the scope and schedule for this report to develop a full experimental design (including appropriate replication) for the example.

However, Kuhn et al. (2012) and Appendix B discuss the steps used in developing a physically based model for U_{BC}. Appendix B illustrates rewriting the model developed by Kuhn et al. (2012) into a mathematically equivalent form to avoid spurious correlation. Appendix B also illustrates generalizing the model by allowing the ϕ_S, u_S, and $u_*\phi_0$ terms to have separate coefficients (c_ϕ, c_u, and c_*) rather than the coefficients (c_θ, c_θ, and $-c_\theta$) corresponding to the θ_s dimensionless group. Generalizing a physically based model in this way provides for assessing the appropriateness of the physically based approach. If fitting the model in Equation (5.6) to experimental data yielded estimates of the coefficients c_ϕ, c_u, and c_* that were substantially different (after accounting for uncertainties) than the c_θ, c_θ, and $-c_\theta$ assumed relationships, it would indicate that an improvement in the physically based model may be needed. Otherwise, restricted least squares methods could be used to force those terms to have the same coefficient except for the sign.

When the LSIT tests are completed and data are available, the methods for evaluating the data (for potential outliers) and fitted models (to see whether they have significant LOFs to the data after accounting for uncertainties in the data) discussed in Section 4.3.3 should then be applied. These are important methods for assessing whether models for mixing performance metrics are adequate for extrapolating to full scale.

5.2.4 Examples and Discussion of Quantifying Uncertainties in Model Coefficients and Predictions of Mixing Performance for the Example

Because there is no appropriate real or simulated data set available with which to fit the example model in Equation (5.6), it is not possible to directly illustrate the methods for quantifying uncertainties in model coefficients and predictions of mixing performance summarized in Section 4.3.4. However, by assuming some intermediate results that might have resulted from the variance component estimation and model fitting, it is possible to illustrate the application of some key formulas in Section 4.3.4.

We assume that applying the REML variance-component estimation methodology discussed in Sections 3.1.3 and 4.3.2 to results of an experimental design (with appropriate replication at each level of restriction on the order of performing tests) yields the following variance component (SD) estimates:

$$SD_{Scale}^{\ln(U_{BC})} = 0.05,\ SD_{Simulant}^{\ln(U_{BC})} = 0.05,\ SD_{SolidsConc}^{\ln(U_{BC})} = 0.05, \text{ and } SD_{Error}^{\ln(U_{BC})} = 0.05 \qquad (5.7)$$

Applying Equation (5.2) yields $SD_{Total}^{\ln(U_{BC})} = 0.100$, as shown in Table 5.1. Hence, for this example, values of U_{BC} from the test matrix would have a total uncertainty of 10 %RSD.

Suppose it is desired to apply the fitted U_{BC} model to predict that metric of mixing performance for a full-scale vessel with a specified set of values for the input parameters of the model in Equation (5.6). Assume that the model-predicted value of $\ln(U_{BC}) = 2.48$, which corresponds to $U_{BC} = 12$ m/s.

Now we illustrate using the methods of Section 4.3.4 (to the extent possible for this limited example) to quantify the total uncertainty (SD) in the preceding predicted value of $\ln(U_{BC})$, and hence of U_{BC}. Per Equations (4.9) and (4.10), the TPSDs are calculated as $TPSD_{Mean} = [FPV_{Mean} + APV]^{0.5}$ and $TPSD_{Individual} = [FPV_{Individual} + APV]^{0.5}$. Suppose that Equations (4.6) and (4.7) yield

$$FPV_{Mean} = 0.020$$
$$FPV_{Individual} = [SD_{Total}^{\ln(U_{BC})}]^2 + FPV_{Mean} = [0.100]^2 + 0.020 = 0.030,$$

respectively. Also, assume that Equation (4.8) yields

$$APV = 0.003$$

under the assumption that the uncertainties in the model input parameters (the vector **x** in Equation (4.8)) are statistically independent, as discussed in Section 4.3.4.4. Then, Equations (4.9) and (4.10) yield

$$TPSD_{Mean} = [FPV_{Mean} + APV]^{0.5} = [0.020 + 0.003]^{0.5} = [0.023]^{0.5} = 0.152$$

$$TPSD_{Individual} = [FPV_{Individual} + APV]^{0.5} = [0.030 + 0.003]^{0.5} = [0.033]^{0.5} = 0.182$$

The above values are SDs of $\ln(U_{BC})$ values. By Equation (5.3), these can be interpreted as RSDs (or %RSDs via multiplying by 100). Hence, for this illustrative example, the predicted U_{BC} value of 12 m/s would have an estimated %RSD = 15.2 (18.2) if it is considered as the prediction of the long-term mean value (individual value) of U_{BC} for the specific set of input parameters used to make the prediction.

Now, suppose that

$$SD_{Scale}^{\ln(U_{BC})} = 0.10,\ SD_{Simulant}^{\ln(U_{BC})} = 0.10,\ SD_{SolidsConc}^{\ln(U_{BC})} = 0.10, \text{ and } SD_{Error}^{\ln(U_{BC})} = 0.10 \qquad (5.8)$$

instead of the values assumed in (5.7). Applying Equation (5.2) yields $SD_{Total}^{\ln(U_{BC})} = 0.200$, as shown in Table 5.1. Assuming $FPV_{Mean} = 0.040$ (twice as large as what was used previously because $SD_{Total}^{\ln(U_{BC})}$ is twice as large), then $FPV_{Individual} = 0.080$. Keeping $APV = 0.003$, then Equations (4.9) and (4.10) yield $TPSD_{Mean} = 0.207$ and $TPSD_{Individual} = 0.288$. Hence, for this revised illustrative example, the predicted U_{BC} value of 12 m/s would have an estimated %RSD = 20.7 (28.8) if it is considered as the prediction of the true, mean value (individual value) of U_{BC} for the specific set of input parameters used to make the prediction.

