ASME VVUQ 20.1-2024

Multivariate Metric for Validation

Supplement to ASME V&V 20-2009

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FOREWORD

In 2009, the ASME V&V 20 Committee published ASME V&V 20, Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer. The Standard presents a verification and validation approach that quantifies the modeling error of a mathematical/computational model for a specified quantity of interest at a specified validation point. This means that the procedure presented in the Standard applies to pointwise validation variables. This Supplement presents a technique to perform a global evaluation of the modeling error of multiple validation variables using the same framework of the pointwise technique: comparison of simulation solutions with experimental data, and includes the experimental, input-parameter and numerical uncertainties that contribute to the validation uncertainty. This multivariate metric can account for uncertainties shared by the multiple validation variables and indicates if discrepancies between simulations and experiments are globally within the validation uncertainties or cannot be explained by the validation uncertainties. Therefore, the interpretation of the results obtained from the multivariate metric requires the knowledge of the validation uncertainties obtained from the pointwise technique; therefore, it works as a complement to the pointwise technique and not as a replacement.

This supplement presents the following:

(a) a short description of the pointwise technique presented in the ASME V&V 20 Standard, to allow the use of this supplement as a self-contained document

(b) the description of the multivariate metric and the definition of a reference value to make the outcome independent of the number of validation variables selected

(c) a simple example illustrating the effect of correlation with discussion and caveats

(d) Nonmandatory Appendix A: a detailed description of the determination of the validation covariance matrix that depends on the experimental, numerical, and input parameter uncertainties for the four types of validation variables considered in the ASME V&V 20-2009 Standard

(e) Nonmandatory Appendix B: the application of the multivariate metric to the example-problem of the ASME V&V 20 Standard

(f) Nonmandatory Appendix C: examples of evaluation of the validation covariance matrix with discussion of the assumptions required for its determination.

Richard Hills is the original author of the first draft of the main body of this document developing the multivariate metric approach. In 2019, a working group comprising Leonard Peltier, Urmila Ghia, Laura Savoldi, Nima Fathi, and Kevin Dowding undertook the task of revising the draft and developing appendices to mature the document as an instructional guide. In 2022, Luís Eça joined the working group. The group finalized the technical contents of this document and ushered this document through review to become a supplement to the ASME V&V 20-2009 standard.

ASME VVUQ 20.1-2024 was approved as an American National Standard on February 26, 2024.

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PREFACE

The ASME VVUQ 20 Subcommittee for Verification, Validation, and Uncertainty Quantification in Computational Fluid Dynamics and Heat Transfer is developing documents that describe techniques that allow users of modelling and simulation, particularly in computational fluid dynamics and heat transfer, to assess the modeling (validation) and numerical (verification) accuracy of their simulations. The following are standards that have been issued or are being developed by this committee as of the issuance of this supplement:

ASME V&V 20, Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer, presents techniques to quantify modeling, numerical, and experimental accuracy for quantities of interest defined by a scalar quantity. The techniques apply to a specified variable at a specified validation point and are based on the comparison of simulation results with experimental data. Simulations and experiments are assumed to have been performed for the same conditions, i.e., same domain, boundary conditions, material properties, and heat transfer coefficients.

ASME VVUQ 20.1, Multivariate Metric for Validation, presents a technique that builds on the pointwise technique of ASME V&V 20 to make a global assessment of the discrepancies between multiple validation variables obtained from experiments and simulations. The metric can be applied to the same validation variable at different locations in space and/or at different time instants, or to different validation variables at the same location and time instant, or even to a combination of both. Furthermore, the multivariate metric can work with experimental, numerical, and input-parameter uncertainties that are independent or shared by the multiple validation set points.

ASME VVUQ 20.2, Regression at an Application Point, extends the technique presented in the ASME V&V 20 to validation variables obtained at an application point where experimental data are not available. The regression is based on a weighted least-squares approach that accounts for uncertainty in the data. The method can be used for both interpolation and extrapolation to ensure that the validation range covers the domain of application. The methodology illustrates how to couple the concepts and procedures presented in ASME V&V 20 with standard statistical techniques.

The ASME VVUQ 20.1 and ASME VVUQ 20.2 supplements may be read as stand-alone documents, but the details of the techniques to estimate experimental, numerical, and input-parameter uncertainties are only presented in ASME V&V 20.

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MULTIVARIATE METRIC FOR VALIDATION

1 PURPOSE

This supplement presents a multivariate metric to determine a global assessment of the discrepancies between experiments and simulations based on pointwise results from multiple validation set points within an application domain. It serves to extend the application of the pointwise or local assessment of the modeling error presented in ASME V&V 20-2009. A set point corresponds to the comparison of simulated and experimental values with their respective uncertainties obtained for a specified variable at a specified validation point.

A reference value is defined to account for the dependence of the multivariate metric on the number of validation set points. The reference value is defined from the expected value of the multivariate metric plus its standard uncertainty. As a consequence, the comparison of the multivariate metric with the reference value indicates if modeling errors are globally smaller than, equal to or larger than the validation uncertainty produced by experimental, numerical and input parameters uncertainties. The application and interpretation of the multivariate metric is similar to the application of the pointwise technique at each of the multiple validation set points.

In this supplement, a summary of the ASME V&V 20-2009 pointwise metric is outlined (para. 4.1), followed by a high-level description and example of the multivariate metric (para. 4.2 and section 5, respectively). To improve clarity in the body of the document, the detailed formulation of the multivariate metric is reserved for Nonmandatory Appendix A, and a detailed example (i.e., fin-tube heat exchanger) covering multiple use-cases is outlined in Nonmandatory Appendix B. Nonmandatory Appendix C presents examples of the choices required in the procedure for using the multivariate metric.

2 SCOPE

The scope of this supplement is similar to the pointwise validation metric described in ASME V&V 20-2009 (see also Eça, Dowding, and Roache, 2022). Therefore, the multivariate metric applies to quantities of interest that are defined by a scalar quantity. The present document describes the formulations of the multivariate metric for each of the four types of validation variables presented in ASME V&V 20-2009: validation variables obtained from a direct measurement (type 1), a combination of other uncorrelated or correlated measured variables in a data reduction equation (types 2 and 3), or in an independent model or analytic equation (type 4).

Multiple set points may be defined for the same validation variable at different locations in space and/or time instants, or by different validation variables at the same location and time instant, or even by a combination of both. Furthermore, the multivariate metric can work with experimental, numerical, and input uncertainties that are independent or shared by the multiple validation set points.

3 MOTIVATION AND INTRODUCTION

ASME V&V 20-2009 presents a validation approach for estimating the model error, δ_{model}, considering experimental, numerical, and input uncertainties in the reported comparison data from an experiment, D, and a simulation S (see also Eça, Dowding, and Roache, 2022). The committee that developed ASME V&V 20-2009 limited its initial consideration to validation for a single validation variable defined by a scalar quantity at a single validation set point. The validation variable can be a single directly measured variable, a single dimensional variable determined from a combination of other measured variables (a data reduction equation), or a single dimensionless variable (such as Nusselt number or friction coefficient) determined from a combination of other variables (measured variables used in an independent model or analytic equation to determine the validation variable). The ASME V&V 20-2009 approach characterizes an interval for δ_{model} as $\delta_{\text{model}} \in (E - u_{\text{val}}, E + u_{\text{val}})$. This interval is centered at the comparison error, E, and has a width proportional to the validation uncertainty u_{val}. E is the difference between the results of the simulation S and experiment D ($E = S - D$), and u_{val} depends on the experimental uncertainty u_D, the numerical uncertainty u_{num}, and the input parameter uncertainty u_{input} that characterize the experimental error δ_D, numerical error δ_{num} and input error δ_{input}, respectively.

This supplement presents a technique to extend the application of the pointwise or local assessment of the modeling error (δ_{model}) presented in ASME V&V 20-2009 to a global assessment of δ_{model} based on pointwise results from multiple validation set points within an application domain. The approach introduces a multivariate r^2 metric that is a weighted-sum-of-squares average of the comparison errors, E_i, where i denotes the ith set point within the multiple set points, i = 1, ..., n, and the weights are related to the contribution to the single set-point validation uncertainties, $u_{\text{val},i}$. Use of the r^2 metric is common in parameter estimation and other engineering disciplines (Beck and Arnold, 1977). It was introduced as a validation metric by Hills and Trucano (1999). This metric has been used in several peer-reviewed articles (Hills, 2006; Hills and Dowding, 2008; Pereira, Eça, and Vaz, 2017) to provide a more holistic, global assessment of model errors.

A multivariate metric is designed to quantify discrepancies between simulation results of a model and experimental data at more than one validation set point. In its most basic form, the multivariate metric provides a weighted sum of squares of the comparison errors obtained at each of the multiple set points. The value of the multivariate metric depends on the number of set points considered and so a reference result is determined from the number of set points and knowledge or assumptions about the modeling error at each of the multiple set points (see para. 4.2.1). The reference result provides a threshold value to assess the statistical significance of the modeling errors when compared to the validation uncertainty, i.e., experimental, numerical, and input-parameter uncertainties. However, one of the main features of the multivariate metric is its ability to incorporate and assess the effect of correlations between the comparison errors across the multiple validation set points. Correlation between simulation results and experimental data at each set point through shared inputs to data reduction equations is also taken into account because it is already included in the pointwise ASME V&V 20-2009 validation metric.

The multivariate metric offers an objective assessment of model performance removing the subjectivity of traditional approaches like comparing isolines from solutions, looking at the scatter of E_i, or comparing color plots which become very complicated for cases with multiple physics of interest. Stated differently, the multivariate metric provides an objective approach for the validation assessment based on the defined performance. For example, Pereira, Eça, and Vaz (2017) calculated the flow around a ship using the time-averaged Navier-Stokes (RANS) equations with 13 different turbulence models. For each of the 13 turbulence-model solutions, they quantified comparison error and validation uncertainty of the velocity components at 654 locations in the propeller plane. These single set-point assessments showed that selection of the optimum turbulence model depended on which set point was selected for assessment. An alternate approach that assesses the overall performance of the 13 models using the full set of 654 data points is more appropriate. As a simple example, one would not compare how well two straight lines with different slopes match a set of data that is linear by comparing the lines at each set point. A global metric is needed for the question, "Which model fits the entire set of data the best?" The multivariate metric provides such a global metric. Pereira, Eça, and Vaz used the multivariate metric to reduce the 654 comparison locations x 13 turbulence models set points to 13 values. This enables ranking of the performance of the 13 turbulence models with an objective approach. Nonetheless, as discussed in para. 4.2.1, comparison of different evaluations of the multivariate metric requires its normalization using a reference value.

Use of the multivariate metric was a topic of workshops at the ASME Verification and Validation Symposiums in 2019 and 2020 (Eça, et al. 2019, 2020). The workshops participants were able to consistently demonstrate that the discrepancies between simulation results and experimental data were globally larger than the validation uncertainty. As Eça et al. (2020) discussed, at some of the validation set points, a wide range of numerical uncertainties were estimated from the same data by the different participants. Nonetheless, the result of the multivariate metric was not significantly affected by the variability in the estimation of the numerical uncertainty for a few validation set points. The workshop also illustrated that the multivariate metric enables a quantitative evaluation of the modeling error of alternative mathematical models for the same problem, which is not easy to be achieved with local evaluation of the modeling error.

While the multivariate metric provides the ability to measure overall behavior of a model relative to a set of experimental data, it does not replace single set-point assessments. For example, a validation data set with a change in physics, such as laminar to turbulence transition, may have single set points exhibiting significant modeling errors that become obscured when included into the multivariate metric. Thus, relying on the multivariate metric alone could lead to a false sense of security in applying the model at other application points within the validation space. Furthermore, increasing the validation uncertainty at the single set points will lead to a decrease of the multivariate metric, i.e., blindly including poor validation cases yields false security. Useful insight is obtained by applying both multivariate metric and single set point measures. Therefore, results of the multivariate metric should be interpreted as a demonstration of discrepancies between simulations and experiments that cannot be explained by the validation uncertainty and not as the sole measure of modeling credibility.

In this supplement, section 4 presents the procedure for development of the multivariate metric, and section 5 illustrates application of the procedure to a comprehensively described example. Section 6 discusses some associated caveats for further clarification. Nonmandatory Appendix A presents the detailed formulation of the multivariate metric, and an example based on the ASME V&V 20-2009 fin-tube heat exchanger is described in Nonmandatory Appendix B. Nonmandatory Appendix C presents examples of the choices required in the procedure for applying the multivariate metric.

4 A MULTIVARIATE METRIC FOR RESULTS FROM MULTIPLE VALIDATION SET POINTS

A multivariate metric is designed to quantify the comparison of simulation results from computational models with experimental data using data from more than one validation set point. The data can be from a variety of sources, for example, multiple set points over time and space for a single multidimensional experiment, data from experiments using the same apparatus at different set points (different flow rates), or data from a combination of variables from a single experiment.

The multivariate metric introduced in para. 4.2 builds upon single set point validation quantification of model comparison error and validation uncertainty using the techniques of ASME V&V 20-2009 (see also Eça, Dowding, and Roache, 2022). A brief overview of the approach described in ASME V&V 20-2009 is presented in para.4.1. A detailed development of the multivariate metric follows in para. 4.2.

4.1 Overview of ASME V&V 20-2009

ASME V&V-20-2009 considers validation for a single validation variable defined by a scalar quantity (see also Eça, Dowding, and Roache, 2022). Therefore, it is mainly focused on, but not limited to, deterministic simulations. An example of its application to stochastic simulations that require the selection of scalar quantities that characterize the distributions is presented in Eça, Dowding, Moorcroft, et al. (2022). The validation metric presented in ASME V&V 20-2009 is based on the comparison error, E, resulting from the comparison of a simulation solution value, S, to the corresponding value, D, from an experiment.

If model inputs are known exactly, the numerical solution is exact (infinite grid iteratively converged to machine accuracy in a machine with an infinite number of digits) and for an equally perfect experiment with exact controls and configuration, then the experimentally observed/derived value is also exact; thus, E is the true model error δ_{model}. In practice, these idealized conditions are impossible to achieve. The ASME V&V 20-2009 method accounts for errors in the simulation results, S, due to uncertainties in the specification of the input parameters, δ_{input} (e.g., uncertainties in boundary conditions, fluid properties, and/or heat transfer coefficients required to perform the simulations), and due to numerical uncertainty, δ_{num} (mesh/time-steps discretization error and iterative convergence error, round-off errors and possibly statistical error if simulations are unsteady and/or stochastic) as well as errors in the experimental outcomes, δ_D. Considering the errors in the simulations (δ_{model}, δ_{num}, and δ_{input}) and in the experiments (δ_D), the relation between δ_{model} and E is as follows:

$$E = S - D = \delta_{\text{model}} + \delta_{\text{num}} + \delta_{\text{input}} - \delta_D \tag{4-1}$$

In principle, $E, S, D, \delta_{\text{model}}, \delta_{\text{num}}, \delta_{\text{input}}$, and δ_D are single-valued numbers. If $\delta_{\text{num}}, \delta_{\text{input}}$, and δ_D are known, the true model error can be calculated from

$$\delta_{\text{model}} = E - \left(\delta_{\text{num}} + \delta_{\text{input}} - \delta_D\right) \tag{4-2}$$

Single values can be calculated only for E, S, and D. An uncertainty is estimated to characterize the unknown errors, δ_{num}, δ_{input}, and δ_D, because the true values are not available. The ASME V&V 20-2009 method characterizes each error source, δ_X, using standard uncertainties $\pm u_X$ and assuming that the expected value of all these errors is zero.

$$-u_{\text{num}} \le \delta_{\text{num}} \le u_{\text{num}} \tag{4-3}$$

$$-u_{\text{input}} \le \delta_{\text{input}} \le u_{\text{input}} \tag{4-4}$$

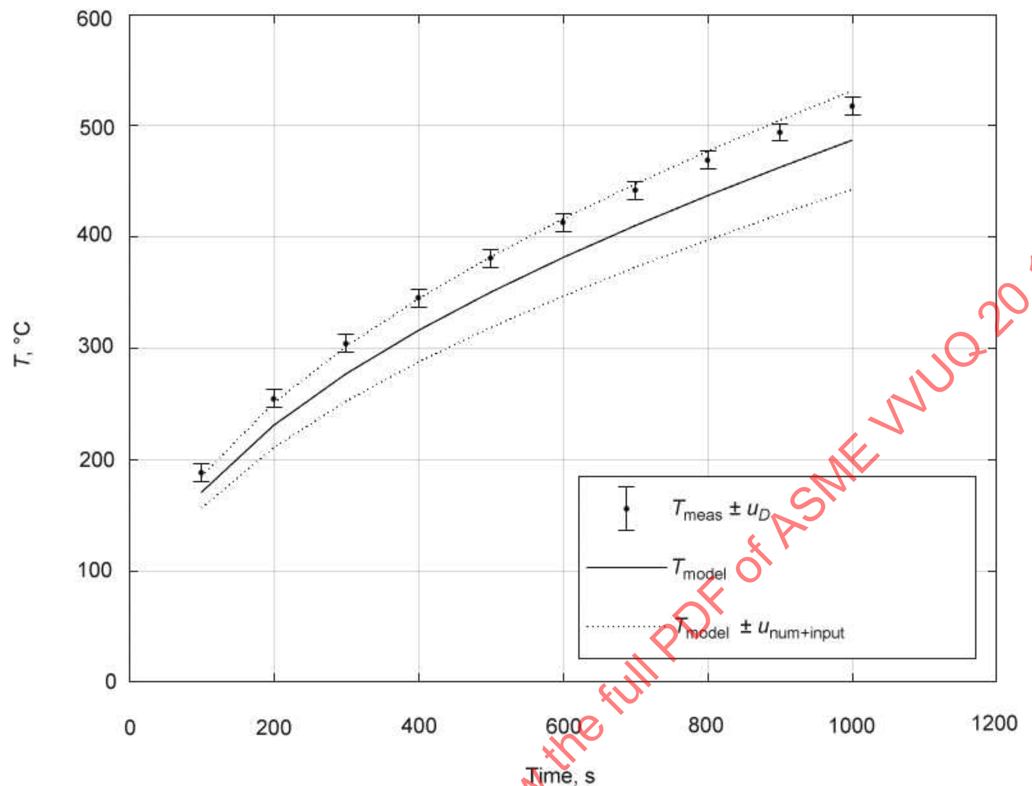
$$-u_D \le \delta_D \le u_D \tag{4-5}$$

The standard uncertainty u_X corresponds conceptually to an estimate of the standard deviation σ of the parent distribution from which δ_X is a single realization.

In eq. (4-3), u_{num} is a measure of the numerical uncertainty that is a consequence of discretization and iterative convergence, round-off error, and possible statistical convergence in the determination of the simulation value, S. Techniques to determine u_{num} are presented in section 2 of ASME V&V 20-2009.

Also, in eq. (4-4), u_{input} is a consequence of the standard uncertainties u_X in the input parameters required to perform the simulation that determines S. It is calculated by propagating the standard uncertainties of the input parameters through the model as discussed in section 3 of ASME V&V 20-2009.

Figure 4.1-1
Temperature *T* as a Function of Time



The determination of the experimental uncertainty u_D is discussed in section 4 of ASME V&V 20-2009. Naturally, the determination of u_D depends on the definition of the validation variable. For example, if the validation variable is an average value calculated from a subset of a population of measurements, u_D will be different from the u_D value corresponding to a validation variable defined by the individual measurements.

The uncertainties are combined into the validation uncertainty u_{val}, which in the simplest case of independence, leads to

$$u_{\text{val}} = \sqrt{u_D^2 + u_{\text{input}}^2 + u_{\text{num}}^2} \tag{4-6}$$

Changes to eq. (4-6) required by shared contributions to these uncertainties are presented in ASME V&V 20-2009.

The outcome of the ASME V&V 20-2009 method is an interval that should contain the model error δ_{model},

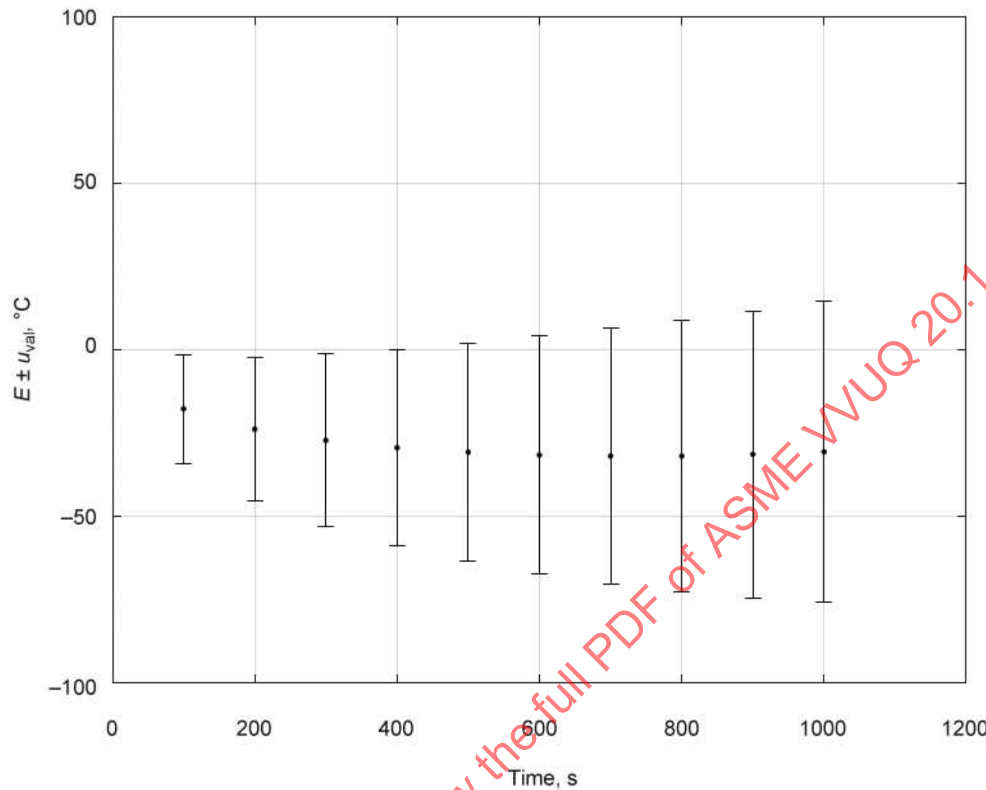
$$\delta_{\text{model}} \in (E - k \cdot u_{\text{val}}, E + k \cdot u_{\text{val}}) \tag{4-7}$$

where the coefficient k is a coverage factor that defines the desired level of confidence. Values for k are typically in the range of 2 to 3 for 95% confidence (ASME V&V 20-2009), but the determination of k requires the knowledge (or assumptions) of the type of distributions that characterize the experimental input-parameters, and numerical errors.

