Foreword: Wording to be added

Add Preface – Main body walks through technique. Details are relegated to appendices to facilitate understanding. The goal is that this Supplement serve as a self-contained primer on this topic.
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1 Purpose

The present 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&V20-2009 [1]. 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 document, a summary of the V&V20-2009 pointwise metric is outlined (Section 4.1), followed by a high-level description and example of the multivariate metric (Sections 4.2 and 5, respectively). To improve clarity in the body of the document, the detailed formulation of the multivariate metric is reserved for Appendix A, and a detailed example (i.e., fin-tube heat exchanger) covering multiple use-cases is outlined in Appendix B. Appendix C presents examples of the choices required in the procedure for using the multivariate metric.

2 Scope

The scope of the present technique is similar to that for the pointwise validation metric described in ASME V&V20-2009 [1, 2]. 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 [1]: 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&V20-2009 [1, 2] presents a validation approach for estimating the model error, $\delta_{\text{model}}$, considering experimental, numerical and input uncertainties in the reported comparison data from an experiment, $D$, and a simulation $S$. The committee that developed [1] 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 V&V20-2009 approach characterizes an interval for $\delta_{\text{model}}$ 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 $u_{\text{val}}$. $E$ is the difference between the results of the simulation $S$ and experiment $D$ ($E = S - D$) and $u_{\text{val}}$ depends on the experimental uncertainty $u_{\text{num}}$ and the input parameter uncertainty $u_{\text{input}}$ that characterize the experimental error $\delta_D$, numerical error $\delta_{\text{num}}$ and input error $\delta_{\text{input}}$, respectively.

The present supplement presents a technique to extend the application of the pointwise or local assessment of the modeling error ($\delta_{\text{model}}$) presented in [1] to a global assessment of $\delta_{\text{model}}$ 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 i-th set point within the multiple set points, $i = 1, \ldots, n$, 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 [3]. It was introduced as a validation metric in 1999 by Hills and Trucano [4]. This metric has been used in several peer-reviewed articles [5, 6, 7] 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 Section 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 V&V20-2009 validation metric [1].

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 [7] 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. In [7], the multivariate metric was used 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 Section 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 [8, 9]. 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 discussed in the 2020 edition [9], 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.

Here in this document, Section 4 presents and discusses 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. Appendix A presents the detailed formulation of the multivariate metric, and an example based on the V&V20-2009 [1] fin-tube heat exchanger is described in Appendix B. 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 Section 4.2 below builds upon single set point validation quantification of model comparison error and validation uncertainty using the techniques of the ASME V&V20-2009 Standard [1, 2]. A brief overview of the approach described in [1] is presented in Section 4.1. A detailed development of the multivariate metric follows in Section 4.2.
4.1 Overview of V&V20-2009

The ASME V&V-20-2009 Standard considers validation for a single validation variable defined by a scalar quantity [1, 2]. 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 [10]. The validation metric presented in ASME V&V20-2009 [1, 2] 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 and thus \( E \) is the true model error \( \delta_{\text{model}} \). In practice, these idealized conditions are impossible to achieve. The V&V20-2009 method accounts for errors in the simulation results, \( S \), due to uncertainties in the specification of the input parameters, \( \delta_{\text{input}} \) (e.g. uncertainties in boundary conditions, fluid properties, and/or heat transfer coefficients required to perform the simulations), and due to numerical uncertainty, \( \delta_{\text{num}} \) (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, \( \delta_D \). Considering the errors in the simulations (\( \delta_{\text{model}}, \delta_{\text{num}} \) and \( \delta_{\text{input}} \)) and in the experiments (\( \delta_D \)), the relation between \( \delta_{\text{model}} \) and \( E \) is as follows:

\[
E = S - D = \delta_{\text{model}} + \delta_{\text{num}} + \delta_{\text{input}} - \delta_D .
\]

Eq. 1

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

\[
\delta_{\text{model}} = E - (\delta_{\text{num}} + \delta_{\text{input}} - \delta_D). \quad \text{Eq. 2}
\]

Single values can be calculated only for \( E, S, \) and \( D \). An uncertainty is estimated to characterize the unknown errors, \( \delta_{\text{num}}, \delta_{\text{input}}, \) and \( \delta_D \), because the true values are not available. The V&V20-2009 method characterizes each error source, \( \delta_X \), using standard uncertainties \( \pm u_X \) and assuming that the expected value of all these errors is zero:

\[
-u_{\text{num}} \leq \delta_{\text{num}} \leq u_{\text{num}} ,
\]

\[
-u_{\text{input}} \leq \delta_{\text{input}} \leq u_{\text{input}} , \quad \text{and}
\]

\[
-u_D \leq \delta_D \leq u_D .
\]

Eq. 3

The standard uncertainty \( u_X \) corresponds conceptually to an estimate of the standard deviation \( \sigma \) of the parent distribution from which \( \delta_X \) is a single realization [1].
In Eq. 3, \( u_{\text{num}} \) is a measure of the numerical uncertainty that is a consequence of discretization and iterative convergence, round-off error and possibly statistical convergence in the determination of the simulation value \( S \). Techniques to determine \( u_{\text{num}} \) are presented in Section 2 of V&V20-2009 [1].

Also, in Eq. 3, \( u_{\text{input}} \) 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 V&V20-2009 [1].

The determination of the experimental uncertainty \( u_D \) is discussed in Section 4 of V&V20-2009 [1]. 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 \( u_{\text{val}} \), which in the simplest case of independence, leads to

\[
  u_{\text{val}} = \sqrt{u_D^2 + u_{\text{input}}^2 + u_{\text{num}}^2}. \tag{Eq. 4}
\]

Changes to Eq. 4 required by shared contributions to these uncertainties are presented in [1].

The outcome of the V&V20-2009 method is an interval that should contain the model error \( \delta_{\text{model}} \),

\[
  \delta_{\text{model}} \in (E - k \cdot u_{\text{val}}, E + k \cdot u_{\text{val}}) \tag{Eq. 5}
\]

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 [1], but the determination of \( k \) requires the knowledge (or assumptions) of the type of distributions that characterize the experimental, input-parameters and numerical errors.

The V&V20-2009 [1] document also provides an example to illustrate the application of the pointwise metric to 10 set points. The results are shown in Figure 1. Experimental data, \( T_{\text{meas}} \), are presented as solid circles with data uncertainty \( u_D \) added as error bars. A corresponding simulation result, \( T_{\text{model}} \), 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 \( u_{\text{num}} \) and \( u_{\text{input}} \) assuming independence,
Following the V&V20-2009 method, a model comparison error $E_i$ and a validation uncertainty $u_{val,i}$ are calculated for each of the 10 set points ($i = 1$ to 10) where an experimental value is available for comparison,

$$
\delta_{\text{model},i} \in [E_i - k \cdot u_{val,i}, E_i + k \cdot u_{val,i}]
$$

The validation results are plotted in Figure 2 with uncertainty evaluated at one standard uncertainty ($k = 1$). For all 10 validation comparisons, $E$ is negative. However, for 7 of the 10 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 $\delta_{\text{model}}$ [2], because the limits of the intervals ($E - u_{val}$ and $E + u_{val}$) have opposite signs. Therefore, at these 7 set points, we can only
conclude that $|\delta_{\text{model}}| < |E - u_{\text{val}}|$. The fact that 7 out of 10 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 7 intervals are not centered at $E = 0$ and the 10 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 10 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 10 different set points and not between experimental, input and numerical uncertainties at a given set point.

The multivariate metric proposed in this document 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 the ASME V&V20-2009 Standard.
4.2 Development of Multivariate Metric $E_{mv}^2$

The multivariate metric presented in this document 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 below.

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 document. The reader should consult references for experimental measurement uncertainty for techniques to quantify correlation [11,12]. 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 over-predicts temperature at one time is likely to over-predict temperature at an adjacent time, see Figure 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, like 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 (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 document 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 \[4\]. 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

$$E_{mv}^2 = E^T V_{val}^{-1} E$$

Eq. 8

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

$$V_{val} = \begin{bmatrix}
    u_{val,1}^2 & \cdots & \rho_{1,n} u_{val,1} u_{val,n} \\
    \vdots & \ddots & \vdots \\
    \rho_{n,1} u_{val,n} u_{val,1} & \cdots & u_{val,n}^2
\end{bmatrix}.$$  

Eq. 9

The off-diagonal terms include the product of the correlation coefficient and the $u_{val,i}$'s at the respective validation set points. The correlation coefficient is defined in introductory statistics textbooks [13]. 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 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-points example. After performing the matrix operations of Eq. 8, the two-set points result can be expressed as the following equation for an ellipse in the $(E_1, E_2)$ space:

$$E_{mv}^2 = \frac{1}{1 - \rho_{1,2} \rho_{2,1}} \left[ \frac{E_1^2}{u_{val,1}^2} + \frac{E_2^2}{u_{val,2}^2} - 2 \frac{\rho_{1,2} \rho_{2,1} E_1 E_2}{u_{val,1} u_{val,2}} \right].$$

Eq. 10
Considering Eq. 10, 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 $u_{val,i}$ has the same dimension as $E_i$), allowing information from set points with different validation variables to be used in the global assessment.

Equation 10 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 $u_{val,1} = u_{val,2}$. 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. 10 reduces to

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

Eq. 11

$E_{mv} = \sqrt{E_{mv}^2}$ 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 goals:

1. Enabling the comparison of $E_{mv}$ values obtained from different number of validation set points;

2. 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 $\delta_{model}$ 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 $\langle E_{mv}^2 \rangle$. 

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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 Sections 4.2.1.1 and 4.2.1.2, respectively.

Two methods are described for calculating a value for $E_{ref}^2$. For normally-distributed comparison errors, the reference value is derived from the $\chi^2$ distribution. A sampling method is proposed if the comparison errors cannot be reasonably described using a normal distribution.

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 $V_{val}$ [5]. 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. 8. The expected value and variance of the $\chi^2(df)$ distribution are

$$\langle E_{mv}^2 \rangle = \langle \chi^2(df) \rangle = df$$

$$u_{E_{mv}^2}^2 = \text{var}(E_{mv}^2) = \text{var}(\chi^2(df)) = 2 \cdot df$$

Eq. 12

The Chi-squared distribution, $\chi^2(df)$, is tabulated in most statistical textbooks [12] and can be evaluated using internal routines from several software packages as for example 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

$$E_{ref}^2 = \langle E_{mv}^2 \rangle + \sqrt{\text{var}(E_{mv}^2)}$$

$$= df + \sqrt{2 \cdot df}.$$  

Eq. 13
4.2.1.2 Non-Normally Distributed Comparison Errors (sampling approach)

If the uncertainty in each set point for $\delta_{model}$ 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 V&V20-2009. 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 $\langle E_{mv}^2 \rangle$

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

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

$$\langle E \rangle = [\langle E_j \rangle_1 : \langle E_j \rangle_n] = [\langle E_j \rangle_i].$$

_eq_14

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

3A. Evaluate $\langle E_{mv}^2 \rangle$ using Eq. 8 using $E = \langle E \rangle$.

4.2.1.2.2 Estimation of $E_{ref}^2$

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 $\langle E_j \rangle_i$, $E_{\text{ref}}^2$ can be calculated from the deviations of $E_{j,i}$ from $\langle E_j \rangle_i$.

The following procedure is used to evaluate $\text{var}(E_{\text{mv}}^2)$ and thus $E_{\text{ref}}^2$:

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

$$E_{\text{ref}}^2_{i,j} = [E_{i,j} - \langle E_j \rangle_i]$$

Eq. 15

2B. Evaluate $[E_{\text{mv}}^2]_i$ for each set point $i$, separately, using Eq. 8 with $E$ replaced by $(E_{\text{ref}}^2)_{i,j}$.

This step provides a distribution of $E_{\text{mv}}^2$ for our hypothetically perfect physics model, given the distributions associated with $u_P$, $u_{\text{num}}$, and $u_{\text{input}}$.

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

4B. Estimate $E_{\text{ref}}^2$ with Eq. 13 using $\langle E_{\text{mv}}^2 \rangle$ and $\sqrt{\text{var}(E_{\text{mv}}^2)}$. The value of $E_{\text{mv}}^2$ can be compared to $E_{\text{ref}}^2$ to compile evidence that the discrepancies can be explained by the estimated uncertainties in its value.

4.2.2 Interpretation of $E_{\text{mv}}^2$

Figure 3 offers a simple demonstration of the interpretation of the metric $E_{\text{mv}}^2$. The solid horizontal line indicates $\langle E_{\text{mv}}^2 \rangle$ given that the expected value for $E_i$ is zero, i.e., $\langle E_i \rangle = 0$, $i = 1, \ldots, n$. Note that $\langle E_{\text{mv}}^2 \rangle$ is nonzero as the value of any realization of $E_{\text{mv}}^2$ cannot be negative. The dashed line represents $E_{\text{ref}}^2$, i.e., $\langle E_{\text{mv}}^2 \rangle$ plus its standard uncertainty $u_{E_{\text{mv}}^2}$.

Consider three scenarios of the metric $E_{\text{mv}}^2$ as quantified by Eq. 8 in Figure 3. The results for Scenarios 1 and 2 indicate that the weighted differences between simulations and measurements, $E_{\text{mv}}^2$, are within the expected value and one standard uncertainty of $\langle E_{\text{mv}}^2 \rangle$, i.e., $E_{\text{mv}}^2 < \langle E_{\text{mv}}^2 \rangle + u_{E_{\text{mv}}^2}$. Nonetheless, Scenario 1 is below $\langle E_{\text{mv}}^2 \rangle$ whereas Scenario 2 is between $\langle E_{\text{mv}}^2 \rangle$ and $E_{\text{ref}}^2$. This suggests that the comparison errors are consistent with the uncertainties as characterized by $V_{\text{val}}$. In contrast, Scenario 3 results in a value for $E_{\text{mv}}^2$ that is several standard uncertainties larger than $\langle E_{\text{mv}}^2 \rangle$, 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 $E_{mv}^2$ on the number of selected set points hinders the comparison presented in Figure 3 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 that exhibit 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 the knowledge of the validation uncertainty and comparison errors at each of the set points. As for the pointwise validation metric [1, 2], 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 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
[7] or multiple test facilities as in the present example. The sensitivity coefficients technique
based on a linearity assumption is illustrated in Section 5.1.1, whereas Section 5.1.2 presents
the application of the sampling approach that is able to deal with non-linearities.

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 equation

$$S(t) = a + bt$$  \hspace{1cm} Eq. 16

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
1.
Table 1. Simulation Model Parameters $a$ and $b$;
Note: $a$ and $b$ are independent and normally distributed

<table>
<thead>
<tr>
<th>Statistic</th>
<th>$a$</th>
<th>$b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>1.00</td>
<td>0.50</td>
</tr>
<tr>
<td>Standard Uncertainty</td>
<td>0.05</td>
<td>0.10</td>
</tr>
</tbody>
</table>

The assumption that $a$ and $b$ are independent implies that the off-diagonal elements in their covariance matrix, $\mathbf{V}_X$, 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 $\mathbf{V}_X$, see Appendix A.

The simulation model (Eq. 16) 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. 8, 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 2.

