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ON THE INTERPRETATION AND SCOPE OF THE V&V 20 STANDARD FOR VERIFICATION AND VALIDATION IN COMPUTATIONAL FLUID DYNAMICS AND HEAT TRANSFER

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ABSTRACT

The goal of this paper is to summarize and clarify the scope and interpretation of the validation procedure presented in the V&V20-2009 ASME Standard. In V&V20-2009, validation is an assessment of the model error, without regard to the assessment satisfying validation requirements. Therefore, validation is not considered as a pass/fail exercise. The purpose of the validation procedure is the estimation of the accuracy of a mathematical model for specified validation variables (also known as quantities of interest, system responses or figures of merit) at a specified validation point for cases in which the conditions of the actual experiment are simulated. The proposed procedure can be applied to variables defined by a scalar.

For the sake of clarity, the paper reiterates the development and assumptions behind the V&V20-2009 procedure that requires the knowledge of the experimental values D and simulation values S at the set point and an estimate of the experimental, numerical and parameter uncertainties. The difference E between S and D is the centre of the interval that should contain the model error (with a certain degree of confidence) and the width of the interval is obtained from the validation uncertainty that is a consequence of the combination of the experimental, numerical and parameter uncertainties.

The paper presents the alternatives to address parameter uncertainty and expands upon the interpretation of the final result. The paper also includes two examples demonstrating the application of the V&V20-2009 validation procedure including one problem from V&V10.1-2012 on solid mechanics.

INTRODUCTION

The ASME V&V Verification and Validation in Computational Modeling and Simulation committee "*coordinates, promotes, and fosters the development of standards that provide procedures for assessing and quantifying the accuracy and credibility of computational models and simulations*" [1]. Four documents have been published: "Guide for Verification and Validation in Computational Solid Mechanics" in 2006 [2], "Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer" in 2009 [3], "An Illustration of the Concepts of Verification and Validation in Computational Solid Mechanics" in 2012 [4] and "Assessing Credibility of Computational Modeling through Verification and Validation: Application to Medical Devices" in 2018 [5]. The first document will be updated to "Standard for Verification and Validation in Computational Solid Mechanics" in March 2020 [6].

These documents present complementary aspects of the use of Verification and Validation: the V&V 10 documents [2, 6] present a conceptual framework and general guidance for implementing the process of computational model V&V, whereas [4] describes a simple example of V&V to illustrate some of the key concepts and procedures presented in [2,6]. The ASME V&V 40 subcommittee has developed a risk-informed credibility assessment framework [5] to provide guidance on how to establish and communicate risk-informed credibility of computational models. The focus of this paper is the document produced by the V&V 20 subcommittee [3] that describes a Verification and Validation approach that quantifies the degree of accuracy of a mathematical/computational model inferred from the comparison of simulated and experimental values obtained for a specified variable at a specified validation point (set point).

In the V&V 20-2009 Standard [3], validation is defined *as the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model*, which is similar to the definition presented in [6] *the process of determining the degree to which the model is an accurate representation of corresponding physical experiments from the perspective of the intended uses of the model*. However, the need to make decisions about the model adequacy in the hierarchical validation procedure proposed in [2,6] requires the definition of validation requirements (step 1) and validation comparisons (step 3) to accept/reject the model components (and the complete model). This pass/fail aspect of validation implied in [2, 6] is not included in V&V20-2009 [3] that presents validation as step 2 of the V&V 10 framework. On the other hand, the V&V10.1 document [4] formulates a comparison of validation variables (also known as quantities of interest, system responses or figures of merit) defined by probability distributions, i.e. a probability density function (and/or a cumulative density function). Whereas V&V20-2009 [3] formulates the comparison of validation variables defined by a scalar, which can be all the individual experiments/simulations available or any property (mean,median,variance,...) of the distributions used by V&V 10. Both V&V10 and V&V 20 account for uncertainties that affect the validation variables. Therefore, there is no incompatibility between the two documents, they formulate different approaches.

The remainder of this paper focus on the clarification of the scope and interpretation of the validation procedure presented in the V&V20-2009 ASME Standard [3]. We review and expand the development and assumptions behind the V&V20-2009 procedure that leads to the estimate of an interval for the model error (with a certain degree of confidence). The difference between the experimental D and simulation S values at the validation set point is used to estimate the centre of the interval that should contain the model error and the combination of the experimental, numerical and parameter uncertainties defines the width of the interval. The paper presents the alternatives to address parameter uncertainty and the interpretation of the final result.

ASME Standards *can be defined as a set of technical definitions and guidelines, "how to" instructions for designers, manufacturers, and user* [7] and *are considered voluntary because they serve as guidelines* [7]. Therefore, the techniques presented in the V&V 2009 Standard do not exclude alternative (reliable) techniques to assess the model error.

The two examples included in [3] and [4] are presented to demonstrate the application of the V&V20-2009 validation procedure. Finally, we will also mention the changes required to apply the V&V10.1 framework to the same examples.

V&V20 VALIDATION PROCEDURE

The goal of the V&V 20-2009 Standard [3] is the estimation of the accuracy of a mathematical model[1] for specified validation variables at a specified validation point for cases in which the conditions of the actual experiment are simulated. As mentioned above, validation variables are also known as quantities of interest, system response quantities or figures of merit. However, to maintain consistency with the V&V 20-2009 Standard [3], validation variable is used in the remainder of this paper.

A specified validation (set) point means that the accuracy of the mathematical model is evaluated for simulations performed for the same domain, fluid properties and boundary conditions of the experiment that provides the physical data. The scope of the V&V 20 Standard is to estimate the accuracy of a mathematical model for a validation variable at a single validation set point. Examples of validation variables are the drag coefficient (integral quantity) or the pressure and skin friction coefficients at a specified location (local quantities) for the flow around an airfoil in a prescribed domain (wind tunnel) at a specified angle of attack and Reynolds number. Assessment of model accuracy at points within a domain other than the selected validation points (e.g., interpolation/extrapolation in a domain of validation) is beyond the scope of the V&V 20-2009 Standard. This topic is also not addressed in the V&V 10 documents [2, 4, 6].