ASME V&V 20-2009 also provides an example to illustrate the application of the pointwise metric to ten set points. The results are shown in Figure 4.1-1. Experimental data, T_{meas}, are presented as solid circles with data uncertainty u_D added as error bars. A corresponding simulation result, T_{model}, is shown as a solid line. Its range of uncertainty due to numerical and input uncertainties, $\pm u_{\text{num+input}}$, is shown using offset dotted lines. For this example, $u_{\text{num+input}}$ is calculated from u_{num} and u_{input} assuming independence,

$$u_{\text{num+input}} = \sqrt{u_{\text{input}}^2 + u_{\text{num}}^2} \tag{4-8}$$

Figure 4.1-2
Comparison Error *E* as a Function of Time



Following the ASME V&V 20-2009 method, a model comparison error E_i and a validation uncertainty $u_{\mathrm{val},i}$ are calculated for each of the ten set points (i = 1 to 10) where an experimental value is available for comparison,

$$\delta_{\mathrm{model},i} \in (E_i - k \cdot u_{\mathrm{val},i}, E_i + k \cdot u_{\mathrm{val},i}) \tag{4-9}$$

The validation results are plotted in Figure 4.1-2 with uncertainty evaluated at one standard uncertainty (k = 1). For all ten validation comparisons, E is negative. However, for seven of the ten set points, the validation uncertainty u_{val} is larger than the comparison error E, and so it is not possible to identify the sign of the modeling error δ_{model} (Eça, Dowding, and Roache, 2022), because the limits of the intervals ($E - u_{\mathrm{val}}$ and $E + u_{\mathrm{val}}$) have opposite signs. Therefore, at these seven set points, the conclusion is $|\delta_{\mathrm{model}}| < |E - u_{\mathrm{val}}|$. The fact that seven out of ten of the estimated intervals contain E = 0 does not imply that there is approximately a 7 in 10 chance that the model simulations are statistically consistent with the data to a range of ± one standard uncertainty. The seven intervals are not centered at E = 0, and the ten evaluations of the modeling error share at least uncertainties in the input parameters and perhaps in the numerical and experimental uncertainties. Therefore, validation uncertainties estimated at the ten set points are correlated because they share the same source of uncertainty and so their values may not be independent. Note that in this case, the correlation is between uncertainties at the ten different set points and not between experimental, input, and numerical uncertainties at a given set point.

The multivariate metric proposed in this supplement provides a global quantitative assessment that indicates if comparison errors are globally smaller than, equal to, or larger than the validation uncertainties using the framework proposed in ASME V&V 20-2009.

4.2 Development of Multivariate Metric E_{mv}^2

The multivariate metric presented in this supplement can account for possible correlations of experimental measurements, input-parameters, and numerical errors at the multiple validation set points. The correlation is quantified by a linear correlation coefficient described in this paragraph.

Correlation may exist between experimental measurement errors at the multiple set points. The specific techniques to experimentally quantify the correlation are beyond the scope of this supplement. The reader should consult references (e.g., Coleman and Steele, 2009; Moffat and Henk, 2021) for experimental measurement uncertainty for techniques to quantify correlation. While measurement correlation is difficult to quantify, the metric can be used to investigate two common cases (independent or perfectly correlated). The dependence of the metric on correlation can be identified. The outcome provides direction on how resources for quantifying the correlation could change the metric.

The comparison errors (and validation uncertainties) for data taken over multiple set points from an experiment or series of experiments using the same apparatus are often correlated, even if there is no correlation between the errors in the measured data. For example, a transient model that overpredicts temperature at one time is likely to overpredict temperature at an adjacent time, see Figure 4.1-2. One would also expect correlation to exist between these comparison errors (and validation uncertainties) evaluated at different spatial locations from the same experiment.

Simulation solution values at multiple set points are always correlated through the input parameter uncertainty. Uncertainty propagation techniques account for the linear correlation of the simulation solution values at multiple validation set points. The correlation of the numerical solution uncertainty, such as the experimental measurement uncertainty, is challenging to quantify. Two common situations, independent (correlation coefficients equal to 0) or perfectly correlated (correlation coefficients equal to 1), can be used to investigate the correlation of the numerical uncertainty at the multiple set points.

Multiple experiments performed using the same apparatus can also lead to correlated comparison errors (and validation uncertainties). Consider the case of data from heat exchanger tests at multiple flow rates. Bias in data over multiple tests may be present due to sensor installation uncertainty (i.e., position errors, thermal contact effects, heat losses from the sensor leads), sensor calibration errors, and environmental biases. Simulation models for the experiment contain uncertainty due to uncertainty in the model parameters, which represent material properties and other characteristics. Unless comparison errors (and validation uncertainties) are taken from independent experiments with the corresponding model solution evaluated at independent values for the model parameters (e.g., independent conditions, properties), the validation data at the different set points will be correlated.

The multivariate metric defined and evaluated in this supplement is based on Least Squares Regression and is commonly called an r^2 metric. This approach takes correlation into account by using a weighted sum of squares of the comparison errors with the weights defined by the inverse of a covariance matrix (Hills and Trucano, 1999). The metric is a summation of the squares of the comparison errors ($E = S - D$) normalized by the uncertainty in the errors represented by the validation uncertainties. The normalized quantities allow for the metric to be compared to a reference value to indicate whether the comparison errors are consistent in magnitude and correlation structure with the validation uncertainties.

Specifically, the metric is

$$E_{mv}^2 = E^T V_{\mathrm{val}}^{-1} E \tag{4-10}$$

Here, E is the vector of comparison errors, $E = [S_i - D_i] = [E_i]$, and V_{val} is the covariance matrix that characterizes the correlation structure between the multiple validation variables.

The covariance matrix V_{val} can be written in an alternative form

$$V_{\mathrm{val}} = \begin{bmatrix} u_{\mathrm{val},1}^2 & \cdots & \rho_{1,n} u_{\mathrm{val},1} u_{\mathrm{val},n} \\ \vdots & \ddots & \vdots \\ \rho_{n,1} u_{\mathrm{val},n} u_{\mathrm{val},1} & \cdots & u_{\mathrm{val},n}^2 \end{bmatrix} \tag{4-11}$$

The off-diagonal terms include the product of the correlation coefficient and the u_{val}'s at the respective validation set points. The correlation coefficient is defined in introductory statistics textbooks (Peck, Olsen, and Devore, 2019). The correlation coefficient is estimated by assessing the effect of errors at the respective set points. Errors that are identically shared between the set points have a correlation coefficient equal to 1. Errors that are independent between set points have a correlation coefficient equal to 0. Techniques are provided in Nonmandatory Appendix A to incorporate the effect of correlation due to shared or independent errors at the multiple validation set points.

For illustrative purposes, it is useful to consider a two set-point example. After performing the matrix operations of eq. (4-10), the two-set points result can be expressed as the following equation for an ellipse in the (E_1, E_2) space:

$$E_{mv}^2 = \left[\frac{1}{1-\rho_{1,2}\rho_{2,1}}\right]\left[\frac{E_1^2}{u_{\mathrm{val},1}^2} + \frac{E_2^2}{u_{\mathrm{val},2}^2} - 2\frac{\rho_{1,2}\rho_{2,1}E_1E_2}{u_{\mathrm{val},1}u_{\mathrm{val},2}}\right] \tag{4-12}$$

Considering eq. (4-12), one can see that E_{mv}^2 is the global length of the multivariate vector for E_i, weighted by significance, i.e., more certain validation experiments are weighted more heavily than less certain validation experiments. This weighting renders the metric dimensionless (because $u_{\mathrm{val},i}$ has the same dimension as E_i), allowing information from set points with different validation variables to be used in the global assessment.

Eq. (4-12) also shows that selecting two points with identically shared errors (i.e., perfectly correlated, $\rho_{1,2} = \rho_{2,1} = 1$) will lead to a singular covariance matrix. For this condition between two set points, the multivariate metric is finite if and only if $E_1 = E_2$ and $u_{\mathrm{val},1} = u_{\mathrm{val},2}$. For conditions where all set points have perfectly correlated errors, it is not appropriate to apply a multivariate metric.

On the other hand, for the special case where E_1 and E_2 are uncorrelated ($\rho_{1,2} = \rho_{2,1} = 0$), eq. (4-12) reduces to

$$E_{mv}^2 = \left[\frac{E_1^2}{u_{\mathrm{val},1}^2} + \frac{E_2^2}{u_{\mathrm{val},2}^2}\right] \tag{4-13}$$

$E_{mv} = \sqrt{E_{mv}^2}$ is a dimensionless quantity that scales with the number of set points, and so it is necessary to introduce a reference value E_{ref}, which has two main purposes as follows:

(a) enabling the comparison of E_{mv} values obtained from different number of validation set points

(b) estimating the discrepancy between simulations and experiments that can be explained by the validation uncertainty, i.e., the experimental, input, and numerical uncertainties

4.2.1 Estimating a Reference Value, E_{ref}, for the Multivariate Metric. The reference value squared E_{ref}^2 is the expected value of E_{mv}^2, denoted $\langle E_{mv}^2 \rangle$ plus its standard uncertainty. Standard uncertainty is included to handle the special case for which $\langle E_i \rangle$ equal to zero. This case would occur if the simulation model perfectly represents the physics of the experiments, if the uncertainties in δ_{model} at each set point are represented by symmetric distributions, if one knew and used the true values for the model parameters and quantities measured to evaluate the E_i, and if the numerical uncertainty associated with the simulation is zero. Note that other measures of central tendency such as mode or median could have been used to define $\langle E_{mv}^2 \rangle$.

The evaluation of $\langle E_{mv}^2 \rangle$ and its standard uncertainty $u_{E_{mv}^2}$ requires knowledge of the underlying distributions for a population of possible comparison errors E_i. The estimation of this standard uncertainty based on normally distributed comparison errors and the use of sampling techniques for more general distributions are presented in paras. 4.2.1.1 and 4.2.1.2, respectively.

Two methods are described in paras. 4.2.1.1 and 4.2.1.2 for calculating a value for E_{ref}^2. For normally distributed comparison errors (para. 4.2.1.1), the reference value is derived from the χ^2 distribution. A sampling method is proposed if the comparison errors cannot be reasonably described using a normal distribution (para. 4.2.1.2).

4.2.1.1 Normally Distributed Comparison Errors (Sensitivity Approach). If the comparison errors E_i at the multiple set points can be represented by a normal distribution, then E_{mv}^2 is distributed as Chi-squared, $\chi^2(df)$, with the degrees of freedom, df, equal to the rank of V_{val} (Hills, 2006). If the measurements are independent, the rank of V_{val} will be equal to the number of measurements. There is no restriction on the independence of the differences, nor requirements for uniform means and standard uncertainties since the differences will be normalized by V_{val} in eq. (4-10). The expected value and variance of the $\chi^2(df)$ distribution are

$$\left\langle E_{mv}^2 \right\rangle = \left\langle \chi^2(df) \right\rangle = df \tag{4-14}$$

$$u_{E_{mv}^2}^2 = \mathrm{var}\left(E_{mv}^2\right) = \mathrm{var}\left(\chi^2(df)\right) = 2 \cdot df \tag{4-15}$$

The Chi-squared distribution, $\chi^2(df)$, is tabulated in most statistical textbooks (NIST/SEMATECH e-Handbook of Statistical Methods) and can be evaluated using internal routines from several software packages, e.g., Microsoft Excel. The sum of the expected value and the standard uncertainty (i.e., square root of the variance) of the $\chi^2(df)$ distribution will be used as a reference value to represent a standard uncertainty range on E_{mv}^2 for normally distributed comparison errors.

$$E_{ref}^2 = \left\langle E_{mv}^2 \right\rangle + \sqrt{\mathrm{var}\left(E_{mv}^2\right)} = df + \sqrt{2 \cdot df} \tag{4-16}$$

4.2.1.2 Nonnormally Distributed Comparison Errors (Sampling Approach). If the uncertainty in each set point for δ_{model} is not normally distributed, E_{mv}^2 will not be represented by $\chi^2(df)$. In this case, a sampling approach is proposed to estimate contributions to E_{ref}.

A general approach to uncertainty quantification is based on Monte Carlo sampling, as presented in ASME V&V 20-2009. This approach allows one to fully account for the effect of nonlinearities in the model and various forms of correlation between the data, between the simulation results, and between data and the simulation results. The sampling approach generates j samples for the differences $E_{j,i}$ between the simulation and experiment for each validation set point, i, due to the uncertainties represented by the probability distributions associated with u_D, u_{num}, and u_{input}.

These samples are used to estimate $\langle E_{mv}^2 \rangle$ and E_{ref}^2.

4.2.1.2.1 Estimation of the Expected Value $\left\langle \boldsymbol{E_{mv}^2} \right\rangle$. To estimate $\langle E_{mv}^2 \rangle$ by sampling, a distribution of the mean values $\langle E_j \rangle_{,i}$ of the differences $E_{j,\,i}$ for each validation set point is calculated and collected into the vector $\langle E \rangle$. The magnitude of this vector accounting for covariances between the validation set points is the estimate of E_{mv}^2. It is calculated using eq. (4-10).

The following procedure is used to calculate E_{mv}^2.

Step 1. Using the samples $E_{j,\,i}$ developed from the methodology defined in ASME V&V20-2009 for each of the n validation set points i = 1, …, n, evaluate the vector of expected values (means) of the differences

$$\left\langle E \right\rangle = \left[\left\langle E_j \right\rangle_{,1} \vdots \left\langle E_j \right\rangle_{,n} \right] = \left[\left\langle E_j \right\rangle_{,i} \right] \tag{4-17}$$

Step 2. Estimate the covariance matrix V_{val} for correlations between elements $\langle E_j \rangle_{,i}$ of $\langle E \rangle$ using the approach outlined in Nonmandatory Appendix A.

Step 3. Evaluate $\langle E_{mv}^2 \rangle$ using eq. (4-10) using $E = \langle E \rangle$.

4.2.1.2.2 Estimation of $\boldsymbol{E_{\mathrm{ref}}^2}$. An estimate of the reference value E_{ref}^2 by sampling is developed to understand the significance of E_{mv}^2. E_{ref}^2 is calculated from an "ideal" distribution, i.e., one with zero model comparison error. Assuming that the distribution of differences for the "ideal" population about a zero mean value is the same as the distribution of population of $E_{j,i}$ about $\langle E_j \rangle_{,i}$, E_{ref}^2 can be calculated from the deviations of $E_{j,i}$ from $\langle E_j \rangle_{,i}$.

The following procedure is used to evaluate E_{mv}^2 and thus E_{ref}^2:

Step 1. Subtract the corresponding set point expected values (means) from each of the j samples of the differences for each validation set point i.

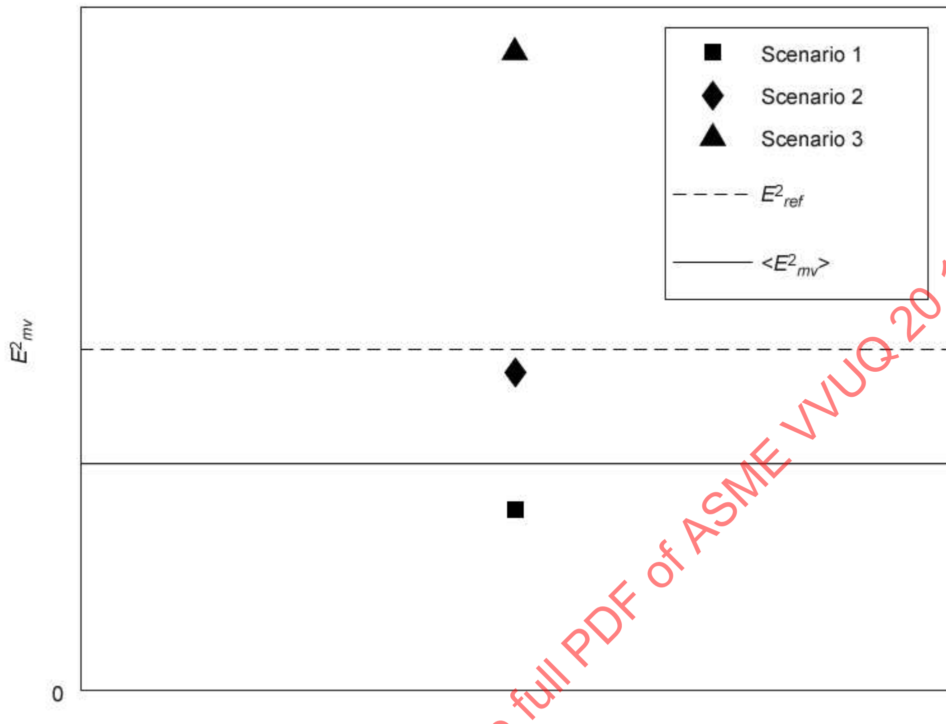
$$\left(E_{\mathrm{ref}}\right)_{j,i} = \left[E_{i,j} - \left\langle E_j \right\rangle_i \right] \tag{4-18}$$

Step 2. Evaluate $[\, E_{mv}^2 \,]_{,i}$ for each set point i, separately, using eq. (4-10) with E replaced by $(E_{\mathrm{ref}})_{\,j,i}$. This step provides a distribution of E_{mv}^2 for our hypothetically perfect physics model, given the distributions associated with u_D, u_{num}, and u_{input}.

Step 3. Evaluate the expected value (i.e., $\langle E_{mv}^2 \rangle$) and variance [i.e., E_{mv}^2] of this sampled population for E_{mv}^2.

Step 4. Estimate E_{ref}^2 with eq. (4-16) using $\langle E_{mv}^2 \rangle$ and $\sqrt{\mathrm{var}\left(E_{mv}^2\right)}$. The value of E_{mv}^2 can be compared to E_{ref}^2 to compile evidence that the discrepancies can be explained by the estimated uncertainties in its value.

Figure 4.2.2-1
Assessment of Three Scenarios



4.2.2 Interpretation of E^2_{mv}. Figure 4.2.2-1 offers a simple demonstration of the interpretation of the metric E^2_{mv}. The solid horizontal line indicates $\langle E^2_{mv} \rangle$ given that the expected value for E_i is zero, i. e., $\langle E_i \rangle = 0$, $i = 1, \ldots, n$. Note that $\langle E^2_{mv} \rangle$ is nonzero as the value of any realization of E^2_{mv} cannot be negative. The dashed line represents E^2_{ref}, i.e., $\langle E^2_{mv} \rangle$ plus its standard uncertainty $u_{E^2_{mv}}$.

Consider three scenarios of the metric E^2_{mv} as quantified by eq. (4-10) in Figure 4.2.2-1. The results for Scenarios 1 and 2 indicate that the weighted differences between simulations and measurements, E^2_{mv} , are within the expected value and one standard uncertainty of $\langle E^2_{mv} \rangle$, i.e., $E^2_{mv} < \left\langle E^2_{mv} \right\rangle + u_{E^2_{mv}}$. Nonetheless, Scenario 1 is below $\langle E^2_{mv} \rangle$ whereas Scenario 2 is between $\langle E^2_{mv} \rangle$ and E^2_{ref} . This suggests that the comparison errors are consistent with the uncertainties as characterized by V_{val}. In contrast, Scenario 3 results in a value for E^2_{mv} that is several standard uncertainties larger than $\langle E^2_{mv} \rangle$, providing evidence that the comparison errors are significant relative to the uncertainties. Furthermore, Scenario 3 provides a global measure of the ratio between comparison error and validation uncertainty.

The dependence of E^2_{mv} on the number of selected set points hinders the comparison presented in Figure 4.2.2-1 when using different numbers of set points.