Table 2. Experimental Data $D$ at 2 Measurement Times, from 3 Independent Facilities

<table>
<thead>
<tr>
<th>Facility</th>
<th>$D_1$ at Time $t_1$</th>
<th>$D_2$ at Time $t_2$</th>
<th>Standard Uncertainty $\mu_D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.65</td>
<td>2.90</td>
<td>0.05</td>
</tr>
<tr>
<td>2</td>
<td>1.35</td>
<td>2.55</td>
<td>0.05</td>
</tr>
<tr>
<td>3</td>
<td>1.45</td>
<td>2.65</td>
<td>0.05</td>
</tr>
</tbody>
</table>

The simulated quantities, $S_i$, and the corresponding differences, $E_i$, are evaluated using the mean values of the input model parameters from Table 1 in Eq. 16, and are listed in Table 3 and Table 4, respectively.
Table 3. Mean Simulation Results $S_i$

<table>
<thead>
<tr>
<th>$t$</th>
<th>$S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_1$</td>
<td>1.5</td>
</tr>
<tr>
<td>$t_2$</td>
<td>2.5</td>
</tr>
</tbody>
</table>

Table 4 Comparison Error $E_i$ at 2 Measurement Times, from 3 Facilities

<table>
<thead>
<tr>
<th>Facility</th>
<th>$t_1 = 1.0$ sec, $E_1$</th>
<th>$t_2 = 3.0$ sec, $E_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-0.15</td>
<td>-0.40</td>
</tr>
<tr>
<td>2</td>
<td>0.15</td>
<td>-0.05</td>
</tr>
<tr>
<td>3</td>
<td>0.05</td>
<td>-0.15</td>
</tr>
</tbody>
</table>

5.1.1 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 Appendix A is an extension of that described in V&V20-2009 for the calculation of $u_{val}$ from estimates of $u_{num}$, $u_{input}$, and $u_D$ for a single set point. Accordingly,

$$V_{val} = V_{num} + V_{input} + V_D.$$  \hspace{1cm} Eq. 17

In Eq. (17), $V_{num}$ is zero since the simulation model, Eq. (16), is a simple algebraic equation, which in this simple example is not even affected by round-off errors. Therefore,

$$V_{num} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$  \hspace{1cm} Eq. 18

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, the present example corresponds to Case 1B presented in 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 Appendix A) using:

$$V_{input} = X_S \cdot V_X \cdot X_S^T.$$  \hspace{1cm} Eq. 19
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:

$$X_S = \begin{bmatrix} \frac{\partial S_1}{\partial a} & \frac{\partial S_1}{\partial b} \\ \frac{\partial S_2}{\partial a} & \frac{\partial S_2}{\partial b} \end{bmatrix} = \begin{bmatrix} 1 & t_1 \\ 1 & t_2 \end{bmatrix} = \begin{bmatrix} 1 & 1 \end{bmatrix}. \quad \text{Eq. 20}$$

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

$$V_X = \begin{bmatrix} (0.05)^2 & 0 \\ 0 & (0.10)^2 \end{bmatrix}. \quad \text{Eq. 21}$$

Evaluation of $V_{input}$ using Eq. 19 gives

$$V_{input} = X_S \cdot V_X \cdot X_S^T = \begin{bmatrix} 0.0125 & 0.0325 \\ 0.0325 & 0.0925 \end{bmatrix}. \quad \text{Eq. 22}$$

The non-zero off-diagonal terms in Eq. 22 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 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 Appendix A) is given by

$$V_D = \begin{bmatrix} (0.05)^2 & 0 \\ 0 & (0.05)^2 \end{bmatrix}. \quad \text{Eq. 23}$$

Given the estimates of $V_{num}$ (Eq. 18), $V_{input}$ (Eq. 22), and $V_D$ (Eq. 23), the matrix $V_{Val}$ is calculated using Eq. 17, as

$$V_{Val} = V_{num} + V_{input} + V_D = \begin{bmatrix} 0.0150 & 0.0325 \\ 0.0325 & 0.0950 \end{bmatrix}. \quad \text{Eq. 24}$$

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. 24. The comparison error, \( E \), and validation uncertainty, \( u_{val} \), are shown in Figure 4 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.

![Figure 4](image)

**Figure 4**  V&V20-2009 validation metric \((E \pm u_{val})\) at the two times for the three facilities

<table>
<thead>
<tr>
<th>Time</th>
<th>( E/u_{val} ), Ratio of comparison error to validation uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Facility 1</td>
<td>Facility 2</td>
</tr>
<tr>
<td>1.0 sec</td>
<td>-1.225</td>
</tr>
<tr>
<td>3.0 sec</td>
<td>-1.298</td>
</tr>
</tbody>
</table>

Table 5. Ratio of comparison error \((E)\) to validation uncertainty \((u_{val})\) at the two-time instants for the three facilities

For comparison of results from the sensitivity approach described in this sub-section and from the sampling approach, which is described in the next sub-section, values for \( E_{mv} = \sqrt{E_{mv}^2} \) are listed in Table 6 for \( V_{input} \) calculated using the sensitivity analysis (described above) and using
sampling, which is described below. The value of $E_{\text{ref}}$ for the sensitivity approach is calculated from Eq. 13 using $df = 2$, yielding $E_{\text{ref}} = 2$.

### 5.1.2 Sampling Approach

This approach applies the sampling methodology described in Appendix A to the linear example for the three facilities and the two time-instants listed in Table 5. The comparison error, $E$, is calculated from the difference between simulations and the measurements.

$$E = \text{mean}_j [S_{i,j} - D_{i,j}] = \text{mean}_j [E_{i,j}]$$  \hspace{1cm} \text{Eq. 25}

Latin Hypercube sampling is used (see [1]) with $n_r = 1000$ 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 model input parameters:

$$S_{i,j} = S_i(a_j, b_j)$$  \hspace{1cm} \text{Eq. 26}

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

$$a_j, b_j = \text{LHS}[N(\text{mean}(a), \text{standard uncertainty}(a)); N(\text{mean}(b), \text{standard uncertainty}(b))]$$  \hspace{1cm} \text{Eq. 27}

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

$$D_{i,j} = D_i + d_{i,j}$$  \hspace{1cm} \text{Eq. 28}

where

$$d_{i,j} = \text{LHS}[N(0, \text{standard uncertainty}(D_i))]$$  \hspace{1cm} \text{Eq. 29}

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

The covariance matrix $V_{\text{Val}}$ is estimated by

$$V_{\text{Val}} = V_{\text{num}} + \text{cov}(E_s)$$  \hspace{1cm} \text{Eq. 30}

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

The quantity $E_{\text{me}}^2$ is calculated using Eq. 8 and the covariance matrix $V_{\text{Val}}$ is estimated from Eq. 30. The value for $E_{\text{ref}}$ for the sampling approach is calculated as described in Section 4.2.1.2 for non-normally distributed comparison errors.
5.1.3 Comparison of Results from Sensitivity and Sampling Approaches

Table 6 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 6 can be reduced by including a larger number of samples (the present example is linear and normal 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.

Table 6. Validation Results for Normally Distributed Simulation Model Parameters

<table>
<thead>
<tr>
<th>Facility</th>
<th>Sensitivity Approach</th>
<th>Sampling Approach</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$E_{mv}$</td>
<td>$E_{ref}$</td>
</tr>
<tr>
<td>1</td>
<td>1.315</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>2.687</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>1.698</td>
<td>2</td>
</tr>
</tbody>
</table>

Figure 5 shows, schematically, the multivariate metric for the three facilities. If $E_{mv} \gg E_{ref}$, then the weighted comparison errors are significantly greater than the validation uncertainties at the multiple set points, given that $\langle E_i \rangle = 0$, $i = 1, ..., n$. 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 $u_{cal}$ at the two validation set points is similar for the three facilities (see Figure 4) and so the multivariate metric is showing that the data of Facility 2 produces the larger modeling errors.
Figure 5  Schematic representation of $E_{mv}$ for three facilities (symbols) using sensitivity approach. The solid line represents the expected value while the dashed line is offset by uncertainty.

Figure 6 illustrates the impact of the correlation characterized by $V_{val}$ on $E_{mv}$. The ellipses shown in Figure 6 represent curves of constant $E_{mv}^2$. The solid curve corresponds to the expected value of $E_{mv}^2$ ($<E_{mv}^2>$) and the dashed curve corresponds to the reference value, $E_{ref}^2$. The corresponding equations for the ellipses in Figure 6a are presented in Eq. 31.

$$E_{mv}^2 = [E_1 \ E_2] \cdot \begin{bmatrix} 0.0150 & 0.0325 \\ 0.0325 & 0.0950 \end{bmatrix}^{-1} \cdot \begin{bmatrix} E_1 \\ E_2 \end{bmatrix}$$

$$= [E_1 \ E_2] \cdot \begin{bmatrix} 257.6 & -88.14 \\ -88.14 & 40.68 \end{bmatrix} \cdot \begin{bmatrix} E_1 \\ E_2 \end{bmatrix}$$

Eq. 31

$$= 257.6 \cdot E_1^2 + 2 \cdot (-88.14) \cdot E_1 \cdot E_2 + 40.68 \cdot E_2^2$$

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 (Fig. 6a), we see that 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 6 presents also the two comparison errors for the three test facilities as listed in Table 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, 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 6b that presents the results obtained ignoring correlation, i.e., setting all the off-diagonal terms in \( V_{Val} \) to zero. In that case, Eq. 8 becomes

\[
E_{mv}^2 = \begin{bmatrix} E_1 & E_2 \end{bmatrix} \cdot \begin{bmatrix} 0.0150 & 0 \\ 0 & 0.0950 \end{bmatrix}^{-1} \cdot \begin{bmatrix} E_1 \\ E_2 \end{bmatrix} = \frac{E_1^2}{0.015} + \frac{E_2^2}{0.095} \quad \text{Eq. 32}
\]

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 6b 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 6b that ignores correlation (by setting the off-diagonal terms to zero) matches the assessment based on the pointwise intervals presented in Figure 4. Facility 1 is the only one that shows two intervals indicating a negative \( \delta_{\text{model}} \) (\( u_{val} \) is the same for the 3 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.
Figure 6  a) Correlated errors in estimates of the true differences and b) the effect of ignoring correlation.
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.

5.2 Summary

A validation metric was presented that 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 simple 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 Appendix B. Appendix A presents the equations required to calculate the covariance matrix for all the definitions of validation variables considered in V&V20-2009 [1].

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 V&V20-2009 [1], 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, $\mathcal{E}^2_{\text{mpv}}$, presented here 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 $V_{\text{Val}}$. V&V20-2009 [1], Section 4, and Appendix A of this supplement provide methodology to estimate the covariance matrix of these validation differences (comparison errors) at the multiple validation set points.

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

- 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;

- The covariance matrix ($V_{\text{Val}}$) 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 $V_{\text{Val}}$, as described in Appendix A.

Therefore, the procedure to obtain $V_{\text{Val}}$ depends on two considerations:

1. Which of the four cases addressed in V&V20-2009 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 [1], whereas the last 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.

The multivariate metric $E^2_{mv}$ produces a weighted distance that is compared to a reference value $E^2_{ref}$ obtained from the expected value of $E^2_{mv}$ 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 $E_{mv}/E_{ref} < 1$ 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 (V&V20-2009 [1]) 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 $E^2_{mv}$-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 $E^2_{mv}$-based metric has a known distribution ($\chi^2$) 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 Section 4.2.1.2 and Appendix A to evaluate the corresponding distribution for the $E^2_{mv}$ 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 Section 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 [1]. 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 simple 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 non-linear 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, as 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.

We recall that the present multivariate metric is an extension of the pointwise estimates of the modeling error provided by the V&V20-2009 [1] 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 document) 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 taken into account. 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 [2], it should be clearly stated once more 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(s) 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).
7 References


APPENDIX A
Methodology to Evaluate the Validation Covariance Matrix, $V_{\text{val}}$

The purpose of this appendix is to present the two techniques available to evaluate the validation covariance matrix $V_{\text{val}}$ (Main Body, Section 4.2, Eq. 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 one on sampling methods. The application of these two techniques to a single set point is presented in sections 3-2 and 3-3 of V&V20-2009 [1]. In this document, we present its application 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 equation (A.1),

$$E_i = S_i(x_1, x_2, \cdots, x_m) - D_i(x_1, x_2, \cdots, x_m), i = 1, \cdots, n$$  (A.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 two considerations:

- The determination of the validation variables. Four cases are considered in V&V20-2009 [1]:

  Case 1: Validation variable is directly measured.

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

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

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

The same four cases are described in this appendix.
Two clarifications must be given about these four cases:

1. 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.

- 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:

  A. No common (shared) errors in the simulation \( (S_1) \) and/or in the experimental measurements \( (D_1) \) at the \( n \) validation set points.

  B. Errors are identically shared at the \( n \) validation set points in the simulation \( (S_1) \) and/or in the experimental measurements \( (D_1) \), 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 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 V&V20-2009 [1].

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

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

![Figure A.1 Logic flow for choosing approach to calculate the validation uncertainty matrix $V_{\text{val}}$.](image)

Table A.1 Contributions to the covariance validation matrix $V_{\text{val}}$ in the sensitivity coefficients approach

<table>
<thead>
<tr>
<th>Section</th>
<th>Case</th>
<th>Contribution to $V_{\text{val}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A.1.1</td>
<td>1A,1B,2A,2B,3A,3B,4A,4B</td>
<td>Numerical uncertainty, $V_{\text{num}}$</td>
</tr>
<tr>
<td>A.1.2</td>
<td>1A,1B</td>
<td>Input parameters uncertainty, $V_{\text{input}}$</td>
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<td>A.1.3</td>
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<td>A.1.4</td>
<td>2A,2B,3A,3B</td>
<td>Correlated experimental and input parameters uncertainty, $V_{\text{input}+D}$</td>
</tr>
<tr>
<td>A.1.5</td>
<td>4A,4B</td>
<td>Input parameters uncertainty of the simulations, $V_{\text{S,input}}$, and of the model that handles the experimental data, $V_{D,input}$.</td>
</tr>
</tbody>
</table>
The calculation of the validation covariance matrix $V_{\text{val}}$ is presented using standard uncertainties to characterize the numerical, input parameters and experimental errors ($u_{\text{num}}$, $u_{\text{input}}$ and $u_D$). Equivalent equations are obtained if expanded uncertainties ($U_{\text{num}}$, $U_{\text{input}}$ and $U_D$) are adopted. Section 6-3 of V&V20-2009 [1] discusses the determination of the coverage factors required to transform standard uncertainties in to expanded uncertainties.

### A.1 Sensitivity coefficients approach

There are four different cases illustrated in figure A.1 that lead to the following expressions:

**Cases 1A and 1B:** Validation variable directly measured with no shared error sources between experiments and simulations.

$$V_{\text{val}} = V_{\text{num}} + V_{\text{input}} + V_D$$  \hspace{1cm} (A.2)

**Cases 2A, 2B, 3A and 3B:** Validation variable computed from a data reduction equation.

$$V_{\text{val}} = V_{\text{num}} + V_{\text{input}} + V_D$$  \hspace{1cm} (A.3)

**Cases 4A and 4B:** Validation variable is evaluated from measured variables analyzed with a model.

$$V_{\text{val}} = V_{\text{num}} + V_{\text{input}} + V_{D,\text{num}} + V_{D,\text{input}}$$  \hspace{1cm} (A.4)

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

These equations have a companion definition of the validation uncertainty $u_{\text{val}}$ for a single set point taken from V&V20-2009 [1]

**Case 1:**

$$u_{\text{val}}^2 = u_{\text{num}}^2 + u_{\text{input}}^2 + u_D^2$$  \hspace{1cm} (A.5)

**Cases 2 and 3:**

$$u_{\text{val}}^2 = u_{\text{num}}^2 + u_{\text{input}}^2$$  \hspace{1cm} (A.6)

**Case 4:**
\[ u_{\text{val}}^2 = u_{S,\text{num}}^2 + u_{S,\text{input}}^2 + u_{D,\text{num}}^2 + u_{D,\text{input}}^2 \]  \hspace{1cm} (A.7)

The expressions to determine the different contributions to the validation covariance matrix \( V_{\text{val}} \) 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). We 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.1.1 Contribution of the numerical uncertainty, \( V_{\text{num}} \) and \( V_{D,\text{num}} \) (cases 1, 2, 3 and 4)**

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

---

**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, \( u_{\text{num},i} \), can be obtained with the techniques described in V&V20-2009 [1]. When there are no shared errors between the \( n \) validation set points, the contribution of the numerical uncertainty to the validation covariance matrix \( V_{\text{num}} \) is defined by equation (A.8).

\[
V_{\text{num}} = \begin{bmatrix}
  u_{\text{num},1}^2 & 0 & \cdots & 0 \\
  0 & u_{\text{num},2}^2 & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \cdots & u_{\text{num},n}^2 
\end{bmatrix} \hspace{1cm} (A.8)
\]