The validation metric adopted by V&V 20-2009 [3] applies to validation variables defined by a scalar. This does not mean that V&V 20-2009 is focused on deterministic simulations. The procedure can be applied to the validation variable obtained in multiple experiments/simulations as in the test case presented in [3] or to the mean, median, variance or any property (global or local) of a probabilistic distribution that can be defined by a scalar. Furthermore, this also does not mean that the proposed procedure "promotes" validation exercises based on single-run experiments and/or single grid simulations. Equivalently to the statement *there can be no validation without experimental data with which to compare the result of the simulation* included in [3], V&V20-2009 cannot be applied without the knowledge of experimental and numerical uncertainties (parameter uncertainties are discussed below) that lead to the validation uncertainty u_{val}. As stated in [3], the estimation of u_{val} is at the core of the methodology presented in V&V20-2009.

The starting point of the V&V20-2009 procedure is the definition of the simulation error δ_S and experimental error δ_D of the selected validation variable:

$$\delta_S = S - \mathbf{T} \tag{1}$$

[1] The mathematical model is defined in the continuum sense. Thus, the model error is separate from, and does not include, discretization/numerical errors.

and

$$\delta_D = D - \mathbf{T} \,. \tag{2}$$

S stands for the simulation value, D is the experimental value and $\mathbf{T}$ is the (unknown) true value. The difference between the simulation S and the experiment D is the comparison error E,

$$E = S - D \,, \tag{3}$$

which is equivalent to the difference between the simulation and experimental errors[2]:

$$E = S - D = (\delta_S + \mathbf{T}) - (\delta_D + \mathbf{T}) = \delta_S - \delta_D \,. \tag{4}$$

No assumptions are made about the way S and D are determined, except that a scalar value is available for both. However, any known signed biases in the experiments are assumed to be removed from the experimental data.

The process of conducting the experiment and measuring the experimental validation variable obviously incurs experimental error. Similarly, the process of simulating the validation variable generates the simulation error δ_S, which includes three contributions:

1. The model error δ_{model} that is a consequence of the continuum modeling assumptions and approximations;
2. The numerical error δ_{num} originates from the numerical solution of the mathematical model;
3. The parameter/input error δ_{input} is the error in S due to inexact boundary conditions, fluid properties and/or heat transfer coefficients.

Introducing these four errors in Eqns.(3) or (4) leads to

$$E = S - D = \delta_{\mathrm{model}} + \delta_{\mathrm{num}} + \delta_{\mathrm{input}} - \delta_D \,. \tag{5}$$

The comparison error E is thus the combination of all errors in the simulation result and in the experimental result. Its sign and magnitude is known once the validation comparison (difference between S and D) is made. The individual error contributions are of unknown sign and magnitude. Each error belongs to a population from which a realization has been taken based on the measured values for the experimental D and simulation S validation variables.

[2]There is a misprint in equation (1-5-4) of the V&V20-2009 Standard. The third $=$ sign should be a $-$.

The goal of the validation procedure is to estimate δ_{model}. Eqn. (5) may be re-arranged to obtain:

$$\delta_{\mathrm{model}} = E - \left(\delta_{\mathrm{num}} + \delta_{\mathrm{input}} - \delta_D\right) \,. \tag{6}$$

The determination of δ_{model} requires the comparison error E and the numerical, input and experimental errors, δ_{num}, δ_{input} and δ_D, which are not known. Therefore, δ_{model} cannot be determined from Eqn. (6) but only estimated using

$$\tilde{\delta}_{\mathrm{model}} = E - \left(\tilde{\delta}_{\mathrm{num}} + \tilde{\delta}_{\mathrm{input}} - \tilde{\delta}_D\right) \,, \tag{7}$$

where $\tilde{\delta}_{\mathrm{model}}$, $\tilde{\delta}_{\mathrm{num}}$, $\tilde{\delta}_{\mathrm{input}}$ and $\tilde{\delta}_D$ become estimates of the unknown errors included in Eqn. (6).

In V&V20-2009 [3], the estimate of the model error is performed using the following assumptions:

- Once the experiment and simulations have been performed to determine D and S, the effect of experimental error on D and numerical, input, and model errors on S are realized fixed quantities ("fossilized") of unknown magnitude;
- Any known signed biases in the experiments and simulations are assumed to be removed;
- Standard uncertainties u_{num}, u_{input} and u_D are estimated to obtain reasonable characterizations of the numerical, input and experimental errors $\tilde{\delta}_{\mathrm{num}}$, $\tilde{\delta}_{\mathrm{input}}$ and $\tilde{\delta}_{\mathrm{D}}$. Uncertainty for the combination of these three errors is u_{val}.

Using a probabilistic description[3] of $\tilde{\delta}_{\mathrm{num}}$, $\tilde{\delta}_{\mathrm{input}}$ and $\tilde{\delta}_{\mathrm{D}}$ based on the mean and standard uncertainty, the expected value of the model error $\hat{\delta}_{\mathrm{model}}$ can be obtained from Eqn. (7) as

$$\hat{\delta}_{\mathrm{model}} = \varepsilon\left[\tilde{\delta}_{\mathrm{model}}\right] = E - \varepsilon\left[\tilde{\delta}_{\mathrm{num}} + \tilde{\delta}_{\mathrm{input}} - \tilde{\delta}_D\right] = E \,, \tag{8}$$

because the expected values of the numerical, input and experimental errors ($\hat{\delta}_{\mathrm{num}}$, $\hat{\delta}_{\mathrm{input}}$ and $\hat{\delta}_{\mathrm{D}}$) are equal to zero, i.e. all known biases have been removed.