Keep in mind that the above example calculations use assumed (i.e., "made up") values of intermediate quantities that in reality must be calculated from the data and the fitted model resulting from an appropriate experimental design with appropriate replication at each level of restriction on the order of performing tests. Based on the amount of data and replication, expanded uncertainties such as a 95% confidence interval or a 95% prediction interval (see Sections 3.3 and 4.3.4.5) could be calculated for each predicted value of U_{BC} (or other mixing performance metrics modeled as a function of test parameters) corresponding to a specific set of input parameter values. Finally, because all of the example calculations use assumed (made up) values that may not represent reality, the results are "for information only."

5.2.5 Discussion of Quantifying Possible Uncertainties Not Observable from Testing Results

Section 4.4 discusses two possible kinds of uncertainty that are not directly observable from testing results. These include 1) a hypothesized model form to represent the relationship

between mixing performance responses and test parameters being incorrect, and 2) differences in scaled test vessels and simulants compared to WTP vessels and actual waste feed materials.

With respect to 1), as noted in Section 4.4.1, the greater the physical understanding of the observed behavior, the greater the ability to assess the validity of a scaling relationship at length scales beyond those tested, and hence the greater the ability to assess the uncertainty in extrapolating to larger scales. The usefulness of the test data is not just from regression to fit models to test data. Test data are equally important for validating a physical conceptual model, which then provides a basis for judging the range of length scales for which the model is valid.

The example model for U_{BC} in Equations (5.5) and (5.6) is a generalization of a physically based model discussed in Appendix B. The functional form of the model is based on a specific hypothesis about the phenomena that determine U_{BC}, as is discussed in Chapters 2 and 4 in Kuhn et al. (2012). This hypothesis resulted not only in the model form in Appendix B (and hence its generalization in Equation (5.5)), but also values of key model coefficients derived concomitantly with the model form. Thus, the model form and its coefficients are an important "expert opinion." In particular, the values of the coefficients c_D, c_ϕ, c_u, and c_* are each expected to fall within a narrow range of values consistent with the physical conceptual model for U_{BC}. Obtaining fitted coefficients substantially inconsistent with these expectations would invalidate the conceptual physical model. Conversely, coefficient values consistent with expectations would tend to validate the model form. To obtain the full weight of expert opinion on the side of validation might require supplemental tests designed to further evaluate detailed expectations implied by the model. For example, that may include observing the time required to clear the bottom in addition to the velocity required ultimately to clear it, or measurements of the rate of erosion of settled solids as a function of jet velocity. Both sets of supplemental data would serve to further validate physical concepts underlying the functional form of the model in Appendix B and its generalization in Equation (5.5). Assuming such experiments add to the confidence in the model form already established by a favorable fit of the model to the anticipated LSIT data set discussed above, the "expert opinion" would be that the phenomena actually controlling the bottom-clearing velocity are as hypothesized. Then, experts could evaluate whether there is any reason for the controlling phenomena to change as the length scale is increased from those of LSIT tests to that of the WTP. If the controlling phenomena do not change between LSIT and WTP tests, the model developed from LSIT data applies at the scale of the WTP, and the uncertainties of model predictions are limited to the uncertainties discussed in Section 4.3.4 and illustrated in Section 5.2.4.

With respect to 2) in the first paragraph, there are two parts to consider. First, there are expected to be small departures from geometric similitude in tanks used for LSIT compared to the corresponding vessels in WTP. Such small departures result from practical considerations, such as the cost of extensive machining to provide shapes matching WTP exactly compared to using standard metal sheet thicknesses and particularly pipe sizes, etc. The resulting inexactitude is correspondingly small and probably not a technical issue. Potential exceptions include

maintaining exact geometric similarity of the PJM arrays (number, relative size, and shape). Experts will need to consider the effect of the resulting change in the flow patterns on the associated transport of solids and ultimately on mixing.

Second, there are expected to be differences between the physical attributes of the slurries tested in LSIT compared to the actual waste in WTP. The most important properties are the average density of solids in the slurry, their settling rate, the rheological properties of the slurry, and the resistance of settled particles to suspension by adjacent fluid motion. These can be matched to the attributes of the WTP waste only approximately because the properties and their variation with solids concentration depend on details such as the particle size density distribution and chemical properties. Experts will need to consider the effect on density differences, settling of different particles, and rheological properties during mixing that might result from the impracticality of exactly matching all aspects of slurries in LSIT to actual WTP waste.

6.0 Summary

This report discusses the statistical methods for quantifying uncertainties in

A) test responses and other parameters that would be measured or calculated in the LSIT

B) estimates of coefficients and predictions of mixing performance from models developed to relate test responses to test parameters.

Testing at a larger scale has been committed to by Bechtel National, Inc., and DOE to "address uncertainties and increase confidence in the projected, full-scale mixing performance and operations"[1] in the WTP.