---

**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 \( V_{\text{num}} \) is defined by equation (A.9).

\[
V_{\text{num}} = \begin{bmatrix}
  u_{\text{num},1}^2 & u_{\text{num},1}u_{\text{num},2} & \cdots & u_{\text{num},1}u_{\text{num},n} \\
  u_{\text{num},1}u_{\text{num},2} & u_{\text{num},2}^2 & \cdots & u_{\text{num},2}u_{\text{num},n} \\
  \vdots & \vdots & \ddots & \vdots \\
  u_{\text{num},1}u_{\text{num},n} & \cdots & u_{\text{num},n}u_{\text{num},2} & u_{\text{num},n}^2 
\end{bmatrix} \hspace{1cm} (A.9)
\]
A.1.2 Contribution of the input uncertainty $V_{\text{input}}$ (case 1)

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

No shared errors between the $n$ validation set points (case 1A)

When there are no input errors shared by the $n$ validation set points, $V_{\text{input}}$ is obtained from equation (A.10).

$$
V_{\text{input}} = \begin{bmatrix} X_{S,1}V_{X,1}X_{S,1}^T & 0 & \cdots & 0 \\
0 & X_{S,2}V_{X,2}X_{S,2}^T & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & X_{S,n}V_{X,n}X_{S,n}^T \end{bmatrix} \quad \text{(A.10)}
$$

where $X_{S,i}$ 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 equation (A.10) are identically 0. The sensitivity coefficients vector originated by the $m$ input variables at each set point $i$, $X_{S,i}$, is a line vector $(1 \times m)$ defined by equation (A.11).

$$
X_{S,i} = \frac{\partial S_i}{\partial x_1} \cdots \frac{\partial S_i}{\partial x_m} \quad \text{(A.11)}
$$

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 equation (A.12).

$$
V_{X,i} = \begin{bmatrix} (u_{x1}^2)_i & 0 & \cdots & 0 \\
0 & (u_{x2}^2)_i & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & (u_{xm}^2)_i \end{bmatrix} \quad \text{(A.12)}
$$

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 equation (A.13).

$$
V_{\text{input}} = X_S V_X X_S^T \quad \text{(A.13)}
$$
\( X \) is a \((n \times m)\) matrix containing the \(m\) sensitivity coefficients at the \(n\) set points defined by equation (A.14) and \( V \) is a \(m \times m\) diagonal matrix including the standard uncertainties of the \(m\) input parameters \(x_j\) squared.

\[
X = \begin{bmatrix}
\frac{\partial S_1}{\partial x_1} & \ldots & \frac{\partial S_1}{\partial x_m} \\
\vdots & \ddots & \vdots \\
\frac{\partial S_n}{\partial x_1} & \ldots & \frac{\partial S_n}{\partial x_m}
\end{bmatrix} \tag{A.14}
\]

\( V \) is defined by equation (A.12) and can be calculated for any of the \(n\) set points.

### A.1.3 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, \( u_{D,j} \), can be obtained at each set point using the techniques described in V&V20-2009 [1].

**No shared errors between the \(n\) validation set points (case 1A)**

For the case that the validation set points do not share experimental errors we have \( V_D \) defined by equation (A.15).

\[
V_D = \begin{bmatrix}
u_{D,1}^2 & 0 & \ldots & 0 \\
0 & u_{D,2}^2 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & u_{D,n}^2
\end{bmatrix} \tag{A.15}
\]

**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 equation (16).

\[
V_D = \begin{bmatrix}
u_{D,1}^2 & u_{D,1}u_{D,2} & \ldots & u_{D,1}u_{D,n} \\
u_{D,2}u_{D,1} & u_{D,2}^2 & \ldots & u_{D,2}u_{D,n} \\
\vdots & \vdots & \ddots & \vdots \\
u_{D,n}u_{D,1} & u_{D,n}u_{D,2} & \ldots & u_{D,n}^2
\end{bmatrix} \tag{16}
\]
A.1.4 Combined contribution of input and experimental uncertainties $V_{\text{input+D}}$ (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. We 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.

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 $V_{\text{input+D}}$ when the $n$ validation set points do not share errors is defined by equation (A.17).

$$
V_{\text{input+D}} = \begin{bmatrix}
V_{\text{input+D}1,1} & 0 & \cdots & 0 \\
0 & V_{\text{input+D}2,2} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & V_{\text{input+D}n,n}
\end{bmatrix}
$$

(A.17)

with

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

(A.18)

The vector containing the sensitivity coefficients of the simulations $X_{S,i}$ is defined by equation (A.11), whereas the vector of sensitivity coefficients of the experiments $X_{D,i}$ is given by equation (A.19).

$$
X_{D,i} = \left[ \frac{\partial D_i}{\partial x_1}, \ldots, \frac{\partial D_i}{\partial x_m} \right]
$$

(A.19)

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 equation (A.12). On the other hand, for shared error between the measured quantities (Case 3), $V_{X,i}$ is determined from equation (A.20).

$$
V_{X,i} = \begin{bmatrix}
(u^2_{x_1})_i & (u_{x_1}u_{x_2})_i & \cdots & (u_{x_1}u_{x_m})_i \\
(u_{x_2}u_{x_1})_i & (u^2_{x_2})_i & \cdots & (u_{x_2}u_{x_m})_i \\
\vdots & \vdots & \ddots & \vdots \\
(u_{x_m}u_{x_1})_i & (u_{x_m}u_{x_2})_i & \cdots & (u^2_{x_m})_i
\end{bmatrix}
$$

(A.20)
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 $V_{\text{input}}$ is determined from equation (A.21).

$$V_{\text{input}} = (X_S - X_D) V_X (X_S - X_D)^T$$  \hspace{1cm} (A.21)

$X_S$ and $X_D$ are $(n \times m)$ matrices that contain the $m$ sensitivity coefficients at the $n$ validation set points. Equation (A.14) defines $X_S$ and $X_D$ is determined from equation (A.22).

$$X_D = \begin{bmatrix} \frac{\partial D_1}{\partial x_1} & \cdots & \frac{\partial D_1}{\partial x_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial D_n}{\partial x_1} & \cdots & \frac{\partial D_n}{\partial x_m} \end{bmatrix}$$  \hspace{1cm} (A.22)

The definition of the $(m \times m)$ matrix $V_X$ is equivalent to the previous section, i.e. $V_X$ is defined by equation (A.12) for case 2 (no shared errors between the measured variables) and $V_X$ is determined from equation (A.20) 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.1.5 Contribution of input uncertainties when experimental value comes from measured variables analyzed with a model, $V_{\text{input}}$, $V_{D,\text{input}}$

In this case there are contributions coming from the $m$ input parameters $x_i$ required for the simulation $V_{\text{input}}$ 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 $V_{\text{input}}$ matrix is presented in section A.1.2 and the determination of $V_{D,\text{input}}$ is similar. Nonetheless, for the sake of clarity, the definitions of $V_{\text{input}}$ and $V_{D,\text{input}}$ are presented below.

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 $V_{\text{input}}$ and $V_{D,\text{input}}$ are defined by equations (A.23) and (A.24).

---

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\[
V_{\text{input}} = \begin{bmatrix}
X_{S,1}V_{X,1}X_{S,1}^T & 0 & \cdots & 0 \\
0 & X_{S,2}V_{X,2}X_{S,2}^T & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & X_{S,n}V_{X,n}X_{S,n}^T
\end{bmatrix}
\] (A.23)

\[
V_{\text{D,input}} = \begin{bmatrix}
X_{D,1}V_{D,1}X_{D,1}^T & 0 & \cdots & 0 \\
0 & X_{D,2}V_{D,2}X_{D,2}^T & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & X_{D,n}V_{D,n}X_{D,n}^T
\end{bmatrix}
\] (A.24)

The \((1 \times m)\) line vector of sensitivity coefficients of the \(m\) input parameters of the simulation \(X_{S,i}\) is defined by equation (A.11), whereas the \((1 \times l)\) line vector of sensitivity coefficients of the \(l\) measured variables used in the model that produces \(D_i\) is defined by equation (A.25).

\[
X_{D,i} = \left[\frac{\partial D_i}{\partial y_1}, \ldots, \frac{\partial D_i}{\partial y_l}\right]
\] (A.25)

The \((m \times m)\) matrix that defines \(V_{X,i}\) is defined by equation (A.12) if the \(m\) input parameters of the simulations are not correlated and by equation (A.20) if they are correlated. The \((l \times l)\) covariance matrix \(V_{D,i}\) is determined by similar definitions, i.e. for \(l\) independent measured variables used in the model that produces \(D_i\) we have \(V_{D,i}\) defined by equation (A.26).

\[
V_{D,i} = \begin{bmatrix}
(u_{y_1}^2)_i & 0 & \cdots & 0 \\
0 & (u_{y_2}^2)_i & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & (u_{y_l}^2)_i
\end{bmatrix}
\] (A.26)

On the other hand, if the \(l\) measured variables are correlated \(V_{D,i}\) is determined from equation (A.27).

\[
V_{D,i} = \begin{bmatrix}
(u_{y_1}^2)_i & (u_{y_1}u_{y_2})_i & \cdots & (u_{y_1}u_{y_1})_i \\
(u_{y_2}u_{y_1})_i & (u_{y_2}^2)_i & \cdots & (u_{y_2}u_{y_1})_i \\
\vdots & \vdots & \ddots & \vdots \\
(u_{y_1}u_{y_1})_i & (u_{y_1}u_{y_2})_i & \cdots & (u_{y_1}^2)_i
\end{bmatrix}
\] (A.27)

\textbf{Shared identical errors between the \(n\) validation set points (case 4B)}

When the errors are shared by the \(n\) validation set points we have \(V_{\text{input}}\) defined by equation (A.28),
\[ \mathbf{V}_{\text{input}} = \mathbf{X}_S \mathbf{V}_X \mathbf{X}_S^T \]  \hspace{1cm} (A.28)

and \( \mathbf{V}_{\text{D,input}} \) given by equation (A.29).

\[ \mathbf{V}_{\text{D,input}} = \mathbf{X}_D \mathbf{V}_D \mathbf{X}_D^T \]  \hspace{1cm} (A.29)

The \((n \times m)\) \( \mathbf{X}_S \) matrix is defined by equation (A.14) and the \((n \times l)\) \( \mathbf{X}_D \) matrix is determined from equation (30).

\[ \mathbf{X}_D = \begin{bmatrix}
\frac{\partial D_1}{\partial y_1} & \cdots & \frac{\partial D_1}{\partial y_l} \\
\vdots & \ddots & \vdots \\
\frac{\partial D_n}{\partial y_1} & \cdots & \frac{\partial D_n}{\partial y_l}
\end{bmatrix} \]  \hspace{1cm} (A.30)

The \((n \times n)\) covariance matrix \( \mathbf{V}_X \) is defined by equation (A.12) if there is no correlation between the \( m \) input variables of the simulation and by equation (A.20) if the \( m \) input variables are correlated. Similarly, for independent measured variables for the determination of \( D_i, \) \( \mathbf{V}_D \) is defined by equation (A.26), whereas the case of correlated measured variables leads to \( \mathbf{V}_D \) determined by equation (A.27).

**A.1.6 Summary of equations required to determine \( \mathbf{V}_{\text{val}} \) with sensitivity analysis**

Table A.2 summarizes all the equations required to calculate \( \mathbf{V}_{\text{val}} \) for the eight cases included in the chart presented in figure A.1. The number of the equation is followed by the corresponding matrix.

**Table A.2 Summary of equation required to calculate the validation uncertainty matrix \( \mathbf{V}_{\text{val}} \).**

<table>
<thead>
<tr>
<th>Case</th>
<th>Equations required</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1A</td>
<td>(A.2)( \mathbf{V}<em>{\text{val}} ), (A.8)( \mathbf{V}</em>{\text{num}} ), (A.10)( \mathbf{V}_{\text{input}} ), (A.11)( \mathbf{X}_S,i ), (A.12)( \mathbf{V}_X,i ) and (A.15)( \mathbf{V}_D )</td>
<td>( \mathbf{V}_{\text{val}} ) is a diagonal matrix</td>
</tr>
<tr>
<td>1B</td>
<td>(A.2)( \mathbf{V}<em>{\text{val}} ), (9)( \mathbf{V}</em>{\text{num}} ), (A.13)( \mathbf{V}_{\text{input}} ), (A.14)( \mathbf{X}_S,i ), (A.12)( \mathbf{V}_X,i ) and (A.16)( \mathbf{V}_D )</td>
<td>( \mathbf{V}_{\text{val}} ) is a full matrix</td>
</tr>
<tr>
<td>2A</td>
<td>(A.3)( \mathbf{V}<em>{\text{val}} ), (A.8)( \mathbf{V}</em>{\text{num}} ), (A.17)( \mathbf{V}_{\text{input+D}} ), (A.11)( \mathbf{X}_S,i ), (A.12)( \mathbf{V}_X,i ) and (A.19)( \mathbf{X}_D,i )</td>
<td>( \mathbf{V}_{\text{val}} ) is a diagonal matrix</td>
</tr>
<tr>
<td>2B</td>
<td>(A.3)( \mathbf{V}<em>{\text{val}} ), (A.9)( \mathbf{V}</em>{\text{num}} ), (A.21)( \mathbf{V}_{\text{input+D}} ), (A.14)( \mathbf{X}_S,i ), (A.12)( \mathbf{V}_X,i ) and (A.22)( \mathbf{X}_D,i )</td>
<td>( \mathbf{V}_{\text{val}} ) is a full matrix</td>
</tr>
</tbody>
</table>
A.2 Procedure to Evaluate Validation Covariance Matrix, $V_{\text{val}}$, 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 $V_{\text{val}}$. Assuming that the propagation of the input uncertainties through the model used in the simulations is independent of the numerical uncertainty, the sampling methodology described in V&V20-2009 [1] leads to equation (A.31) for the definition of each entry of the validation covariance matrix.

\[
[V_{\text{val}}]_{i,k} \approx [V_{\text{num}}]_{i,k} + \frac{1}{n_r - 1} \sum_{i=1}^{n_r} \sum_{k=1}^{n_r} (E_{i,l} - \bar{E}_i) (E_{k,K} - \bar{E}_k) \tag{A.31}
\]

$V_{\text{num}}$ is obtained from the equations presented in Section A.1.1, $n_r$ is the number of random samples over population, $E_{i,l}$ is the $l^{th}$ sample from the population values associated with the uncertainties, $u_{\text{input}}$ and $u_D$ of set point $i$, $E_{k,K}$ is the $K^{th}$ sample from the population values associated with the uncertainties, $u_{\text{input}}$ and $u_D$ at set point $k$, $\bar{E}_i$ and $\bar{E}_k$ 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.31) estimates the contribution to $V_{\text{val}}$ 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 V&V20-2009 [1]. 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 non-normally 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.2 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 equations (A.32) and (A.33).

\[
E_{i,j} = S_{i,j}(x_{1,j}, x_{2,j}, \ldots, x_{m,j}) - D_{i,j}(x_{1,j}, x_{2,j}, \ldots, x_{m,j}), i = 1, \ldots, n \tag{A.32}
\]

\[
E_{k,K} = S_{k,K}(x_{1,K}, x_{2,K}, \ldots, x_{m,K}) - D_{k,K}(x_{1,K}, x_{2,K}, \ldots, x_{m,K}), i = 1, \ldots, n \tag{A.33}
\]

The samples of the input parameter uncertainties are independently generated, i.e., independent sample sets \([x_{1,l}, x_{2,l}, \ldots, x_{m,l}]\) 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.2 2 Shared identical errors between the \(n\) validation set points (case 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 equation (A.31).

A.3 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 \(\delta_{model}\), i.e. all input parameters are hardwired to the model and so \(\delta_{input}\) is merged with \(\delta_{model}\). This leads to a validation uncertainty \(u_{val}^2\) defined by equation (A.34).

\[
u_{val}^2 = u_{num}^2 + u_D^2 \tag{A.34}
\]

Therefore, the validation covariance matrix defined by equation (35) includes only numerical uncertainty \((V_{num})\) and experimental uncertainty \((V_D)\), which have been presented in sections A.1.1 and A.1.3.

\[
V_{val} = V_{num} + V_D \tag{A.35}
\]
If the errors are not shared at the \( n \) validation set points, the validation covariance matrix \( V_{\text{val}} \) is defined by equations (A.8) and (A.15). However, if the errors are identically shared at the \( n \) validation set points the three matrices, \( V_{\text{num}} \), \( V_{\text{p}} \) and \( V_{\text{val}} \) will be singular (have a zero determinant). Therefore, the multivariate metric cannot be calculated. However, in such conditions, the modeling error at the \( n \) set points should lead to similar comparison errors (\( E \)) and validation uncertainties (\( U_{\text{val}} \)) and so a multivariate metric is not required to assess the global modeling error.