A solution that improves interpretability is obtained from the ratio of E_{mv} to E_{ref}, which does not depend on the number of selected set points. E_{mv}/E_{ref} is a quantitative measure of the modeling error that indicates validation assessments based on global differences between experiments and simulations. Obtaining $E_{mv}/E_{ref} < 1$ only means that modeling errors are globally smaller than the validation uncertainties. Therefore, the interpretation of the value of E_{mv}/E_{ref} requires knowledge of the validation uncertainty and comparison errors at each of the set points. As for the pointwise validation metric (ASME V&V 20-2009; Eça, Dowding, and Roache, 2022), the level of the modeling errors can be as high as the sum of comparison errors and validation uncertainties. On the other hand, when the ratio E_{mv}/E_{ref} is much larger than unity, it provides quantitative assessment of the global level of the modeling errors when compared to the validation uncertainty. Note that the confidence level used in the pointwise evaluation of the numerical, input, and experimental uncertainties is

Table 5-1
Simulation Model Parameters *a* and *b*

Statistic	*a*	*b*
Mean	1.00	0.50
Standard uncertainty	0.05	0.10

GENERAL NOTE: Parameters a and b are independent and normally distributed.

embedded in the determination of the contributions to the covariance matrix, and so it is also reflected in the outcome of the multivariate metric.

Therefore, for analysis purposes, it is recommended to use the ratio E_{mv}/E_{ref} for quantitative assessments as it removes the dependence on degrees of freedom, i.e., the number of validation set points.

5 EXAMPLE OF THE APPLICATION OF THE MULTIVARIATE METRIC SHOWING THE EFFECTS OF CORRELATION

This section steps through an example for determining the multivariate metric to objectively assess simulation results from a very simple two-parameter linear algebraic model using validation measurement data from a test facility at multiple correlated set points in time. The data may be values for time instants from a time series of temperature, velocity magnitude, or any other scalar quantity. There are no restrictions on whether the data are instantaneous values or statistics such as averages or variances; however, such details are fundamental to estimate the uncertainty in the reported measurement data, u_D, and input u_{input}, and numerical u_{num} uncertainties in the simulation results. The main purpose of this section is to illustrate the use of the multivariate metric in a simple example and to point out the consequences of ignoring correlation between the multiple validation set points.

A second purpose of this section is to illustrate the use of the multivariate metric to objectively compare simulation results to experimental measurement data across multiple sources of simulation or experimental data, which can be multiple mathematical models as illustrated in Pereira, Eça, and Vaz (2017) or multiple test facilities as in the present example. The sensitivity coefficients technique based on a linearity assumption is illustrated in para. 5.1, whereas para. 5.2 presents the application of the sampling approach that handles nonlinearities.

Consider evaluation of the multivariate metric for a very simple example of a two-parameter linear algebraic model using validation measurement data at multiple set points. The simulation model consists of the following equation:

$$S(t) = a + bt \tag{5-1}$$

where S represents the result computed from the simulation model, and a and b are input parameters in the model. The result, S, is to be compared with the measured quantity, D, at validation set points defined by time, t. For this example, the mean values of the model input parameters a and b and their measurement uncertainties are assumed to be normally distributed and independent, and their means and standard uncertainties are as listed in Table 5-1.

The assumption that a and b are independent implies that the off-diagonal elements in their covariance matrix, V_X, are zero. Note that the parameters a and b will be correlated if a least-squares procedure is used to estimate the two parameters simultaneously. In that case, standard statistical packages provide estimates of the corresponding covariance matrix of the simulation inputs. This correlation affects estimation of the covariance matrix V_X; see Nonmandatory Appendix A.

The simulation model [eq. (5-1)] is to be tested using data from each of three test facilities with measurements available at two times, t_1 and t_2, from each facility. Because of differences in experimental approaches, equipment, personnel, and environmental conditions, one would reasonably expect variability across the three facilities. The multivariate metric, eq. (4-10), will be evaluated using the data from each facility to assess the variability of the measured results from facility to facility.

Measurements are taken at the two times, $t_1 = 1.0$ sec and $t_2 = 3.0$ sec. The corresponding data for the three facilities and their standard uncertainties are listed in Table 5-2.

The simulated quantities, S_i, and the corresponding differences, E_i, are evaluated using the mean values of the input model parameters from Table 5-1 in eq. (5-1), and are listed in Tables 5-3 and 5-4, respectively.

Table 5-2
Experimental Data D at Two Measurement Times From Three Independent Facilities

Facility (D_i at Time t_i)	D_1 (for t_1 = 1.0 s)	D_2 (for t_2 = 3.0 s)	Standard Uncertainty, u_D
1	1.65	2.90	0.05
2	1.35	2.55	0.05
3	1.45	2.65	0.05

Table 5-3
Mean Simulation Results, S_i

t_i	S_i
t_1	1.5
t_2	2.5

Table 5-4
Comparison Error, E_i, at Two Measurement Times From Three Facilities

Facility	E_1 (for t_1 = 1.0 s)	E_2 (t_2 = 3.0 s)
1	−0.15	−0.40
2	0.15	−0.05
3	0.05	−0.15

5.1 Sensitivity Approach

The covariance matrix V_{val} for the multivariate matrix is estimated from contributions due to V_{num}, the numerical uncertainty in the simulations; V_{input}, the input-parameters uncertainty in the simulations; and V_D, the uncertainty in the experimental data. The method described in detail in Nonmandatory Appendix A is an extension of that described in ASME V&V 20-2009 for the calculation of u_{val} from estimates of u_{num}, u_{input}, and u_D for a single set point. Accordingly,

$$V_{val} = V_{num} + V_{input} + V_D \tag{5-2}$$

In eq. (5-1), V_{num} is zero since the simulation model, eq. (4-18), is a simple algebraic equation, which in this simple example is not affected by round-off errors. Therefore,

$$V_{num} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \tag{5-3}$$

The validation variable, D, is directly measured and since the same input parameters are used for each facility, there are identical shared errors between the validation set points for the simulation inputs. Therefore, errors in the input parameters will have the same effect on the simulation of each facility. Furthermore, this example corresponds to Case 1B presented in Nonmandatory Appendix A. In the sensitivity method, that is based on a linear approach, the input parameters covariance matrix V_{input} is estimated from the matrix of sensitivity coefficients X_S and the covariance matrix for the input parameters V_X (see Nonmandatory Appendix A) using the following:

$$V_{input} = X_S \cdot V_X \cdot X_S^T \tag{5-4}$$

For this simple example, the simulation model is linear, and so it is straightforward to determine the sensitivity matrix of S with respect to the parameters $X_1 = a$ and $X_2 = b$ for the two-time instants:

$$X_S = \begin{bmatrix} \dfrac{\partial S_1}{\partial a} & \dfrac{\partial S_1}{\partial b} \\ \dfrac{\partial S_2}{\partial a} & \dfrac{\partial S_2}{\partial b} \end{bmatrix} = \begin{bmatrix} 1 & t_1 \\ 1 & t_2 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 3 \end{bmatrix} \tag{5-5}$$

The covariance matrix V_X for a and b is evaluated using the standard uncertainties given in Table 5-1. Since a and b are independent, the off-diagonal elements of this matrix are zero.

$$V_X = \begin{bmatrix} (0.05)^2 & 0 \\ 0 & (0.10)^2 \end{bmatrix} \tag{5-6}$$

Evaluation of V_{input} using eq. (5-4) gives

$$V_{\text{input}} = X_S \cdot V_X \cdot X_S^T = \begin{bmatrix} 0.0125 & 0.0325 \\ 0.0325 & 0.0925 \end{bmatrix} \tag{5-7}$$

The nonzero off-diagonal terms in eq. (5-7) signify that the two simulated values S_1 and S_2 are correlated.

The standard uncertainty, u_D, for the measurements from each test facility is listed in Table 5-2. The measurements are taken at different facilities and do not share error sources at the two-time instants. The covariance matrix, V_D, for the measurements (Case 1A of Nonmandatory Appendix A) is given by

$$V_D = \begin{bmatrix} (0.05)^2 & 0 \\ 0 & (0.05)^2 \end{bmatrix} \tag{5-8}$$

Given the estimates of V_{num} [eq. (5-3)], V_{input} [eq. (5-7)], and V_D [eq. (5-8)], the matrix V_{val} is calculated using eq. (5-5), as

$$\begin{aligned} V_{\text{val}} &= V_{\text{num}} + V_{\text{input}} + V_D \\ &= \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0.0125 & 0.0325 \\ 0.0325 & 0.0925 \end{bmatrix} + \begin{bmatrix} (0.05)^2 & 0 \\ 0 & (0.05)^2 \end{bmatrix} \\ &= \begin{bmatrix} 0.0150 & 0.0325 \\ 0.0325 & 0.0950 \end{bmatrix} \end{aligned} \tag{5-9}$$

Note that V_{Val} is applicable for all three facilities because the standard deviations of the measurements at the two-time instants are identical in all facilities, and so V_D is equal for the three facilities.

The standard validation uncertainty, u_{val}, for each measurement time is the square root of the corresponding diagonal term of the matrix in eq. (5-9). The comparison error, E, and validation uncertainty, u_{val}, are shown in Figure 5.1-1 at the two measurement times t_1 = 1 sec and t_2 = 3 sec, and the ratio E/u_{val} is presented in Table 5.1-1.

For comparison of results from the sensitivity approach described in this paragraph and from the sampling approach, which is described in the next paragraph, values for $E_{mv} = \sqrt{E_{mv}^2}$ are listed in Table 5.3-1 for V_{input} calculated using the sensitivity analysis (para. 5.1) and using sampling, which is described in para. 5.2. The value of E_{ref} for the sensitivity approach is calculated from eq. (4-16) using df = 2, yielding E_{ref} = 2.

5.2 Sampling Approach

This approach applies the sampling methodology described in Nonmandatory Appendix A to the linear example for the three facilities and the two time-instants listed in Table 5.1-1. The comparison error, E, is calculated from the difference between simulations and the measurements.

$$E = \text{mean}_j\left[S_{i,j} - D_{i,j}\right] = \text{mean}_j\left[E_{i,j}\right] \tag{5-10}$$

Latin Hypercube sampling (LHS) is used (see ASME V&V 20-2009) with n_r = 1,000 realizations to estimate the effect of model parameter uncertainty and measurement error on the simulation and experimental data, respectively. The simulation values are estimated by sampling the following model input parameters:

$$S_{i,j} = S_i\left(a_j, b_j\right) \tag{5-11}$$

The uncertainty in the model parameters is defined with normal distributions using statistics from Table 5-1.

$$\begin{aligned} a_j, b_j = \text{LHS}[&N(\text{mean}(a), \text{standard uncertainty}(a); \\ &N(\text{mean}(b), \text{standard uncertainty}(b)] \end{aligned} \tag{5-12}$$

Figure 5.1-1
ASME V&V 20-2009 Validation Metric ($E \pm u_{val}$) at the Two Times for the Three Facilities

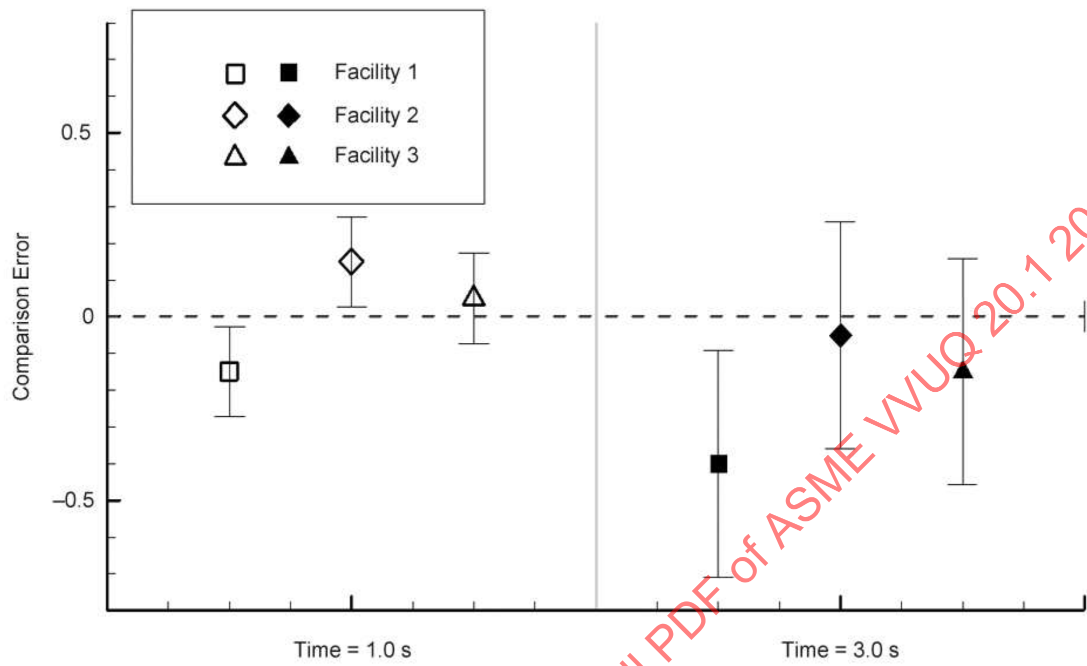


Table 5.1-1
Ratio of Comparison Error, E, to Validation Uncertainty, u_{val}, at the Two Time Instants for the Three Facilities

Time, s	E/u_{val}, Ratio of Comparison Error to Validation Uncertainty		
	Facility 1	Facility 2	Facility 3
1.0	−1.225	1.225	0.408
3.0	−1.298	−0.162	−0.487

Latin Hypercube sampling is also used to estimate the effect of measurement error for the experimental data.

$$D_{i,j} = D_i + d_{i,j} \tag{5-13}$$

$$d_{i,j} = \text{LHS}[N(0, \text{standard uncertainty}(D_i))] \tag{5-14}$$

The experimental data, D_i at the measurement times, t_i, are listed in Table 5-2. The statistics of the measurement error are also listed in Table 5-2.

The covariance matrix V_{Val} is estimated by

$$V_{\text{val}} = V_{\text{num}} + \text{cov}(E_s) \tag{5-15}$$

where (E_s) are the sampled values for the comparison errors.

The quantity E_{mv}^2 is calculated using eq. (4-10) and the covariance matrix V_{Val} is estimated from eq. (5-15). The value for E_{ref} for the sampling approach is calculated as described in para. 4.2.1.2 for nonnormally distributed comparison errors.

5.3 Comparison of Results from Sensitivity and Sampling Approaches

Table 5.3-1 lists the values of $E_{mv} = \sqrt{E_{mv}^2}$ and E_{ref} calculated using the sensitivity and sampling approaches. The small differences observed between the Latin Hypercube results ("Sampling Approach") and the sensitivity-based results in Table 5.3-1 can be reduced by including a larger number of samples. The present example is linear and normal

Table 5.3-1
Validation Results for Normally Distributed Simulation Model Parameters

Facility	Sensitivity Approach		Sampling Approach	
	E_{mv}	E_{ref}	E_{mv}	E_{ref}
1	1.315	2	1.313	1.992
2	2.687	2	2.793	1.992
3	1.698	2	1.758	1.992

distributions are assumed for input and experimental uncertainties and so statistical convergence will lead to the same results of the sensitivity approach. For the present number of samples, the results are nearly the same.

Figure 5.3-1 schematically shows the multivariate metric for the three facilities. If $E_{mv} \gg E_{\text{ref}}$, then the weighted comparison errors are significantly greater than the validation uncertainties at the multiple set points, given that $\langle E_i \rangle = 0$, $i = 1, \ldots, n$. The results indicate that the value of the multivariate metric for test Facility 1 and Facility 3 lie within the reference bound E_{ref}, and that for Facility 2 lies outside this bound. Therefore, Facility 2 is the only one for which the discrepancies between experiments and simulations are globally larger than the validation uncertainty. Note that, in this example, the level of u_{val} at the two validation set points is similar for the three facilities (see Figure 5.1-1) and so the multivariate metric is showing that the data of Facility 2 produces the larger modeling errors.

Figure 5.3-2 illustrates the impact of the correlation characterized by V_{val} on E_{mv}. The ellipses shown in Figure 5.3-2 represent curves of constant E_{mv}^2. The solid curve corresponds to the expected value of $E_{mv}^2 \left(< E_{mv}^2 > \right)$ and the dashed curve corresponds to the reference value, E_{ref}^2. The corresponding equations for the ellipses in Figure 5.3-2, illustration (a) are presented in eq. (5-16).

$$\begin{aligned} E_{mv}^2 &= [E_1 \quad E_2] \cdot \begin{bmatrix} 0.0150 & 0.0325 \\ 0.0325 & 0.0950 \end{bmatrix}^{-1} \cdot \begin{bmatrix} E_1 \\ E_2 \end{bmatrix} \\ &= [E_1 \quad E_2] \cdot \begin{bmatrix} 257.6 & -88.14 \\ -88.14 & 40.68 \end{bmatrix} \cdot \begin{bmatrix} E_1 \\ E_2 \end{bmatrix} \\ &= 257.6 \cdot E_1^2 + 2 \cdot (-88.14) \cdot E_1 \cdot E_2 + 40.68 \cdot E_2^2 \end{aligned} \quad (5\text{-}16)$$

where E_1 and E_2 are the comparison errors at $t_1 = 1$ and $t_2 = 3$, respectively.

The inclination of the major axis of the ellipse and the relative length of the major and minor axes provides a graphical representation of the correlation between the comparison errors at the two validation set points (E_1 at $t_1 = 1\ s$ and E_2 at $t_2 = 3\ s$). For the case of normally distributed differences, these ellipses correspond to curves of constant joint probability of comparison errors, assuming $\langle E_i \rangle = 0$, $i = 1, 2$. For the present model [Figure 5.3-2, illustration (a)], high values of E_1 tend to correspond to high values for E_2. Likewise, low E_1 tends to correspond to low E_2. This means that the errors in the estimation of $\delta_{\text{model},1}$ and $\delta_{\text{model},2}$ are positively correlated, which affects the global evaluation of the comparison errors and validation uncertainties obtained at the two set points.

Figure 5.3-2 presents also the two comparison errors for the three test facilities as listed in Table 5-4, where the difference E_1 (at $t = t_1 = 1$) is plotted along the abscissa, and E_2 (at $t = t_2 = 3$) is plotted along the ordinate. As for the comparison presented in Figure 5.3-1, the point corresponding to Facility 1 is within the solid ellipse (E_{mv}^2), that for Facility 3 is within the dashed ellipse (E_{ref}^2), and the point for Facility 2 is outside both ellipses. Because of the correlation induced by the simple linear simulation model, the E_{mv}^2 for Facility 1 is lower than that for the other two facilities, even though this point is more than twice the Euclidian distance from $E_{mv}^2 = 0$ (e.g., $E_1 = 0$, $E_2 = 0$).

The discrepancy introduced by ignoring this correlation is illustrated in Figure 5.3-2, illustration (b) that presents the results obtained ignoring correlation, i.e., setting all the off-diagonal terms in V_{val} to zero. In that case, eq. (4-10) becomes

$$E_{mv}^2 = [E_1 \quad E_2] \cdot \begin{bmatrix} 0.0150 & 0 \\ 0 & 0.0950 \end{bmatrix}^{-1} \cdot \begin{bmatrix} E_1 \\ E_2 \end{bmatrix} = \frac{E_1^2}{0.015} + \frac{E_2^2}{0.095} \tag{5-17}$$

The ellipses that represent the expected value of E_{mv}^2 and the reference value E_{ref}^2 have the two axes parallel to the E_1 and E_2 axes and so they lead to a different ordering of the comparison between the simulations and the test facilities. Figure 5.3-2, illustration (b) indicates that the agreement between the measurements and simulation results is best for Facility 1 when correlation is considered, but worst when correlation is ignored. In this example with only two set points, it is possible to see that the evaluation of Figure 5.3-2, illustration (b) that ignores correlation (by setting the off-diagonal terms to zero) matches the assessment based on the pointwise intervals presented in Figure 5.1-1. Facility 1 is the only one that shows two intervals indicating a negative δ_{model} (u_{val} is the same for the three facilities), which agrees with the positive correlation between the two validation set points. However, Facility 1 also leads to the largest values of comparison errors at the two validation set points. Therefore, if correlation is ignored, the largest discrepancies between simulations and experiments are obtained for Facility 1.

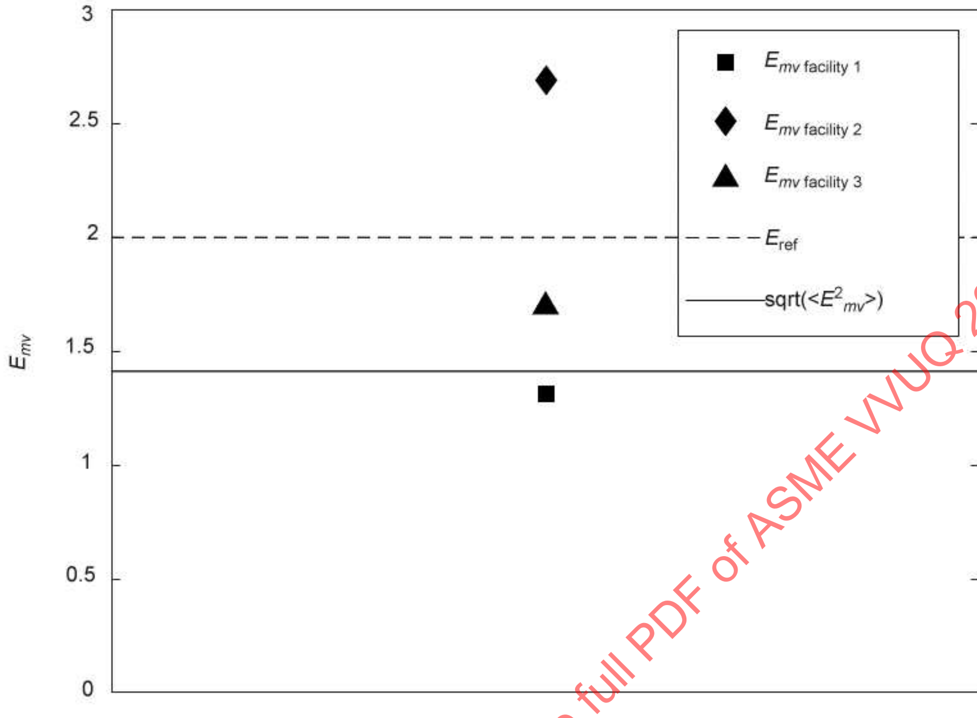
5.4 Summary

A validation metric presented is designed to characterize modeling errors when data is considered from multiple validation set points. Correlation in comparison errors across multiple validation set points is induced by simulation models that possess more than one uncertain model parameter and may be present even if the measurements are not correlated. Examples of correlated comparison errors include measurements from different spatial locations or data from time responses. Although not demonstrated, the metric presented can be applied without modification to multiple types of measurements as well as measurements of the same type at the same or multiple set points. The normalization by the inverse of the covariance matrix has the effect of scaling the comparison errors, in addition to making them dimensionless. For example, one may measure temperature and pressure at the same or at different set points for simultaneous use in the metric. Observed pressure comparison errors and observed temperature comparison errors are expected to be correlated, for example, if they are associated with the same constitutive model (e.g., the ideal gas law).