Current plans for the LSIT involve testing PJM technology in three scaled vessels with nominal diameters of 43 in., 8 ft, and 14 ft. It is anticipated that LSIT would use several test responses to quantify mixing performance, including *ECR*, U_{BC},[2] blending criteria, no solids accumulation during pump-out, and sampling requirements.

There may be practical restrictions on the order of performing LSIT tests over the three scales, including those listed in Table 6.1. Such restrictions on the order of performing tests

Table 6.1. Possible Practical Restrictions on the Order of Performing LSIT Tests

Restriction Number	Restriction on the Order of Performing Tests
1	Performing all tests for a given test vessel size (scale) before switching to a different test vessel size
2	Performing all tests with a given simulant for a given test vessel size before switching to a different simulant
3	Performing all tests with a given solids concentration for a given test vessel size and a given simulant before switching to a different solids concentration
4	Performing all tests with varying nozzle-jet velocities for a given combination of test vessel size, simulant, and solids concentration before switching to a different combination

[1] Hazen H. September 2011. *Contract No. DE-AC27-01RV14136- Hanford Tank Waste Treatment and Immobilization Plant, Memorandum of agreement (MOA) 24590-QL-WA49-00001, - Directive subcontractor change notice No. 119 for WA39LSIT testing*, CCN237865, Bechtel National, Inc., Richland, Washington.
[2] The minimum PJM nozzle-jet velocity required to achieve bottom motion of solids.

complicate the error structure of the resulting test data, compared to the simpler error structure that would apply if the tests could be performed in a completely randomized order. Specifically, instead of a single uncertainty component for a completely randomized data structure, there are k + 1 uncertainty components when there are k restrictions on the order of performing tests. Also, the restrictions cause subgroups of the test response values to have nonzero covariances. Appendix A gives the matrix-vector formulas for the variance-covariance matrices of the *ECR* and U_{BC} test responses under the more complicated error structure. The more complicated error structure that exists when there are restrictions on the order of performing tests must be accounted for in developing the LSIT experimental design and in analyzing the data (including developing models to predict mixing performance as a function of scale and other LSIT test parameters).

Sections 2.3 and 2.4 present possible additive and multiplicative data structures of LSIT test responses for *ECR* and U_{BC}. The data structures discussed in Sections 2.3 and 2.4 assume that restrictions 1–4 in Table 6.1 apply for *ECR* and restrictions 1–3 in Table 6.1 apply for U_{BC}. Estimates of the SDs for an additive data structure and the %RSD for a multiplicative data structure are:

- ***ECR Additive***: SD^{ECR}_{Scale}, $SD^{ECR}_{Simulant}$, $SD^{ECR}_{SolidsConc}$, $SD^{ECR}_{NozzleVel}$, and SD^{ECR}_{Error}
- ***ECR Multiplicative***: $\%RSD^{ECR}_{Scale}$, $\%RSD^{ECR}_{Simulant}$, $\%RSD^{ECR}_{SolidsConc}$, $\%RSD^{ECR}_{NozzleVel}$, and $\%RSD^{ECR}_{Error}$
- ***U_{BC} Additive***: $SD^{U_{BC}}_{Scale}$, $SD^{U_{BC}}_{Simulant}$, $SD^{U_{BC}}_{SolidsConc}$, and $SD^{U_{BC}}_{Error}$
- ***U_{BC} Multiplicative***: $\%RSD^{U_{BC}}_{Scale}$, $\%RSD^{U_{BC}}_{Simulant}$, $\%RSD^{U_{BC}}_{SolidsConc}$, and $\%RSD^{U_{BC}}_{Error}$

where the *Scale*, *Simulant*, *SolidsConc*, and *NozzleVel* subscripts correspond to the restrictions 1–4 in Table 6.1, respectively. The *Error* subscript refers to the uncertainties within test combinations of *Scale*, *Simulant*, and *SolidsConc* (for U_{BC}), as well as *NozzleVel* (for *ECR*).

The LSIT experimental design (i.e., the test matrix, including replicates; order of performing the tests; etc.) must be developed to provide for quantifying the uncertainties in A) and B) above and reducing the uncertainties in B). Statistical OED methods guided by subject-matter knowledge provide for distributing test parameter combinations (tests) over the test parameter space to provide optimal support for the model forms that may be fitted to the test-response data. Including replicates at each level of restriction on the order of performing tests provides for quantifying the SDs associated with the sources of uncertainty in the data. Statistical experimental design methods provide for determining the amount of replication needed to estimate as precisely as possible the SDs given a specified limit on the total number of tests.

The guidance document ASME PTC 19.1-2005 (*Test Uncertainty*, ASME 2006) discusses many useful methods for quantifying uncertainties in test responses and parameters that are discussed in this report. Section 3.2 discusses the error propagation methodology for calculating the uncertainty in a parameter expressed as a known function of other uncertain parameters. Section 3.3 discusses the concepts of combined uncertainties (combining estimates of uncertainty from all sources into a single total uncertainty) and expanded uncertainties (uncertainties with a multiplier chosen to provide a specified level of statistical confidence). However, uncertainties resulting from restrictions on the order of performing tests in a test matrix are not directly addressed by ASME (2006). Hence, statistical methods from other references (e.g., Montgomery et al. 2001; Goos et al. 2006; Kowalski et al. 2007) are also required.