The variance of $\tilde{\delta}_{\mathrm{model}}$ is given by

$$V\left[\tilde{\delta}_{\mathrm{model}}\right] = V\left[\tilde{\delta}_{\mathrm{num}} + \tilde{\delta}_{\mathrm{input}} - \tilde{\delta}_D\right] \,, \tag{9}$$

since E is a fixed number. On the other hand, the determination of $V\left[\tilde{\delta}_{\mathrm{num}} + \tilde{\delta}_{\mathrm{input}} - \tilde{\delta}_D\right]$ depends on possible correlations between the (unknown) numerical, input and experimental errors. Although V&V 20-2009 [3] describes complex dependencies between the three different error sources, in the simplest situation, $\tilde{\delta}_{\mathrm{num}}$, $\tilde{\delta}_{\mathrm{input}}$ and $\tilde{\delta}_{\mathrm{D}}$ are independent leading to the familiar

[3]Probabilistic distributions are identified by $\tilde{}$, whereas expected values are designated by $\hat{}$ or ε.

root sum squared (RSS) summation for the determination of the validation uncertainty u_{val}

$$u_{\text{val}}^2 = V\left[\tilde{\delta}_{\text{num}} + \tilde{\delta}_{\text{input}} - \tilde{\delta}_D\right] = u_{\text{num}}^2 + u_{\text{input}}^2 + u_D^2 \,. \quad (10)$$

Thus, the interval that characterizes the estimated model error is given by

$$E - u_{\text{val}} \le \delta_{\text{model}} \le E + u_{\text{val}} \,. \quad (11)$$

We recall that according to Eqn. (8) the comparison error E is equal to the expected value of the model error $\hat{\delta}_{\text{model}}$. Such statement seems to be in conflict with Eqn. (5) that shows that E is the sum of four errors. However, the expected values of three of those four errors ($\hat{\delta}_{\text{num}}$, $\hat{\delta}_{\text{input}}$ and $\hat{\delta}_{\text{D}}$) are equal to zero and so there is no inconsistency in the result obtained from Eqn. (8). The contributions of these errors to the procedure comes from their uncertainties, which contribute to u_{val}.

The estimation of u_{val} is thus at the core of the methodology presented in the V&V20-2009 Standard and so the evaluation of the numerical, input and experimental uncertainties is a fundamental part of the quality of the validation procedure and their assessment will naturally be penalized by careless experimental and/or simulation work. Large uncertainties for the simulation numerical errors, simulation input errors and experimental measurement errors will result in a poor estimate of δ_{model}, i.e. a large range of possible values for the error of the mathematical model.

Handling Input/parameter uncertainties

The estimation of the input/parameter uncertainty requires the propagation through the model equations of uncertainties in the boundary conditions, fluid properties and/or heat transfer coefficients. Section 3 of [3] describes a local and a global uncertainty propagation procedure to estimate u_{input}.

The handling of δ_{input} in a validation exercise may have many different choices. Nonetheless, there are two limiting situations:

1. All input parameters are "hard-wired" and so they are considered part of the model, which means that $\delta_{\text{input}} = 0$ by definition;
2. Input uncertainties are estimated for all input parameters appearing in the model differential equations, which means that δ_{model} will contain only the error of the general model equations.

As discussed in section C-6 of [3], the first option corresponds to the "strong-model" that considers all input parameters fixed in the model. On the other hand, the second alternative corresponds to the "weak-model" (or model form) that includes only the mathematical formulation of the problem (*e.g., the incompressible Navier-Stokes equations, or the Fourier law of heat conduction*, [3]).

Naturally, the number of input parameters taken into account for the determination of δ_{input} is a users choice. However, it should be emphasized that δ_{input} is never neglected. If an uncertain input parameter is considered fixed, its contribution to the simulation error becomes part of δ_{model}, whereas propagating the input uncertainty through the model equation will put its contribution in δ_{input} . Therefore, the way input/parameter errors are handled defines only if they are considered as a contribution to the model error or as a separate error.

Expanded uncertainties and degree of confidence

As discussed in section 6-3 of V&V20-2009 [3], the standard uncertainties u may be multiplied by a coverage factor k to obtain an expanded uncertainty $U_{\%}$. The expanded uncertainty

$$U_{\%} = ku. \quad (12)$$

provides a band at a given confidence level (typically 95%) for an interval that should contain the model error δ_{model}.

The determination of the coverage factor k requires an assumption (or the knowledge) about the probability distributions that characterize $\tilde{\delta}_{\text{num}}$, $\tilde{\delta}_{\text{input}}$ and $\tilde{\delta}_{\text{D}}$. V&V20-2009 presents examples of parent error distributions and discusses the determination of k. For the three distributions considered in [3] (uniform, triangular and Gaussian), k is typically a number in the range of 2 to 3. To counteract a common misrepresentation of V&V20-2009 due to common presumptions, we emphasize here that V&V20-2009 methodology is NOT limited to assumption of Gaussian (normal) distribution.

The replacement of the standard uncertainty u_{val} in Eqn. (11) by the expanded uncertainty $U_{(\text{val},\%)}$ leads to

$$E - U_{(\text{val},\%)} \le \delta_{\text{model}} \le E + U_{(\text{val},\%)} \,. \quad (13)$$

The choice of coverage factor does not affect the comparison error E which is the center of the interval including δ_{model}, which depends only on S and D. However, the width of the estimated interval ($2U_{(\text{val},\%)}$) is directly proportional to the coverage factor k. Therefore, the estimated upper limit of the interval ($(\hat{\delta}_{\text{model}})_{max} = E + U_{(\text{val},\%)}$) and lower limit of the interval ($(\hat{\delta}_{\text{model}})_{min} = E - U_{(\text{val},\%)}$) values of the model error depend on k. This means that $(\hat{\delta}_{\text{model}})_{max}$ and $(\hat{\delta}_{\text{model}})_{min}$ depend on the required confidence level and on the type of probability distribution of the combination of experimental, numerical and input errors and so they depend on choices and/or assumptions of the user.

Interpretation of the V&V20-2009 procedure

The validation procedure presented in the V&V 20-2009 standard [3] defines a validation metric at the set point. For a specific validation variable at specified conditions (the set point), it defines an interval that should contain the model error (for example) roughly 95 times out of 100 if the uncertainty of the combined errors are represented by $U_{(\mathrm{val},95)}$,

$$E - U_{(\mathrm{val},95)} \leq \delta_{\mathrm{model}} \leq E + U_{(\mathrm{val},95)} \; . \tag{14}$$

The comparison error E corresponds to the centre of the interval containing the model error (Eqn. (8)) and $U_{(\mathrm{val},95)}$ is the validation uncertainty using expanded numerical, input and experimental uncertainties that require the definition of the appropriate coverage factor k. If numerical, experimental and input uncertainties are independent

$$U_{(\mathrm{val},95)} = \sqrt{(U^2_{(\mathrm{num},95)} + U^2_{(\mathrm{input},95)} + U^2_{(\mathrm{D},95)}} \; . \tag{15}$$

Alternatively, Eqn. (11) using standard deviations can be used without the need to make any assumption about the underlying error distributions. However, the knowledge of the degree of confidence in the interval that should contain δ_{model} would still require assumption/knowledge of error distributions.