The example presented illustrates the importance of accounting for correlation. Ignoring correlation can lead to incorrect conclusions about the observed comparison errors. Incorporating correlation allows one to address integrated effects at multiple set points and multiple measurement types. A more detailed example of the application of the multivariate metric using validation results from multiple set points is presented in Nonmandatory Appendix B. Nonmandatory Appendix A presents the equations required to calculate the covariance matrix for all the definitions of validation variables considered in ASME V&V 20-2009.

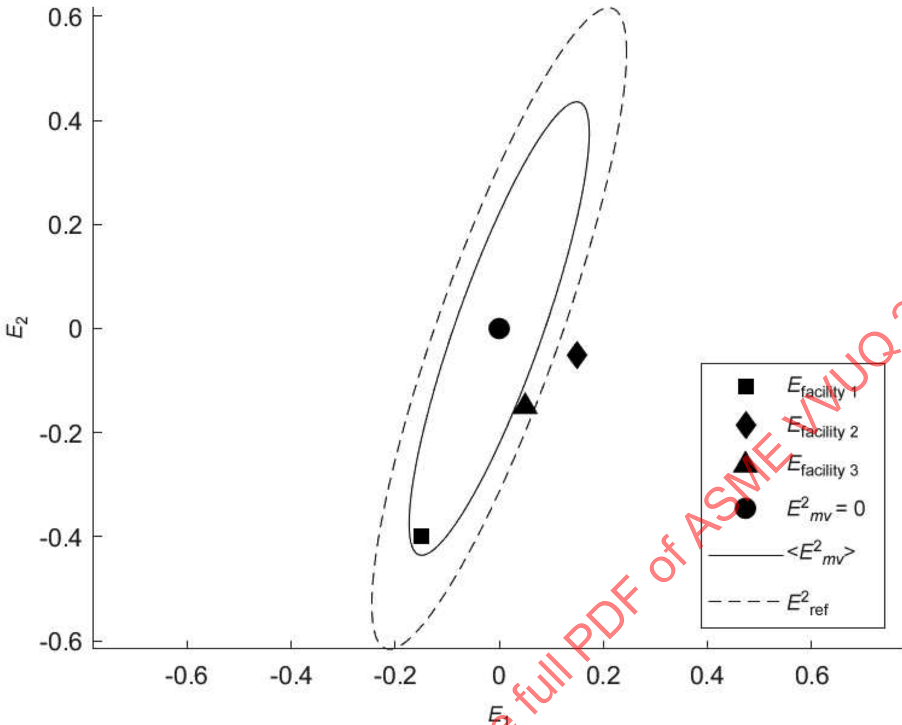
The correlation structure induced by even the simplest models (linear in this case) complicates the multivariate comparison of measurement data with model simulation results because equally probable measurement-simulation differences (comparison errors) do not lie at a constant distance from the origin, i.e., they are represented by ellipses that have orientations of the major and minor axes that depend on the correlation between the results at different validation set points. The normalization by V_{val} accounts for the shapes of these ellipses.

Figure 5.3-1
Schematic Representation of E_{mv} for Three Facilities (Symbols) Using Sensitivity Approach

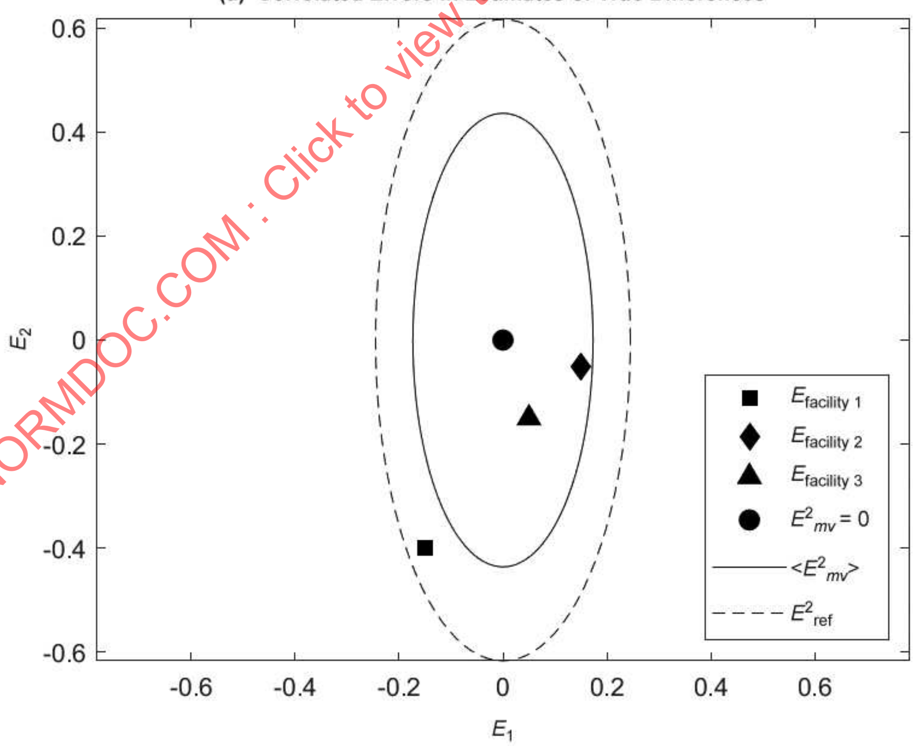


GENERAL NOTE: The solid line represents the expected value while the dashed line is offset by uncertainty.

Figure 5.3-2
Correlated Errors in Estimates of the True Differences and the Effect of Ignoring Correlation



(a) Correlated Errors in Estimates of True Differences



(b) Effect of Ignoring Correlation

6 DISCUSSION AND CAVEATS

Different approaches can be used to compare simulation results with experimental measurements obtained at multiple set points. The methodology presented herein represents an approach to define a multivariate metric for such a comparison. The methodology chosen utilizes the concepts and procedures presented in ASME V&V 20-2009, coupled with standard statistical techniques.

A multivariate metric allows one to characterize the comparison errors relative to the uncertainties at multiple validation set points. The weighted multivariate metric, E_{mv}^2 , is a standard regression measure of distance between simulation model results, S_i, and experimental data, D_i, at multiple set points, with the uncertainty in the validation data characterized by a covariance matrix V_{val}. ASME V&V 20-2009, section 4, and Nonmandatory Appendix A of this supplement provide methodology to estimate the covariance matrix of these validation differences (comparison errors) at the multiple validation set points.

(a) Evaluating the multivariate metric for application to multiple validation set points requires the following information:

(1) comparison errors E at each set point, i.e., the difference between the simulation results and the experimental data at each of the multiple validation set points.

(2) the covariance matrix (V_{val}) for these comparison errors. The covariance matrix depends on the numerical, input, and experimental uncertainties, and the knowledge if errors at the multiple set points are shared (correlated) or not shared (independent). Note that the existence of correlation between input and experimental uncertainties at a given set point also influences the calculation of V_{val}, as described in Nonmandatory Appendix A.

(b) The procedure to obtain V_{val} depends on the following two considerations:

(1) which of the four cases addressed in ASME V&V 20-2009 defined the validation variables: direct measurement (Case 1); result of a data reduction equation using several uncorrelated or correlated measured variables (Cases 2 and 3); or the outcome of measured variables analyzed with a model different from that used in the simulations (Case 4)

(2) the relationship between comparison errors (i.e., differences between the numerical and experimental values) at the multiple validation set points, i.e., if these errors are assumed to be independent (not shared) or identical (shared)

The first consideration was already addressed in ASME V&V 20-2009, whereas the second one is a consequence of the assessment performed at multiple validation set points. It must be emphasized that the use of the appropriate method for calculating the covariance matrix is essential for the outcome of the procedure. The "simplest approach" that ignores correlation and input uncertainty may lead to a misleading conclusion, whereas including correlation when none exists may lead to an equally misleading conclusion. Therefore, the determination of the covariance matrix must be carried out with great care, i.e., selecting the most appropriate choice to take into account uncertainties and possible correlations. This is not always a trivial exercise, and it may depend on the definition of the different validation variables included in the multivariate metric.

(c) The multivariate metric E_{mv}^2 produces a weighted distance that is compared to a reference value E_{ref}^2 obtained from the expected value of E_{mv}^2 plus its standard deviation. The ratio between these two quantities provides a global assessment of the error in the simulation model result. If the ratio is smaller than or close to unity, the comparison errors at multiple set points may not be significant relative to validation uncertainty. The estimation of modeling errors depends on comparison errors and validation uncertainties. On the other hand, if the ratio is much larger than unity, the discrepancies between simulations and experiments are mainly due to modeling errors and may indicate significant model bias.

It must be emphasized that the metric is not a quantity that provides a pass/fail outcome of a validation exercise. Obtaining $E_{mv}/E_{\mathrm{ref}} < 1$ is not the goal of the multivariate metric. When the metric provides an indication of modeling errors significantly larger than validation uncertainties (i.e., the ratio E_{mv}/E_{ref} is significantly larger than 1), it must be complemented with the pointwise information (ASME V&V 20-2009) of the level of validation uncertainties (main-diagonal entries of the covariance matrix) to obtain a global estimate of the modeling error.

A criticism of any E_{mv}^2 -based metric, whether weighted or not, is that this measure of distance is more sensitive to the larger differences between model prediction and experimental data because the E's at the different validation set points are squared. Another issue that occurs in regression is that an E_{mv}^2 -based metric has a known distribution (χ^2) only if the differences are normally distributed. For the case of the multivariate metric, the requirement for normally distributed differences can be removed if one utilizes the sampling approach discussed in para. 4.2.1.2 and Nonmandatory Appendix A to evaluate the corresponding distribution for the E_{mv}^2 based metric.

There is a significant advantage in accounting for the covariance between the E's at different validation set points. The approach presented in para. 4.2 transforms the comparison errors across multiple set points into a single measure by accounting for correlation. This results in an increased ability to resolve the effect of model error when compared to set-point by set-point evaluation as defined in ASME V&V 20-2009. As a result, one is more likely to resolve discrepancies that are not explained by the validation uncertainty using a properly defined multivariate metric, compared to measures applied at individual validation set points, as illustrated in the example presented in section 5.

However, because the validation differences are combined appropriately into a single measure based on the covariance matrix (i.e., linear correlation), the combined representation is approximate if the correlation is nonlinear across multiple set points. For example, if system physics changes between two time-measurements, resulting in a nonlinear relation between the errors at these times, the combining may not be appropriate. In such cases, one can apply the multivariate metric evaluation to subsets of the full domain where the subset is chosen based on similar physics. Similar situations may appear in transient responses, for example, in the heating of a liquid that leads to evaporation. In that case, the multivariate metric may be applied to different windows of time that correspond to the same physics.

Recall that the present multivariate metric is an extension of the pointwise estimates of the modeling error provided by the ASME V&V 20-2009 procedure. It provides a global quantification of the differences between experiments (physical reality) and simulations (modeling) that can deal with possible correlations between the n set points used in its evaluation. The ratio between the multivariate metric and a reference value (also discussed in this supplement) leads to the ability to identify discrepancies between simulations and experiments that are globally larger than the numerical, input, and experimental uncertainties.

However, to have a global quantification of the modeling error, the level of the pointwise validation uncertainties must be considered. Increasing the validation uncertainty at the single set points leads to a decrease of the multivariate metric, but this decrease is not caused by an improvement in modeling accuracy. As for the pointwise metric (Eça, Dowding, and Roache, 2022), it should be emphasized that the goal of the multivariate metric is not to obtain a value smaller than the reference value (ratio E_{mv}/E_{ref} smaller than unity). If the level of the validation uncertainties is unacceptably large, a ratio smaller than unity only indicates that, globally, the modeling error should be smaller than the sum of comparison errors and validation uncertainties. The ratio E_{mv}/E_{ref} should not be used as a pass/fail threshold of the validation exercise. The metric does provide a quantitative global assessment of the modeling error when it is much larger than one. Attribution of the source or sources of the global modeling error can only be made through the validation uncertainties (that depend on numerical, input, and experimental uncertainties at each set point realization and on the associated confidence level).

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NONMANDATORY APPENDIX A METHODOLOGY TO EVALUATE THE VALIDATION COVARIANCE MATRIX, V_{val}

A-1 INTRODUCTION

The purpose of this Appendix is to present the two techniques available to evaluate the validation covariance matrix V_{val} [para 4.2, eq. (4-9)], which includes contributions from the numerical input parameters and experimental uncertainties. The first technique is based on the sensitivity coefficients approach and the second on sampling methods. The application of these two techniques to a single set point is presented in sections 3-2 and 3-3 of ASME V&V 20-2009. This Standard presents the application of these techniques to the multivariate metric applied to n validation set points.

The validation covariance matrix characterizes the correlation structure due to input, numerical, and measurement errors for the comparison errors E_i obtained at n validation set points that are defined by eq. (A-1-1),

$$E_i = S_i(x_1, x_2, \cdots, x_m) - D_i(x_1, x_2, \cdots, x_m),\ i = 1, \cdots, n \tag{A-1-1}$$

S_i and D_i are the values of the validation variables at the n validation set points obtained from experiments (D_i) and simulations (S_i) containing m input variables.

The specific form of the equations to evaluate the validation matrix contributions depends on the following:

(a) the determination of the validation variables. Four cases are considered in ASME V&V 20-2009:

(1) Case 1: validation variable is directly measured.

(2) Case 2: validation variable is a result defined by a data reduction equation with no shared error sources between the measured variables.

(3) Case 3: validation variable is a result defined by a data reduction equation with shared error sources between the measured variables.

(4) Case 4: the result of a simulation is compared to a validation variable evaluated from measured variables analyzed with a model.

These four cases are described in this Appendix.

NOTES:

(1) For the four cases, the sharing of error sources mentioned above is related to the experimental data and input parameters of the simulations at each set point.

(2) In Case 4, the model used in the simulations is independent from the model applied to the measured variables to obtain the experimental validation variable.

(b) the existence of shared numerical input parameters or experimental errors at the n validation set points included in the determination of V_{val}. Two bounding cases are considered:

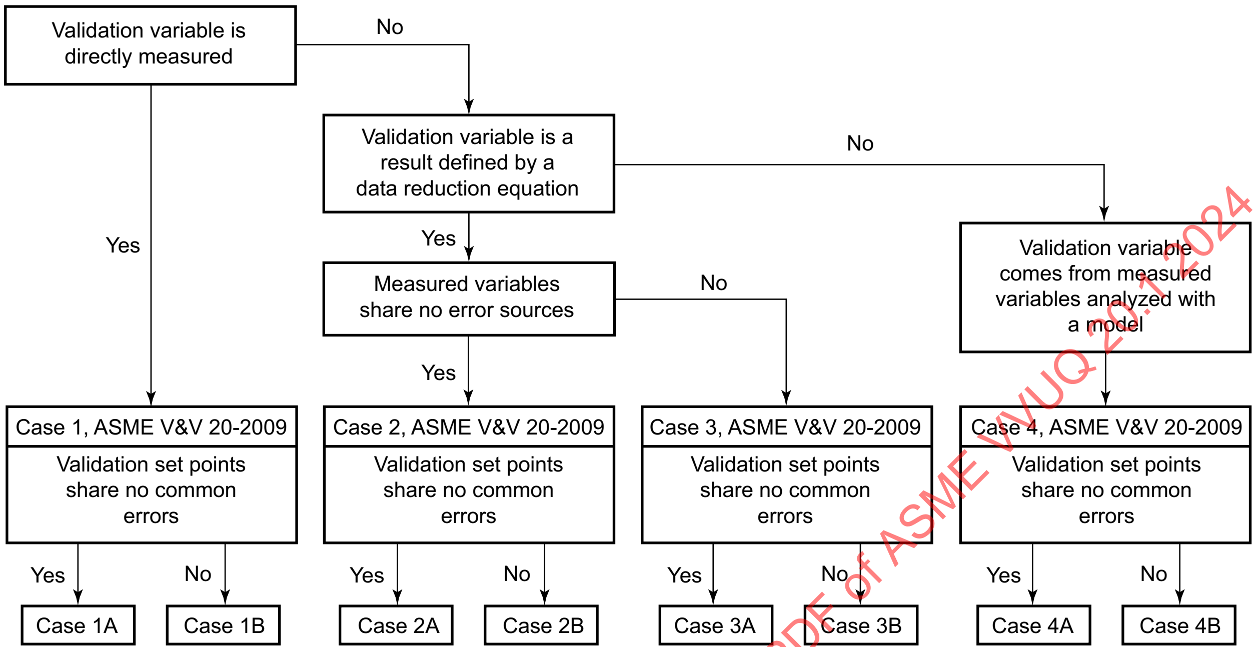
(1) no common (shared) errors in the simulation (S_i) and/or in the experimental measurements (D_i) at the n validation set points.

(2) errors are identically shared at the n validation set points in the simulation (S_i) and/or in the experimental measurements (D_i), i.e., errors are the same at the n validation set points.

These two assumptions are bounding for the relationship between errors at the multiple validation set points, as the case of no shared errors has a correlation coefficient of zero, whereas the case of identical shared errors has a correlation coefficient of one. The error sharing between the n validation set points is different from the error sharing that distinguishes the four cases described in ASME V&V20-2009. It is a consequence of the application of the multivariate metric to multiple set points and so it is not addressed in ASME V&V 20-2009.

The flowchart in Figure A-1-1 provides a decision tree to identify the appropriate cases and bounding assumptions for the relationship between errors at the validation set points. Note that this flowchart does not cover all the possible situations of a validation exercise. For example, it is assumed that the direct measurement of a validation variable guarantees that numerical input parameters and experimental contributions to the validation covariance matrix are independent. Naturally, such assumption may not always apply to directly measured validation variables.

Figure A-1-1
Logic Flow for Choosing Approach to Calculate the Validation Uncertainty Matrix, V_{val}



However, it is not difficult to adjust each situation using the several possibilities described in the flowchart of Figure A-1-1.

The equations that define the validation covariance matrix V_{val} and its contributions are presented in this Appendix for all the cases included in Figure A-1-1. To avoid unnecessary repetitions, the equations are organized per contribution to V_{val}. Section A-2 is dedicated to the sensitivity coefficients approach with the different contributions to V_{val} organized as illustrated in Table A-1-1. The sampling technique is described in section A-3. Finally, section A-4 presents important remarks about the calculation of V_{val} for the strong version of simulation models, i.e., for the cases that assume that all input parameters are hard wired, so there is no input uncertainty.

The calculation of the validation covariance matrix V_{val} is presented using standard uncertainties to characterize the numerical input parameters and experimental errors (u_{num}, u_{input}, and u_D). Equivalent equations are obtained if expanded uncertainties (u_{num}, u_{input}, and u_D) are adopted. Section 6-3 of ASME V&V 20-2009 discusses the determination of the coverage factors required to transform standard uncertainties in to expanded uncertainties.

Table A-1-1
Contributions to the Covariance Validation Matrix, V_{val}, in the Sensitivity Coefficients Approach

Paragraph	Case	Contribution to V_{val}
A-2.1	1A, 1B, 2A, 2B, 3A, 3B, 4A, 4B	Numerical uncertainty, V_{num}
A-2.2	1A, 1B	Input parameters uncertainty, V_{input}
A-2.3	1A, 1B	Experimental uncertainty, V_D
A-2.4	2A, 2B, 3A, 3B	Correlated experimental and input parameters uncertainty, $V_{input+D}$
A.-2.5	4A, 4B	Input parameters uncertainty of the simulations, $V_{S,input}$, and of the model that handles the experimental data, $V_{D,input}$

A-2 Sensitivity Coefficients Approach

(a) The four different cases illustrated in Figure A-1-1 lead to the following equations:

(1) Cases 1A and 1B: validation variable directly measured with no shared error sources between experiments and simulations.

$$V_{\mathrm{val}} = V_{\mathrm{num}} + V_{\mathrm{input}} + V_D \tag{A-2-1}$$

(2) Cases 2A, 2B, 3A, and 3B: validation variable computed from a data reduction equation.

$$V_{\mathrm{val}} = V_{\mathrm{num}} + V_{\mathrm{input}+D} \tag{A-2-2}$$

(3) Cases 4A and 4B: validation variable is evaluated from measured variables analyzed with a model.

$$V_{\mathrm{val}} = V_{\mathrm{num}} + V_{\mathrm{input}} + V_{D,\mathrm{num}} + V_{D,\mathrm{input}} \tag{A-2-3}$$

In case 4, V_{num} and $V_{\mathrm{D,num}}$ correspond to numerical uncertainties from two different models: V_{num} refers to the model used to obtained the results of the simulations S_i, whereas the $V_{D,\mathrm{num}}$ contribution comes from the model applied to measured quantities to obtain D_i.