Assuming an appropriate experimental design with adequate replication at the different levels of restriction on the order of performing tests, the method for estimating the associated SDs for a given test response is discussed in Section 3.1.3. Section 3.1.4 discusses how replicate measurements may be averaged to effectively reduce the magnitude of SD^{Y}_{Error} or $\%RSD^{Y}_{Error}$, where Y is a given test response. Section 3.1.5 gives the formulas for quantifying the total uncertainty (SD or %RSD) in values of the test responses ECR and U_{BC}, assuming the data structures in Table 6.1, as discussed previously. For example, if U_{BC} has a multiplicative data structure, the total %RSD is given by

$$\%RSD^{U_{BC}}_{Total} = [(\%RSD^{U_{BC}}_{Scale})^2 + (\%RSD^{U_{BC}}_{Simulant})^2 + (\%RSD^{U_{BC}}_{SolidsConc})^2 + (\%RSD^{U_{BC}}_{Error})^2]^{0.5} \quad (6.1)$$

where the notation is as defined previously.

Section 4 presents and discusses methods for reducing and quantifying the uncertainties of full-scale mixing performance using models developed from LSIT data. Section 4.1 discusses two approaches for developing the experimental design for LSIT. Section 4.2 discusses the OED method for generating test parameter combinations to

- adequately "cover" the test parameter space (which may be expressed in terms of dimensional and/or dimensionless parameters)

- provide support for fitting models of the forms that might be required to adequately represent the dependence of mixing performance on test parameters, including scale.

Section 4.2 also discusses and illustrates what is meant by replicates at each level of restriction on the order of performing tests, and describes approaches that would provide sufficient numbers of replicates at each level of restriction without having too large a total number of tests.

Section 4.3.1 discusses the development of model forms for test responses as functions of test parameters (dimensional, and/or dimensionless). It also describes 1) the concept of spurious

correlation, (which can result in a model form appearing to fit experimental data better than it actually does), and 2) methods for re-expressing models to mathematically equivalent forms to avoid spurious correlation. Section 4.3.2 discusses the FGLS methodology for fitting models to data that have more complicated error structures because of restrictions on the order of performing tests. Section 4.3.3 discusses methods for evaluating how well a model form fits a given data set, and whether the uncertainties in model predictions are within the uncertainty of the data. Section 4.3.4 presents matrix-vector formulas for quantifying uncertainties in model coefficients and model predictions of mixing performance. The total uncertainty in a model prediction comprises fitting prediction uncertainty (uncertainty resulting from fitting model coefficients to experimental data) and application prediction uncertainty (uncertainty resulting from uncertainties in the model parameter values used to make the prediction). The variance components associated with these two sources of model prediction uncertainty are denoted *FPV* and *APV*, respectively. The *FPV* can be calculated considering the predicted value to be an estimate of 1) the true, unknown mean for the given set of input parameter values (denoted FPV_{Mean}), or 2) an individual test result (denoted $FPV_{Individual}$).

Section 5 presents example applications and discussions of the methods for quantifying uncertainties discussed in Sections 3 and 4. For the examples in Section 5, it is assumed that models for mixing performance metrics have a multiplicative structure (e.g., power-law models) with multiplicative errors. Then, taking the natural logarithm of both sides of the model yields an additive model form with additive errors.

Table 5.1 in Section 5.1.1 lists the values of $SD_{Total}^{\ln(ECR)}$ and $SD_{Total}^{\ln(U_{BC})}$ that result from the formulas

$$SD_{Total}^{\ln(ECR)} = [(SD_{Scale}^{\ln(ECR)})^2 + (SD_{Simulant}^{\ln(ECR)})^2 + (SD_{SolidsConc}^{\ln(ECR)}) + (SD_{NozzleVel}^{\ln(ECR)})^2 + (SD_{Error}^{\ln(ECR)})^2]^{0.5} \quad (6.2)$$

$$SD_{Total}^{\ln(U_{BC})} = [(SD_{Scale}^{\ln(U_{BC})})^2 + (SD_{Simulant}^{\ln(U_{BC})})^2 + (SD_{SolidsConc}^{\ln(U_{BC})}) + (SD_{Error}^{\ln(U_{BC})})^2]^{0.5}, \quad (6.3)$$

where the SDs on the right-hand sides of the equations take all possible combinations of the values 0.05 and 0.10. The approximate relationship

$$SD[\ln(y)] \approx RSD(y) \quad (6.4)$$

indicates that the SDs on both sides of Equations (6.2) and (6.3) can be interpreted as %RSDs (i.e., 100 × RSD). Hence, the values of 0.05 or 0.10 for SDs on the right-hand sides of the equations correspond to %RSD values of 5% or 10%. The $SD_{Total}^{\ln(ECR)}$ values from Equation (6.2) range from 0.112 to 0.224 (11.2 to 22.4 %RSD), while the $SD_{Total}^{\ln(U_{BC})}$ values from Equation (6.3)

range from 0.100 to 0.200 (10 to 20 %RSD). The $SD_{Total}^{\ln(U_{BC})}$ values are smaller than the $SD_{Total}^{\ln(ECR)}$ values because the latter have one extra estimated SD ($SD_{NozzleVel}^{\ln(ECR)}$) that contributes to the total SD.

Section 5.1.2 contains an example illustrating application of the error propagation methods from Section 3.2 to calculate the uncertainty in the estimated PJM nozzle velocity based on uncertainties of the input parameters in an equation used to estimate the PJM nozzle velocity.