There are two main observations about the outcome of the procedure (independent of the $U_{(\mathrm{val},\%)}$ chosen):

1. The goal of V&V20 is to estimate δ_{model}. **It is not** to obtain $E \leq U_{(\mathrm{val},95)}$. Satisfying this inequality is always possible and trivial. Increasing numerical and/or experimental uncertainties is sufficient to achieve it;
2. $U_{(\mathrm{val},95)}$ reflects the quality of the validation assessment and not the accuracy of the model (i.e. δ_{model}) [10]. The validation uncertainty depends only on the numerical, input and experimental uncertainties and so its level reflects quality of the experiments and simulations **not** the quality of the model.

Eqn. (14) estimates an interval that should contain δ_{model} with a confidence level of 95%, i.e. it provides estimates of the lowest $(\hat{\delta}_{\mathrm{model}})_{min}$ and largest $(\hat{\delta}_{\mathrm{model}})_{max}$ values of δ_{model} at the set point with a confidence level of 95%. Although the present interpretation of this metric could finish here, it might be useful to analyze the consequences of the relative values of E and $U_{(\mathrm{val},95)}$ on δ_{model}.

As illustrated in Fig. 1, there are three possible cases:

1. $|E| \gg U_{(\mathrm{val},95)}$ leads to $\delta_{\mathrm{model}} \approx E$;
2. $|E| \ll U_{(\mathrm{val},95)}$ gives $|\delta_{\mathrm{model}}| \leq U_{(\mathrm{val},95)}$, which still gives an interval for δ_{model} but it does not identify the sign of the model error;
3. If $|E|$ and $U_{(\mathrm{val},95)}$ do not satisfy either of the two conditions above, we can only say that $|\delta_{\mathrm{model}}| < |E| + U_{(\mathrm{val},95)}$. However, there is a slight difference between the cases where $|E|$ is larger or smaller than $U_{(\mathrm{val},95)}$,
   (a) $|E| \geq U_{(\mathrm{val},95)}$ indicates that the sign of δ_{model} is equal to the sign of E, because $(\hat{\delta}_{\mathrm{model}})_{min}$ and $(\hat{\delta}_{\mathrm{model}})_{max}$ have the same sign;
   (b) $|E| < U_{(\mathrm{val},95)}$ does not allow to estimate the sign of δ_{model}, because $(\hat{\delta}_{\mathrm{model}})_{min}$ and $(\hat{\delta}_{\mathrm{model}})_{max}$ have different signs.

From a validation perspective, the first case is the desired outcome because the goal of the procedure is to estimate δ_{model}. On the other hand, the second case is a consequence of a poor quality validation exercise that may be easily misinterpreted, because it suggests a relation between the true δ_{model} and $U_{(\mathrm{val},95)}$ when none exists. Nonetheless, it provides an interval for the model error that was not available without the validation exercise. However, the reduction of $U_{(\mathrm{val},95)}$ is not dependent on the model. It requires improvements in the numerical and/or experimental accuracies and/or in the specification of the input parameters. The area to target for improving the validation assessment can be determined by the relative size of $U_{(\mathrm{num},95)}$, $U_{(\mathrm{input},95)}$ and $U_{(\mathrm{D},95)}$ along with the resources required to reduce them. It should also be noted that the second case is the only one that is in agreement (rigorously for $E = 0$) with the ITTC (2002) validation methodology [8] for ship hydrodynamics that claims "validation at the $U_{(\mathrm{val},95)}$ level" when $|E| < U_{(\mathrm{val},95)}$. As mentioned above, satisfying such inequality cannot be the goal of the validation exercise.

The interpretation given above for the V&V 2009 Validation procedure still includes fuzzy statements in the definitions of cases one and two. Although such an approach is common in science and engineering, it requires subjective decisions of the user. Therefore, to obtain a computable algorithm the $\gg$, $\ll$ and $\approx$ signs must be converted into unambiguous quantities.

The proposed algorithmic version of the outcome of V&V 2009 is:

$$\begin{array}{llll}
1 & |E| > CU_{\mathrm{val},\%} & \Rightarrow & \delta_{\mathrm{model}} = E \; ; \\
3a & CU_{\mathrm{val},\%} \geq |E| \geq U_{\mathrm{val},\%} & \Rightarrow & |\delta_{\mathrm{model}}| < |E| + U_{\mathrm{val},\%} \\
 & & & \text{and } \mathrm{sign}(\delta_{\mathrm{model}}) = \mathrm{sign}(E) \; ; \\
3b & U_{\mathrm{val},\%} \geq |E| \geq \frac{1}{C} U_{\mathrm{val},\%} & \Rightarrow & |\delta_{\mathrm{model}}| < |E| + U_{\mathrm{val},\%} \\
 & & & \text{and } \mathrm{sign}(\delta_{\mathrm{model}}) \text{ unknown} \; ; \\
2 & \frac{1}{C} U_{\mathrm{val},\%} \geq |E| & \Rightarrow & |\delta_{\mathrm{model}}| < U_{\mathrm{val},\%} \\
 & & & \text{and } \mathrm{sign}(\delta_{\mathrm{model}}) \text{ unknown} \; .
\end{array}$$

The constant C is typically equal to 10 (one order of magnitude). However, if there are no high risk decisions involved, $C = 10$ would be unnecessarily conservative for many problems due to several conservative aspects inherent to the methodology.