A.4 References

APPENDIX B

Example Problem: Fin-Tube Heat Exchanger

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 they are presented in the following tables. Example calculations are performed using Excel (Microsoft Office 365 ProPlus, Ver. 1803) with default precision. Results are reported rounded to 2 digits after the decimal point except for small numbers (< 1) which are reported using scientific notation rounded to 2 digits past the decimal point.

The organization of this section is as follows:

- Section B.1: Reporting of the validation case
- Section B.2: Reporting of the experimental data
- Section B.3: Reporting of simulation model
- Section B.4: Evaluation of the pointwise V&V20-2009 metric
- Section B.5: Evaluation of the multivariate metric $E$

B.1 Validation Example

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

The experimental data used in this Section are synthetic values generated per Section 7-3.2 of the ASME V&V20-2009 Standard. Use of synthetic, rather than experimental, data facilitates “teaching” because dependencies can be controlled to provide “clean” results to demonstrate and document effects.

B.2 Experimental Data and Uncertainties

Six experiments are conducted which vary the inflow temperature, $T_i$, from ~70°C to ~ 92°C. The outflow temperature, $T_o$, and the ambient temperature, $T_\infty$, are measured.
The data reduction defined in Eq. (B.1):

$$q_D = \rho Q C_p (T_i - T_o)$$  \hspace{1cm} (B.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, $\rho$, 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.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.2. Additional parameters, $X_i = \{T_o, k_t, k_f, h_i, h_f, \text{and } h_o\}$, are included in Table B.2 to support discussion of the simulation model in Section B.3. $k_t$ and $k_f$ are the thermal conductivities of the tube and fin. $h_i, h_f, \text{and } h_o$ are convective heat transfer coefficients for the inner surface of the tube, the fin, and the outer surface of the tube, respectively. The flow temperatures, $T_i$ and $T_o$ have shared systematic sources.
Table B.2 Random and systematic uncertainties for input parameters $X_i$

<table>
<thead>
<tr>
<th>Input Parameter Standard Uncertainties</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_i$</td>
</tr>
<tr>
<td>$T_i$  °C</td>
</tr>
<tr>
<td>$T_0$  °C</td>
</tr>
<tr>
<td>$Q$  m³/s</td>
</tr>
<tr>
<td>$\rho$ kg/m³</td>
</tr>
<tr>
<td>$c_p$ J/kg°C</td>
</tr>
<tr>
<td>$T_{\infty}$ °C</td>
</tr>
<tr>
<td>$k_f$ W/m°C</td>
</tr>
<tr>
<td>$h_i$ W/m°C</td>
</tr>
<tr>
<td>$h_f$ W/m°C</td>
</tr>
<tr>
<td>$h_o$ W/m°C</td>
</tr>
</tbody>
</table>

Because the heat transfer rate, $q_D$, is calculated from the data reduction Eq. (B.1), data uncertainty, $u_{q_D}$, is quantified as input parameter uncertainty from uncertain inputs when propagated through the data reduction equation. For this example, $u_{q_D}$ is calculated using the method of sensitivity coefficients described in Section 4-2.2 of the ASME V&V20-2009 Standard [1], see Section 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.2) using the data reduction Eq. (B.1):

$$X_i \frac{\partial q_D}{\partial X_i} = \begin{bmatrix} T_i \frac{\partial q_D}{\partial T_i} \\ T_0 \frac{\partial q_D}{\partial T_0} \\ Q \frac{\partial q_D}{\partial Q} \\ \rho \frac{\partial q_D}{\partial \rho} \\ c_p \frac{\partial q_D}{\partial c_p} \end{bmatrix} = \begin{bmatrix} \rho c_p T_i \\ -\rho c_p T_0 \\ \rho c_p (T_i - T_0) \\ -\rho c_p (T_i - T_0) \end{bmatrix}$$

(B.2)
An example of the calculation of the sensitivity coefficient for parameter $T_i$ for Experiment 1 of Table B.1 is defined in Eq. (B.3):

$$T_i \frac{\partial q_D}{\partial T_i} = \rho Q C_p T_i = \left(990 \frac{kg}{m^3}\right) \left(6.21 \times 10^{-6} \frac{m^3}{s}\right) \left(4180 \frac{J}{kg{\degree}C}\right)(70.44 \, ^{\circ}C)(W) = 1810.18 \, W$$ \hspace{1cm} (B.3)

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

### Table B.3  Calculated sensitivity coefficients for the experiments reported in Table B.1.

<table>
<thead>
<tr>
<th>Exp.</th>
<th>$T_i \cdot \frac{\partial q_D}{\partial T_i}$</th>
<th>$T_o \cdot \frac{\partial q_D}{\partial T_o}$</th>
<th>$Q \cdot \frac{\partial q_D}{\partial Q}$</th>
<th>$\rho \cdot \frac{\partial q_D}{\partial \rho}$</th>
<th>$C_p \cdot \frac{\partial q_D}{\partial C_p}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1810.18</td>
<td>-1732.32</td>
<td>77.87</td>
<td>77.87</td>
<td>77.87</td>
</tr>
<tr>
<td>2</td>
<td>1900.01</td>
<td>-1800.34</td>
<td>99.67</td>
<td>99.67</td>
<td>99.67</td>
</tr>
<tr>
<td>3</td>
<td>1943.85</td>
<td>-1836.78</td>
<td>107.08</td>
<td>107.08</td>
<td>107.08</td>
</tr>
<tr>
<td>4</td>
<td>2073.84</td>
<td>-1948.75</td>
<td>125.09</td>
<td>125.09</td>
<td>125.09</td>
</tr>
<tr>
<td>5</td>
<td>2256.61</td>
<td>-2114.56</td>
<td>142.05</td>
<td>142.05</td>
<td>142.05</td>
</tr>
<tr>
<td>6</td>
<td>2380.68</td>
<td>-2223.44</td>
<td>157.24</td>
<td>157.24</td>
<td>157.24</td>
</tr>
</tbody>
</table>

#### B.2.1 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 Section 4-2.2 of the ASME V&V20-2009 Standard [1]. Per Eq. 4-2-4 of the Standard, $u_{q_D}$ is the root-sum-square of uncertainties from random, $s_{q_D}$, and systematic, $b_{q_D}$, sources.

$$u_{q_D}^2 = s_{q_D}^2 + b_{q_D}^2$$ \hspace{1cm} (B.4)

Equation 4-2-6 of the ASME V&V20-2009 Standard [1] provides the propagation equation for random uncertainty, $s_{q_D}$. The equation, in matrix notation, is

$$s_{q_D}^2 = X_D^T V_X(rnd) X_D$$ \hspace{1cm} (B.5)

$X_D$ is the matrix of sensitivity coefficients for an experimental result as written in Eq. (B.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 $s_X^2$ along the diagonal (Eq. (B.6)): 50
Using sensitivity coefficients from Table B.3, \( X_D \) for Experiment 1 is defined in Eq. (B.7):

\[
X_D = \begin{bmatrix}
1810.18 \\
-1732.32 \\
77.87 \\
77.87 \\
77.87
\end{bmatrix}
\]

Using uncertainties from Table B.2, \( V_X(rnd) \) is defined in Eq. (B.8):

\[
V_X(rnd) = \begin{bmatrix}
4.90E-7 & 0 & 0 & 0 & 0 \\
0 & 4.90E-7 & 0 & 0 & 0 \\
0 & 0 & 2.50E-5 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

The calculation of \( s_{qD}^2 \) for Experiment 1 is defined in Eq. (B.9):

\[
s_{qD}^2 = [1810.18 \ -1732.32 \ 77.87 \ 77.87 \ 77.87] \times
\begin{bmatrix}
4.90E-7 \\
0 \\
0 \\
0 \\
0
\end{bmatrix}
\begin{bmatrix}
1810.18 \\
-1732.32 \\
77.87 \\
77.87 \\
77.87
\end{bmatrix}
\]

which yields (Eq. (B.10))

\[
s_{qD} = \sqrt{s_{qD}^2} = \sqrt{3.23 W^2} = 1.80 W
\]

Calculated values for \( s_{qD} \) for each experiment are reported in Table B.4.

The propagation equation for systematic uncertainty, \( b_{qD} \), is provided in Equation 4-2-5 of the ASME V&V20-2009 Standard [1]. The equation, in matrix form, is defined in Eq. (B.11):

\[
b_{qD}^2 = X_D^T V_X(sys) X_D
\]
Table B.4  Random, systematic, and total data uncertainties for the experimental data

<table>
<thead>
<tr>
<th>Exp.</th>
<th>$s_{qd}$</th>
<th>$b_{qd}$</th>
<th>$u_{qd}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$W$</td>
<td>$W$</td>
<td>$W$</td>
</tr>
<tr>
<td>1</td>
<td>1.80</td>
<td>1.17</td>
<td>2.15</td>
</tr>
<tr>
<td>2</td>
<td>1.90</td>
<td>1.50</td>
<td>2.42</td>
</tr>
<tr>
<td>3</td>
<td>1.95</td>
<td>1.61</td>
<td>2.53</td>
</tr>
<tr>
<td>4</td>
<td>2.09</td>
<td>1.88</td>
<td>2.81</td>
</tr>
<tr>
<td>5</td>
<td>2.28</td>
<td>2.14</td>
<td>3.13</td>
</tr>
<tr>
<td>6</td>
<td>2.41</td>
<td>2.37</td>
<td>3.38</td>
</tr>
</tbody>
</table>

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

$$V_x(sys) = \begin{bmatrix} b_{T_l}^2 & b_{T_l}b_{T_o} & 0 & 0 & 0 \\ b_{T_l}b_{T_o} & b_{T_o}^2 & 0 & 0 & 0 \\ 0 & 0 & b_{b_0}^2 & 0 & 0 \\ 0 & 0 & 0 & b_{b_p}^2 & 0 \\ 0 & 0 & 0 & 0 & b_{v_p}^2 \end{bmatrix}$$ (B.12)

$T_l$ and $T_o$ are correlated because they share identical systematic error sources. Using uncertainties from Table B.2, $V_x(sys)$ is

$$V_x(sys) = \begin{bmatrix} 1.96E-6 & 1.96E-6 & 0 & 0 & 0 \\ 1.96E-6 & 1.96E-6 & 0 & 0 & 0 \\ 0 & 0 & 1.00E-4 & 0 & 0 \\ 0 & 0 & 0 & 2.50E-5 & 0 \\ 0 & 0 & 0 & 0 & 1.00E-4 \end{bmatrix}$$ (B.13)

The calculation of $b_{qd}^2$ for Experiment 1 is

$$b_{qd}^2 = \begin{bmatrix} 1810.18 & -1732.32 & 77.87 & 77.87 & 77.87 \\ 1.96E-6 & 1.96E-6 & 0 & 0 & 0 \\ 1.96E-6 & 1.96E-6 & 0 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} 1810.18 \\ -1732.32 \\ 0 \\ 0 \\ 0 \end{bmatrix} \times \begin{bmatrix} 1810.18 \\ -1732.32 \\ 77.87 \\ 77.87 \\ 77.87 \end{bmatrix}$$ (B.14)

which yields Eq. (B.15):

$$b_{qd} = \sqrt{b_{qd}^2} = \sqrt{1.38 W^2} = 1.17 W$$ (B.15)
Calculated values for \( s_{q_D} \) for each experiment are reported in Table B.4.

\( u_{q_D} \) for Experiment 1 is the combined value of \( s_{q_D} \) (Eq. (B.10)) and \( b_{q_D} \) (Eq. (B.15)):  
\[
 u_{q_D} = \sqrt{3.23 W^2 + 1.38 W^2} = 2.15 W 
\]  
(B.16)

Calculated values for \( u_{q_D} \) for each experiment are reported in Table B.4.

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

![Figure B.1 Experimentally determined total heat transfer as a function of inflow temperature.](image)

**B.3 Simulation Model**

The simulation model for the fin-tube heat exchanger is described in Section 7-3.3 of the ASME V&V20-2009 Standard [1]. Details are provided in Mandatory Appendix 1. 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 Section 7-3.5.1 of the Standard, introducing a known systematic model error.

**B.3.1 Simulation Results**

Simulations for the set point conditions of Table B.1 are performed. Simulation parameters, set-point conditions, and simulation results, \( q_s \), are reported in Table B.5. Simulation results are
compared to the experimental data in Figure B.2. The simulation results exceed the
experimental measurements for $T_i \lesssim 74^\circ F$ and are less than the experimental measurements
for $T_i \gtrsim 74^\circ F$.

Table B.5 Simulation Parameters, Set-Point Conditions, and Results

<table>
<thead>
<tr>
<th>Simulation Case</th>
<th>$T_i$ (°C)</th>
<th>$T_\infty$ (°C)</th>
<th>$Q$ (m³/s)</th>
<th>$\rho$ (kg/m³)</th>
<th>$C_p$ (kJ/kg°C)</th>
<th>$T_o$ (°C)</th>
<th>$q_s$ (W/m°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>70.44</td>
<td>21.66</td>
<td>6.21E-06</td>
<td>990</td>
<td>4180</td>
<td>67.41</td>
<td>98.61</td>
</tr>
<tr>
<td>2</td>
<td>73.58</td>
<td>22.14</td>
<td>6.24E-06</td>
<td>990</td>
<td>4180</td>
<td>69.72</td>
<td>104.00</td>
</tr>
<tr>
<td>3</td>
<td>75.52</td>
<td>21.99</td>
<td>6.22E-06</td>
<td>990</td>
<td>4180</td>
<td>71.36</td>
<td>108.22</td>
</tr>
<tr>
<td>4</td>
<td>80.57</td>
<td>21.88</td>
<td>6.22E-06</td>
<td>990</td>
<td>4180</td>
<td>75.71</td>
<td>118.66</td>
</tr>
<tr>
<td>5</td>
<td>87.53</td>
<td>22.08</td>
<td>6.23E-06</td>
<td>990</td>
<td>4180</td>
<td>82.02</td>
<td>132.31</td>
</tr>
<tr>
<td>6</td>
<td>91.90</td>
<td>22.11</td>
<td>6.26E-06</td>
<td>990</td>
<td>4180</td>
<td>85.83</td>
<td>141.12</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Simulation Case</th>
<th>$k_t$ (W/m°C)</th>
<th>$k_f$ (W/m°C)</th>
<th>$h_i$ (W/m°C)</th>
<th>$h_f$ (W/m°C)</th>
<th>$h_o$ (W/m°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>386</td>
<td>204</td>
<td>150</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>2</td>
<td>386</td>
<td>204</td>
<td>150</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>3</td>
<td>386</td>
<td>204</td>
<td>150</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>4</td>
<td>386</td>
<td>204</td>
<td>150</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>5</td>
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<td>150</td>
<td>6</td>
<td>6</td>
</tr>
<tr>
<td>6</td>
<td>386</td>
<td>204</td>
<td>150</td>
<td>6</td>
<td>6</td>
</tr>
</tbody>
</table>

Figure B.2 Simulation results and experimental observations for heat transfer as functions of
inflow temperature.
The ASME V&V20-2009 Standard [1] quantifies the degree of accuracy of a simulation model for a specified validation variable at a specified validation point (setpoint condition) using comparison error, $E$ (Eq. 1-5-1 of the Standard), and validation uncertainty, $u_{val}$ (Eq. 1-5-10 of the Standard), as the validation metrics. Quantification of comparison error is discussed in Section B.4.1. Quantification of validation uncertainty is discussed in Section B.4.2.

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.6. Uncertainty due to numerics, $u_{num}$, is reported to be 0.07$W$ for each of the simulation results.