Section 5.2 presents applications and discussion of the methods (in Section 4) for quantifying uncertainties of full-scale mixing performance using an example model for U_{BC},

$$U_{BC} = c_{WTP} D^{c_D} \phi_S^{c_\phi} u_S^{c_u} (u_* \phi_0)^{c_*}, \tag{6.5}$$

where D = diameter of the scaled test vessel
ϕ_S = volume fraction of solids in the vessel
u_S = nominal settling velocity of the particles as they settle on to the floor of the vessel
u_*, ϕ_0 = material properties of the layer of settled solids

and c_{WTP}, c_D, c_ϕ, c_u, and c_* are coefficients to be estimated by fitting the model to experimental data. To avoid spurious correlation, a physically based model developed by Kuhn et al. (2012) was re-expressed in the mathematically equivalent form in Equation (6.5), as discussed in Appendix B. Because Equation (6.5) has a multiplicative structure and is under the assumption that the error structure is multiplicative, taking the natural logarithm of both sides yields

$$\ln(U_{BC}) = \ln(c_{WTP}) + c_D \ln(D) + c_\phi \ln(\phi_S) + c_u \ln(u_S) + c_* \ln(u_* \phi_0) \tag{6.6}$$

where all notation is as previously defined. Assuming that the experimental design would be subject to restrictions 1–3 on the order of performing tests given in Table 6.1, the model term(s) in (6.6) associated with each error term are

Scale: $\ln(D)$
Simulant: $\ln(u_S)$, $\ln(u_* \phi)$
Solids Concentration: $\ln(\phi_S)$.

It was beyond the scope of work summarized in this report to develop an experimental design (including a test matrix) for this U_{BC} example. Section 5.2.2 briefly discusses the steps of the process that would be used to develop an experimental design.

There are no existing data sets from previous tank mixing studies that 1) were conducted accounting for the restrictions on the order of performing tests, and 2) included appropriate replication. Hence, there were no existing data that could be used to illustrate the model fitting and evaluation methods discussed in Section 4.3. Because developing an experimental design for the example model was beyond the scope of the effort, it was not possible to simulate a data set using specified model coefficient values and estimates of the SDs for the multiple sources of uncertainty associated with restrictions on the order of performing tests. However, Section 5.2.3 discusses development of the example model in Equation (6.5) and notes that model evaluation methods could be applied if a data set were available.

Section 5.2.4 contains examples and discussion of the methods in Section 4.3.4 for quantifying uncertainties in model predictions of mixing performance. Because no real or simulated data were available, some intermediate values were assumed that would normally be obtained by analyzing data from an experimental design with appropriate replication. Assuming

$$\hat{\sigma}_{Scale}^{\ln(U_{BC})} = 0.05\,,\ \hat{\sigma}_{Simulant}^{\ln(U_{BC})} = 0.05\,,\ \hat{\sigma}_{SolidsConc}^{\ln(U_{BC})} = 0.05\,,\text{ and }\ \hat{\sigma}_{Error}^{\ln(U_{BC})} = 0.05 \qquad (6.7)$$

and applying Equation (6.3) yields $SD_{Total}^{\ln(U_{BC})} = 0.100$. This can be interpreted, via Equation (6.4), as U_{BC} values from the test matrix having a total uncertainty of 10 %RSD.

Suppose the fitted U_{BC} model Equation (6.6) was available and used to predict U_{BC} for a full-scale vessel with a specified set of values for the input parameters of the model. Assume that the model-predicted value of $\ln(U_{BC}) = 2.48$, which corresponds to $U_{BC} = 12$ m/s. As shown in Section 5.2.4, Equations (4.6) and (4.7) yield $FPV_{Mean} = 0.020$ and $FPV_{Individual} = 0.030$, respectively. Then, assuming that Equation (4.8) yields $APV = 0.003$, Equations (4.9) and (4.10) yield

$$TPSD_{Mean} = [FPV_{Mean} + APV]^{0.5} = [0.020 + 0.003]^{0.5} = [0.023]^{0.5} = 0.152$$

$$TPSD_{Individual} = [FPV_{Individual} + APV]^{0.5} = [0.030 + 0.003]^{0.5} = [0.033]^{0.5} = 0.182,$$

respectively. The above values are *TPSD*s of the predicted value $\ln(U_{BC}) = 2.48$. Via Equation (6.4), these can be interpreted as %RSD =15.2 if the predicted value of $U_{BC} = 12$ m/s is considered a prediction of the long-term mean value, and %RSD = 18.2 if it is considered a prediction of an individual value.

A second example in Section 5.2.4 uses 0.10 instead of 0.05 for each of the four SDs in Equation (6.7). The results are $TPSD_{Mean} = 0.207$ and $TPSD_{Individual} = 0.288$. Via Equation (6.4), these can be interpreted as %RSD values of 20.7 if the predicted value of $U_{BC} = 12$ m/s is considered a prediction of the long-term mean value, and 28.8 if it is considered a prediction of an individual value.