(b) These equations have a companion definition of the validation uncertainty u_{val} for a single set point taken from ASME V&V 20-2009.

(1) Case 1

$$u_{\mathrm{val}}^2 = u_{\mathrm{num}}^2 + u_{\mathrm{input}}^2 + u_D^2 \tag{A-2-4}$$

(2) Cases 2 and 3

$$u_{\mathrm{val}}^2 = u_{\mathrm{num}}^2 + u_{\mathrm{input}+D}^2 \tag{A-2-5}$$

(3) Case 4

$$u_{\mathrm{val}}^2 = u_{S,\mathrm{num}}^2 + u_{S,\mathrm{input}}^2 + u_{D,\mathrm{num}}^2 + u_{D,\mathrm{input}}^2 \tag{A-2-6}$$

The expressions to determine the different contributions to the validation covariance matrix V_{val} are presented below for the two limiting cases: validation set points do not share error sources (correlation coefficients equal to zero, cases 1A, 2A, 3A, and 4A); validation set points share error sources (correlation coefficients equal to one, cases 1B, 2B, 3B, and 4B). Recall that this choice is related to the conditions at the *n* validation set points and not to the way each validation variable is determined.

A-2.1 Contribution of the Numerical Uncertainty, V_{num} and $V_{D,\mathrm{num}}$ (Cases 1, 2, 3, and 4)

The contribution of the numerical uncertainty in cases 1, 2, and 3 leads to V_{num}, whereas two contributions exist for case 4, V_{num} and $V_{D,\mathrm{num}}$. The expressions for the determination of these two matrices are similar. Therefore, only the equations for V_{num} are presented. Expressions for $V_{D,\mathrm{num}}$ are easily obtained replacing the numerical standard uncertainty at each set point $u_{\mathrm{num},i}$ by $u_{D,\mathrm{num},i}$.

(a) *No Shared Errors Between the n Validation Set Points (Cases 1A, 2A, 3A, and 4A).* The standard uncertainty of the numerical error at each set point, $u_{\mathrm{num},i}$, can be obtained with the techniques described in ASME V&V 20-2009. When there are no shared errors between the *n* validation set points, the contribution of the numerical uncertainty to the validation covariance matrix V_{num} is defined by eq. (A-2-7).

$$V_{\text{num}} = \begin{bmatrix} u_{\text{num},1}^2 & 0 & \cdots & 0 \\ 0 & u_{\text{num},2}^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & u_{\text{num},n}^2 \end{bmatrix} \tag{A-2-7}$$

(b) Shared Identical Errors Between the n Validation Set Points (Cases 1B, 2B, 3B, and 4B). For the case the numerical errors are shared by the n set points, the contribution of the numerical uncertainty to the validation covariance matrix V_{num} is defined by eq. (A-2-8).

$$V_{\text{num}} = \begin{bmatrix} u_{\text{num},1}^2 & u_{\text{num},1}u_{\text{num},2} & \cdots & u_{\text{num},1}u_{\text{num},n} \\ u_{\text{num},2}u_{\text{num},1} & u_{\text{num},2}^2 & \cdots & u_{\text{num},2}u_{\text{num},n} \\ \vdots & \vdots & \ddots & \vdots \\ u_{\text{num},n}u_{\text{num},1} & u_{\text{num},n}u_{\text{num},2} & \cdots & u_{\text{num},n}^2 \end{bmatrix} \tag{A-2-8}$$

A-2.2 Contribution of the Input Uncertainty, V_{input} (Case 1)

In case 1, the contributions of the numerical input and experimental uncertainties to the validation uncertainty is independent and so V_{input} depends only on uncertainties of the m input parameters $u_{\text{input},j}$.

(a) No Shared Errors Between the n Validation Set Points (Case 1A). When there are no input errors shared by the n validation set points, V_{input} is obtained from eq. (A-2-9).

$$V_{\text{input}} = \begin{bmatrix} X_{S,1}V_{X,1}X_{S,1}^{T} & 0 & \cdots & 0 \\ 0 & X_{S,2}V_{X,2}X_{S,2}^{T} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & X_{S,n}V_{X,n}X_{S,n}^{T} \end{bmatrix} \tag{A-2-9}$$

where X_{Si} is the sensitivity matrix for the simulation and $V_{X,i}$ is the covariance matrix of the simulation inputs, both at set point i. Since there are no shared errors, off-diagonal entries in eq. (A-2-9) are identically 0. The sensitivity coefficients vector originated by the m input variables at each set point i, X_{Si}, is a line vector ($1 \times m$) defined by eq. (A-2-10).

$$X_{S,i} = \begin{bmatrix} \frac{\partial S_i}{\partial x_1} & \cdots & \frac{\partial S_i}{\partial x_m} \end{bmatrix} \tag{A-2-10}$$

The covariance matrix $V_{X,i}$ is an ($m \times m$) matrix defined by the standard uncertainties of the input parameters at each set point i as presented in eq. (A-2-11).

$$V_{X,i} = \begin{bmatrix} \left(u_{x_1}^2\right)_i & 0 & \cdots & 0 \\ 0 & \left(u_{x_2}^2\right)_i & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \left(u_{x_m}^2\right)_i \end{bmatrix} \tag{A-2-11}$$

(b) Shared Identical Errors Between the n Validation Set Points (Case 1B). If input parameter errors are shared by all validation set points, i.e., the n $V_{X,i}$ matrices are all equal, the contribution of the input uncertainty to the validation covariance matrix is defined by eq. (A-2-12).

$$V_{\text{input}} = X_S V_X X_S^T \tag{A-2-12}$$

X_S is a $(n \times m)$ matrix containing the m sensitivity coefficients at the n set points defined by eq. (A-2-13), and V_X is a $m \times m$ diagonal matrix including the standard uncertainties of the m input parameters x_j squared.

$$X_S = \begin{bmatrix} \frac{\partial S_1}{\partial x_1} & \cdots & \frac{\partial S_1}{\partial x_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial S_n}{\partial x_1} & \cdots & \frac{\partial S_n}{\partial x_m} \end{bmatrix} \tag{A-2-13}$$

V_x is defined by eq. (A-2-11) and can be calculated for any of the n set points.

A-2.3 Contribution of the Experimental Uncertainty, V_D (Case 1)

When the experimental measurement does not share any errors with the simulation and the validation variables are directly measured, the contribution of the experimental uncertainty to the validation covariance matrix is independent of the input uncertainty. The standard uncertainty of the measurement, u_{D_i}, can be obtained at each set point using the techniques described in ASME V&V 20-2009.

(a) No Shared Errors Between the n Validation Set Points (Case 1A). For the case that the validation set points do not share experimental errors, V_D is defined by eq. (A-2-14).

$$V_D = \begin{bmatrix} u_{D,1}^2 & 0 & \cdots & 0 \\ 0 & u_{D,2}^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & u_{D,n}^2 \end{bmatrix} \tag{A-2-14}$$

(b) Shared Identical Errors Between the n Validation Set Points (Case 1B). If the experimental errors are shared at the n validation set points, the contribution of the experimental uncertainty to the validation covariance matrix V_D is defined by eq. (A-2-15).

$$V_D = \begin{bmatrix} u_{D,1}^2 & u_{D,1}u_{D,2} & \cdots & u_{D,1}u_{D,n} \\ u_{D,2}u_{D,1} & u_{D,2}^2 & \cdots & u_{D,2}u_{D,n} \\ \vdots & \vdots & \ddots & \vdots \\ u_{D,n}u_{D,1} & u_{D,n}u_{D,2} & \cdots & u_{D,n}^2 \end{bmatrix} \tag{A-2-15}$$

A-2.4 Combined Contribution of Input and Experimental Uncertainties, $V_{input+D}$ (Cases 2 and 3)

When the validation variable is a result defined by a data reduction equation, the contribution of input parameters and experimental uncertainties to the validation covariance matrix is done simultaneously. There are slight differences between the cases with (case 3) and without (case 2) shared errors between the measured quantities that will be pointed out below. Recall that the distinction between cases 2 and 3 is different from the possible correlations between the n validation set points used in the multivariate metric.

(a) No Shared Errors Between the n Validation Set Points (Cases 2A and 3A). The contribution of the combined effect of input parameters and experimental uncertainty to the validation covariance matrix $V_{input+D}$ when the n validation set points do not share errors is defined by eq. (A-2-16).

$$V_{input+D} = \begin{bmatrix} V_{(input+D)_{1,1}} & 0 & \cdots & 0 \\ 0 & V_{(input+D)2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & V_{(input+D)_{n,n}} \end{bmatrix} \tag{A-2-16}$$

with

$$V_{(\text{input}+D)_{i,i}} = (X_{S,i} - X_{D,i})V_{X,i}(X_{S,i} - X_{D,i})^T \tag{A-2-17}$$

The vector containing the sensitivity coefficients of the simulations $X_{S,i}$ is defined by eq. (A-2-10), whereas the vector of sensitivity coefficients of the experiments $X_{D,i}$ is given by eq. (A-2-18).

$$X_{D,i} = \begin{bmatrix} \frac{\partial D_i}{\partial x_1} & \cdots & \frac{\partial D_i}{\partial x_m} \end{bmatrix} \tag{A-2-18}$$

The covariance matrix $V_{X,i}$ depends on the existence of shared errors between the measured quantities required to obtain the validation variable. For the case of no shared errors (case 2), $V_{X,i}$ is defined by eq. (A-2-11). On the other hand, for shared error between the measured quantities (Case 3), $V_{X,i}$ is determined from eq. (A-2-19).

$$V_{X,i} = \begin{bmatrix} \left(u_{x_1}^2\right)_i & \left(u_{x_1}u_{x_2}\right)_i & \cdots & \left(u_{x_1}u_{x_m}\right)_i \\ \left(u_{x_2}u_{x_1}\right)_i & \left(u_{x_2}^2\right)_i & \cdots & \left(u_{x_2}u_{x_m}\right)_i \\ \vdots & \vdots & \ddots & \vdots \\ \left(u_{x_m}u_{x_1}\right)_i & \left(u_{x_m}u_{x_2}\right)_i & \cdots & \left(u_{x_m}^2\right)_i \end{bmatrix} \tag{A-2-19}$$

(b) Shared Identical Errors Between the n Validation Set Points (Cases 2B and 3B). In the case the n validation points share identical errors, the contribution of the combined effect of input and experimental uncertainties to the validation covariance matrix $V_{\text{input}+D}$ is determined from eq. (A-2-20).

$$V_{\text{input}+D} = (X_S - X_D)V_X(X_S - X_D)^T \tag{A-2-20}$$

X_S and X_D are $(n \times m)$ matrices that contain the m sensitivity coefficients at the n validation set points. eq. (A-2-13) defines X_S and X_D is determined from eq. (A-2-21).

$$X_D = \begin{bmatrix} \frac{\partial D_1}{\partial x_1} & \cdots & \frac{\partial D_1}{\partial x_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial D_n}{\partial x_1} & \cdots & \frac{\partial D_n}{\partial x_m} \end{bmatrix} \tag{A-2-21}$$

The definition of the $(m \times m)$ matrix V_X is equivalent to the previous section, i.e., V_X is defined by eq. (A-2-11) for case 2 (no shared errors between the measured variables), and V_X is determined from eq. (A-2-19) in case 3 (shared errors between the measured variables). We recall that this distinction between cases 2 and 3 is related to the way the validation variables are determined and not to sharing of errors between the n validation set points.

A-2.5 Contribution of Input Uncertainties When Experimental Value Comes From Measured Variables Analyzed With a Model, V_{input}, $V_{D,\text{input}}$

In this case there are contributions coming from the m input parameters x_j required for the simulation V_{input} and from the l experimental variables, y_k used in the model that produces the experimental results D_i, $V_{D,\text{input}}$. Note that the model used to post-process the measured variables is independent from the model used in the simulations.

The determination of the V_{input} matrix is presented in para. A-2.2 and the determination of $V_{D,\text{input}}$ is similar. Nonetheless, for the sake of clarity, the definitions of V_{input} and $V_{D,\text{input}}$ are presented below.

(a) No Shared Errors Between the n Validation Set Points (Case 4A). When there are no shared errors between the n validation set points, the $(n \times n)$ matrices V_{input} and $V_{D,\text{input}}$ are defined by eqs. (A-2-22) and (A-2-23).

$$V_{\text{input}} = \begin{bmatrix} X_{S,1}V_{X,1}X_{S,1}^T & 0 & \cdots & 0 \\ 0 & X_{S,2}V_{X,2}X_{S,2}^T & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & X_{S,n}V_{X,n}X_{S,n}^T \end{bmatrix} \tag{A-2-22}$$

$$V_{D,\text{input}} = \begin{bmatrix} X_{D,1}V_{D,1}X_{D,1}^T & 0 & \cdots & 0 \\ 0 & X_{D,2}V_{D,2}X_{D,2}^T & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & X_{D,n}V_{D,n}X_{D,n}^T \end{bmatrix} \tag{A-2-23}$$

The (1 × m) line vector of sensitivity coefficients of the m input parameters of the simulation $X_{S,i}$ is defined by eq. (A-2-10), whereas the (1 × l) line vector of sensitivity coefficients of the l measured variables used in the model that produces D_i is defined by eq. (A-2-24).

$$X_{D,i} = \begin{bmatrix} \frac{\partial D_i}{\partial y_1} & \cdots & \frac{\partial D_i}{\partial y_l} \end{bmatrix} \tag{A-2-24}$$

The (m × m) matrix that defines $V_{X,i}$ is defined by eq. (A-2-11) if the m input parameters of the simulations are not correlated and by eq. (A-2-19) if they are correlated. The (l × l) covariance matrix $V_{D,i}$ is determined by similar definitions, i.e., for l independent measured variables used in the model that produces D_i, $V_{D,i}$ is defined by eq. (A-2-25).

$$V_{D,i} = \begin{bmatrix} \left(u_{y_1}^2\right)_i & 0 & \cdots & 0 \\ 0 & \left(u_{y_2}^2\right)_i & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \left(u_{y_l}^2\right)_i \end{bmatrix} \tag{A-2-25}$$

On the other hand, if the l measured variables are correlated $V_{D,i}$ is determined from eq. (A-2-26).

$$V_{D,i} = \begin{bmatrix} \left(u_{y_1}^2\right)_i & \left(u_{y_1}u_{y_2}\right)_i & \cdots & \left(u_{y_1}u_{y_l}\right)_i \\ \left(u_{y_2}u_{y_1}\right)_i & \left(u_{y_2}^2\right)_i & \cdots & \left(u_{y_2}u_{y_l}\right)_i \\ \vdots & \vdots & \ddots & \vdots \\ \left(u_{y_l}u_{y_1}\right)_i & \left(u_{y_l}u_{y_2}\right)_i & \cdots & \left(u_{y_l}^2\right)_i \end{bmatrix} \tag{A-2-26}$$

(b) Shared Identical Errors Between the n Validation Set Points (Case 4B). When the errors are shared by the n validation set points, V_{input} is defined by eq. (A-2-27),

$$V_{\text{input}} = X_S V_X X_S^T \tag{A-2-27}$$

and $V_{D,\text{input}}$ given by eq. (A-2-28).

$$V_{D,\text{input}} = X_D V_D X_D^T \tag{A-2-28}$$

The (n × m) X_S matrix is defined by eq. (A-2-13) and the (n × l) X_D matrix is determined from eq. (A-2-29).

Table A-2.6-1
Summary of Equations Required to Calculate the Validation Uncertainty Matrix, V_{val}

Case	Equations Required	Comments
1A	V_{val}: (A-2-1); V_{num}: (A-2-7); V_{input}: (A-2-9); $X_{S,i}$: (A-2-10); $V_{X,i}$: (A-2-11); and V_D: (A-2-14)	V_{val} is a diagonal matrix
1B	V_{val}: (A-2-1); V_{num}: (4-11); V_{input}: (A-2-12); $X_{S,i}$: (A-2-13); $V_{X,i}$: (A-2-11); and V_D : (A-2-15)	V_{val} is a full matrix
2A	V_{val}: (A-2-2); V_{num}: (A-2-7); $V_{input+D}$: (A-2-16); $X_{S,i}$: (A-2-10); $V_{X,i}$: (A-2-11); and $X_{D,i}$: (A-2-18)	V_{val} is a diagonal matrix
2B	V_{val}: (A-2-2); V_{num}: (A-2-8); $V_{input+D}$: (A-2-20); $X_{S,i}$: (A-2-13); $V_{X,i}$: (A-2-11); and $X_{D,i}$: (A-2-21)	V_{val} is a full matrix
3A	V_{val}: (A-2-2); V_{num}: (A-2-7); $V_{input+D}$: (A-2-16); $X_{S,i}$: (A-2-10); $V_{X,i}$: (A-2-19); and $X_{D,i}$: (A-2-18)	V_{val} is a diagonal matrix
3B	V_{val}: (A-2-2); V_{num}: (A-2-8); $V_{input+D}$: (A-2-20); $X_{S,i}$: (A-2-13); $V_{X,i}$: (A-2-19); and $X_{D,i}$: (A-2-21)	V_{val} is a full matrix
4A	V_{val}: (A-2-3); V_{num}, $V_{D,num}$: (A-2-7); V_{input}: (A-2-22); $V_{D,input}$: (A-2-23); $X_{S,i}$: (A-2-10); $X_{D,i}$: (A-2-24); $V_{X,i}$: (A-2-11) or (A-2-19); $V_{D,i}$: (A-2-25) or (A-2-26)	V_{val} can be diagonal or full matrix
4B	V_{val}: (A-2-3); V_{num}, $V_{D,num}$: (A-2-8); V_{input}: (A-2-27); $V_{D,input}$: (A-2-28); $X_{S,i}$: (A-2-13); $X_{D,i}$: (A-2-29); $V_{X,i}$: (A-2-11) or (A-2-19); $V_{D,i}$: (A-2-25) or (A-2-26)	V_{val} is a full matrix

$$X_D = \begin{bmatrix} \frac{\partial D_1}{\partial y_1} & \cdots & \frac{\partial D_1}{\partial y_l} \\ \vdots & \ddots & \vdots \\ \frac{\partial D_n}{\partial y_1} & \cdots & \frac{\partial D_n}{\partial y_l} \end{bmatrix} \tag{A-2-29}$$

The $(n \times n)$ covariance matrix V_X is defined by eq. (A-2-11) if there is no correlation between the m input variables of the simulation and by eq. (A-2-19) if the m input variables are correlated. Similarly, for independent measured variables for the determination of D_i, V_D is defined by eq. (A-2-25), whereas the case of correlated measured variables leads to V_D determined by eq. (A-2-26).

A-2.6 Summary of Equations Required To Determine V_{val} With Sensitivity Analysis

Table A-2.6-1 summarizes all the equations required to calculate V_{val} for the eight cases included in the chart presented in Figure A-1-1. The matrix is followed by the corresponding equation number.

A-3 PROCEDURE TO EVALUATE VALIDATION COVARIANCE MATRIX, V_{val}, THROUGH RANDOM SAMPLING

When the distributions that characterize the uncertainties of the input parameters and the experimental data are known, Monte Carlo sampling can also be used to estimate the covariance matrix V_{val}. If the propagation of the input uncertainties through the model used in the simulations is independent of the numerical uncertainty, the sampling methodology described in ASME V&V 20-2009 leads to eq. (A-3-1) for the definition of each entry of the validation covariance matrix.

$$[V_{\mathrm{val}}]_{i,k} \approx [V_{\mathrm{num}}]_{i,k} + \frac{1}{n_r - 1} \sum_{I=1,K=1}^{n_r} (E_{i,I} - \overline{\overline{E}}_i)(E_{k,K} - \overline{\overline{E}}_k) \tag{A-3-1}$$

V_{num} is obtained from the equations presented in para. A-2.1; n_r is the number of random samples over population; $E_{i,I}$ is the I^{th} sample from the population values associated with the uncertainties, u_{input} and u_D of set point i; $E_{k,K}$ is the K^{th} sample from the population values associated with the uncertainties, u_{input} and u_D at set point k; $\overline{\overline{E}}_i$ and $\overline{\overline{E}}_i$ are the mean values over the n_r samples at set points i and k; and the subscripts i, k indicate the i^{th}, k^{th} element of the corresponding matrix.

Equation (A-3-1) estimates the contribution to V_{val} of two validation set points, i and k. Details of the sampling techniques applied at each set point (i and k) for cases 1, 2, 3, and 4 are described in section 5 of ASME V&V 20-2009. However, as described in the previous section using sensitivity analysis, the relationship between the errors at the n validation set points also affects the sampling approach.

The sampling approach accounts for correlation between the errors characterized by u_D and u_{input} and allows for nonnormally distributed experimental data and simulation model parameters. The sampling method does not make any assumption about the properties of the model used in the simulations.