### Table B.6 Sensitivity coefficients for the simulation result

<table>
<thead>
<tr>
<th>Simulation Case</th>
<th>$T_i \cdot \partial q_S / \partial T_i$</th>
<th>$T_{\infty} \cdot \partial q_S / \partial T_{\infty}$</th>
<th>$Q \cdot \partial q_S / \partial Q$</th>
<th>$\rho \cdot \partial q_S / \partial \rho$</th>
<th>$C_p \cdot \partial q_S / \partial C_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>141.69</td>
<td>-43.79</td>
<td>3.96</td>
<td>3.96</td>
<td>3.97</td>
</tr>
<tr>
<td>2</td>
<td>148.76</td>
<td>-44.77</td>
<td>4.18</td>
<td>4.18</td>
<td>4.19</td>
</tr>
<tr>
<td>3</td>
<td>152.68</td>
<td>-44.46</td>
<td>4.37</td>
<td>4.37</td>
<td>4.38</td>
</tr>
<tr>
<td>4</td>
<td>162.89</td>
<td>-44.23</td>
<td>4.78</td>
<td>4.78</td>
<td>4.80</td>
</tr>
<tr>
<td>5</td>
<td>176.96</td>
<td>-44.65</td>
<td>5.33</td>
<td>5.33</td>
<td>5.34</td>
</tr>
<tr>
<td>6</td>
<td>185.80</td>
<td>-44.71</td>
<td>5.66</td>
<td>5.66</td>
<td>5.67</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Simulation Case</th>
<th>$k_t \cdot \partial q_S / \partial k_t$</th>
<th>$k_f \cdot \partial q_S / \partial k_f$</th>
<th>$h_i \cdot \partial q_S / \partial h_i$</th>
<th>$h_f \cdot \partial q_S / \partial h_f$</th>
<th>$h_o \cdot \partial q_S / \partial h_o$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.50E-02</td>
<td>1.88E-01</td>
<td>48.55</td>
<td>3.79</td>
<td>41.45</td>
</tr>
<tr>
<td>2</td>
<td>1.60E-02</td>
<td>1.99E-01</td>
<td>51.59</td>
<td>4.03</td>
<td>44.04</td>
</tr>
<tr>
<td>3</td>
<td>1.70E-02</td>
<td>2.07E-01</td>
<td>53.67</td>
<td>4.20</td>
<td>45.82</td>
</tr>
<tr>
<td>4</td>
<td>1.80E-02</td>
<td>2.27E-01</td>
<td>58.85</td>
<td>4.60</td>
<td>50.24</td>
</tr>
<tr>
<td>5</td>
<td>2.00E-02</td>
<td>2.53E-01</td>
<td>65.62</td>
<td>5.13</td>
<td>56.03</td>
</tr>
<tr>
<td>6</td>
<td>2.10E-02</td>
<td>2.70E-01</td>
<td>70.01</td>
<td>5.47</td>
<td>59.77</td>
</tr>
</tbody>
</table>

### B.4 V&V20-2009 Metric

Validation metric defined in the ASME V&V20-2009 [1] 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 the next section.
### B.4.1 Comparison Error $E$

The metric in V&V-20-2009 standard is based on comparison error, $E$, and the validation uncertainty, $u_{val}$. Comparison error, $E$, is defined in the ASME V&V20-2009 Standard [1]. Per Eq. 1-5-1 as

$$E = q_S - q_D$$  \hspace{1cm} (B.17)

The comparison error is computed with $q_S$ from Tables B.3-B.5 and $q_D$ from Table B.1. Results are reported in Section B.4.3 of this appendix.

### B.4.2 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, $u_{input+D}$, which affects both the simulation result and the comparison data, see V&V20-2009 Standard [1]:

$$u_{val}^2 = u_{num}^2 + u_{input}^2$$  \hspace{1cm} (B.18)

#### B.4.2.1 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 V&V-20-2009 [1]. The uncertainty was estimated to be 0.07 $W$ for each of the simulation results, therefore $u_{num}$ is defined in Eq. (B.19) as:

$$u_{num} = 0.07 W$$  \hspace{1cm} (B.19)

#### B.4.2.2 Simulation Input Parameter Uncertainty

The variable $u_{input}$ has random, $u_{input+D}(rnd)$, and systematic, $u_{inp} (sys)$, error sources which combine also as a root-sum-square is defined in Eq. (B.20):

$$u_{input+D}^2 = u_{input+D}(rnd)^2 + u_{input}^2 (sys)$$  \hspace{1cm} (B.20)

The propagation equation for the random uncertainty $u_{inp} (rnd)$ is obtained from Eq. (B.21) as follows:

$$u_{input}^2 (rnd) = (X_S - X_D)^T V_X(rnd) (X_S - X_D)$$  \hspace{1cm} (B.21)
The sensitivity matrices for $X_S$ and $X_D$ are defined in Eq. (B.22):

$$X_S = \begin{bmatrix}
T_i \frac{\partial q_S}{\partial T_i} & 0 & Q \frac{\partial q_S}{\partial Q} & \rho \frac{\partial q_S}{\partial \rho} & C_p \frac{\partial q_S}{\partial C_p} \\
0 & T_o \frac{\partial q_D}{\partial T_o} & Q \frac{\partial q_D}{\partial Q} & \rho \frac{\partial q_D}{\partial \rho} & C_p \frac{\partial q_D}{\partial C_p}
\end{bmatrix}$$

$X_D = \begin{bmatrix}
T_i \frac{\partial q_D}{\partial T_i} & T_o \frac{\partial q_D}{\partial T_o} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}$

Using values from Table B.6 and Table B.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.23) as follows:

$$X_S = \begin{bmatrix}
141.69 \\
0 \\
3.96 \\
3.96 \\
3.97 \\
-43.79 \\
1.50E-02 \\
1.88E-01 \\
48.55 \\
3.79 \\
41.45
\end{bmatrix}, \quad X_D = \begin{bmatrix}
1810.18 \\
-1732.32 \\
77.87 \\
77.87 \\
77.87 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{bmatrix}, \quad X_S - X_D = \begin{bmatrix}
-1668.49 \\
1732.32 \\
73.91 \\
73.91 \\
73.90 \\
-43.79 \\
1.50E-02 \\
1.88E-01 \\
48.55 \\
3.79 \\
41.45
\end{bmatrix}$$
\( V_X(rnd) \) is the covariance matrix for the random uncertainties in the input parameters (Eq. (B.24)):

\[
V_X(rnd) =
\begin{bmatrix}
\begin{array}{cccccccccc}
\frac{s^2_i}{s^2_j} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{s^2_i}{s^2_j} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{s^2_i}{s^2_j} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{s^2_i}{s^2_j} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{s^2_i}{s^2_j} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{s^2_i}{s^2_j} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{s^2_i}{s^2_j} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{s^2_i}{s^2_j} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{s^2_i}{s^2_j} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{s^2_i}{s^2_j}
\end{array}
\end{bmatrix}
\] (B.24)

Using values from Table B.2, \( V_X(rnd) \) is defined in Eq. (B.25):

\[
V_X(rnd) =
\begin{bmatrix}
4.90E-7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 4.90E-7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2.50E-5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\] (B.25)

The calculation of \( u^2_{\text{input}}(rnd) \) for Experiment 1 is
which yields Eq. (B.27):

\[ \sigma_{\text{input}+\text{D}}(\text{rnd}) = \sqrt{\sigma_{\text{input}}^2(\text{rnd})} = \sqrt{2.97 W^2} = 1.72 W \] (B.27)

Calculated values for \( \sigma_{\text{input}+\text{D}}(\text{rnd}) \) for each experiment are reported in Table B.7.

The propagation equation for the random uncertainty \( \sigma_{\text{input}}(\text{sys}) \) is defined as follows:

\[ \sigma_{\text{input}}^2(\text{sys}) = (X_S - X_D)^T V_X(\text{sys})(X_S - X_D) \] (B.28)

\( V_X(\text{sys}) \) is the covariance matrix for the systematic uncertainties in the input parameters (Eq. (B.29))

\[
V_X(\text{sys}) = \begin{bmatrix}
    b_i^2 & b_i^2 b_{\text{re}} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    b_i^2 b_{\text{re}} & b_{\text{re}}^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & b_{\theta}^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & b_{\phi}^2 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & b_{\psi}^2 & 0 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & b_{\phi e}^2 & 0 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & b_{\phi t}^2 & 0 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & b_{\phi r}^2 & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_{\phi t}^2 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_{\phi r}^2 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\] (B.29)
Using values from Table B.2, $V_X(s_{ys})$ is defined in Eq. (B.30):

$$V_X(s_{ys}) =$$

\[
\begin{bmatrix}
1.96E-06 & 1.96E-06 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1.96E-06 & 1.96E-06 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2.50E-05 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1.00E-04 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 2.50E-03 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2.50E-03 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1.00E-02 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.00E-02 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.00E-02 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.00E-02 & 0 \\
\end{bmatrix}
\]  

(B.30)

The calculation of $u_{input}^2 (s_{ys})$ for Experiment 1 yields Eq. (B.31):

$$u_{input} (s_{ys}) = \sqrt{u_{input+D}^2 (s_{ys})} = \sqrt{42.32 W^2} = 6.51 W$$  

(B.31)

Calculated values for $u_{input+D} (s_{ys})$ for each experiment are reported in Table B.7.

$u_{input}$ for Experiment 1 is the combined values of $u_{input} (r_{nd})$ (Eq. (B.27)) and $u_{input} (s_{ys})$ (Eq.(B.31)):

$$u_{input+D} = \sqrt{2.97 W^2 + 42.32 W^2} = \sqrt{45.29 W^2} = 6.73 W$$  

(B.32)

Calculated values for $u_{input}$ for each experiment are reported in Table B.7.

**B.4.2.3 Estimated intervals at each Validation Set Point**

The validation uncertainty, $u_{val}$, is calculated by combining $u_{num}$ (Eq. (B.19)) and $u_{input+D}$ (Eq. (B.32)) as a root-sum-square value, see Eq. (B.18):

$$u_{val} = \sqrt{u_{num}^2 + u_{input}^2} = \sqrt{4.90E-03 W^2 + 45.29 W^2} = \sqrt{45.29 W^2} = 6.73 W$$  

(B.33)

Calculated values for $u_{val}$ for each experiment are reported in Table B.7.

Calculated values for $E$, $u_{num}$, $u_{input} (r_{nd})$, $u_{input+ (s_{ys})}$, $u_{input}$, and $u_{val}$ are reported in Table B.7. A plot of the comparison error, $E$, with $u_{val}$ as uncertainty bars is shown in Figure B.3.
Table B.7 Comparison error and validation uncertainty estimated using the method of sensitivity coefficients

<table>
<thead>
<tr>
<th>Simulation Case</th>
<th>$q_E$</th>
<th>$q_d$</th>
<th>$E$</th>
<th>$u_{input}$</th>
<th>$u_{sys}$</th>
<th>$u_{total}$</th>
<th>$u_{val}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>W</td>
<td>W</td>
<td>W</td>
<td>W</td>
<td>W</td>
<td>W</td>
<td>W</td>
</tr>
<tr>
<td>1</td>
<td>98.61</td>
<td>77.87</td>
<td>20.74</td>
<td>21.03%</td>
<td>0.07</td>
<td>1.72</td>
<td>6.51</td>
</tr>
<tr>
<td>2</td>
<td>104.00</td>
<td>99.67</td>
<td>4.33</td>
<td>4.16%</td>
<td>0.07</td>
<td>1.82</td>
<td>6.96</td>
</tr>
<tr>
<td>3</td>
<td>108.22</td>
<td>107.08</td>
<td>1.14</td>
<td>1.05%</td>
<td>0.07</td>
<td>1.87</td>
<td>7.25</td>
</tr>
<tr>
<td>4</td>
<td>118.66</td>
<td>125.09</td>
<td>-6.43</td>
<td>-5.42%</td>
<td>0.07</td>
<td>2.00</td>
<td>7.97</td>
</tr>
<tr>
<td>5</td>
<td>132.31</td>
<td>142.05</td>
<td>-9.74</td>
<td>-7.36%</td>
<td>0.07</td>
<td>2.19</td>
<td>8.89</td>
</tr>
<tr>
<td>6</td>
<td>141.12</td>
<td>157.24</td>
<td>-16.12</td>
<td>-11.42%</td>
<td>0.07</td>
<td>2.32</td>
<td>9.51</td>
</tr>
</tbody>
</table>

Figure B.3 Comparison error as a function of inflow temperature with bars showing the range of $u_{val}$.

B.5 Multivariate Metric

B.5.1 Multivariate Metric Calculated with Sensitivity Analysis

The multivariate metric, $E_{mv}$, is defined in Eq. (B.34) of this supplement. It is the magnitude of the comparison error vector, $E$, over multiple validation set points accounting for correlations between the setpoints.

$$E_{mv}^2 = E^T V_{val}^{-1} E,$$  \hspace{1cm} (B.34)

where
\[ E = [S_1 - D_1 \vdots S_n - D_n] = [E_1 \vdots E_n] \]  \hspace{1cm} (B.35)

and

\[ E_{mv} = \sqrt{E_{mv}^2}. \]  \hspace{1cm} (B.36)

\( E \) 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. Section 4.2.1 provides methods to calculate \( E_{ref} \). The ratio \( \frac{E_{mv}}{E_{ref}} \) removes the dependence on the number of validation set points so is used in this section as a metric for comparison of results and interpretation.

B.5.1.1 Contributions to Validation Covariance Matrix

The validation covariance matrix \( V_{val} \) is a generalization of \( u_{val}^2 \) to multivariate applications. Appendix A explains that the approach to compute \( V_{val} \) depends on whether the validation variable

- is directly measured (Case 1 of V&V20-2209 [1]),
- is a result defined by a data reduction equation where the measured variables share no error sources (Case 2 of V&V20-2209 [1]),
- is a result defined by a data reduction equation where the measured variables share identical error sources (Case 3 of V&V20-2209 [1]), or
- comes from measured variables analyzed with a model (Case 4 of V&V20-2209 [1]).

and depends on whether

A. there are no common errors between the validation set points or
B. there are shared identical errors between the validation set points.

This logic flow is depicted graphically in Figure A.1 of Appendix A.

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, \( V_{input} \). Therefore, for the fin-tube heat exchanger example, \( V_{val} \) is defined in Eq. (B.37):
\[ V_{Val} = V_{num} + V_{input+D} \]  \hspace{1cm} \text{(B.37)}

Two approaches are demonstrated for the calculation of the uncertainty due to input parameters, \( V_{input+D} \). One approach uses sensitivity coefficients which is valid for systems with locally linear behavior in the validation space. The other approach uses sampling which captures non-linear 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.5.1.1.1 Numerical Uncertainty, \( V_{num} \)**

Two possibilities for calculation of \( V_{num} \) are discussed in Section A.1.1 of appendix A. For the fin-tube heat exchanger example, uncertainty due to numerics, \( u_{num} \), is reported to be 0.07 W for each of the simulation results and independence is assumed. Therefore, the diagonal form is used in Eq. (B.38) for calculating \( V_{num} \):

\[
V_{num} = \begin{bmatrix}
0.07^2 & 0 & \cdots & 0 \\
0 & 0.07^2 & \cdots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & 0.07^2 & 0
\end{bmatrix} = \begin{bmatrix}
4.90E-03 & 0 & \cdots & 0 \\
0 & 4.90E-03 & \ddots & \vdots \\
\vdots & \ddots & \ddots & 4.90E-03 \\
0 & \cdots & 0 & 4.90E-03
\end{bmatrix} \hspace{1cm} \text{(B.38)}
\]

**B.5.1.1.2 Input Parameter Uncertainty, \( V_{input+D} \)**

Random and systematic input parameter uncertainties are reported in Table B.2. Because random uncertainties are independent, the covariance array for random uncertainties, \( V_{X(rnd)} \), is diagonal. Systematic uncertainties may share common error sources, therefore, may be dependent. The covariance array for systematic uncertainties, \( V_{X(sys)} \), will have non-zero off diagonal terms for contributions which share error sources. Because of the potential differences in array structures, random and systematic uncertainties are addressed separately in Eq. (B.39):

\[
V_{input+D} = V_{input+D(rnd)} + V_{input+D(sys)} \hspace{1cm} \text{(B.39)}
\]

**Random Uncertainties**

The method to calculate contributions to \( V_{Val} \) from random error sources is found by following the flow logic in Figure A.1 of appendix A as follows:
(a) Choose from [Case 1, Case 2, Case 3, Case 4].
(b) Because heat flux is not directly measured,
   (1) Case 1 does not apply: [Case 1, Case 2, Case 3, Case 4],
   (c) Because heat flux is a result defined by a data reduction equation. Case 4 does not apply: [Case 1, Case 2, Case 3, Case 4].
   (d) Because random uncertainties are independent, Cases 3 does not apply: [Case 1, Case 2, Case 3, Case 4].
   (e) Therefore, Case 2 applies.
(f) Choose from [Case 2A, Case 2B].
(g) Because random error sources are independent, Case 2B does not apply: [Case 2A, Case 2B].
(h) Therefore, follow Case 2A.