In conclusion, LSIT testing is planned to be performed in three scaled test vessels, with the order of performing the tests expected to be subject to several restrictions. Such restrictions result in a more complicated variance-covariance matrix for the data (which has the sum of all relevant variance components in the diagonal elements of the matrix, and nonzero covariances in several off-diagonal elements). The nonzero covariances are also sums of certain variance components. Hence, estimating the whole variance-covariance matrix requires estimating only the multiple variance components associated with the restrictions on the order of performing the tests. The experimental design for LSIT must be constructed to adequately "cover" the test parameter space (in dimensional and/or nondimensional parameter space) so as to provide support for fitting the model forms hypothesized. The experimental design must also include sufficient replication at each level of restriction to provide for quantifying the associated variance components. Then, statistical methods can be applied to fit the physically based models to the experimental data, and to evaluate the data for outliers and the models for adequate fits. Initially hypothesized model forms may be revised based on model evaluation methods. When final fitted versions of physically based models are obtained that fit the data within its uncertainty, they can then be used to predict mixing performance for full-scale vessels. Statistical methods for quantifying uncertainties of model predictions can be applied to attach uncertainties to predicted values of the mixing performance metrics.

7.0 References

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Appendix A

Variance-Covariance Matrices for Example LSIT Data Structures of *ECR* and U_{BC} Test Responses

Appendix A

Variance-Covariance Matrices for Example LSIT Data Structures of *ECR* and U_{BC} Test Responses

Section A.1 displays the variance-covariance matrices for the effective clearing radius (*ECR)* test response assuming the Large Scale Integrated Testing (LSIT) data structure discussed in Section 2.3. Section A.2 displays the variance-covariance matrices for the U_{BC} test response assuming the LSIT data structure discussed in Section 2.4.

A.1 Variance-Covariance Matrices for the *ECR* Test Response with an Example LSIT Data Structure

The variance-covariance matrix corresponding to the additive data structure for *ECR* in Equation (2.8) of Section 2.3 is given by

$$\mathbf{V}_{ECR} = \sigma^2_{Scale}\mathbf{ZZ}'+\sigma^2_{Simulant}\mathbf{PP}'+\sigma^2_{SolidsConc}\mathbf{QQ}'+\sigma^2_{NozzleVel}\mathbf{RR}'+\sigma^2_{Error}\mathbf{I}_n \qquad \text{(A.1)}$$

where $\mathbf{Z}$ is an $n \times b$ matrix with i^{th} row equal to $\mathbf{z_i}$, $\mathbf{P}$ is an $n \times c$ matrix with i^{th} row equal to $\mathbf{p_i}$, $\mathbf{Q}$ is an $n \times d$ matrix with ith row equal to $\mathbf{q_i}$, $\mathbf{R}$ is an $n \times e$ matrix with i^{th} row equal to $\mathbf{r_i}$, and $\mathbf{I}_n$ is an $n \times n$ identity matrix (i.e., with ones on the diagonal and zeroes elsewhere). The constant n is the number of test runs in the experimental design (i.e., test matrix), while the constants b, c, d, and e are respectively the numbers of distinct scaled test vessels, simulants, solids concentration levels and nozzle velocity levels in the experiment. Further, $\mathbf{z}_i$ is an indicator vector with a one in the k^{th} position if the i^{th} run involves the k^{th} scale and zero otherwise. Similarly, $\mathbf{p}_i$ is an indicator vector with a one in the k^{th} position if the i^{th} run involves the k^{th} simulant (within a scale) and zero otherwise. The vectors $\mathbf{q}_i$ and $\mathbf{r}_i$ are similarly defined for solids concentration and nozzle velocity. The variances σ^2_{Scale}, $\sigma^2_{Simulant}$, $\sigma^2_{SolidsConc}$, and $\sigma^2_{NozzleVel}$ are the variance components associated with the corresponding restrictions on the order of performing tests. The variance σ^2_{Error} is associated with the random errors in the test response for a given set of values of all other test parameters.

With the multiplicative structure for *ECR* in Equation (2.7) of Section 2.3, the modeling approach could be to take the natural logarithm of both sides so that the model and error structure are then additive. The variance-covariance matrix for that approach would then have the same form as in Equation (A.1), except that σ^2_{Scale}, $\sigma^2_{Simulant}$, $\sigma^2_{SolidsConc}$, $\sigma^2_{NozzleVel}$, and σ^2_{Error} would be for natural logarithm transformations of *ECR*.

A.2 Variance-Covariance Matrices for the U_{BC} Test Response with an Example LSIT Data Structure

The variance-covariance matrix corresponding to the additive data structure for U_{BC} in Equation (2.11) of Section 2.4 is given by

$$\mathbf{V} = \sigma^2_{Scale}\mathbf{ZZ}'+\sigma^2_{Simulant}\mathbf{PP}'+\sigma^2_{SolidsConc}\mathbf{QQ}'+\sigma^2_{Error}\mathbf{I}_n \qquad \text{(A.2)}$$

where the notation is as defined in Section A.1.

With the multiplicative structure for U_{BC} in Equation (2.12) of Section 2.4, the modeling approach could be to take the natural logarithm of both sides so that the model and error structure are then additive. The variance-covariance matrix for that approach would then have the same form as in Equation (A.2), except that σ^2_{Scale}, $\sigma^2_{Simulant}$, $\sigma^2_{SolidsConc}$, and σ^2_{Error} would be for natural logarithm transformations of U_{BC}.