A-3.1 No Shared Errors Between the *n* Validation Set Points (Cases 1A, 2A, 3A, and 4A)

When there are no shared errors between the n validation set points, the samples over the input parameters are independently generated to obtain the distributions of comparison errors. As an example, the input parameter uncertainties of the m input parameters at the n validation set points are sampled as illustrated in eqs. (A-3-2) and (A-3-3).

$$E_{i,I} = S_{i,I}(x_{1,I}, x_{2,I}, \ldots, x_{m,I}) - D_{i,I}(x_{1,I}, x_{2,I}, \ldots, x_{m,I}),\ i = 1, \ldots, n \tag{A-3-2}$$

$$E_{k,K} = S_{k,K}(x_{1,K}, x_{2,K}, \ldots, x_{m,K}) - D_{i,K}(x_{1,K}, x_{2,K}, \ldots, x_{m,K}),\ i = 1, \ldots, n \tag{A-3-3}$$

The samples of the input parameter uncertainties are independently generated, i.e., independent sample sets $[x_{1,I}, x_{2,I} \ldots x_{m,I}]$ and $[x_{1,K}, x_{2,K} \ldots x_{m,K}]$ are generated to evaluate the comparison error at the two validation set points i and k.

A-4 TWO SHARED IDENTICAL ERRORS BETWEEN THE *n* VALIDATION SET POINTS (CASES 1B, 2B, 3B, and 4B)

When there are shared identical errors between the validation set points, the samples over the input uncertainties would be identical, which means that the same sampling of the m input variables is used at all the n validation set points, i.e., $I \equiv K$ in eq. (A-3-1).

A-5 VALIDATION COVARIANCE MATRIX, V_{val}, FOR THE STRONG VERSION OF THE MODEL

The strong version of model absorbs all errors of the input parameters in δ_{model}, i.e. all input parameters are hardwired to the model and so δ_{input} is merged with δ_{model}. This leads to a validation uncertainty u_{val}^2 defined by eq. (A-5-1).

$$u_{val}^2 = u_{num}^2 + u_D^2 \tag{A-5-1}$$

Therefore, the validation covariance matrix defined by eq. (A-5-2) includes only numerical uncertainty (V_{num}) and experimental uncertainty (V_D), which have been presented in paras. A-2.1 and A-2.3.

$$V_{val} = V_{num} + V_D \tag{A-5-2}$$

If the errors are not shared at the n validation set points, the validation covariance matrix V_{val} is defined by eqs. (A-2-7) and (A-2-14). However, if the errors are identically shared at the n validation set points, the three matrices, V_{num}, V_D, and V_{val} will be singular (have a zero determinant). Therefore, the multivariate metric cannot be calculated. In such conditions, the modeling error at the n set points should lead to similar comparison errors (E) and validation uncertainties (U_{val}) and so a multivariate metric is not required to assess the global modeling error.

NONMANDATORY APPENDIX B
EXAMPLE PROBLEM: FIN-TUBE HEAT EXCHANGER

B-1 INTRODUCTION

The purpose of this Appendix is to illustrate the application of the multivariate metric to quantitatively compare a computational model to experimental data at multiple set points. The multivariate metric discussed in section 4 is used. Example calculations are shown.

A set number of significant digits from the calculation inputs have not been tracked. The precision of the input data is as presented in the following tables. Example calculations are performed using Excel (Microsoft Office 365 ProPlus, version 1803) with default precision. Results are rounded to two digits after the decimal point except for small numbers (< 1), which are reported using scientific notation rounded to two digits past the decimal point.

The organization of this Appendix is as follows:

(a) Section B-2: reporting of the validation case
(b) Section B-3: reporting of the experimental data
(c) Section B-4: reporting of simulation model
(d) Section B-5: evaluation of the pointwise ASME V&V 20-2009 metric
(e) Section B-6: evaluation of the multivariate metric E

B-2 VALIDATION EXAMPLE

The validation case is the fin-tube heat exchanger used as an example problem in ASME V&V 20-2009. Figure 1-4-1 of ASME V&V20-2009 provides a schematic of the geometry identifying relevant geometric features and parameters.

The experimental data used in this Appendix are synthetic values generated per para. 7-3.2 of the ASME V&V 20-2009. Use of synthetic rather than experimental data facilitates "teaching" because dependencies can be controlled to provide "clean" results to demonstrate and document effects.

B-3 EXPERIMENTAL DATA AND UNCERTAINTIES

Six experiments are conducted that vary the inflow temperature, T_i, from ~70°C to ~ 92°C. The outflow temperature, T_o, and the ambient temperature, T_∞, are measured. See Table B-3-1.

The data reduction defined in eq. (B-3-1) is used to calculate the heat transfer rate, q_D, from the measured values T_i and T_o given the fluid flow rate, Q, the fluid density, ρ, and the specific heat, C_p. For a given flow condition, an increase in the inlet temperature yields an increase in the fluid temperature thus an increase in the outlet temperature measurement. Set point conditions and results for each experiment are summarized in Table B-3-1.

$$q_D = \rho Q C_p (T_i - T_o) \tag{B-3-1}$$

The Fin-Tube Heat Exchanger example assumes that replicate experiments are not performed to quantify data and parameter uncertainties. Instead, the experimental apparatus and data collection are assumed to be well characterized and to have well characterized uncertainties. Estimates of the random and systematic uncertainties for the input parameters, $X_i = \{T_i, T_o, Q, \rho, \text{and } C_p\}$, are reported in Table B-3-2. Additional parameters, $X_i = \{T_\infty, k_t, k_f, h_i, h_f, \text{and } h_o\}$, are included in Table B-3-2 to support discussion of the simulation model in section B-4. The variables k_t and k_f are the thermal conductivities of the tube and fin. The variables h_i, h_f, and h_o are convective heat transfer coefficients for the inner surface of the tube, fin, and outer surface of the tube, respectively. The flow temperatures T_i and T_o have shared systematic sources.

Because the heat transfer rate, q_D, is calculated from the data reduction eq. (B-3-1), data uncertainty, u_{qD}, is quantified as input parameter uncertainty from uncertain inputs when propagated through the data reduction equation. For this example, u_{qD} is calculated using the method of sensitivity coefficients described in para. 4-2.2 of ASME V&V 20-2009; see para. 5-2.1.

The sensitivity coefficients, $X_i \frac{\partial q_D}{\partial X_i}$, for parameters X_i are calculated analytically in eq. (B-3-2) using the data reduction of eq. (B-3-1).

$$X_i \frac{\partial q_D}{\partial X_i} = \begin{bmatrix} T_i \frac{\partial q_D}{\partial T_i} \\ T_o \frac{\partial q_D}{\partial T_o} \\ Q \frac{\partial q_D}{\partial Q} \\ \rho \frac{\partial q_D}{\partial \rho} \\ C_p \frac{\partial q_D}{\partial C_p} \end{bmatrix} = \begin{bmatrix} \rho Q C_p T_i \\ -\rho Q C_p T_o \\ \rho Q C_p (T_i - T_o) \\ \rho Q C_p (T_i - T_o) \\ \rho Q C_p > (T_i - T_o >) \end{bmatrix} \tag{B-3-2}$$

An example of the calculation of the sensitivity coefficient for parameter T_i for Experiment 1 of Table B-3-1 is defined in eq. (B-3-3).

$$T_i \frac{\partial q_D}{\partial T_i} = \rho Q C_p T_i = \left(990 \frac{\text{kg}}{\text{m}^3}\right)\left(6.21 \times 10^{-6} \frac{\text{m}^3}{s}\right)\left(4180 \frac{\text{J}}{\text{kg}\,°\text{C}}\right)(70.44°\text{C})(W) = 1810.18W \tag{B-3-3}$$

The computed sensitivity coefficients, $X_i \frac{\partial q_D}{\partial X_i}$, for each experiment are reported in Table B-3-3.

B-3.1 Experimental Data Uncertainty

Data uncertainty, u_{q_D}, for the heat transfer rate, q_D, for each experiment is computed rigorously using the method of sensitivity coefficients as described in para. 4-2.2 of ASME V&V 20-2009. Per eq. (4-2-4) of ASME V&V 20-2009, u_{qD} is the root-sum-square of uncertainties from random, s_{q_D}, and systematic, b_{qD}, sources.

$$u_{q_D}^2 = s_{q_D}^2 + b_{q_D}^2 \tag{B-3-4}$$

Equation (4-2-6) of ASME V&V 20-2009 provides the propagation equation for random uncertainty, s_{qD}. The equation in matrix notation is

$$s_{q_D}^2 = X_D^T V_X(rnd) X_D \tag{B-3-5}$$

X_D is the matrix of sensitivity coefficients for an experimental result as written in eq. (B-3-2). V_X (rnd) is the covariance matrix for the random uncertainties in the input parameters. Because cross-correlations of random parameters are zero, V_X (rnd) is a diagonal matrix with entries $s_{X_i}^2$ along the diagonal [eq. (B-3-6)].

$$V_X(\text{rnd}) = \begin{bmatrix} s_{T_i}^2 & 0 & 0 & 0 & 0 \\ 0 & s_{T_o}^2 & 0 & 0 & 0 \\ 0 & 0 & s_Q^2 & 0 & 0 \\ 0 & 0 & 0 & s_\rho^2 & 0 \\ 0 & 0 & 0 & 0 & s_{C_p}^2 \end{bmatrix} \tag{B-3-6}$$

Using sensitivity coefficients from Table B-3-3, X_D for Experiment 1 is defined in eq. (B-3-7).

$$X_D = \begin{bmatrix} 1810.18 \\ -1732.32 \\ 77.87 \\ 77.87 \\ 77.87 \end{bmatrix} W \tag{B-3-7}$$

Similar expressions are used for each experiment. Using uncertainties from Table B-3-2, V_X (rnd) is defined in eq. (B-3-8).

$$V_X(\text{rnd}) = \begin{bmatrix} 4.90\,\text{E}{-07} & 0 & 0 & 0 & 0 \\ 0 & 4.90\,\text{E}{-07} & 0 & 0 & 0 \\ 0 & 0 & 2.50\,\text{E}{-05} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \tag{B-3-8}$$

The calculation of $s_{q_D}^2$ for Experiment 1 is defined in eq. (B-3-9).

$$s_{q_D}^2 = [1810.18 \quad -1732.32 \quad 77.87 \quad 77.87 \quad 77.87] \times \begin{bmatrix} 4.90\,\text{E}{-07} & 0 & 0 & 0 & 0 \\ 0 & 4.90\,\text{E}{-07} & 0 & 0 & 0 \\ 0 & 0 & 2.50\,\text{E}{-05} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} 1810.18 \\ -1732.32 \\ 77.87 \\ 77.87 \\ 77.87 \end{bmatrix} W^2 \tag{B-3-9}$$

$$= 3.23W^2$$

which yields eq. (B-3-10).

$$s_{q_D} = \sqrt{s_{q_D}^2} = \sqrt{3.23W^2} = 1.80W \tag{B-3-10}$$

Calculated values for s_{q_D} for each experiment are reported in Table B-3.1-1.

The propagation equation for systematic uncertainty, b_{q_D}, is provided in eq. 4-2-5 of ASME V&V 20-2009. The equation in matrix form is defined in eq. (B-3-11).

$$b_{q_D}^2 = X_D^T V_X(\text{sys}) X_D \tag{B-3-11}$$

V_X (sys) is the covariance matrix for systematic uncertainties with non-zero off-diagonal terms for correlated parameters as follows:

$$V_X(\text{sys}) = \begin{bmatrix} b_{T_i}^2 & b_{T_i}b_{T_o} & 0 & 0 & 0 \\ b_{T_i}b_{T_o} & b_{T_o}^2 & 0 & 0 & 0 \\ 0 & 0 & b_Q^2 & 0 & 0 \\ 0 & 0 & 0 & b_\rho^2 & 0 \\ 0 & 0 & 0 & 0 & b_{C_p}^2 \end{bmatrix} \tag{B-3-12}$$

T_i and T_o are correlated because they share identical systematic error sources. Using uncertainties from Table B-3-2, V_X (sys) is

$$V_X(\text{sys}) = \begin{bmatrix} 1.96\,\text{E}{-06} & 1.96\,\text{E}{-06} & 0 & 0 & 0 \\ 1.96\,\text{E}{-06} & 1.96\,\text{E}{-06} & 0 & 0 & 0 \\ 0 & 0 & 1.00\,\text{E}{-04} & 0 & 0 \\ 0 & 0 & 0 & 2.50\,\text{E}{-05} & 0 \\ 0 & 0 & 0 & 0 & 1.00\,\text{E}{-04} \end{bmatrix} \tag{B-3-13}$$

The calculation of $b^2_{q_D}$ for Experiment 1 is

$$b^2_{q_D} = [1810.18 \quad -1732.32 \quad 77.87 \quad 77.87 \quad 77.87] \times \begin{bmatrix} 1.96\,E{-06} & 1.96\,E{-06} & 0 & 0 & 0 \\ 1.96\,E{-06} & 1.96\,E{-06} & 0 & 0 & 0 \\ 0 & 0 & 1.00\,E{-04} & 0 & 0 \\ 0 & 0 & 0 & 2.50\,E{-05} & 0 \\ 0 & 0 & 0 & 0 & 1.00\,E{-04} \end{bmatrix} \times \begin{bmatrix} 1810.18 \\ -1732.32 \\ 77.87 \\ 77.87 \\ 77.87 \end{bmatrix} W^2 = 1.38W^2 \tag{B-3-14}$$

which yields eq. (B-3-15).

$$b_{q_D} = \sqrt{b^2_{q_D}} = \sqrt{1.38W^2} = 1.17\ W \tag{B-3-15}$$

Calculated values for s_{q_D} for each experiment are reported in Table B-3.1-1.

u_{q_D} for Experiment 1 is the combined value of s_{q_D} [eq. (B-3-10)] and b_{q_D} [eq. (B-3-15)] as follows:

$$u_{q_D} = \sqrt{3.23W^2 + 1.38W^2} = 2.15\ W \tag{B-3-16}$$

Calculated values for u_{qD} for each experiment are reported in Table B-3.1-1.

A plot of q_D versus T_i is presented in Figure B-3.1-1. The range of u_{qD} is included on the plot as uncertainty bars on the data; however, values of u_{qD} are sufficiently small to be occluded by the symbol.

Table B-3-1
Measured Flow Conditions and Calculated Total Heat Transfer Rate

Example	Experiment	Set Point Conditions					Results	
		T_i, °C	T_∞, °C	Q, m^3/s	ρ, kg /m^3	C_p, J/kg°C	T_o, °C	q_D, W
1	1	70.440	21.660	6.210 E−06	990	4180	67.410	77.870
2	4	73.580	22.140	6.240 E−06	990	4180	69.720	99.670
3	5	75.520	21.990	6.22 0E−06	990	4180	71.360	107.080
4	7	80.570	21.880	6.220 E−06	990	4180	75.710	125.090
5	9	87.530	22.080	6.230 E−06	990	4180	82.020	142.050
6	10	91.900	22.110	6.260 E−06	990	4180	85.830	157.240

Table B-3-2
Random and Systematic Uncertainties for Input Parameters, X_i

X_i	Input Parameter Standard Uncertainties	
	Random, S_{Xi}	Systematic, b_{X_i}
T_i, °C	0.07%	0.14%
T_o, °C	0.07%	0.14%
Q, m^3/s	0.50%	1.00%
ρ, kg/m^3	...	0.50%
C_p, J/kg°C	...	1.00%
T_∞, °C	...	1.00%
k_t, W/m°C	...	5.00%
k_f, W/m°C	...	5.00%
h_i, W/m°C	...	10.00%
h_f, W/m°C	...	10.00%
h_o, W/m°C	...	10.00%

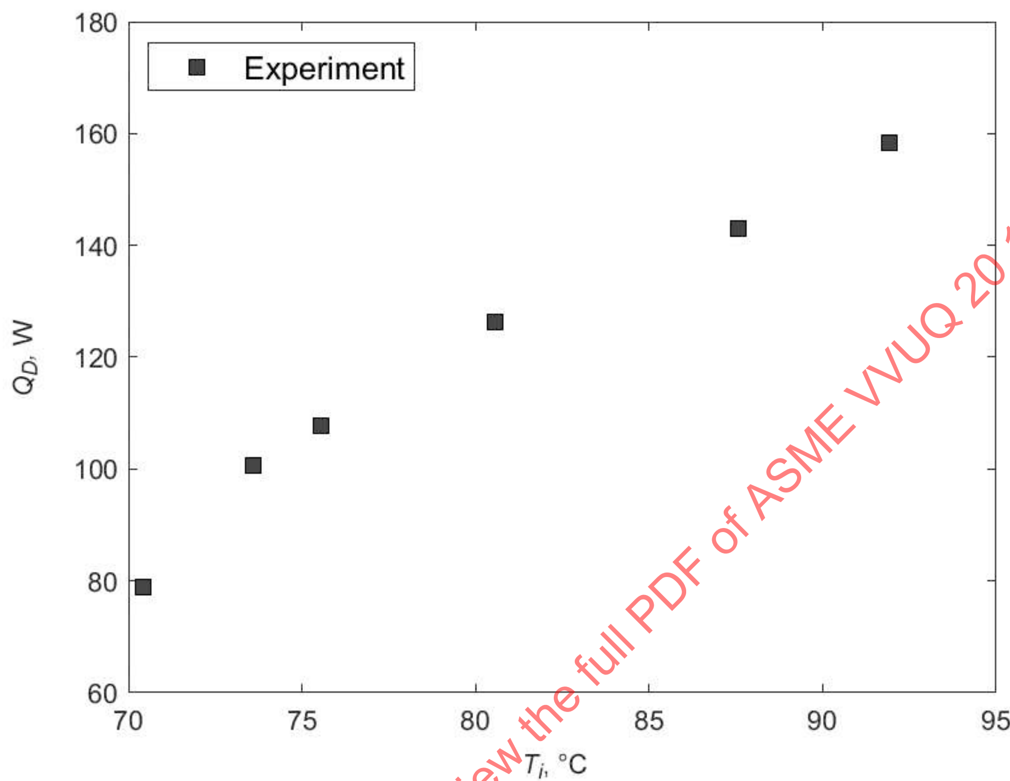
Table B-3-3
Calculated Sensitivity Coefficients for the Experiments Reported in Table B-3-1

Experiment	Scaled Sensitivity Coefficients				
	$T_i \cdot \partial q_D/\partial T_i$, W	$T_o \cdot \partial q_D/\partial T_o$, W	$Q \cdot \partial q_D/\partial Q$, W	$\rho \cdot \partial q_D/\partial \rho$, W	$C_p \cdot \partial q_D/\partial C_p$, W
1	1810.18	−1732.32	77.87	77.87	77.87
2	1900.01	−1800.34	99.67	99.67	99.67
3	1943.85	−1836.78	107.08	107.08	107.08
4	2073.84	−1948.75	125.09	125.09	125.09
5	2256.61	−2114.56	142.05	142.05	142.05
6	2380.68	−2223.44	157.24	157.24	157.24

Table B-3.1-1
Random, Systematic, and Total Data Uncertainties for the Experimental Data

Experiment	Standard Uncertainties			
			u_{qD}	
	S_{qD}, W	b_{qD}, W	W	%
1	1.80	1.17	2.15	2.76
2	1.90	1.50	2.42	2.43
3	1.95	1.61	2.53	2.36
4	2.09	1.88	2.81	2.25
5	2.28	2.14	3.13	2.20
6	2.41	2.37	3.38	2.15

Figure B-3.1-1
Experimentally Determined Total Heat Transfer as a Function of Inflow Temperature



B-4 SIMULATION MODEL

The simulation model for the fin-tube heat exchanger is described in para. 7-3.3 of ASME V&V 20-2009. Details are provided in ASME V&V 20-2009, Mandatory Appendix I. The simulation model differs from the model used to derive the synthetic data by a modification to the contact conductance at the fin/tube interface, see para. 7-3.5.1 of ASME V&V 20-2009, introducing a known systematic model error.

B-4.1 Simulation Results

Simulations for the set point conditions of Table B-3-1 are performed. Simulation parameters, set-point conditions, and simulation results, q_s, are reported in Table B-4.1-1. Simulation results are compared to the experimental data in Figure B-4.1-1. The simulation results exceed the experimental measurements for $T_i \lesssim 74$°F and are less than the experimental measurements for $T_i \gtrsim 74$°F.

ASME V&V20-2009 quantifies the degree of accuracy of a simulation model for a specified validation variable at a specified validation point (set point condition) using comparison error, E [eq. (1-5-1) of ASME V&V20-2009 , and validation uncertainty, u_{val} [eq. 1-5-10 of ASME V&V20-2009], as the validation metrics. Quantification of comparison error is discussed in para. B-5.1. Quantification of validation uncertainty is discussed in para. B-5.2.

The method of sensitivity coefficients is used to calculate input parameter uncertainties. The sensitivity coefficients for each parameter X_i of the simulation model result q_s are computed numerically using central finite-differences. The finite-difference perturbation size is specified to be the same as the standard uncertainty (deviation) in each parameter to approximate the gradient in the range of the uncertainty. The calculated sensitivity coefficients are provided in Table B-4.1-2. Uncertainty due to numerics, u_{num}, is reported to be $0.07W$ for each of the simulation results.