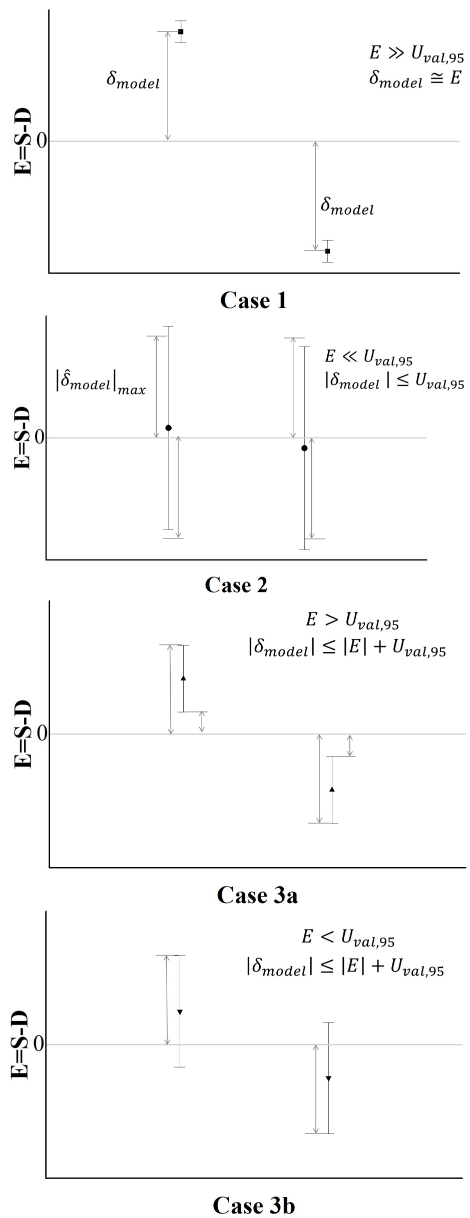

FIGURE 1. Examples of different relative values of comparison error E (symbols) and validation uncertainty $U_{(\mathrm{val},95)}$ (uncertainty interval). Arrows identify the model error δ_{model} or its maximum $|\hat{\delta}_{\mathrm{model}}|_{\mathrm{max}}$ and minimum $|\hat{\delta}_{\mathrm{model}}|_{\mathrm{min}}$ values. Case 1 $\rightarrow |E| \gg U_{(\mathrm{val},95)}$; Case 2 $\rightarrow |E| \ll U_{(\mathrm{val},95)}$; Case 3 $\rightarrow |E|$ and $U_{(\mathrm{val},95)}$ are of the same order of magnitude, 3a $\rightarrow |E| \geq U_{(\mathrm{val},95)}$; 3b $\rightarrow |E| < U_{(\mathrm{val},95)}$.

As for example, the double-counting when numerical, experimental and input errors are assumed to be independent or when the signed estimated numerical error is converted into a $\pm$ symmetric uncertainty. Therefore, $C = 7$ is proposed in [9].

The outcome of the V&V 2009 validation procedure is an assessment of the model error δ_{model}. The decision of whether or not a given model error is acceptable for a specific application (or what do we do with that information) is a different kind of problem. It is an engineering management decision that cannot be addressed in general. Depending on the purpose of the use of the model, one can imagine situations where the assessment of δ_{model} provided by any of the four options of the algorithm above leads to an acceptable or to an unacceptable model.

EXAMPLES OF APPLICATION

Heat transfer validation example from V&V20-2009

The example presented in [3] is based on a model to determine the heat transfer rate q (validation variable) of a fin-tube heat exchanger composed of a fully developed flow of a hot fluid inside a round tube. As illustrated in [3], square fins are attached to the outside tube wall to enhance the heat transfer to the surrounding cooling air at temperature T_∞. The operating condition is defined by the Reynolds number of the flow inside the tube Re, inlet temperature of the hot fluid T_i and T_∞. The Re number depends on the fluid density ρ and viscosity μ, volumetric flow rate Q and inner tube diameter d_1. Details of the geometry and flow conditions are given in [3] (Table 7-3-1).

The experimental value of the validation variable q_D is obtained from

$$q_D = \rho Q C_p \left(T_i - T_o\right) \, , \tag{16}$$

where C_p is the specific heat of the hot fluid and T_i and T_o are the bulk fluid temperatures at the inlet and outlet of the heat exchanger, respectively. Therefore, the experimental determination of q_D requires three measured quantities (Q, T_i and T_o) and two fluid properties (ρ and C_p).

The simulation is based on the numerical solution of the partial differential equation that expresses linear steady heat conduction with convective boundary conditions. In [3], two models are tested: one assuming perfect contact at the interface of the tube and fin (designated by S1) and a second model that includes a contact conductance at the fin/tube interface (designated by S2). Details of the model domain, equations, and boundary conditions as well as discretization techniques and solution algorithm are given in [3]. For the present illustration, the most important feature of the model is the equation that determines the simulated value of the validation variable q_S

$$q_S = \rho Q C_p \left(T_o - T_\infty\right) \left[exp\left(\frac{\overline{\mathrm{U}}_1 A_1}{\rho Q C_p}\right) - 1 \right] \, , \tag{17}$$

where $\overline{\mathrm{U}}_1$ is the axially averaged overall heat transfer coefficient and A_1 is the wetted area of the tube's inner surface. The de-

TABLE 1. Simulation results, numerical and input uncertainties for the mean value of q using a model with (S1) and without (S2) contact conductance at the fin/tube interface.

Model	q_S(W)	u_{num}(W)	u_{input}(W)
S1	97.2	0.07	6.37
S2	73.8	0.01	5.18

termination of $\overline{\mathrm{U}}_1$ requires the knowledge of the convective heat transfer coefficients on the inside h_1 and outside h_2 of the bare tube, the thermal conductivity of the tube k_t, the thermal conductivity of the fin k_f and the convective heat transfer coefficient on the fin surface h_f. Model S2 requires also the contact conductance at the fin/tube interface h_c. Therefore, the model(s) input parameters include experimentally measured data (Q, T_i and T_∞), fluid properties (ρ and C_p), material properties (k_t and k_f), convective heat transfer coefficients (h_1, h_2 and h_f) and for model S2 the contact conductance h_c.