We now illustrate the matrices in the variance-covariance matrix formula in Equation (A.2), for an example[(1)] with the U_{BC} response and a balanced experiment with 16 total runs. This includes eight runs at each of the two different scales (conducted as two whole plots), two simulants (run as two sub-plots within each whole plot), two solids concentrations conducted as sub-sub-plots within each sub-plot, and finally an application of the process incrementing nozzle velocity to determine U_{BC} for each of the pairs of eight combinations of scale, simulant, and solids concentrations. The matrices $\sigma^2_{Scale}\mathbf{ZZ}'$, $\sigma^2_{Simulant}\mathbf{PP}'$, $\sigma^2_{SolidsConc}\mathbf{QQ}'$, and $\sigma^2_{Error}\mathbf{I}_n$ are shown in Figures A.1 to A.4, respectively. These matrices assume the data are ordered such that

- Scale varies least frequently (i.e., tests 1-8 are at one scale, and tests 9-16 are at the second scale)
- Simulant varies next most frequently (i.e., tests 1–4 and 9–12 use the first simulant, while tests 5–8 and 13–16 use the second simulant)
- Solids concentration varies the next most frequently (i.e., tests 1, 2, 5, 6, 9, 10, 13, 14 use the first solids concentration, while tests 3, 4, 7, 8, 11, 12, 15, and 16 use the second solids concentration)
- The measurement process to determine U_{BC} varies the most frequently (i.e., is replicated twice for each of tests 1–16).

(1) This example was not constructed to be realistic, but rather to be simple enough to produce a variance-covariance matrix whose component matrices could be displayed.

This order was selected for simplicity in displaying the matrices. In practice, the order of testing the values of each test parameter should be randomized within each level of restriction on the order of performing tests.

Finally, recall that this example for U_{BC} with two values for each test parameter and no replication was chosen solely to keep the total number of tests to a bare minimum to enable illustrating the forms of the matrices, which when added together, form the variance-covariance matrix for the data. In reality, the appropriate numbers of values of each test parameter would be investigated, and some (e.g., partial) replication would be required at each level of restriction on the order of performing the tests. The specific combinations of test parameters and the replications comprising an actual test matrix should be determined using statistical experimental design methods and software (which account for the complicated split-plot structure of the data) in combination with subject-matter expertise.

$$
\begin{bmatrix}
\sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale} & \sigma^2_{Scale}
\end{bmatrix}
$$

Figure A.1. The $\sigma^2_{Scale}\mathbf{ZZ}'$ Matrix from Equation (A.2) for the U_{BC} Example

$$
\begin{bmatrix}
\sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant} & \sigma^2_{Simulant}
\end{bmatrix}
$$

Figure A.2. The $\sigma^2_{Simulant}\mathbf{PP}'$ Matrix from Equation (A.2) for the U_{BC} Example

$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0	0	0	0	0	0	0	0	0	0	0
0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0	0	0	0	0	0	0	0	0
0	0	0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0	0	0	0	0	0	0
0	0	0	0	0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0	0	0	0	0
0	0	0	0	0	0	0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0	0	0
0	0	0	0	0	0	0	0	0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0
0	0	0	0	0	0	0	0	0	0	0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$
0	0	0	0	0	0	0	0	0	0	0	0	0	0	$\sigma^2_{SolidsConc}$	$\sigma^2_{SolidsConc}$

Figure A.3. The $\sigma^2_{SolidsConc}\mathbf{QQ}'$ Matrix from Equation (A.2) for the U_{BC} Example

σ^2_{Error}	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	σ^2_{Error}	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	σ^2_{Error}	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	σ^2_{Error}	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	σ^2_{Error}	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	σ^2_{Error}	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	σ^2_{Error}	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	σ^2_{Error}	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	σ^2_{Error}	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	σ^2_{Error}	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	σ^2_{Error}	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	σ^2_{Error}	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	σ^2_{Error}	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	σ^2_{Error}	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	σ^2_{Error}	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	σ^2_{Error}

Figure A.4. The $\sigma^2_{Error}\mathbf{I}_n$ Matrix from Equation (A.2) for the U_{BC} Example

Appendix B

Development of a Physical Model for U_{BC}

Appendix B

Development of a Physical Model for U_{BC}

The Hanford Waste Treatment and Immobilization Plant (WTP) is being designed and built to pre-treat and vitrify a large portion of the waste stored in the Hanford Site's 177 underground waste storage tanks. Several process vessels will hold the waste at various processing stages. These vessels have mixing[(1)] system requirements to maintain conditions in which hydrogen gas accumulation remains below acceptable limits, and mixing within the vessels is sufficient to make sure that pump transfer and normal operations occur reliably. WTP uses pulse jet mixing (PJM) technology for slurry mixing applications. There is a suction phase, during which process liquid is drawn into the PJM from the vessel. That is followed by the drive phase, during which air in the PJM is pressurized, discharging the PJM liquid contents at high velocity into the vessel, causing mixing to occur. A PJM system differs fundamentally from many industrial mixers. In a sense, PJMs alternate between mixing success and failure during every pulse cycle. During the refill phase, some of the solids settle from the slurry, which nominally is a failure in mixing, but during the drive phase all of the solids can be resuspended. The extent to which settled solids are cleared from the vessel floor and resuspended can be linked fundamentally to the momentum flow rate out of the PJM during the drive phase.