Table B-4.1-1
Simulation Parameters, Set-Point Conditions, and Results

Simulation Case	Simulation Conditions					Results						
	T_i, °C	T_∞, °C	Q, m^3/s	ρ, kg/m^3	C_p, J/kg°C	T_o, °C	q_S, W	k_t, W/m°C	k_f, W/m°C	h_i, W/m°C	h_f, W/m°C	h_o, W/m°C
1	70.44	21.66	6.21 E−06	990	4180	67.41	98.61	386	204	150	6	6
2	73.58	22.14	6.24 E−06	990	4180	69.72	104.00	386	204	150	6	6
3	75.52	21.99	6.22 E−06	990	4180	71.36	108.22	386	204	150	6	6
4	80.57	21.88	6.22 E−06	990	4180	75.71	118.66	386	204	150	6	6
5	87.53	22.08	6.23 E−06	990	4180	82.02	132.31	386	204	150	6	6
6	91.90	22.11	6.26 E−06	990	4180	85.83	141.12	386	204	150	6	6

Figure B-4.1-1
Simulation Results and Experimental Observations for Heat Transfer as Functions of Inflow Temperature

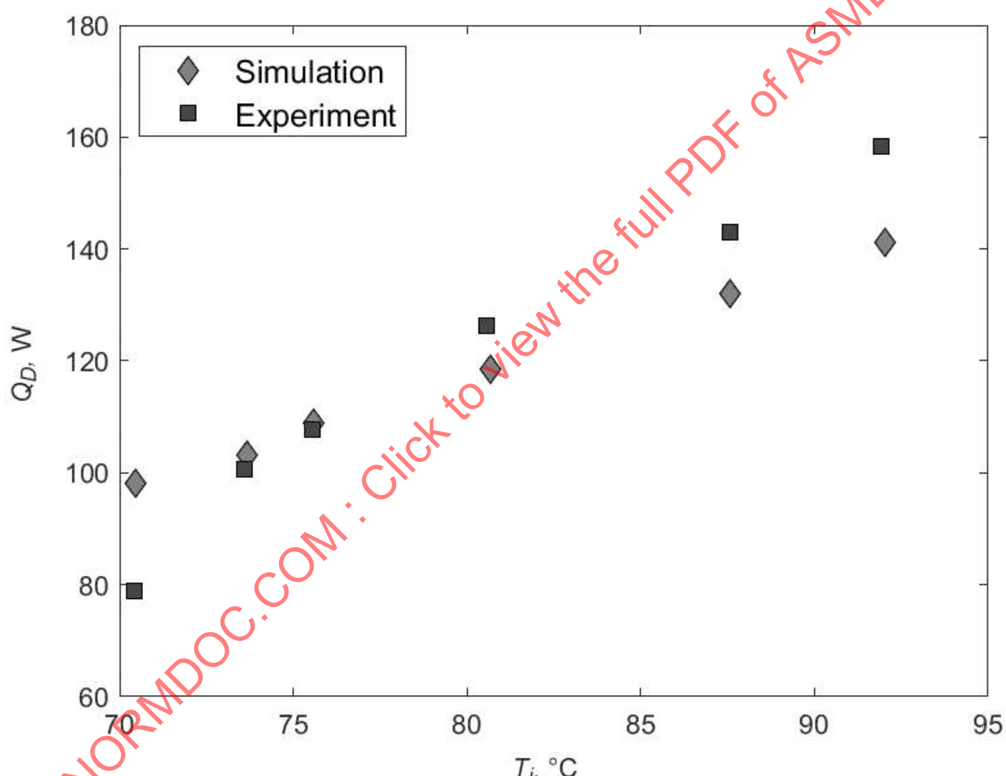


Table B-4.1-2
Sensitivity Coefficients for the Simulation Result

Simulation Case	Scaled Sensitivity Coefficients									
	$T_i \cdot \partial q_S / \partial T_i$, W	$T_\infty \cdot \partial q_S / \partial T_\infty$, W	$Q \cdot \partial q_S / \partial Q$, W	$\rho \cdot \partial q_S / \partial \rho$, W	$C_p \cdot \partial q_S / \partial C_p$, W	$k_t \cdot \partial q_S / \partial k_t$, W	$k_f \cdot \partial q_S / \partial k_f$, W	$h_i \cdot \partial q_S / \partial h_i$, W	$h_f \cdot \partial q_S / \partial h_f$, W	$h_o \cdot \partial q_S / \partial h_o$, W
1	141.69	−43.79	3.96	3.96	3.97	1.50 E−02	1.88 E−01	48.55	3.79	41.45
2	148.76	−44.77	4.18	4.18	4.19	1.60 E−02	1.99 E−01	51.59	4.03	44.04
3	152.68	−44.46	4.37	4.37	4.38	1.70 E−02	2.07 E−01	53.67	4.20	45.82
4	162.89	−44.23	4.78	4.78	4.80	1.80 E−02	2.27 E−01	58.85	4.60	50.24
5	176.96	−44.65	5.33	5.33	5.34	2.00 E−02	2.53 E−01	65.62	5.13	56.03
6	185.80	−44.71	5.66	5.66	5.67	2.10 E−02	2.70 E−01	70.01	5.47	59.77

B-5 ASME V&V 20-2009 METRIC

Validation metric defined in ASME V&V 20-2009 is applied in this section. The metric will be computed at each validation set point. These results will be compared to the multivariate metric that is computed in B-5.1.

B-5.1 Comparison Error, *E*

The metric in ASME V&V 20-2009 is based on comparison error, E, and the validation uncertainty, u_{val}. Comparison error, E, is defined in ASME V&V 20-2009. Per eq. (1-5-1) as

$$E = q_S - q_D \tag{B-5-1}$$

The comparison error is computed with q_s from Tables B-3-3, B-3.1-1, and B-4.1-1 and q_D from Table B-3-1. Results are reported in Table B-5.2.2-1.

B-5.2 Validation Uncertainty, u_{val}

The validation uncertainty u_{val} is calculated as the root-sum-square of uncertainty due to numerics, u_{num}, and uncertainty due to uncertain input parameters, $u_{\text{input}+D}$, which affects both the simulation result and the comparison data; see ASME V&V 20-2009.

$$u_{\text{val}}^2 = u_{\text{num}}^2 + u_{\text{input}+D}^2 \tag{B-5-2}$$

B-5.2.1 Numerical Uncertainty. For the fin-tube heat exchanger simulations, uncertainty due to numerics, u_{num}, is estimated with a mesh refinement study using the approach reported in ASME V&V 20-2009. The uncertainty was estimated to be 0.07W for each of the simulation results, therefore u_{num} is defined in eq. (B-5-3) as follows:

$$u_{\text{num}} = 0.07W \tag{B-5-3}$$

B-5.2.2 Simulation Input Parameter Uncertainty. The variable $u_{\text{input}+D}$ has random, $u_{\text{input}+D}$ (rnd), and systematic, $u_{\text{input}+D}$ (sys), error sources that combine also as a root-sum-square is defined in eq. (B-5-4).

$$u_{\text{input}+D}^2 = u_{\text{input}+D}^2(\text{rnd}) + u_{\text{input}+D}^2(\text{sys}) \tag{B-5-4}$$

The propagation equation for the random uncertainty $u_{\text{input}+D}$ (rnd) is obtained from eq. (B-5-5) as follows:

$$u_{\text{input}+D}^2(\text{rnd}) = (X_S - X_D)^T \, V_X(\text{rnd})(X_S - X_D) \tag{B-5-5}$$

The sensitivity matrices for X_S and X_D are defined in eq. (B-5-6).

$$X_S = \begin{bmatrix} T_i \frac{\partial q_S}{\partial T_i} \\ 0 \\ Q \frac{\partial q_S}{\partial Q} \\ \rho \frac{\partial q_S}{\partial \rho} \\ C_p \frac{\partial q_S}{\partial C_p} \\ T_\infty \frac{\partial q_S}{\partial T_\infty} \\ k_t \frac{\partial q_S}{\partial k_t} \\ k_f \frac{\partial q_S}{\partial k_f} \\ h_i \frac{\partial q_S}{\partial h_i} \\ h_f \frac{\partial q_S}{\partial h_f} \\ h_o \frac{\partial q_S}{\partial h_o} \end{bmatrix} \text{ and } X_D = \begin{bmatrix} T_i \frac{\partial q_D}{\partial T_i} \\ T_o \frac{\partial q_D}{\partial T_o} \\ Q \frac{\partial q_D}{\partial Q} \\ \rho \frac{\partial q_D}{\partial \rho} \\ C_p \frac{\partial q_D}{\partial C_p} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{B-5-6}$$

Using values from Table B-4.1-2 and Table B-3-3, the sensitivity vectors for X_S and X_D and the difference vector X_S–X_D for Experiment 1 are defined in eq. (B-5-7) as follows:

$$X_S = \begin{bmatrix} 141.69 \\ 0 \\ 3.96 \\ 3.96 \\ 3.97 \\ -43.79 \\ 1.50\text{E}{-02} \\ 1.88\text{E}{-01} \\ 48.55 \\ 3.79 \\ 41.45 \end{bmatrix} W, \; X_D = \begin{bmatrix} 1810.18 \\ -1732.32 \\ 77.87 \\ 77.87 \\ 77.87 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} W, \text{ and } X_S - X_D = \begin{bmatrix} -1668.49 \\ 1732.32 \\ -73.91 \\ -73.91 \\ -73.90 \\ -43.79 \\ 1.50\text{E}{-02} \\ 1.88\text{E}{-01} \\ 48.55 \\ 3.79 \\ 41.45 \end{bmatrix} W \tag{B-5-7}$$

V_X (rnd) is the covariance matrix for the random uncertainties in the input parameters [eq. (B-5-8)].

$$V_X(\text{rnd}) = \begin{bmatrix} s_{T_i}^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & s_{T_0}^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & s_Q^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & s_p^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{C_p}^2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{T_\infty}^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & s_{k_t}^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & s_{k_f}^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s_{h_i}^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & S_{h_f}^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & s_{h_0}^2 \end{bmatrix} \tag{B-5-8}$$

Using values from Table B-3-2, V_X (rnd) is defined in eq. (B-5-9).

$$V_X(\text{rnd}) = \begin{vmatrix} 4.90\text{E}{-7} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4.90\text{E}{-7} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2.50\text{E}{-5} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix} \tag{B-5-9}$$

The calculation of $u_{\text{input}+D}^2(\text{rnd})$ for Experiment 1 is

$$\begin{aligned} & u_{\text{input}+D}^2(\text{rnd}) \\ &= [-1668.49 \quad 1732.32 \quad -73.91 \quad -73.91 \quad -73.90 \quad -43.79 \quad 1.50\text{E}{-02} \quad 1.88\text{E}{-01} \quad 48.55 \quad 3.79 \quad 41.45] \\ & \times \begin{vmatrix} 4.90\,\text{E}{-07} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4.90\,\text{E}{-07} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2.50\,\text{E}{-05} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix} \times \begin{bmatrix} -1668.49 \\ 1732.32 \\ -73.91 \\ -73.91 \\ -73.90 \\ -43.79 \\ 1.50\,\text{E}{-02} \\ 1.88\,\text{E}{-01} \\ 48.55 \\ 3.79 \\ 41.45 \end{bmatrix} W^2 = 2.97 W^2 \end{aligned} \tag{B-5-10}$$

which yields eq. (B-5-11).

$$u_{\text{input}+D}(\text{rnd}) = \sqrt{u_{\text{input}+D}^2(\text{rnd})} = \sqrt{2.97 W^2} = 1.72\ W \tag{B-5-11}$$

Calculated values for $u_{\text{input}+D}$ (rnd) for each experiment are reported in Table B-5.2.2-1.
The propagation equation for the random uncertainty $u_{\text{input}+D}$ (sys) is defined as follows:

$$u_{\text{input}+D}^2(\text{sys}) = (X_S - X_D)^T\ V_X(\text{sys})(X_S - X_D) \tag{B-5-12}$$

V_X (sys) is the covariance matrix for the systematic uncertainties in the input parameters [eq. (B-5-13)].

$$V_X(\text{sys}) = \begin{bmatrix} b_{T_i}^2 & b_{T_i}b_{T_o} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ b_{T_i}b_{T_o} & b_{T_o}^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & b_Q^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & b_\rho^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & b_{C_p}^2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & b_{T_\infty}^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & b_{k_t}^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_{k_f}^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_{h_i}^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_{h_f}^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_{h_o}^2 \end{bmatrix} \quad \text{(B-5-13)}$$

Using values from Table B-3-2, V_X (sys) is defined in eq. (B-5-14).

$$V_X(\text{sys}) = \quad \text{(B-5-14)}$$

$$\begin{bmatrix} 1.96\,\text{E}{-06} & 1.96\,\text{E}{-06} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1.96\,\text{E}{-06} & 1.96\,\text{E}{-06} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1.00\,\text{E}{-04} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.50\,\text{E}{-05} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1.00\,\text{E}{-04} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.00\,\text{E}{-04} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2.50\,\text{E}{-03} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2.50\,\text{E}{-03} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.00\,\text{E}{-02} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.00\,\text{E}{-02} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.00\,\text{E}{-02} \end{bmatrix}$$

The calculation of $u_{\text{input}+D}^2(\text{sys})$ for Experiment 1 yields eq. (B-5-15).

$$u_{\text{input}+D}(\text{sys}) = \sqrt{u_{\text{input}+D}^2(\text{sys})} = \sqrt{42.32W^2} = 6.51\ W \quad \text{(B-5-15)}$$

Calculated values for $u_{\text{input}+D}$ (sys) for each experiment are reported in Table B-5.2.2-1.

$u_{\text{input}+D}$ for Experiment 1 is the combined values of $u_{\text{input}+D}$ (rnd) [eq. (B-5-11)] and $u_{\text{input}+D}$ (sys) [eq.(B-5-15)] as follows:

$$u_{\text{input}+D} = \sqrt{2.97W^2 + 42.32W^2} = \sqrt{45.29W^2} = 6.73\ W \quad \text{(B-5-16)}$$

Calculated values for $u_{\text{input}+D}$ for each experiment are shown in Table B-5.2.2-1.

B-5.2.3 Estimated Intervals at Each Validation Set Point. The validation uncertainty, u_{val}, is calculated by combining u_{num} [eq. (B-5-3)] and $u_{\text{input}+D}$ [eq. (B-5-16)] as a root-sum-square value, [see eq. (B-5-2)] as follows:

$$u_{\text{val}} = \sqrt{u_{\text{num}}^2 + u_{\text{input}+D}^2} = \sqrt{4.90E-03W^2 + 45.29W^2} = \sqrt{45.29W^2} = 6.73\ W \quad \text{(B-5-17)}$$

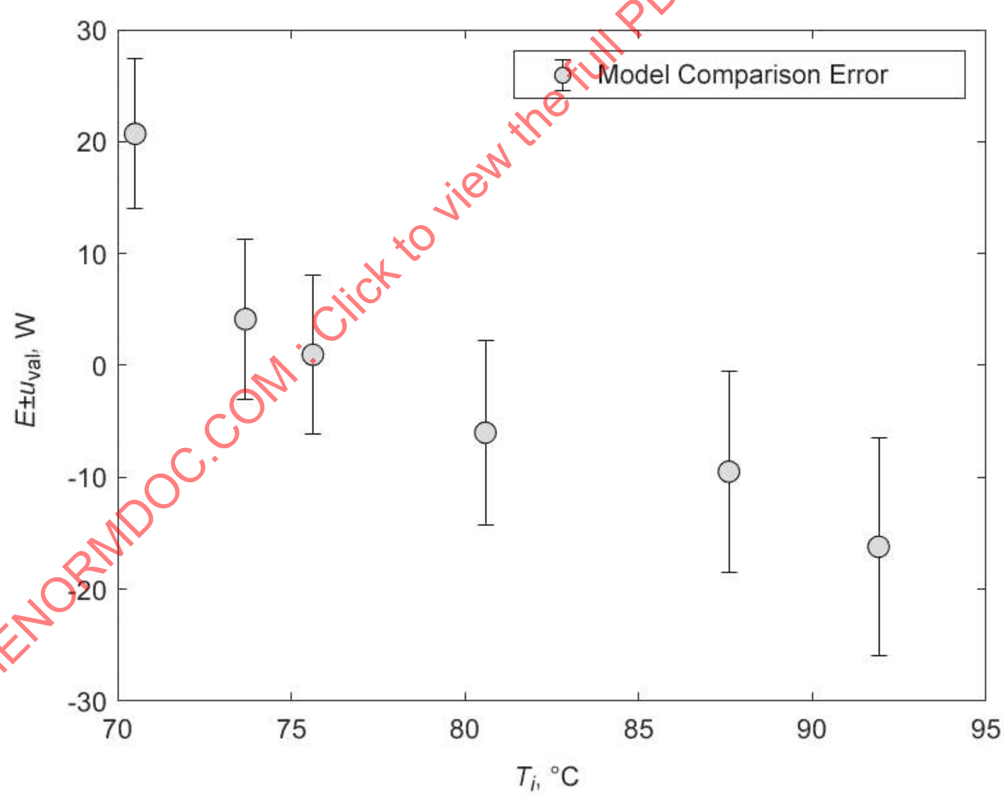
Calculated values for u_{val} for each experiment are reported in Table B-5.2.2-1.

Calculated values for E, u_{num}, $u_{\text{input}+D}$(rnd), $u_{\text{input}+D}$(sys), $u_{\text{input}+D}$, and u_{val} are reported in Table B-5.2.2-1. A plot of the comparison error, E, with u_{val} as uncertainty bars is shown in Figure B-5.2.3-1.

Table B-5.2.2-1
Comparison Error and Validation Uncertainty Estimated Using the Method of Sensitivity Coefficients

Simulation Case	Model Comparison Error and Validation Uncertainty									
	q_s, W	q_D, W	E		u_{num}, W	$u_{input+D}$			u_{val}	
			W	%		(rnd) W	(sys) W	Total W	W	%
1	98.61	77.87	20.74	21.03	0.07	1.72	6.51	6.73	6.73	6.82
2	104.00	99.67	4.33	4.16	0.07	1.82	6.96	7.19	7.19	6.91
3	108.22	107.08	1.14	1.05	0.07	1.87	7.25	7.49	7.49	6.92
4	118.66	125.09	−6.43	−5.42	0.07	2.00	7.97	8.22	8.22	6.93
5	132.31	142.05	−9.74	−7.36	0.07	2.19	8.89	9.16	9.16	6.92
6	141.12	157.24	−16.12	−11.42	0.07	2.32	9.51	9.79	9.79	6.94

Figure B-5.2.3-1
Comparison Error as a Function of Inflow Temperature With Bars Showing the Range of u_{val}



B-6 MULTIVARIATE METRIC

B-6.1 Multivariate Metric Calculated With Sensitivity Analysis

The multivariate metric, E_{mv}, is defined in eq. (B-6-1). It is the magnitude of the comparison error vector, E, over multiple validation set points accounting for correlations between the set points.

$$E_{mv}^2 = E^T V_{\mathrm{val}}{}^{-1} E \tag{B-6-1}$$

where

$$\mathrm{E}=\begin{bmatrix} S_1 - D_1 \\ \vdots \\ S_n - D_n \end{bmatrix} = \begin{bmatrix} E_1 \\ \vdots \\ E_n \end{bmatrix} \tag{B-6-2}$$

$$E_{mv} = \sqrt{E_{mv}^2} \tag{B-6-3}$$

E is the array of comparison errors. V_{val} is the validation covariance matrix.

Because the magnitude of E_{mv} depends on the number of validation set points used to compute it (see section 4), a reference value, E_{ref}, is used for normalization. Paragraph 4.2.1 provides methods to calculate E_{ref}. The ratio $\frac{E_{mv}}{E_{\mathrm{ref}}}$ removes the dependence on the number of validation set points and is used in this section as a metric for comparison of results and interpretation.

B-6.1.1 Contributions to Validation Covariance Matrix. The validation covariance matrix V_{val} is a generalization of u_{val}^2 to multivariate applications. Nonmandatory Appendix A explains that the approach to compute V_{val} depends on the following:

(a) whether the validation variable

(1) is directly measured (Case 1 of ASME V&V 20-2009)

(2) is a result defined by a data reduction equation where the measured variables share no error sources (Case 2 of ASME V&V 20-2009)

(3) is a result defined by a data reduction equation where the measured variables share identical error sources (Case 3 of ASME V&V 20-2009)

(4) comes from measured variables analyzed with a model (Case 4 of ASME V&V 20-2009)

(b) whether there are no common errors between the validation set points or there are shared identical errors between the validation set points.

This logic flow is depicted graphically in Nonmandatory Appendix A, Figure A-1-1.

Like u_{val}^2 , V_{val} has uncertainty contributions due to numerics, V_{num}, input parameters, V_{input}, and experimental data, V_D, which are independent when the comparison data are directly measured. When the comparison data are calculated using a data reduction equation, like heat flux q_D for the fin-tube heat exchanger example, the uncertainties due to uncertain input parameters and V_{input} and V_D are calculated together, $V_{\mathrm{input}+D}$. Therefore, for the fin-tube heat exchanger example, V_{val} is defined in eq. (B-6-4).

$$V_{\mathrm{val}} = V_{\mathrm{num}} + V_{\mathrm{input}+D} \tag{B-6-4}$$

Two approaches are demonstrated for the calculation of the uncertainty due to input parameters, $V_{\mathrm{input}+D}$. One approach uses sensitivity coefficients that are valid for systems with locally linear behavior in the validation space. The other approach uses sampling that captures nonlinear behaviors. Because a linear model is sufficient to capture the effects of the systematic error introduced by the change in contact conductance for the fin-tube heat exchanger example, the results from the sensitivity coefficient approach and from sampling will be similar.