In [3], the validation methodology is applied to the data obtained from each of the 10 synthetic experiments available and to the mean value of q. Such approach is enabled by the availability of the simulation input parameters (Q, T_i and T_∞) for each of the experimental realizations. For the sake of simplicity, the present description is restricted to the value obtained for the mean value of q. Furthermore, in [3], experimental, input and validation standard uncertainties are estimated using propagation and sampling techniques. Without any loss of generality, only the data obtained from the propagation approach is presented. All details of the determination of experimental, numerical, input and validation uncertainties given in [3] are not repeated in this paper. Nonetheless, the basic assumptions required for their determination are recalled.

The estimated experimental standard uncertainty u_D includes random contributions for Q, T_i and T_o and systematic contributions for all five variables (ρ, Q, C_p, T_i and T_o) [3]. The systematic uncertainties of T_i and T_o are perfectly correlated and all other contributions are uncorrelated. The experimental data for the validation variable are $q_D = 74.9$W and $u_D = 2.17$W (2.9%).

For both models, the numerical uncertainty u_{num} is estimated using the Grid Convergence Index [11] applied to two grid triplets that cover a grid refinement ratio of approximately 4. For the selected level of grid refinement, the estimated numerical uncertainties are at least one order of magnitude smaller than u_D for both models. The outcome of the simulations for the two models is summarized in table 1.

The simulation input parameter uncertainty u_{input} depends on random uncertainties of Q and bulk fluid temperature T_{fl} (related to T_i) and on systematic uncertainties from all input variables including thermal conductivity coefficients (k_t and k_f), convective heat transfer coefficients (h_1, h_2 and h_f), fluid properties (ρ and C_p), operating conditions (Q, T_{fl} and T_∞) and contact conductance (h_c) for model S2. Using the standard uncertainties given in [3] for the ten/eleven input variables, the estimated values for the simulation input parameter uncertainty are given in Table 1.

The determination of the comparison error (Eqn. (3)) for the validation variable $E(q)$ is straightforward using q_D, q_{S1} and q_{S2}. On the other hand, the estimation of the width of the interval that should contain δ_{model} with a given degree of confidence requires further assumptions. For the sake of simplicity, but without any loss of generality, we will assume Gaussian error distributions and 95% confidence level to determine $U_{(\mathrm{val},95)} = 2u_{\mathrm{val}}$. Three different situations for the determination of u_{val} are analyzed:

1. Strong model that considers all input variables part of the model ($u_{\mathrm{input}} = 0$)

$$\left(U_{(\mathrm{val},95)}\right)_0 = 2\sqrt{u_D^2 + u_{\mathrm{num}}^2} \, .$$

2. Input parameter uncertainty quantified for all input parameters assuming that u_D, u_{num} and u_{input} are independent[4].

$$\left(U_{(\mathrm{val},95)}\right)_1 = 2\sqrt{u_D^2 + u_{\mathrm{num}}^2 + u_{\mathrm{input}}^2} \, .$$

3. Eqns. (16) and (17) show that there are several variables that affect u_D and u_{input} (Q, T_i, ρ and C_p). Therefore, u_{val} should not be determined from Eqn. (10). V&V20-2009 [3] describes in detail the determination of u_{val} taking into account the shared uncertainties and correlations between input/measured variables. The propagation equation includes contributions of five different types: uncertain parameters that impact both the simulation and experimental values of q; uncertain parameters that only affect q_S; uncertainty parameters that only affect q_D; numerical uncertainty and correlated bias errors that impact both the simulation and experiment.

In the present example, the validation uncertainties obtained with the second and third alternatives differ only 0.05% of q_D and so only $\left(U_{(\mathrm{val},95)}\right)_1$ is presented. However, this is no guarantee that assuming independent contributions is always reasonable (even if it is more conservative). As discussed in [3], the value of u_{val} is dominated by the contributions of input parameters that affect only the simulation and so the double accounting from ignoring shared error sources has a negligible effect on u_{val}.

[4] As stated in [3], u_D and u_{input} are correlated, but such approach is often used in practical applications. Furthermore, [3] also shows that the effect of correlation is negligible.

TABLE 2. Comparison error, validation uncertainties with $\left(U_{(\text{val},95)}\right)_1$ and without $\left(U_{(\text{val},95)}\right)_0$ input parameter uncertainties and estimated intervals that contain δ_{model} of the validation variable (mean value of q) for the models without (S1) and with (S2) contact conductance at the fin/tube interface. Comparison error E is normalized by the experimental result $q_D = 74.9$W.

$\delta_{\text{input}} = 0$

Model	E (%)	$\left(U_{(\text{val},95)}\right)_0$ (%)	δ_{model} (%)
S1	29.8	5.79	[24.0 ; 35.6]
S2	-1.47	5.79	[−7.26 ; 4.32]

$\delta_{\text{input}} \neq 0$

Model	E (%)	$\left(U_{(\text{val},95)}\right)_1$ (%)	δ_{model} (%)
S1	29.8	18.0	[11.8 ; 47.8]
S2	-1.47	15.0	[−16.5 ; 13.5]

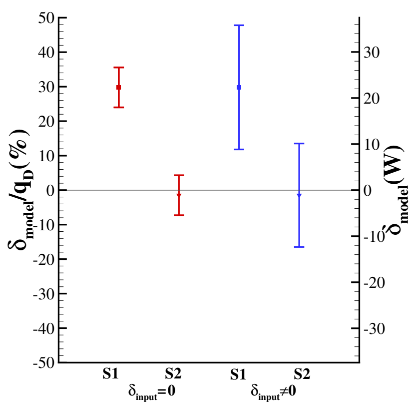

FIGURE 2. Estimated intervals that contain δ_{model} of the validation variable (mean value of q) for the models without (S1) and with (S2) contact conductance at the fin/tube interface.

Table 2 presents the comparison error E, validation uncertainties with $\left(U_{(\text{val},95)}\right)_1$ and without $\left(U_{(\text{val},95)}\right)_0$ input parameter uncertainties and the corresponding intervals that should contain δ_{model} with 95 % confidence. Results are presented for the models without (S1) and with (S2) contact conductance at the fin/tube interface in percentage of the experimental value of the validation variable q_D. Fig. 2 presents the same data in graphical form.