**Case 2A:**

$V_{\text{input}+D}(\text{rnd})$ is calculated as follows:

$$V_{\text{input}+D}(\text{rnd}) =
\begin{bmatrix}
(X_{S,1} - X_{D,1})^T V_{X,1}(\text{rnd})(X_{S,1} - X_{D,1}) & 0 & 0 \\
0 & \ddots & 0 \\
0 & 0 & (X_{S,n} - X_{D,n})^T V_{X,n}(\text{rnd})(X_{S,n} - X_{D,n})
\end{bmatrix} \quad (B.40)$$

The sensitivity matrices $X_{S,i}$ and $X_{D,i}$ are defined in Eq. (B.41):
\[ X_{s,i} = \begin{bmatrix} T_i \frac{\partial q_{s,i}}{\partial T_i} \\ 0 \\ Q \frac{\partial q_{s,i}}{\partial Q} \\ \rho \frac{\partial q_{s,i}}{\partial \rho} \\ C_p \frac{\partial q_{s,i}}{\partial C_p} \\ k_t \frac{\partial q_{s,i}}{\partial k_t} \\ k_f \frac{\partial q_{s,i}}{\partial k_f} \\ h_t \frac{\partial q_{s,i}}{\partial h_t} \\ h_f \frac{\partial q_{s,i}}{\partial h_f} \\ h_o \frac{\partial q_{s,i}}{\partial h_o} \end{bmatrix} \quad \text{and} \quad X_{D,i} = \begin{bmatrix} T_i \frac{\partial q_{D,i}}{\partial T_i} \\ T_0 \frac{\partial q_{D,i}}{\partial T_0} \\ Q \frac{\partial q_{D,i}}{\partial Q} \\ \rho \frac{\partial q_{D,i}}{\partial \rho} \\ C_p \frac{\partial q_{D,i}}{\partial C_p} \\ k_t \frac{\partial q_{D,i}}{\partial k_t} \\ k_f \frac{\partial q_{D,i}}{\partial k_f} \\ h_t \frac{\partial q_{D,i}}{\partial h_t} \\ h_f \frac{\partial q_{D,i}}{\partial h_f} \\ h_o \frac{\partial q_{D,i}}{\partial h_o} \end{bmatrix} \] (B.41)

where \( q_{s,i} \) and \( q_{D,i} \) are \( q_s \) and \( q_D \) for the \( i^{th} \) Experiment. The covariance matrices, \( V_{x,i}(\text{rnd}) \), for this example are identical, \( V_{x,1}(\text{rnd}) = V_{x,2}(\text{rnd}) = \cdots = V_{x,n}(\text{rnd}) = V_x(\text{rnd}) \). \( V_x(\text{rnd}) \) is given by Eq. (B.24).

**Example: Setpoint Experiments 3 and 5**

The matrix to be calculated is in Eq. (B.42):

\[
V_{\text{input+D}}(\text{rnd}) = \\
\begin{bmatrix}
(X_{S,3} - X_{D,3})^T V_{x,3}(\text{rnd})(X_{S,3} - X_{D,3}) & 0 \\
0 & (X_{S,5} - X_{D,5})^T V_{x,5}(\text{rnd})(X_{S,5} - X_{D,5})
\end{bmatrix}
\] (B.42)
Using values from Table B.6 and Table B.3, the sensitivity vectors $X_{S,3}$ and $X_{D,3}$ and the difference vector $X_{S,3} - X_{D,3}$ for Experiment 3 are defined in the following set of equations (Eq. (B.43)):

$$
X_{S,3} = \begin{bmatrix} 152.68 \\ 0 \\ 4.37 \\ 4.38 \\ 4.37 \\ -44.46 \\ 1.70E-02 \\ 2.07E-01 \\ 53.67 \\ 4.20 \\ 45.82 \end{bmatrix} \quad W, \quad X_{D,3} = \begin{bmatrix} 1943.85 \\ -1836.78 \\ 107.08 \\ 107.08 \\ 107.08 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad W, \quad X_{S,3} - X_{D,3} = \begin{bmatrix} -1791.17 \\ 1836.78 \\ -102.71 \\ -102.70 \\ -102.71 \\ -44.46 \\ 1.70E-02 \\ 2.07E-01 \\ 53.67 \\ 4.20 \\ 45.82 \end{bmatrix} \quad W \quad (B.43)
$$

$V_{X}(rnd)$ is given in Eq. (B.25). The value of $V_{input+D}(rnd)[1,1]$ is

$$
(X_{S,3} - X_{D,3})^T V_{X,3}(rnd)(X_{S,3} - X_{D,3}) = 3.49 \quad W^2 \quad (B.44)
$$

Calculations for Setpoint Experiment 5 are similar. The final matrix $V_{input+D}(rnd)$ is

$$
V_{input+D}(rnd) = \begin{bmatrix} 3.49 \\ 0 \\ 0 \\ 4.78 \end{bmatrix} \quad W^2 \quad (B.45)
$$

Systematic Uncertainties

The method to calculate contributions to $V_{input+D}$ from systematic error sources is found from the flow logic in Figure A.1 of Appendix A as follows:

1. Choose from [Case 1, Case 2, Case 3, Case 4].
2. Because heat flux is not directly measured,
   a. Case 1 does not apply: [Case 1, Case 2, Case 3, Case 4].
3. Because heat flux is a result defined by a data reduction equation,
   a. Case 4 does not apply: [Case 1, Case 2, Case 3, Case 4].
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),
   a. Cases 2 does not apply: [Case 1, Case 2, Case 3, Case 4].
5. Therefore, Case 3 applies.
6. Choose from [Case 3A, 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),
   a. Case 3A does not apply: [Case 3A, Case 3B].
8. Therefore, follow Case 3B.

**Case 3B**

$V_{input+D(sys)}$ is calculated in Eq. (B.46):

$$V_{input+D} = (X_S - X_D)^T V_X (X_S - X_D) \quad \text{(B.46)}$$

The sensitivity matrices $X_S$ and $X_D$ are defined in Eq. (B.47):

$$X_S = \begin{bmatrix} T_i \frac{\partial q_s}{\partial T_i} \\ 0 \\ Q \frac{\partial q_s}{\partial Q} \\ \rho \frac{\partial q_s}{\partial \rho} \\ C_p \frac{\partial q_s}{\partial C_p} \\ T_\infty \frac{\partial q_s}{\partial T_\infty} \end{bmatrix} \quad \text{and} \quad X_D = \begin{bmatrix} T_i \frac{\partial q_d}{\partial T_i} \\ T_\infty \frac{\partial q_d}{\partial T_\infty} \\ Q \frac{\partial q_d}{\partial Q} \\ \rho \frac{\partial q_d}{\partial \rho} \\ C_p \frac{\partial q_d}{\partial C_p} \end{bmatrix} \quad \text{(B.47)}$$

where $q_s$ and $q_d$ are vectors of the setpoint experiments being evaluated. The covariance matrix, $V_s(sys)$, is provided in Eq. (B.29).
Example: Setpoint Experiments 3 and 5

Using values from Table 6 and Table 3, the sensitivity vectors for $X_S$ and $X_D$ and the difference vector $X_S - X_D$ for Setpoint Experiments 3 and 5 are defined in Eq. (B.48):

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

$$X_S - X_D = \begin{bmatrix} -1791.17 & -2079.65 \\ 1836.78 & 2114.56 \\ -102.71 & -136.72 \\ -102.70 & -136.71 \\ -102.71 & -136.72 \\ -44.46 & -44.65 \\ 1.70E-02 & 2.00E-02 \\ 2.07E-01 & 2.53E-01 \\ 53.67 & 65.62 \\ 4.20 & 5.13 \\ 45.82 & 56.03 \end{bmatrix} \quad W \quad (B.48)$$

$V_X(sys)$ is given in Eq. (B.30). The matrix $V_{input+D}(sys)$ is obtained in Eq. (B.49):

$$V_{input+D}(sys) = (X_S - X_D)^T V_X(X_S - X_D) = \begin{bmatrix} 52.55 & 64.47 \\ 64.47 & 79.12 \end{bmatrix} W^2 \quad (B.49)$$
B.5.1.2 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, $V_{input+D}$, see Eq. (B.37).

For Setpoint Experiments 3 and 5, the $V_{val}$ matrix calculated in Eq. (B.50) using the method of sensitivity coefficients is the sum of Eqs. (B.38), (B.45) and (B.49):

$$V_{val} = V_{num} + V_{input+D} = V_{num} + V_{input+D}(rnd) + V_{input+D}(sys)$$

$$= \begin{bmatrix} 4.90E-03 & 0 \\ 0 & 4.90E-03 \end{bmatrix} W^2 + \begin{bmatrix} 3.49 & 0 \\ 0 & 4.78 \end{bmatrix} W^2 + \begin{bmatrix} 52.55 & 64.47 \\ 64.47 & 79.12 \end{bmatrix} W^2 = \begin{bmatrix} 56.04 & 64.47 \\ 64.47 & 83.90 \end{bmatrix} W^2 \tag{B.50}$$

The inverse of $V_{val}$ is defined in Eq. (B.51):

$$V_{val}^{-1} = \begin{bmatrix} 1.54E-01 & -1.18E-01 \\ -1.18E-01 & 1.03E-01 \end{bmatrix} W^{-2} \tag{B.51}$$

The corresponding $V_{val}$ matrix calculated in Eq. (B.52) using the sampling method is:

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

$$= \begin{bmatrix} 63.41 & 75.53 \\ 75.53 & 101.36 \end{bmatrix} W^2 \tag{B.52}$$

The inverse of $V_{val}$ from sampling is defined be Eq. (B.53):

$$V_{val}^{-1} = \begin{bmatrix} 1.40E-01 & -1.05E-01 \\ -1.05E-01 & 8.78E-02 \end{bmatrix} W^{-2} \tag{B.53}$$

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. min verse using MS Excel, Office 365 ProPlus) are retained.

B.5.1.3 Multivariate Metric Results

In this section, 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 setpoints is explored. A later section shows the results using sampling.

Comparison error $E$ for the validation set points is reported in Table B.7. For Set Points 3 and 5, as examples, the vector $E$ is defined in Eq. (B.54):

$$E = \begin{bmatrix} S_3 - D_3 \\ S_5 - D_5 \end{bmatrix} = \begin{bmatrix} 108.22 - 106.96 \\ 132.31 - 141.85 \end{bmatrix} W = \begin{bmatrix} 1.14 \\ -9.74 \end{bmatrix} W \tag{B.54}$$
B.5.1.3.1 Accounting for Correlation in the Comparison Errors

The matrix $V_{val}$ for setpoints 3 and 5 which is provided in Eq. (B.50) is used here to obtain Eq. (B.55):

$$V_{val} = \begin{bmatrix} 56.04 & 64.47 \\ 64.47 & 83.90 \end{bmatrix} W^2 \quad (B.55)$$

The inverse matrix $V_{val}^{-1}$ which is provided in Eq. (B.51) gives us Eq. (B.56)

$$V_{val}^{-1} = \begin{bmatrix} 1.54E-01 & -1.18E-01 \\ -1.18E-01 & 1.03E-01 \end{bmatrix} W^{-2} \quad (B.56)$$

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

$$E_{mv}^2 = E^T V_{val}^{-1} E = \begin{bmatrix} 1.14 & -9.74 \end{bmatrix} \cdot \begin{bmatrix} 1.54E-01 & -1.18E-01 \\ -1.18E-01 & 1.03E-01 \end{bmatrix} \cdot \begin{bmatrix} 1.14 \\ -9.74 \end{bmatrix} = 12.57 \quad (B.57)$$

The value $E_{mv}$ is obtained by taking the square root of $E_{mv}^2$ in Eq. (B.58)

$$E_{mv} = \sqrt{E_{mv}^2} = \sqrt{12.57} = 3.55 \quad (B.58)$$

As discussed in Section 2.2.1, 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. 13 of Section 4.2.1:

$$E_{ref}^2 = df + \sqrt{2df} = 2 + \sqrt{2 \cdot 2} = 2 + 2 = 4 \quad (B.59)$$

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

$$E_{ref} = \sqrt{E_{ref}^2} = \sqrt{4} = 2 \quad (B.60)$$

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 $E_{mv}^2$:

$$\frac{E_{mv}}{E_{ref}} = \frac{3.55}{2} = 1.78 \quad (B.61)$$

The observation that $E_{mv}/E_{ref} > 1$ is an indication that the model results show a significant systematic error relative to the experiment due ostensibly 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.5.1.3.2 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. Were one to treat the validation set points as independent, the calculation of \( E_{\text{mv}} \) becomes

- Use the validation matrix from Eq. (B.55) setting the off-diagonal entries to zero (Eq. (B.62)):
  \[
  V_{\text{val}} = \begin{bmatrix} 56.04 & 0 \\ 0 & 83.90 \end{bmatrix} W^2
  \]  
  \[\text{(B.62)}\]

- Calculate the inverse matrix \( V_{\text{val}}^{-1} \) as defined in Eq. (B.63):
  \[
  V_{\text{val}}^{-1} = \begin{bmatrix} 1.78E-02 & 0 \\ 0 & 1.19E-02 \end{bmatrix} W^{-2}
  \]  
  \[\text{(B.63)}\]

- Calculate \( E_{\text{mv}}^2 \) via matrix multiplication (Eq. (B.64)):
  \[
  E_{\text{mv}}^2 = E^T V_{\text{val}}^{-1} E = \begin{bmatrix} 1.14 & -9.74 \end{bmatrix} \begin{bmatrix} 1.78E-02 & 0 \\ 0 & 1.19E-02 \end{bmatrix} \begin{bmatrix} 1.14 \\ -9.74 \end{bmatrix} = 1.15
  \]  
  \[\text{(B.64)}\]

- Calculate \( E_{\text{mv}} \) from the square root of \( E_{\text{mv}}^2 \):
  \[
  E_{\text{mv}} = \sqrt{E_{\text{mv}}^2} = \sqrt{1.15} = 1.07
  \]  
  \[\text{(B.65)}\]

- Compare to \( E_{\text{ref}} \)
  \[
  \frac{E_{\text{mv}}}{E_{\text{ref}}} = \frac{1.07}{2} = 0.54
  \]  
  \[\text{(B.66)}\]

The interpretation of \( E_{\text{mv}}/E_{\text{ref}} < 1 \) would be 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.5.2 Multivariate Metric Calculated with Sampling

The multivariate metric does not change when sampling is used. The same expression given in Eq. (B.35) 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., $V_{input+D}$, will use sampling instead of a sensitivity approach.

**B.5.2.1 Input Parameter Uncertainty, $V_{input+D}$**

The sampling to estimate $V_{input+D}$, twenty data points for $q_{Si}$ and $q_{Di}$ were constructed for each of set point conditions using the Latin hypercube sampling approach described in the ASME V&V20-2009 Standard. The subscript “$i$” denotes the sample index. These data are provided in Table B.8.

The choice of 20 sample points is based on providing a relatively small dataset 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.