B-6.1.1.1 Numerical Uncertainty, V_{num}. Two possibilities for calculation of V_{num} are discussed in Nonmandatory Appendix A, para. A-2.1. For the fin-tube heat exchanger example, uncertainty due to numerics, u_{num}, is reported to be $0.07W$ for each of the simulation results and independence is assumed. Therefore, the diagonal form is used in eq. (B-6-5) for calculating V_{num}.

$$V_{\text{num}} = \begin{bmatrix} 0.07^2 & 0 & \cdots & 0 \\ 0 & 0.07^2 & & \\ \vdots & & \ddots & \\ 0 & & & 0.07^2 \end{bmatrix} = \begin{bmatrix} 4.90\,\text{E}{-03} & 0 & \cdots & 0 \\ 0 & 4.90\,\text{E}{-03} & & \\ \vdots & & \ddots & \\ 0 & & & 4.90\,\text{E}{-03} \end{bmatrix} \tag{B-6-5}$$

B-6.1.1.2 Input Parameter Uncertainty, $V_{\text{input+}D}$. Random and systematic input parameter uncertainties are reported in Table B-3-2. Because random uncertainties are independent, the covariance array for random uncertainties, $V_X(\text{rnd})$, is diagonal. Systematic uncertainties may share common error sources and, therefore, may be dependent. The covariance array for systematic uncertainties, $V_X(sys)$, will have nonzero off diagonal terms for contributions that share error sources. Because of the potential differences in array structures, random and systematic uncertainties are addressed separately in eq. (B-6-6).

$$V_{\text{input}+D} = V_{\text{input}+D}(\text{rnd}) + V_{\text{input}+D}(\text{sys}) \tag{B-6-6}$$

B-6.1.1.2.1 Random Uncertainties

(a) The method to calculate contributions to V_{val} from random error sources is found by following the flow logic in Nonmandatory Appendix A, Figure A-1-1 as follows:

(1) Choose from Case 1, Case 2, Case 3, or Case 4.
(2) Because heat flux is not directly measured, Case 1 does not apply.
(3) Because heat flux is a result defined by a data reduction equation, Case 4 does not apply.
(4) Because random uncertainties are independent, Case 3 does not apply.
(5) Therefore, Case 2 applies.
(6) Choose from Case 2A or Case 2B.
(7) Because random error sources are independent, Case 2B does not apply.
(8) Therefore, follow Case 2A.

(b) *Case 2A.* $V_{\text{input+}D}(\text{rnd})$ is calculated as follows:

$$V_{\text{input}+D}(\text{rnd}) = \begin{bmatrix} (X_{S,1} - X_{D,1})^T V_{x,1}(\text{rnd})(X_{S,1} - X_{D,1}) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & (X_{S,n} - X_{D,n})^T V_{X,n}(\text{rnd})(X_{S,n} - X_{D,n}) \end{bmatrix} \tag{B-6-7}$$

The sensitivity matrices $X_{S,i}$ and $X_{D,i}$ are defined in eq. (B-6-8).

$$X_{S,i} = \begin{bmatrix} T_i \frac{\partial q_{S,i}}{\partial T_i} \\ 0 \\ Q \frac{\partial q_{S,i}}{\partial Q} \\ \rho \frac{\partial q_{S,i}}{\partial \rho} \\ C_p \frac{\partial q_{S,i}}{\partial C_p} \\ T_\infty \frac{\partial q_{S,i}}{\partial T_\infty} \\ k_t \frac{\partial q_{S,i}}{\partial k_t} \\ k_f \frac{\partial q_{S,i}}{\partial k_f} \\ h_i \frac{\partial q_{S,i}}{\partial h_i} \\ h_f \frac{\partial q_{S,i}}{\partial h_f} \\ h_o \frac{\partial q_{S,i}}{\partial h_o} \end{bmatrix} \text{ and } X_{D,i} = \begin{bmatrix} T_i \frac{\partial q_{D,i}}{\partial T_i} \\ T_o \frac{\partial q_{D,i}}{\partial T_o} \\ Q \frac{\partial q_{D,i}}{\partial Q} \\ \rho \frac{\partial q_{D,i}}{\partial \rho} \\ C_p \frac{\partial q_{D,i}}{\partial C_p} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{B-6-8}$$

where $q_{S,i}$ and $q_{D,i}$ are q_S and q_D for the ith experiment. The covariance matrices, $V_{X,j}(\text{rnd})$, for this example are identical, $V_{x,1}(\text{rnd}) = V_{x,2}(\text{rnd}) = \ldots = V_{x,n}(\text{rnd}) = V_x(\text{rnd}) \cdot V_x(\text{rnd})$. $V_X(\text{rnd})$ is given by eq. (B-5-8).

(-1) Example: Set-Point Experiments 3 and 5. The matrix to be calculated is shown in eq. (B-6-9).

$$V_{\text{input}+D}(\text{rnd}) = \begin{bmatrix} (X_{S,3} - X_{D,3})^T V_{x,3}(\text{rnd})(X_{S,3} - X_{D,3}) & 0 \\ 0 & (X_{S,5} - X_{D,5})^T V_{X,5}(\text{rnd})(X_{S,5} - X_{D,5}) \end{bmatrix} \tag{B-6-9}$$

Using values from Table B-4.1-1 and Table B-3-3, the sensitivity vectors $X_{S,3}$ and $X_{D,3}$ and the difference vector $X_{S,3} - X_{D,3}$ for set-point experiment 3 are defined in the following set of equations [eq. (B-6-10)]:

$$X_{S,3} = \begin{bmatrix} 152.68 \\ 0 \\ 4.37 \\ 4.38 \\ 4.37 \\ -44.46 \\ 1.70\text{ E}{-02} \\ 2.07\text{ E}{-01} \\ 53.67 \\ 4.20 \\ 45.82 \end{bmatrix} W, \quad X_{D,3} = \begin{bmatrix} 1943.85 \\ -1836.78 \\ 107.08 \\ 107.08 \\ 107.08 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} W, \quad \text{and } X_{S,3} - X_{D,3} = \begin{bmatrix} -1791.17 \\ 1836.78 \\ -102.71 \\ -102.70 \\ -102.71 \\ -44.46 \\ 1.70\text{ E}{-02} \\ 2.07\text{ E}{-01} \\ 53.67 \\ 4.20 \\ 45.82 \end{bmatrix} W \tag{B-6-10}$$

$V_X(\text{rnd})$ is given in eq. (B-5-9). The value of $V_{\text{input}+D}(\text{rnd})[1,1]$ is

$$(X_{S,3} - X_{D,3})^T V_{x,3}(rnd)(X_{S,3} - X_{D,3}) = 3.49\ W^2 \tag{B-6-11}$$

Calculations for set-point experiment 5 are similar. The final matrix $V_{\text{input}+D}(\text{rnd})$ is

$$V_{\text{input}+D}(\text{rnd}) = \begin{bmatrix} 3.49 & 0 \\ 0 & 4.78 \end{bmatrix} W^2 \tag{B-6-12}$$

B-6.1.1.2.2 Systematic Uncertainties

(a) The method to calculate contributions to $V_{\text{input}+D}$ from systematic error sources is found from the flow logic in Nonmandatory Appendix A, Figure A-1-1 as follows:

(1) Choose from Case 1, Case 2, Case 3, or Case 4.

(2) Because heat flux is not directly measured, Case 1 does not apply.

(3) Because heat flux is a result defined by a data reduction equation, Case 4 does not apply.

(4) Because heat flux is computed using the measured variables inflow temperature, T_i, outflow temperature, T_o, and volumetric flow rate, Q, where the measured variables T_i and T_o share common systematic error sources (e.g., measurements in the same facility with the same instruments), Case 2 does not apply.

(5) Therefore, Case 3 applies.

(6) Choose from Case 3A or Case 3B.

(7) Because the validation set points may have common systematic error sources (e.g. measurements in the same facility with the same instruments), Case 3A does not apply.

(8) Therefore, follow Case 3B.

(b) *Case 3B.* $V_{\text{input}+D}(\text{sys})$ is calculated in eq. (B-6-13).

$$V_{\text{input}+D} = (X_S - X_D)^T V_x (X_S - X_D) \tag{B-6-13}$$

The sensitivity matrices X_S and X_D are defined in eq. (B-6-14).

$$X_S = \begin{bmatrix} T_i\frac{\partial q_S}{\partial T_i} \\ 0 \\ Q\frac{\partial q_S}{\partial Q} \\ \rho\frac{\partial q_S}{\partial \rho} \\ C_p\frac{\partial q_S}{\partial C_p} \\ T_\infty\frac{\partial q_S}{\partial T_\infty} \\ k_t\frac{\partial q_S}{\partial k_t} \\ k_f\frac{\partial q_S}{\partial k_f} \\ h_i\frac{\partial q_S}{\partial h_i} \\ h_f\frac{\partial q_S}{\partial h_f} \\ h_o\frac{\partial q_S}{\partial h_o} \end{bmatrix} \text{ and } X_D = \begin{bmatrix} T_i\frac{\partial q_D}{\partial T_i} \\ T_o\frac{\partial q_D}{\partial T_o} \\ Q\frac{\partial q_D}{\partial Q} \\ \rho\frac{\partial q_D}{\partial \rho} \\ C_p\frac{\partial q_D}{\partial C_p} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{B-6-14}$$

where q_s and q_D are vectors of the set point experiments being evaluated. The covariance matrix, $V_x(\text{sys})$ is provided in eq. (B-5-13).

(-1) Example: Set-Point Experiments 3 and 5. Using values from Table 5.3-1 and Table 5-3, the sensitivity vectors for X_S and X_D and the difference vector $X_S - X_D$ for set-point experiments 3 and 5 are defined in eq. (B-6-15) as follows:

$$X_S = \begin{bmatrix} 152.68 & 176.96 \\ 0 & 0 \\ 4.37 & 5.33 \\ 4.38 & 5.34 \\ 4.37 & 5.33 \\ -44.46 & -44.65 \\ 1.70\text{ E}-02 & 2.00\text{ E}-02 \\ 2.07\text{ E}-01 & 2.53\text{ E}-01 \\ 53.67 & 65.62 \\ 4.20 & 5.13 \\ 45.82 & 56.03 \end{bmatrix} W, \quad X_D = \begin{bmatrix} 1943.85 & 2256.61 \\ -1836.78 & -2114.56 \\ 107.08 & 142.05 \\ 107.08 & 142.05 \\ 107.08 & 142.05 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} W, \text{ and}$$

$$X_S - X_D = \begin{bmatrix} -1791.17 & -2079.65 \\ 1836.78 & 2114.56 \\ -102.71 & -136.72 \\ -102.70 & -136.71 \\ -102.71 & -136.72 \\ -44.46 & -44.65 \\ 1.70\text{ E}-02 & 2.00\text{ E}-02 \\ 2.07\text{ E}-01 & 2.53\text{ E}-01 \\ 53.67 & 65.62 \\ 4.20 & 5.13 \\ 45.82 & 56.03 \end{bmatrix} W \tag{B-6-15}$$

V_x(sys) is given in eq. (B-5-14). The matrix $V_{\text{input}+D}$(sys) is obtained in eq. (B-6-16).

$$V_{\text{input}+D}(sys) = (X_S - X_D)^T V_x (X_S - X_D) = \begin{bmatrix} 52.55 & 64.47 \\ 64.47 & 79.12 \end{bmatrix} W^2 \tag{B-6-16}$$

B-6.1.2 Calculation of Validation Covariance Matrix. The validation covariance matrix, V_{val}, is the sum of the covariance matrices for uncertainty due to numerics, V_{num}, and uncertainty due to uncertain input parameters, $V_{\text{input}+D}$, see eq. (B-6-4).

For set-point experiments 3 and 5, the V_{val} matrix calculated in eq. (B-6-17) using the method of sensitivity coefficients is the sum of eqs. (B-6-4), (B-6-12), and (B-6-16):

$$\begin{aligned} V_{\text{val}} &= V_{\text{num}} + V_{\text{input}+D} = V_{\text{num}} + V_{\text{input}+D}(\text{rnd}) + V_{\text{input}+D}(sys) \\ &= \begin{bmatrix} 4.90\text{E}-03 & 0 \\ 0 & 4.90\text{E}-03 \end{bmatrix} W^2 + \begin{bmatrix} 3.49 & 0 \\ 0 & 4.78 \end{bmatrix} W^2 + \begin{bmatrix} 52.55 & 64.47 \\ 64.47 & 79.12 \end{bmatrix} W^2 = \begin{bmatrix} 56.04 & 64.47 \\ 64.47 & 83.90 \end{bmatrix} W^2 \end{aligned} \tag{B-6-17}$$

The inverse of V_{val} is defined in eq. (B-6-18):

$$V_{\text{val}}^{-1} = \begin{bmatrix} 1.54\text{ E}-01 & -1.18\text{ E}-01 \\ -1.18\text{ E}-01 & 1.03\text{ E}-01 \end{bmatrix} W^{-2} \tag{B-6-18}$$

The corresponding V_{val} matrix calculated in eq. (B-6-19) using the sampling method is

$$\begin{aligned} V_{\text{val}} = V_{\text{num}} + V_{\text{input}+D} &= \begin{bmatrix} 4.90\text{ E}-03 & 0 \\ 0 & 4.90\text{ E}-03 \end{bmatrix} W^2 + \begin{bmatrix} 63.41 & 75.53 \\ 75.53 & 101.36 \end{bmatrix} W^2 \\ &= \begin{bmatrix} 63.41 & 75.53 \\ 75.53 & 101.36 \end{bmatrix} W^2 \end{aligned} \tag{B-6-19}$$

The inverse of V_{val} from sampling is defined in eq. (B-6-20):

$$V_{\text{val}}^{-1} = \begin{bmatrix} 1.40\text{ E}-01 & -1.05\text{ E}-01 \\ -1.05\text{ E}-01 & 8.78\text{ E}-02 \end{bmatrix} W^{-2} \tag{B-6-20}$$

NOTE: The inverse matrices are provided for checking purposes. When used for calculation of the multivariate metric below, all digits from the matrix inversion function (e.g., minimum verse using Microsoft Excel, Office 365 ProPlus) are retained.

B-6.1.3 Multivariate Metric Results. Calculation of the multivariate metric, E_{mv}, and the reference value, E_{ref}, is demonstrated using the Method of Sensitivity Coefficients. In addition, the effect of neglecting correlations between the set points is explored. Paragraph B-6.2 shows the results using sampling.

Comparison error E for the validation set points is reported in Table B-5.2.2-1. For set points 3 and 5, as examples, the vector E is defined in eq. (B-6-21).

$$E = \begin{bmatrix} S_3 - D_3 \\ S_5 - D_5 \end{bmatrix} = \begin{bmatrix} 108.22 - 106.96 \\ 132.31 - 141.85 \end{bmatrix} W = \begin{bmatrix} 1.14 \\ -9.74 \end{bmatrix} W \tag{B-6-21}$$

B-6.1.3.1 Accounting for Correlation in the Comparison Errors. The matrix V_{val} for set points 3 and 5, which is provided in eq. (B-6-17), is used to obtain eq. (B-6-22).

$$V_{\text{Val}} = \begin{bmatrix} 56.04 & 64.47 \\ 64.47 & 83.90 \end{bmatrix} W^2 \tag{B-6-22}$$

The inverse matrix V_{val}^{-1} , which is provided in eq. (B-6-15) gives eq. (B-6-23).

$$V_{\text{val}}^{-1} = \begin{bmatrix} 1.54\,\text{E}{-01} & -1.18\,\text{E}{-01} \\ -1.18\,\text{E}{-01} & 1.03\,\text{E}{-01} \end{bmatrix} W^{-2} \tag{B-6-23}$$

E_{mv}^2 is computed via matrix multiplication as follows:

$$E_{mv}^2 = \text{E}^{\text{T}} V_{\text{val}}{}^{-1} E = [1.14 \quad -9.74] \cdot \begin{bmatrix} 1.54\,\text{E}{-01} & -1.18\,\text{E}{-01} \\ -1.18\,\text{E}{-01} & 1.03\,\text{E}{-01} \end{bmatrix} \cdot \begin{bmatrix} 1.14 \\ -9.74 \end{bmatrix} = 12.57 \tag{B-6-24}$$

The value E_{mv} is obtained by taking the square root of E_{mv}^2 in eq. (B-6-25).

$$E_{mv} = \sqrt{E_{mv}^2} = \sqrt{12.57} = 3.55 \tag{B-6-25}$$

As discussed in para. B-6.1, the value of E_{mv} is a function of the rank of V_{val}; therefore, a reference value, E_{ref}, is used to interpret E_{mv} relative to expected standard uncertainty range on E_{mv}^2 . Setting df (degrees of freedom) to the rank of V_{val} (here, df = 2), E_{ref}^2 is calculated using eq. (4-16).

$$E_{\text{ref}}^2 = df + \sqrt{2df} = 2 + \sqrt{2 \cdot 2} = 2 + 2 = 4 \tag{B-6-26}$$

The value of E_{ref} is obtained by taking the square root of E_{ref}^2 :

$$E_{\text{ref}} = \sqrt{E_{\text{ref}}^2} = \sqrt{4} = 2 \tag{B-6-27}$$

The ratio E_{mv}/E_{ref} is then an indication of the extent to which the model, represented by E_{mv}, conforms to the expectation for E_{mv}, E_{ref}, within one standard uncertainty on E_{mv}^2:

$$\frac{E_{mv}}{E_{\text{ref}}} = \frac{3.55}{2} = 1.78 \tag{B-6-28}$$

The determination that $E_{mv}/E_{\text{ref}} > 1$ is an indication that the model results show a significant systematic error relative to the experiment due to missing model physics. For the fin-tube heat exchanger example problem, the missing physics is the modification to the contact conductance at the fin-tube interface.

B-6.1.3.2 Neglecting Correlation in the Comparison Errors. The modification to the contact conductance in the fin-tube heat exchanger problem is a common error shared by each of the validation set points. If the validation set points were treated as independent, E_{mv} is calculated by the following:

Step 1. Use the validation matrix from eq. (B-6-22) setting the off-diagonal entries to zero [eq. (B-6-29)].

$$V_{\text{val}} = \begin{bmatrix} 56.04 & 0 \\ 0 & 83.90 \end{bmatrix} W^2 \tag{B-6-29}$$

Step 2. Calculate the inverse matrix V_{val}^{-1} as defined in eq. (B-6-30).

$$V_{\text{val}}^{-1} = \begin{bmatrix} 1.78\text{E}{-02} & 0 \\ 0 & 1.19\text{E}{-02} \end{bmatrix} W^{-2} \tag{B-6-30}$$

Step 3. Calculate E_{mv}^2 via matrix multiplication [eq. (B-6-31)].

$$E_{mv}^2 = E^T V_{\text{val}}{}^{-1}\,\text{E} = [1.14 \quad -9.74] \cdot \begin{bmatrix} 1.78\,\text{E}{-02} & 0 \\ 0 & 1.19\,\text{E}{-02} \end{bmatrix} \cdot \begin{bmatrix} 1.14 \\ -9.74 \end{bmatrix} = 1.15 \tag{B-6-31}$$

Step 4. Calculate E_{mv} from the square root of E_{mv}^2.

$$E_{mv} = \sqrt{E_{mv}^2} = \sqrt{1.15} = 1.07 \tag{B-6-32}$$

Step 5. Compare to E_{ref}.

$$\frac{E_{mv}}{E_{\text{ref}}} = \frac{1.07}{2} = 0.54 \tag{B-6-33}$$

The interpretation of $E_{mv}/E_{\text{ref}} < 1$ is that there is no indication that the model results show a significant systematic error relative to the experiment. The significance of the modification to the contact conductance at the fin-tube interface would be missed.

B-6.2 Multivariate Metric Calculated With Sampling

The multivariate metric does not change when sampling is used. The same expression given in eq. (B-6-2) is used to evaluate the metric for sampling. The same procedure is also used to compute the numerical uncertainty. The procedures to estimate experimental data uncertainty and simulation input uncertainty, i.e., $V_{\text{input}+D}$, will use sampling instead of a sensitivity approach.

B-6.2.1 Input Parameter Uncertainty, $V_{\text{input}+D}$. In the sampling to estimate $V_{\text{input}+D}$, twenty data points for q_{S_i} and q_{D_i} were constructed for each of set point conditions using the Latin hypercube sampling approach described in ASME V&V 20-2009. The subscript i denotes the sample index. These data are provided in Table B-6.2.1-1.

The choice of 20 sample points is based on providing a relatively small data set that can be used as a practice problem by copying data out of the printed document. No sensitivity assessment was used to establish convergence of statistics. Another sample set with 320 sample points was constructed to show the difference in statistics between a small and a large sample set. Those data are not reported. The sole requirement was that the large sample set have a much greater number of samples than 20. No justification of 320 is intended based on based concerns for rigorous convergence of statistics.

$V_{\text{input}+D}$ is the covariance of the variabilities of the sample comparison errors, E_i, for set-point experiment i about its mean value $\overline{E_i}$. Defining the deviation vector as $E_i' = E_i - \overline{E}_i$ and the matrix of deviation vectors in a multivariate assessment as E', V_{val} is given by eq. (B-6-34).

$$V_{\text{input}+D} = \frac{1}{n_r - 1} E'^T E' \tag{B-6-34}$$

where n_r is the number of samples in the sample set.