For the strong version of the models ($\delta_{\text{input}} = 0$), it is clear that the inclusion of the contact conductance reduces δ_{model}, as expected. However, from the validation perspective there are slight changes between the two estimated intervals. For S1, the validation uncertainty is smaller than the comparison error (Case 3a) and so there is an indication that the model over predicts the validation variable. On the other hand, $\left(U_{(\text{val},95)}\right)_0 > |E|$ for S2 (Case 3b) and so the model error may be positive or negative. In both cases, the validation uncertainty is dominated by the experimental uncertainty and so the reduction of the width of the intervals that contain δ_{model} (11.6%) can only be achieved by improving the quality of the experiment.

Adding δ_{input} to $\left(U_{(\text{val},95)}\right)_1$ instead of including it in δ_{model} leads to a significant growth of the validation uncertainty. Therefore, the width of the intervals that should contain δ_{model} increases significantly, from 11.6% to 36.0% (S1) and 30.0% (S2). Results obtained for the S1 model still correspond to Case 3a suggesting that the over prediction of the validation variable is a consequence of missing physics in the model. On the other hand, for the model including contact conductance (S2) the data correspond to Case 2 with the validation uncertainty much larger than the comparison error. As depicted in Fig. 2, the estimated intervals for the two models overlap.

As discussed in [3], one of the main advantages of the V&V20-2009 methodology is that it provides information to trace the origin of unacceptable validation uncertainties. Therefore, it shows where are improvements required: experiments, numerical simulations or definition of input parameters.

Cantilever beam validation example from V&V10.1-2012

The validation exercise described in [4] is an elastic, hollow, tapered, cantilever, box beam under a uniform loading applied over half the length of the beam. The validation variable is the transverse tip deflection of the beam w. Details of the geometry are given in [4], including the constraints to apply at the "fixed-end" of the beam, where the rotational constraint is assumed to vary linearly with the magnitude of the moment reaction.

The validation variable is measured directly using a displacement transducer, which is the simplest of the four alternatives described in [3] for validation variables.

The simulations are based on the numerical solution of the equation of static Bernoulli-Euler beam theory, which requires the experimental values of the modulus of elasticity[5] of the beam material Y and the flexibility of the linear rotational spring restraining the beam at its constrained end f_r. Beam geometry and loading are assumed to have exact values.

As in the previous example, the numerical uncertainty is estimated with the GCI [11] using a grid triplet. However, the simulations for the estimation of u_{num} are performed with $f_r = 0$. Nonetheless, as mentioned in [4], the contribution of the support rotation to the tip deflection can simply be added to that due to beam deformation. Therefore, it is expected that u_{num} is similar to that obtained with $f_r > 0$. Using the data presented in [4] the estimated value of u_{num} is only 0.05% of the estimate of the exact

[5]The notation is not identical to [4] to avoid confusion with the comparison error.

TABLE 3. Experimental and simulated values of the validation variable w and experimental and input standard uncertainties for approach 1 presented in [4]. Cantilever beam validation example.

w_D (mm)	w_S (mm)	u_D (mm)	u_{input} (mm)
-15.0	-14.2	0.25	0.24

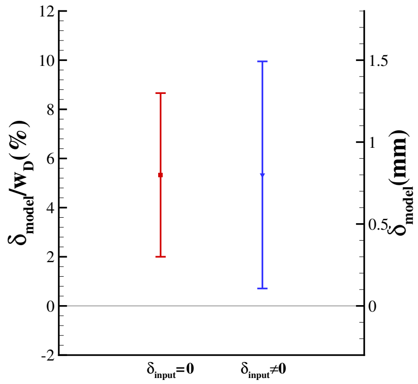

FIGURE 3. Estimated intervals that contain δ_{model} of the validation variable (mean value of w) for the approach 1 presented in [4] of the cantilever beam validation example. Reference value is the experimental value w_D.

solution of the mathematical model (with $f_r = 0$). This value is sufficiently small to be ignored in the determination of u_{val}.

For the experimental and input uncertainties, two different approaches are presented in [4]: values obtained from subject matter experts (approach 1); experimental uncertainty is estimated from 10 replicates of the measurement using 10 nominal identical beams and input uncertainty is estimated using extra experiments and simulations (approach 2).

Approach 1 In this approach there is an experimental result w_D from a single experiment and a simulation result w_S with a negligible numerical uncertainty performed with the nominal value of Y and f_r derived from a single additional experiment.

In such conditions, rigorous application of the V&V20-2009 procedure cannot be performed because there is no direct knowledge of u_D and u_{input} and so it is not possible to estimate u_{val}. Unfortunately, such conditions are not unusual in many practical applications that replace proper estimation of u_D and u_{input} by information obtained from subject matter experts to perform "quantitative" estimates of the model error. The data provided in [4] is summarized in Table 3.

Assuming normal probability density functions for experimental and input uncertainties, as suggested in [4], the intervals that should contain the model error with 95% confidence are presented in Table 4 and Fig. 3. For both alternatives, $|E| > U_{val}$ (Case 3a) and so the results suggest that the model error is positive. In this case, estimated experimental and input parameter uncertainties are similar and so $\left(U_{(\text{val},95)}\right)_1$ does not have a dominant contribution. However, it must be reinforced that replacing direct estimation of experimental and input parameter uncertainties by information obtained from subject matter experts is not a recommended approach for validation exercises.

TABLE 4. Comparison error, validation uncertainties $\left(U_{(\text{val},95)}\right)$ with and without input parameter uncertainties and estimated intervals that contain δ_{model} of the validation variable (mean value of w) for approach 1 presented in [4] of the cantilever beam validation example. Reference value is the experimental value $w_D = -15.0$(mm).

δ_{input}	E (%)	$\left(U_{(\text{val},95)}\right)$ (%)	δ_{model} (%)
0	5.33	3.33	[2.00 ; 8.66]
$\neq 0$	5.33	4.62	[0.71 ; 9.95]

Approach 2 The second approach reported in [4] uses 10 replicates of the measurement using 10 nominal identical beams to estimate the experimental uncertainty. As stated in [4], *the uncertainty in the response of the beam is due to random and systematic uncertainty in the multiple experimental measurements as well as variability in the properties of the test article*. The reported values of the mean tip deflection and standard deviation of the 10 experiments are -15.4mm and 0.57mm, respectively.