$V_{input+D}$ is the covariance of the variabilities of the sample comparison errors, $E_i$, for Setpoint Experiment $i$ about their 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. 67:

$$V_{input+D} = \frac{1}{n_r - 1} E'^T E' \quad \text{(B.67)}$$

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

**Example: Set point Experiments 3 and 5**

Using the data from Table B.8, $E_3$, $\overline{E_3}$, and $E_3'$, for Setpoint Experiment 3 are defined in Eq. (B.68):
Similarly, $E_5$, $E_5'$, and $E_5''$, for Setpoint Experiment 5 are defined in Eq. (B.69):

$$
E_5 = \begin{bmatrix}
-13.11 \\
-8.26 \\
-5.80 \\
0.68 \\
10.44 \\
-10.55 \\
0.47 \\
-14.64 \\
-3.01 \\
-19.26 \\
-6.80 \\
-16.33 \\
6.56 \\
-5.61 \\
-11.54 \\
-30.74 \\
-15.33 \\
-15.79 \\
-3.52 \\
-25.02
\end{bmatrix} W, \quad \bar{E}_5 = -9.36 W \rightarrow E_5' = \begin{bmatrix}
-3.75 \\
1.10 \\
3.56 \\
10.04 \\
19.80 \\
-1.19 \\
9.83 \\
-5.28 \\
6.35 \\
-9.90 \\
2.56 \\
-6.97 \\
15.92 \\
3.75 \\
-2.18 \\
-21.38 \\
-5.97 \\
-6.43 \\
5.84 \\
-15.66
\end{bmatrix} W \quad (B.69)
$$
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Table B.8 Latin Hypercube Sampling Data
The corresponding matrix $E'$ is defined in Eq. (B.70):

$$
E' = \begin{bmatrix}
-3.01 & -3.75 \\
-1.21 & 1.10 \\
-1.88 & 3.56 \\
11.83 & 10.04 \\
14.89 & 19.80 \\
-0.11 & -1.19 \\
6.69 & 9.83 \\
-2.71 & -5.28 \\
4.25 & 6.35 \\
-6.13 & -9.90 \\
1.77 & 2.56 \\
-7.11 & -6.97 \\
17.75 & 15.92 \\
-1.17 & 3.75 \\
-5.26 & -2.18 \\
-12.77 & -21.38 \\
-5.20 & -5.97 \\
-2.29 & -6.43 \\
2.61 & 5.84 \\
-11.02 & -15.66
\end{bmatrix} W \tag{B.70}
$$

Evaluation of Eq. 67, using $E'$ from Eq. (B.70) yields Eq. (B.71):

$$
V_{input+D} = \frac{1}{n_r - 1} E'^T E' = \begin{bmatrix} 63.41 & 75.53 \\
75.53 & 101.36 \end{bmatrix} W^2 \tag{B.71}
$$

B.5.2.2 Multivariate Metric Results

The vector $E$ is derived from the average of $E_i = q_{si} - q_{di}$ over the twenty samples for each of the validation setpoints: $\langle E \rangle = \langle E \rangle_i = \langle q_{si} - q_{di} \rangle = \langle q_{si} \rangle - \langle q_{di} \rangle$, see Appendix A, Eq. (A.31). Using set points 3 and 5 for demonstration and the mean data from Table B.8, the vector $E$ is defined in Eq. (B.72):

$$
\langle E \rangle = \begin{bmatrix} \langle q_{s3} \rangle - \langle q_{d3} \rangle \\
\langle q_{s5} \rangle - \langle q_{d5} \rangle \end{bmatrix} = \begin{bmatrix} 108.32 - 106.88 \\
132.43 - 141.79 \end{bmatrix} W = \begin{bmatrix} 1.44 \\
-9.36 \end{bmatrix} W \tag{B.72}
$$

B.5.2.2.1 Accounting for Correlation of the Comparison Errors

The matrix $V_{Val}$ for setpoints 3 and 5 from sampling is provided in Eq. (B.52):
\[ V_{val} = \begin{bmatrix} 63.41 & 75.53 \\ 75.53 & 101.36 \end{bmatrix} W^2 \] (B.73)

The inverse matrix \( V_{val}^{-1} \) is provided in Eq. (B.53):

\[ V_{val}^{-1} = \begin{bmatrix} 1.40E-01 & -1.05E-01 \\ -1.05E-01 & 8.78E-02 \end{bmatrix} W^{-2} \] (B.74)

\( E_{mv}^2 \) is calculated via matrix multiplication

\[
E_{mv}^2 = (E)^T V_{val}^{-1} E = [1.44 -9.36] \cdot \begin{bmatrix} 1.40E-01 & -1.05E-01 \\ -1.05E-01 & 8.75E-02 \end{bmatrix} \cdot [-9.36] = 10.80 \] (B.75)

The value \( E_{mv} \) is obtained by taking the square root of \( E_{mv}^2 \):

\[ E_{mv} = \sqrt{E_{mv}^2} = \sqrt{10.80} = 3.29 \] (B.76)

The process to calculate the reference value, \( E_{ref} \), for the sampling approach is described in section 2.2.1.2.2, Eq. 15. Begin by defining the matrix \( E_{perfect} \) whose columns are the deviation vectors, \( E_i' \), defined in Section 5.5.2.1 of Appendix B. \( E_{perfect} \) for setpoints 3 and 5 is provided in Eq. (B.70).

Calculate \( E_{mv,i}^2 \) for each row \( i \) of \( E_{perfect} \) separately. For row \( i = 1 \), as an example, \( E_{perfect,1} \) is

\[ E_{perfect,1} = [-3.01 \ -3.75] \]

\( E_{mv,1}^2 \) is calculated in Eq. (B.77):

\[
E_{mv,1}^2 = E_{perfect,1} V_{val}^{-1} E_{perfect,1}^T = [-3.01 \ -3.75] \cdot \begin{bmatrix} 1.40E-01 & -1.05E-01 \\ -1.05E-01 & 8.78E-02 \end{bmatrix} \cdot [-3.01 \ -3.75] = 0.15 \] (B.77)

Performing similar operations for each row yields the column vector \( E_{mv}^2 \) as follows:
The expected value \( \langle E^2_{mv} \rangle \) is the mean value of the sample population \( E^2_{mv,i} \) (Eq. (B.79)):

\[
\langle E^2_{mv} \rangle = \frac{1}{20} \sum_{i=1}^{20} E^2_{mv,i} = 1.90
\]  

(B.79)

The variance, \( \text{var}(E^2_{mv}) \), of the sample population for \( E^2_{mv} \) is defined in Eq. (B.80):

\[
\text{var}(E^2_{mv}) = \frac{1}{19} \sum_{i=1}^{20} (E^2_{mv,i} - \langle E^2_{mv} \rangle)^2 = 4.00
\]  

(B.80)

The standard uncertainty \( u_{E^2_{mv}} \) of the sample population for \( E^2_{mv} \) is the square root of the variance \( \text{var}(E^2_{mv}) \):

\[
u_{E^2_{mv}} = \sqrt{\text{var}(E^2_{mv})} = \sqrt{4.00} = 2.00
\]  

(B.81)

The value of \( E^2_{ref} \) is defined in Eq. (B.82):

\[
E^2_{ref} = \langle E^2_{mv} \rangle + u_{E^2_{mv}} = 1.90 + 2.00 = 3.90
\]  

(B.82)

The value of \( E_{ref} \) is obtained by taking the square root of \( E^2_{ref} \):

\[
E_{ref} = \sqrt{E^2_{ref}} = \sqrt{3.90} = 1.97
\]  

(B.83)
The ratio $E_{mv}/E_{ref}$ is defined in Eq. (B.84):

$$\frac{E_{mv}}{E_{ref}} = \frac{3.29}{1.97} = 1.67 \quad (B.84)$$

This value is close to the value of $E_{mv}/E_{ref} = 1.77$, see Eq. (B.61), calculated using the Method of Sensitivity Coefficients. Sampling also confirms that there is a significant systematic error relative to the experiment due ostensibly to missing model physics.

**B.5.2.2.2 Neglecting Correlation of the Comparison Errors**

The calculation of $E_{mv}$ by sampling neglecting common errors is

- Use the validation matrix from Eq. (B.73) setting the off-diagonal entries to zero:
  $$V_{val} = \begin{bmatrix} 63.41 & 0 \\ 0 & 101.36 \end{bmatrix} W^2 \quad (B.85)$$

- Calculate the inverse matrix $V_{val}^{-1}$
  $$V_{val}^{-1} = \begin{bmatrix} 1.58E-02 & 0 \\ 0 & 9.87E-03 \end{bmatrix} W^{-2} \quad (B.86)$$

- Calculate $E_{mv}^2$ via matrix multiplication
  $$E_{mv}^2 = \langle E \rangle V_{val}^{-1} \langle E \rangle = \begin{bmatrix} 1.44 & -9.36 \end{bmatrix} \begin{bmatrix} 1.58E-02 & 0 \\ 0 & 9.87E-03 \end{bmatrix} \begin{bmatrix} 1.44 \\ -9.36 \end{bmatrix} = 0.90 \quad (B.87)$$

- Calculate $E_{mv}$ from the square root of $E_{mv}^2$:
  $$E_{mv} = \sqrt{E_{mv}^2} = \sqrt{0.90} = 0.95 \quad (B.88)$$

- Compare to $E_{ref}$
  $$E_{ref} = 2.11 \quad (B.89)$$

- Calculate $E_{ref}$ using $V_{val}^{-1}$ from Eq. (B.86):
  $$\frac{E_{mv}}{E_{ref}} = \frac{0.95}{2.11} = 0.45 \quad (B.90)$$

This value is close to the value of $E_{mv}/E_{ref} = 0.54$, see Eq. (B.66), calculated using the Method of Sensitivity Coefficients. Neglecting common errors would lead to the incorrect interpretation that the model does not show significant systematic errors relative to the experiment.
B.5.3 Overall Summary

The multivariate metric $E_{mv}$, the reference value, $E_{ref}$, and ratio $E_{mv}/E_{ref}$ are calculated for 5 combinations of the setpoint data using the Method of Sensitivity Coefficients and using Sampling, accounting for common errors between the setpoints. Two sample sets were generated. One set, with 20 samples, is reported in Table 8. The other set, not shown, has 320 samples. The choice of 320 samples for this demonstration is not an outcome of a rigorous uncertainty quantification. It is meant only to show how the results might change/converge with a large difference in sample size. No further conclusions about sample size and converge of the sample results should be drawn. The results are reported in Table B.9.

Table B.9 Summary of Multivariate Metric Estimates

<table>
<thead>
<tr>
<th>Included Setpoints</th>
<th>Sensitivity</th>
<th>Sampling</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$E_{mv}$/$E_{ref}$</td>
<td>$E_{mv}$/$E_{ref}$</td>
</tr>
<tr>
<td>2-Point (3,5)</td>
<td>2.00</td>
<td>1.97</td>
</tr>
<tr>
<td>3-Point (1,3,5)</td>
<td>2.33</td>
<td>2.33</td>
</tr>
<tr>
<td>3-Point (2,3,5)</td>
<td>2.33</td>
<td>2.20</td>
</tr>
<tr>
<td>4-Point (1,2,4,6)</td>
<td>2.61</td>
<td>2.51</td>
</tr>
<tr>
<td>6-Point All</td>
<td>3.08</td>
<td>2.99</td>
</tr>
</tbody>
</table>

Results from the sensitivity approach and the sampling approach are similar. One might think that the two approaches should always converge, however, non-linear differences are only captured by the sampling technique. In general, the results will not be the same. The good agreement between the results computed using sensitivity coefficients and the results computed using sampling is an outcome of a nearly linear response of the systematic difference between the simulation result and the experiment for the example problem.

A value for $E_{mv}/E_{ref}$ significantly greater than 1 is evidence that the differences observed between the simulation model results and experimental data are not consistent with uncertainty included in the metric ($V_{val}$). Table B.9 shows that $E_{mv}/E_{ref}$ is greater than 1 for all combinations of set point data but is significantly greater than 1 for combinations (1, 3, & 5), (1, 2, 4, & 6), and (1, 2, 3, 4, 5, & 6). The conclusion is that the simulation model results are inconsistent with the experimental data providing evidence of missing physics. However, for a limited range of data (the combination of set points 3 & 5, for example), the inconsistency may not be strongly evident. This quantification might support a decision to qualify the model for use for an intended purpose within a limited parameter range. It may also support an assessment of bounds on the range of accuracy of the model within a range of application.
Ratios of the results from the Sensitivity assessment to the Sampling assessment are shown in Table B.10. These ratios (sensitivity result/sampling result) are meant only to convey convergence of sampling approaches with increasing sample size.

The data show that, for the combinations of setpoints considered, a maximum difference of 6% is observed between $E_{ref}$ from sampling using the 20 samples dataset and the theoretical value for $E_{ref}$, assuming individual estimates for $\delta_{model}$ can be represented by normal distributions, see discussion in Section 2. This difference reduces to 1% when the sample size is increased to 320 samples. Similarly, the maximum difference between $E_{mv}/E_{ref}$ from sampling to the sensitivity assessment result reduces from 25% for the 20 samples dataset to 6% for the 320 samples dataset.

Table B.10 Summary of Multivariate Metric Estimates

<table>
<thead>
<tr>
<th>Included Setpoints</th>
<th>20 Samples</th>
<th>320 Samples</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-Point (3,5)</td>
<td>1.02</td>
<td>1.01</td>
</tr>
<tr>
<td>3-Point (1,3,5)</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>3-Point (2,3,5)</td>
<td>1.06</td>
<td>1.00</td>
</tr>
<tr>
<td>4-Point (1,2,4,6)</td>
<td>1.04</td>
<td>1.01</td>
</tr>
<tr>
<td>6-Point All</td>
<td>1.03</td>
<td>1.01</td>
</tr>
</tbody>
</table>

B.6 References

APPENDIX C
Examples of Evaluation of the Validation Covariance Matrix, \( V_{val} \)

The application of the multivariate metric presented in this document requires the calculation of the comparison errors \( E_i \) at \( n \) validation set points (Eq. A.1) and the evaluation of the validation covariance matrix \( V_{val} \). As for the point wise evaluation of the scalar validation uncertainty \( u_{val} \) described in ASME-V&V20-2009 [1], the selection of the appropriate expressions to determine \( V_{val} \) depends on the process used to measure the \( n \) validation variables included in the multivariate metric, which can exhibit four different options (see Figure A.1). However, the evaluation of the validation covariance matrix also depends on the possible sharing of experimental, numerical and input parameters uncertainties at the \( n \) set points. Therefore, Appendix A has presented different expressions for the calculation of \( V_{val} \) using sensitivity coefficients or sampling techniques. The purpose of this appendix, Appendix C, is to illustrate the use of Appendix A for the evaluation of \( V_{val} \) for three simple examples. The example included in Appendix B illustrates the use of sensitivity coefficients and sampling techniques. Therefore, in appendix C, we will restrict these examples to the sensitivity coefficients technique.

The three examples presented in this appendix show that the procedure for calculating the multivariate metric is strongly dependent on the techniques and assumptions used to obtain the experimental and simulation data. Each example contains three sections: the definition of the problem; the selection of the quantities of interest, and the discussion of options in the procedure for determination of the validation covariance matrix \( V_{val} \).

C.1 Pressure distribution on an airfoil

In engineering applications using lifting surfaces, one of the most important flow features is the pressure distribution on the surface of airfoils and/or wings. Therefore, from the simulations point of view, it involves the estimation of modeling errors at multiple set points.

C.1.1 Problem definition

For the first example, we consider the flow around an Eppler 387 airfoil at an angle of attack of \( \alpha = 1^\circ \) and Reynolds number of \( e = 3 \times 10^5 \). This problem was also the test case for the 2\textsuperscript{nd} Workshop for the Assessment of a Multivariate Metric for Validation at multiple set points [2].
For this flow problem, measurements were performed in a wind-tunnel, and the two-dimensional experimental data is reported in [3]. Simulations were performed by numerically solving the Reynolds-averaged Navier-Stokes (RANS) equations using eddy-viscosity and local correlation transition models in the domain illustrated in Figure 1, with the boundary conditions shown in this figure. The fluid is assumed to be incompressible, and mean flow quantities are defined with time-averaging and so the simulated flow is statistically steady and two-dimensional. Any differences between the computational domain size and the wind tunnel dimensions are neglected, and fluid properties and imposed inflow boundary conditions are assumed to have exact values. Therefore, any errors introduced by these assumptions are incorporated in the modeling error. The only uncertain parameter considered in this example, is the angle of attack that is assumed to be measured with an accuracy of ±0.2° (the measuring accuracy is not reported in [3]). Details of the simulations are reported in [2,4].

\[ V_y = 0, \frac{\partial \phi}{\partial y} = 0 \]

\[ p = 0 \]

\[ \frac{\partial \phi}{\partial x} = 0 \]

\[ V_x = V_\infty \]

\[ V_y = 0 \]

\[ \frac{\partial \phi}{\partial y} = 0 \]

Figure C.1: Domain and boundary conditions for the simulation of the flow around the Eppler 387 airfoil at an angle of attack of \( \alpha = 1^\circ \) and Reynolds number of \( Re = 3 \times 10^5 \). \( \phi \) designates the dependent variables that are not explicitly given.