Thus, it is essential to predict the minimum momentum flow rate at which settled solids are cleared from the bottom of a WTP vessel. One approach is presented by Kuhn et al. (2012) based on 1) the expected behavior of the radial wall jet on the vessel flow induced by the PJM momentum, and 2) certain hypotheses about the relationship of shear stress action on the settled solids to the rate of erosion of the solids. See Sections 2.2.2 and 2.2.3 of Kuhn et al. (2012) for details. The result is the expression

$$\sqrt{K_{BC}} = c_0 r^{c_r} \left(r/H\right)^{c_H} d_S^{c_S} \left(1+\theta_S\right)^{c_\theta} \tag{B.1}$$

where K_{BC} = minimum kinematic momentum flow from the PJM that clears the settled solids (termed the "bottom clearing" condition)

r = radius from the centerline of the PJM out to the collision of the radial wall jet with those from surrounding PJMs

H = distance from the PJM nozzle to the vessel floor

(1) Mixing refers to the mobilization and subsequent suspension of undissolved solids within a vessel. Mixing can have varying results: 1) a fully-mixed vessel where the solids concentration is uniform throughout the vessel, 2) a partially mixed vessel where there is a solids concentration gradient that is higher at the bottom of the vessel, or 3) a poorly mixed vessel where the solids are disturbed but remain on or near the bottom of the vessel.

d_S = nominal diameter of the particles forming the settled solids
θ_S = dimensionless group as defined in Equation (B.2).

and c_0, c_r, c_H, c_S, and c_θ are coefficients to be estimated by fitting the model to data. Also in Equation (B.1), θ_S is given by

$$\theta_S = \frac{\phi_S u_S t_S}{(u_* \phi_0) t_D} \tag{B.2}$$

where ϕ_S = volume fraction of solids in the vessel
u_S = nominal settling velocity of the particles as they settle on to the floor of the vessel
t_S = time during which the particles settle
u_*, ϕ_0 = material properties of the layer of settled solids
t_D = time available for the PJM momentum to clear the settled solids.

Kuhn et al. (2012) evaluated θ_S by assuming that the product $(u_* \phi_0)$ is small enough that $\theta_S >> 1$, in which case the $(1 + \theta_S)$ in Equation (B.1) may be replaced by θ_S. Doing that and then substituting Equation (B.2) into Equation (B.1) yields

$$\sqrt{K_{BC}} = c_0 r^{c_r} \left(\mathrm{r/H}\right)^{c_H} d_S^{c_S} \phi_S^{c_\theta} u_S^{c_\theta} \mathrm{t_S^{c_\theta}} \left(u_* \phi_0\right)^{-c_\theta} t_D^{-c_\theta} \tag{B.3}$$

The radius r can be estimated by assuming each PJM clears the same area of settled solids

$$r = \left(D / 2\sqrt{N_J}\right) \tag{B.4}$$

where D is the diameter of the vessel and N_J is the number of PJMs in the vessel. The momentum flow rate is the product of the volumetric flow rate and the velocity. Evaluating this at the PJM nozzle gives

$$\sqrt{K_{BC}} = \sqrt{\frac{\pi}{4}}\, d_J U \tag{B.5}$$

where d_J is the diameter of the PJM nozzle and U is the PJM nozzle velocity. Substituting Equations (B.4) and (B.5) into Equation (B.3) yields

$$\sqrt{\frac{\pi}{4}} d_J U_{BC} = c_0 \left(D / 2\sqrt{N_J}\right)^{c_r} \left(\mathrm{D/H}\right)^{c_H} \left(2\sqrt{N_J}\right)^{-c_H} \phi_S^{c_\theta} u_S^{c_\theta} \mathrm{t_S^{c_\theta}} \left(u_* \phi_0\right)^{-c_\theta} t_D^{-c_\theta} \tag{B.6}$$

If the Large Scale Integrated Testing were going be done using Approach 1 discussed in Section 4.1, consider the tests associated with a single type of WTP vessel. All tests would be done for one set of parameters specified to maintain geometric similitude. Regarding the parameters considered here, the values of the ratios d_J/D and H/D would be kept constant at the values of the ratio in the WTP vessel. Thus we would have

$$d_J / D = (d_J / D)_{WTP} \tag{B.7}$$

$$H/D = (H/D)_{WTP} \tag{B.8}$$

$$N_J = (N_J)_{WTP} \tag{B.9}$$

Also, the ratio t_S/t_D would be kept constant at its value for that WTP vessel, so that

$$(t_S / t_D) = (t_S / t_D)_{WTP} \tag{B.10}$$

Substituting Equations (B.7) to (B.10) into Equation (B.6) and solving for U_{BC} yields

$$U_{BC} = c_{WTP} D^{c_r - 1} \phi_S^{c\theta} u_S^{c\theta} (u_* \phi_0)^{-c\theta} \tag{B.11}$$

where

$$c_{WTP} = c_0 \sqrt{\frac{4}{\pi}} \left(2\sqrt{N_J}\right)_{WTP}^{-c_r} (d_J / D)_{WTP}^{-1} (\mathrm{D/H})_{WTP}^{cH} \left(2\sqrt{N_J}\right)_{WTP}^{-cH} (t_S / t_D)_{WTP}^{c\theta} \tag{B.12}$$

is a constant depending on the identity of the WTP vessel on which the testing is based.

If the form of the model Equation (B.11) is correct, but one wants to assess whether ϕ_S, u_S, and $(u_*\phi_0)$ all have coefficients equal to c_θ or its negative, the following generalized form of Equation (B.11) may be considered

$$U_{BC} = c_{WTP} D^{cD} \phi_S^{c\phi} u_S^{cu} (u_* \phi_0)^{c*} \tag{B.13}$$

where ϕ_S, u_S, and $(u_*\phi_0)$ have been given different exponents (coefficients). In this equation, we assume the components of the product $(u_*\phi_0)$ cannot be distinguished physically from the tests done to check the functional form for U_{BC}. Hence, this product is treated as a single parameter.

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