Input parameter uncertainty (in Y and f_r) is addressed with extra experiments and simulations. The variability in Y *is due to inherent variations in the material, and these variations cannot be eliminated in the production of the beam or in the validation experiment* [4]. On the other hand, the variability of f_r *is a combination of experimental measurement uncertainty and variability in repeatedly attaching the special beam to the test fixture* [4].

For Y, replicate experiments are performed on coupon samples taken from the same material, whereas a mixture of experiments performed on a specially made and instrumented beam combined with high-fidelity simulations (parameter estimation) is used to estimate the uncertainty in the support flexibility f_r. In both cases, Y and f_R are described by normal probability density functions. The mean value of Y differs 1.6% from the nominal value (used in approach 1) and its standard deviation is 5.1% of the nominal value, whereas the mean value of f_r is identical to the value used in approach 1 and the standard deviation is 5.1% of the mean value. The effect of these uncertainties in the input parameters is propagated through the mathematical/computational

TABLE 5. Experimental and simulated values of the validation variable w and experimental and input standard uncertainties for approach 2 presented in [4]. Cantilever beam validation example.

w_D (mm)	w_S (mm)	u_D (mm)	u_{input} (mm)
-15.4	-14.1	0.57	0.65

model using Monte Carlo simulations to obtain a mean value of -14.1mm and a standard deviation of 0.65mm. Although not stated in [4], we will assume that a normal PDF is a good fit to the distribution obtained for the tip deflection.

The determination of the comparison error E for the mean value of the ten individual experiments is straightforward. However, the determination of the validation uncertainty for the mean deflection is more delicate. Unlike the example of [3], the different sources of experimental uncertainty are not known and so assumptions have to be made for the estimation of u_D for the mean value of the 10 measurements. If experimental uncertainty is dominated by random contributions, the standard deviation of the mean would be equal to the standard deviation of the N samples divided by $\sqrt{N}$. On the other hand, if systematic uncertainties are dominant the standard uncertainty of the mean is not affected by N. The same reasoning applies to u_{input} for the mean tip deflection.

In the absence of the required information, we take a conservative approach and assume that u_D and u_{input} for the mean tip deflection are equal to the reported values of the standard deviations of the (normal) PDF's that characterize w_D and w_S. Table 5 summarizes the values required for the application of the V&V20-2009 procedure.

Table 6 and Fig. 4 present the comparison errors and validation uncertainties with and without input uncertainties included in the validation uncertainty. The validation uncertainties obtained from subject matter experts are smaller than those estimated from replicate experiments and extra simulations, which leads to an increase of the intervals width when compared to approach 1. As a consequence, the estimate that includes u_{input} in $U_{(\mathrm{val},95)}$ exhibits a validation uncertainty larger than the absolute value of the comparison error (Case 3b) and so in that case the model error may be positive or negative.

The V&V10 framework

Although the focus of this paper is V&V20-2009, we point out the three main differences between the procedure presented above and the application of the V&V10 approach as described in [4]:

1. Validation requirements should be established to decide if the model is acceptable.
2. The validation variable is represented by a cumulative distribution function (CDF) for both experiments and simulations, which is a consequence of a probability density function (PDF).
3. The model error is assessed by the area metric that depends on the absolute value of the difference between the CDF's of the experiments and simulations.

TABLE 6. Comparison error, validation uncertainties $\left(U_{(\mathrm{val},95)}\right)$ with and without input parameter uncertainties and estimated intervals that contain δ_{model} of the validation variable (mean value of w) for the approach 2 presented in [4] of the cantilever beam validation example. Reference value is the experimental value $w_D = -15.4$(mm).

δ_{input}	E (%)	$\left(U_{(\mathrm{val},95)}\right)_0$ (%)	δ_{model} (%)
0	8.44	7.40	[1.04 ; 15.84]
$\neq 0$	8.44	11.2	[−2.76 ; 19.6]

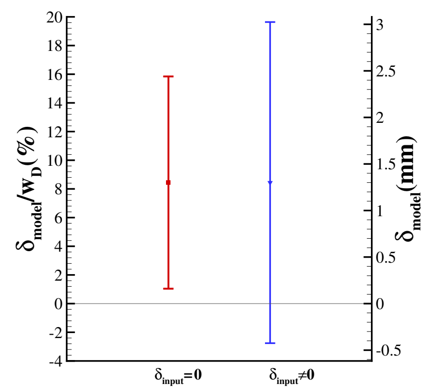

FIGURE 4. Estimated intervals that contain δ_{model} of the validation variable (mean value of w) for the approach 2 presented in [4] of the cantilever beam validation example. Reference value is the experimental value w_D.

This means that using the approach described in [4], the experimental and simulated values of the validation variables are distributions and the evaluation of the model error is a scalar.

FINAL REMARKS

There are four main observations that must be repeated to avoid the misuse of V&V20-2009:

1. The procedure **cannot** be applied without the estimates of experimental and numerical uncertainties. Input parameter uncertainties can be included in the model error (strong ver-

sion of the model) or accounted for in the validation procedure;
2. The purpose of the procedure **is not** to obtain $|E| < U_{\text{val},\%}$. The goal is to estimate δ_{model} and so the desired result is $|E| \gg U_{\text{val},\%}$, which determines a precise estimate of δ_{model}. Note that if we want to improve the precision of the estimate of δ_{model}, we must focus solely on reducing $U_{\text{val},\%}$.
3. The value of the validation uncertainty does not reflect the quality of the model. u_{val} depends on the quality of the experiment u_D, quality of the numerical simulations u_{num} and definition of the input parameters u_{input}.
4. There is no assumption about the probability distributions that characterize the experimental, numerical and input parameter uncertainties. However, the determination of the degree of confidence of the estimated interval requires the knowledge (or assumptions) about the type of distribution (that can be **any** distribution).

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