C.1.2 Quantity of interest

The selected quantity of interest is the time-averaged pressure coefficient defined by
where \( p \) is the static pressure, \( p_{ref} \) is the reference pressure, \( \rho \) is the fluid density and \( V_\infty \) is the velocity of the incoming flow. Naturally, the three flow variables included in Eq. (C.1) are time-averaged quantities. The comparison error is evaluated at 56 locations on the surface (28 on the upper surface and 28 on the lower surface) of the airfoil where measurements are available.

**C.1.3 Evaluation of \( V_{val} \)**

The first step in the calculation procedure for \( V_{val} \) is to identify which of the 4 cases considered for the measurement of the experimental data applies to the selected quantity of interest.

**C.1.3.1 Assumptions for Cases 2 and 3**

The definition of \( C_p \) (Eq. (C.1)) at a location on the surface of the airfoil involves four different quantities: \( p, p_{ref}, \rho \) and \( V_\infty \). Therefore, if all these quantities are assumed to be affected by uncertainties, and the pressure coefficient is obtained from a data reduction equation, then the situation corresponds either to Case 2 or to Case 3 depending on whether the measurements are correlated or not, and \( V_{val} \) is determined from Eq. (A.3). If the measurement of the fluid density \( \rho \) also affects the experimental determination of \( V_\infty \), the measured variables share uncertainties, and so the procedure for Case 3 should be followed. On the other hand, if independent measurements are performed for these four variables, Case 2 procedure should be followed.

**C.1.3.2 Assumptions for Case 1**

In [2], it is suggested to use Case 1 that corresponds to evaluating \( V_{val} \) from Eq. (A.2). This means that \( C_p \) was “directly measured”. This assumption is a consequence of considering that \( \rho \) and \( V_\infty \) are exact values (no measurement uncertainty) and that \( (p - p_{ref}) \) is directly measured, which is common practice in wind tunnel experiments. We will follow this assumption (that was also adopted in the simulations reported in [2]) for the remainder of this example.

The evaluation of \( V_{val} \) for Case 1 involves independent contributions from numerical \( V_{num} \), input-parameter \( V_{input} \) and experimental uncertainties \( V_D \), Eq. (A.2).

Numerical uncertainty is determined for the simulation results at each of the 56 locations where the comparison error is evaluated, using a least-squares version [5] of the Grid Convergence Index [6]. Iterative and round-off errors are reduced to negligible levels when
compared to the discretization error, and so it is assumed that numerical errors at the 56 locations on the airfoil surface are independent. This means that $V_{\text{num}}$ is calculated from Eq. (A.8). The assumption of no shared numerical errors at the 56 validation points is justified by the fact that discretization errors are evaluated independently at each validation point. On the other hand, in cases that include a non-negligible contribution of the iterative error to the numerical uncertainty, errors may be shared by the different validation points. However, estimation of the correlation coefficients (Appendix A only describes the limiting situations of no correlation or fully correlated) may be difficult to quantify. Nonetheless, it is possible to assess the influence of this assumption determining the value of the multivariate metric with or without shared numerical uncertainties. Furthermore, correlation coefficients between 0 (without correlation) and 1 (perfect correlation) can be easily tested.

The contribution of the input parameter uncertainty to the validation covariance matrix is a consequence of the uncertainty in the measurement of the angle of attack. Naturally, this input parameter uncertainty is shared by all the validation variables and so $V_{\text{input}}$ is calculated using Eq. (A.13). The $\mathbf{X}_S$ array is defined by Eq. (A.14) and, in this simple case, $V_X$ is just the standard deviation of the measurement of the angle of attack squared.

The determination of the contribution of the experimental uncertainty to $V_{\text{val}}$ may be performed with or without shared error sources. If the 56 pressure differences $(p - p_{\text{ref}})$ are measured with the same pressure sensor, the 56 measurements share the same experimental errors and $V_D$ should be determined from Eq. (A.16). On the other hand, if independent measurements are performed for each of the 56 locations, Eq. (A.15) is the correct option to determine $V_D$.

As illustrated in this example, several choices and assumptions have to be made for the determination of the validation covariance matrix. Some of them are identical to those required for the application of the point wise V&V20-2009 procedure. However, possible correlation between the numerical, input-parameter and experimental uncertainties at the 56 validation set points must be assessed to apply the multivariate metric to multiple set points.

### C.2 Pressure drop for a fully developed flow in a smooth pipe

The second example focuses on the pressure drop in fully developed flow in a smooth pipe of diameter $D$ and length $L$, as illustrated in Figure 2. The goal of the example is to determine the friction factor for this flow at different flow rates, which for a fixed diameter $D$ and fluid kinematic viscosity $\nu = \mu/\rho$ corresponds to different Reynolds numbers. A reference solution for this is obtained from the empirical correlation proposed by Colebrook [8].
C.2.1 Problem definition

The geometry of the simulation of the fully developed flow in a smooth circular pipe is illustrated in Figure 2. Flow conditions are specified by the flow rate and a mean flow field that only exhibits axial velocity components and a mean velocity profile that does not change along the pipe.

![Figure C.2: Illustration of a fully-developed flow in a circular pipe of diameter $D$ and length $L$. $\tau_w$ is the shear-stress at the wall and the pressure drop is $\Delta p = p_{\text{in}} - p_{\text{out}}$.](image)

As for the previous example, the Reynolds-Averaged continuity and momentum equations have been selected to perform the simulations [8]. In this example, simulations are performed with two-equation and three-equation eddy-viscosity models. Time averaging is applied to define the mean flow and the fluid is assumed to be incompressible. The multivariate metric allows a quantitative assessment of the turbulence models tested. A detailed description of the simulations is presented in [8].

In this example, the geometric definition of the pipe, fluid properties and flow rate are assumed to be exact quantities, and so there is no input uncertainty in the simulations. In such conditions, the application of the multivariate metric must be done carefully. If experimental uncertainties are perfectly correlated at the multiple set points, the contribution of the “experimental uncertainty” to the covariance matrix is a singular matrix. Similarly, for perfectly shared numerical uncertainties at the multiple set points, the contribution of the numerical uncertainties to $V_{vai}$ is also a singular matrix. Therefore, $V_{vai}$ may be a singular matrix which would mean that the multivariate metric cannot be applied. However, in such conditions the evaluation of modeling errors at the multiple set points should be equivalent and so the multivariate is not required.

C.2.2 Quantity of interest

The selected quantity of interest is the friction factor defined as the nondimensional pressure gradient for the pipe, and is given as
\[ f = \frac{\Delta p}{\frac{1}{2} \rho V^2 L}, \]  
(C.2)

where \( \rho \) is the density of the fluid, \( L \) is the length of the pipe and \( V \) is the mean velocity, which is obtained from the volumetric flow rate and the cross-sectional area of the pipe, and \( \Delta p \) is the pressure drop over the pipe length \( L \).

The friction factor can also be expressed in terms of the wall shear stress \( \tau_w \) using the equilibrium between the pressure force and the friction force:

\[ \Delta p \frac{\pi D^2}{4} = \tau_w \pi D L. \]  
(C.3)

Substituting Eq. (C.3) into Eq. (C.2) leads to the following expression for the friction factor \( f \):

\[ f = \frac{4\tau_w}{\frac{1}{2} \rho V^2}. \]  
(C.4)

The empirical correlation proposed by Colebrook [7] is given by

\[ \frac{1}{\sqrt{f}} = -2\log_{10} \left( \frac{\epsilon}{3.7D} + \frac{2.51}{Re \sqrt{f}} \right), \]  
(C.5)

where \( \epsilon \) is the wall roughness (assumed to be zero in this example) and \( Re \) is the Reynolds number based on the pipe diameter, mean velocity and fluid kinematic viscosity. In the present example, it is assumed that the quantities required to determine \( f \) are exact. However, there is uncertainty in the reference value of \( f \) associated with the process that led to Eq. (C.5).

The friction factor \( f \) is determined for three different flow rates for the same geometry (corresponding to a ratio between the largest and smallest Reynolds number of 2.67).

C.2.3 Evaluation of \( V_{val} \)

The determination of the quantity of interest \( f \) from the Colebrook correlation (Eq. (C.5)) depends on two quantities: \( D \) and \( Re \). The Reynolds number depends on the pipe diameter, flow rate and kinematic viscosity of the fluid. Therefore, as for the previous example, the determination of \( V_{val} \) depends on the assumptions made in obtaining these quantities.

C.2.3.1 Assumptions for Case 1

As mentioned above, \( D, V \) and \( \nu \) are assumed to be exact values and so this example corresponds to Case 1. If any of the quantities required to determine \( f \) are not exact, this
example can correspond to Cases 2 or 3. However, in those cases, the uncertainty originating from the quantities required to obtain \( f \) need to be combined with the uncertainty of the correlation used to obtain the reference result.

With these assumptions, \( V_{\text{val}} \) is determined from Eq. (A.2) as the previous example. However, the calculation of \( V_{\text{val}} \) is different from the first example presented above because \( V_{\text{input}} = 0 \).

Numerical uncertainty is determined for each of the flow rates and turbulence models using a least-squares version [5] of the Grid Convergence Index [6]. As for the previous example, it is assumed that iterative and round-off error contributions to the numerical uncertainty are negligible and so \( V_{\text{num}} \) is a diagonal matrix calculated from Eq. (A.8).

In this example, there is no contribution from the input-parameter uncertainty \( V_{\text{input}} \), because geometric properties of the pipe, fluid properties and flow rate are assumed to be exact. However, the reference data obtained from the Colebrook correlation does not produce exact values due to the process of deriving the correlation from experimental data, and so we will have a contribution from \( V_{D} \). Hence, two different options are possible:

a) ignoring correlation in the error sources that produce the uncertainty in the reference results for the three flow rates from the Colebrook formula, i.e., estimated uncertainties for each flow rate are independent;

b) including correlation in the error sources that produce the uncertainty in the reference results for the three flow rates.

Option a) leads to \( V_{D} \) becoming a diagonal matrix determined by Eq. (A.15), whereas Option b) leads to a full \( V_{D} \) matrix determined by Eq. (A.16). For either of these options, the validation covariance matrix is given by \( V_{\text{val}} = V_{\text{num}} + V_{D} \). Application of the multivariate metric with Option a) is straightforward because \( V_{\text{val}} \) is a diagonal matrix.

However, for Option b) the results of the multivariate metric may be misleading because the determinant of \( V_{\text{val}} \) tends to zero with the reduction of the numerical uncertainty. Therefore, the quantitative comparison of the three turbulence models must be performed carefully. If \( V_{\text{val}} \cong V_{D} \), the validation covariance matrix becomes singular and the multivariate metric cannot be applied. In fact, in these conditions the comparison between simulations and reference values at the three set points (three flow rates) would become equivalent. If comparison errors and validation uncertainties for the three flow rates are not equivalent, the assumption of fully-correlated uncertainties at the three set points is not observed.
C.3 Skin friction coefficient for a turbulent flow over a flat plate

In viscous flow simulations, one of the main goals is the determination of the friction force that results from the shear-stress, \( \tau_w \), at the wall. In turbulent flow, it is difficult to measure the mean velocity sufficiently close to the wall to determine \( \tau_w \) from its definition,

\[
\tau_w = \mu \left( \frac{\partial V_t}{\partial y_n} \right)_{y_n},
\]

where \( \mu \) is the dynamic viscosity of the fluid, \( V_t \) is velocity component parallel to the wall and \( y_n \) is the direction perpendicular to the wall. One of the most popular experimental techniques to determine \( \tau_w \) is the Clauser plot \[9\] that is based on the log-law region of the mean velocity profile. This means that experimental data is used as the input for a model that determines the dimensionless shear-stress at the wall that corresponds to the skin friction coefficient.

C.3.1 Problem definition

The original goal of this problem \[10\] was to assess the performance of RANS turbulence models in the simulation of non-equilibrium boundary-layers. In this appendix, its purpose is to illustrate an example that requires the Case 4 option.

A NACA 0012 airfoil was installed in the center of a wind tunnel at different angles of attack and Reynolds number of \( Re = 2 \times 10^6 \). The presence of the airfoil imposes favorable and adverse pressure gradients on the boundary-layer developing on the wind tunnel wall. Experimental data includes pressure distribution on the wind tunnel wall, and profiles of mean velocity, turbulence kinetic energy \( k \) and Reynolds shear-stresses \(-\rho \overline{u_x v_y}\) at seven different locations \[10\]. Mean velocity profiles were measured with an array of pitot tubes, whereas turbulence quantities \( k \) and \(-\rho \overline{u_x v_y}\) were measured with Particle Image Velocimetry (PIV).

Simulations reported in \[10\] were based on the Reynolds-averaged Navier-Stokes (RANS) equations using several RANS turbulence models. The fluid is assumed to be incompressible and mean flow quantities are defined with time-averaging and so the simulated flow is statistically steady. A computational domain similar to that depicted in Figure 1 is proposed in \[10\] to perform two-dimensional simulations with a uniform inlet velocity profile. Details of the simulations are reported in \[10\].

C.3.2 Quantity of interest

The quantity of interest for this example is the skin friction coefficient,
\[ C_f = \frac{\tau_w}{\frac{1}{2} \rho V_{\infty}^2}, \quad \text{(C.7)} \]

where \( V_{\infty} \) is the velocity of the incoming flow and \( \rho \) is the fluid density. The determination of the shear-stress directly from Eq. (C.6) is not possible, because there are no velocity measurements sufficiently close to the wall. Therefore, the evaluation of \( C_f \) is based on the log-law [9]

\[ \frac{V_t}{u_t} = \frac{1}{\kappa} \ln \left( \frac{u_t y_n}{v} \right) + B, \quad \text{(C.8)} \]

where \( V_t \) is the mean velocity component parallel to the wall, \( u_t \) is the friction velocity

\[ u_t = \sqrt{\frac{\tau_w}{\rho}} = V_{\infty} \frac{C_f}{2}, \quad \text{(C.9)} \]

\( \kappa = 0.41 \) and \( B = 5 \). Substituting Eq. (C.9) in Eq. (C.8) leads to

\[ \frac{V_t}{V_{\infty}} = \sqrt{\frac{C_f}{2}} \frac{1}{\kappa} \ln \left( \frac{y_n}{c} \right) + \sqrt{\frac{C_f}{2}} \left( \frac{1}{\kappa} \ln \left( \sqrt{\frac{C_f V_{\infty} c}{2}} \right) + B \right). \quad \text{(C.10)} \]

Eq. (C.10) allows the determination of \( C_f \) from the slope of the mean velocity profile represented as a function \( \ln \left( \frac{y_n}{c} \right) \).

**C.3.3 Evaluation of \( V_{val} \)**

The determination of the skin friction coefficient from Eq. (C.10) corresponds to Case 4. The measured quantities are mean velocity components \( V_t \) and distances to the wall \( y_n \) that are used in the log-law equation to obtain \( C_f \). This means that \( V_{val} \) is obtained from Eq. (A.4) that includes four contributions \( V_{num} \), \( V_{input} \), \( V_{D,num} \) and \( V_{D,input} \). The calculation of \( V_{num} \) and \( V_{input} \) is similar to that discussed Sections 1 and 2 for the other examples. Furthermore, \( V_{D,num} \) and \( V_{D,input} \) are contributions from the solution of Eq. (C.10) using the experimental data. Here, \( V_{D,num} \) corresponds to the numerical accuracy of the slope obtained from the fit to the data, and \( V_{D,input} \) is a consequence of the experimental uncertainties of the variables used in Eq. (C.10).

It should be noted that simulations may determine \( C_f \) from Eq. (C.7) or (C.10) when simulations are performed without wall functions. If simulations are performed with wall functions, experiments and simulations must determine the quantity of interest with the same
However, if $\tau_w$ is calculated with Eq. (C.6) (no wall functions), the comparison between experiments and simulations is affected by the post-processing technique used to determine the quantity of interest. In that case, it may be useful to determine $V_1$ at the experimentally measured distances to the wall $y_n$ and determine $C_f$ from Eq. (C.10).

C.4 References


