CFD VALIDATION EXPERIMENTS: WHAT'S THE DIFFERENCE?

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1 INTRODUCTION

Nuclear safety calculations have traditionally been performed using control-volume-based safety codes such as RELAP [1] and TRACE [2]. However, the capabilities of Computation Fluid Dynamics (CFD) have grown steadily since its inception, making it a very attractive alternative tool for design and safety calculations in nuclear power applications. While it is not practical to use CFD to simulate all of the components and coupled physics in a full nuclear reactor, it can provide much more detailed information about a small portion of the plant than safety codes.

Before CFD can be used for decision making, the uncertainty of the calculations must be found. To quantify the uncertainty of the calculations, the code and solution must be "Verified" (a process that will not be discussed here but is described in detail in [3, 4] and elsewhere) and the model "Validated" against experimental data. While it may be tempting to use experimental results found in published literature for validation, such a practice can lead to unacceptable uncertainties because the values of important model inputs are typically not included in journal articles. In particular, validation experiments that are relevant to nuclear energy generation are a necessity. This article will discuss some of the unique aspects of CFD validation experiments based on the literature and the author's recent experiences. We will begin by discussing the validation process, then distinguishing validation experiments from traditional experiments. The unique features, benefits, and requirements of validation experiments will then be discussed.

2 VALIDATION

While the specifics of how validation is performed are outside the scope of this paper. a very simple statement of the process could be matching the system response of a model to an experiment where the inputs of the model (the boundary conditions, inflow conditions, fluid properties, etc.) are matched to the experiment. The American Institute of Aeronautics and Astronautics, the American Society of Mechanical Engineers and the U.S. Department of Defense each use the same definition of validation: "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." [4–6]. The interpretation of the phrase "intended uses of the model" remains somewhat controversial. Here we use the term "validation" to mean any intended use of the model, regardless of the level of complexity of the system or the physics involved. With the topic of this article being

CFD validation, we will concentrate on relatively simple systems and physics, such as occur in the separate effects tests defined below.

2.1 CFD Validation and the Validation Hierarchy

The idea of performing validation through a “building block” approach was was developed in the 1980s and 1990s in the aerodynamics and nuclear community [3]. Validation is typically performed using an approach that divides the engineering system of interest into three or four progressively simpler levels of complexity (or tiers): subsystem cases, benchmark cases, and unit problems. The lowest tier is referred to as “separate effects testing” in the nuclear energy community. This paper will focus on the lower tier, in which the geometry is simplified and high-resolution measurements are made because these are the problems for which CFD is typically used.

2.2 Goal of Validation Experiments

The purpose of performing a validation experiment is to provide the information required to quantify the uncertainty of a mathematical model. In the vast majority of cases, the model will be solved numerically. The accuracy of the code and the numerical solution is the domain of verification, which also forms part of the total uncertainty of a simulation. Confirming that the code is written correctly (code verification) and is solving the partial differential equations sufficiently accurately (solution verification) provide one part of the model’s uncertainty. Verification will not be discussed in this article, but we note that there are many excellent sources on verification including [3, 7].

Validation is used to determine the accuracy of the physics model that the code is solving. Validation experiments provide the information necessary to determine the accuracy of the physics model.

3 TRADITIONAL EXPERIMENTS

Traditional experiments have been divided into three general categories based on the goal of each [8, 9] which are described in the following sections.

3.1 Discovery Experiments

Discovery (or physical discovery) experiments are conducted to improve the fundamental understanding of some physical process and their results are commonly published in journals. Examples include experiments to determine the characteristics of transient convection [10], or to measure fundamental fluid turbulence characteristics in two-phase flow [11].

3.2 Model Calibration Experiments

Model calibration, or model tuning experiments are conducted to construct, improve, or determine parameters in mathematical models. Examples include (a) experiments measuring reaction rate parameters in reacting or detonating flows, (b) experiments calibrating parameters in a turbulence mode, and (c) experiments calibrating mass diffusion rate parameters in a mass-transport chemistry model.

3.3 Acceptance Tests

Acceptance tests are experiments that determine the reliability, performance, or safety of components, subsystems, or complete systems. Examples include (a) tests of new combustor designs in gas turbine engines, (b) tests of multi-element flap designs for a new wing, and (c) safety tests of the emergency cooling systems in nuclear reactors.

4 VALIDATION EXPERIMENTS

Only recently have experiments been performed with the specific purpose of providing data for validation. A validation experiment is conducted in order to determine the predictive capability of a mathematical model of a physical process. In other words, a validation experiment is designed, executed, and analyzed in order to quantitatively determine the ability of the model and its embodiment in a computer code to simulate a well-characterized physical process.

In a validation experiment, the model builder or computational analyst is the primary customer. It was not until the last two decades that scientific computing matured to a point where it could even be considered an independent stakeholder or customer in experimental activities. During this time, model builders and CFD analysts have had very limited success using one of the three types of traditional experiments for model validation because the level of detail of reported information is typically insufficient.

Another unique aspect of validation experiments is that traditional experiments place a great deal of emphasis on repeatability of an experiment and the quality of the inflow conditions. Measurements of physical processes can only be reliably repeated by other experimenters when a controlled environment is used. Also, the results may only be considered general with an idealized inflow.

For validation experiments, the characterization of the experiment is the primary goal. By characterization we mean measuring all important characteristics of the experiment necessary for input to the simulation of the experiment. Simulations require detailed information both of fluid properties and detailed information concerning the boundary conditions, (e.g., inflow velocity and free-stream turbulence distributions). In other words, assuming that all data are acquired simultaneously, control and repeatability of the experiment are less important in a validation experiment than precisely measuring the conditions that impact the modeling of this particular experiment. For example, in an uncontrolled experiment, such as atmospheric flow around a city, the critical issue is measuring the important features of geometry, initial conditions, and boundary conditions that exist during the time frame of the validation experiment.

In some cases, it may not be possible to acquire all data simultaneously. For instance, inflow data and system response data may be acquired at separate times using the same measurement system. In this circumstance, it is essential that conditions be recorded *and* repeated as closely as possible. This can be challenging as common laboratory HVAC systems allow the room temperature to fluctuate over large temperature ranges and atmospheric pressure varies from one day to the next. One solution is to trigger data acquisition based on room conditions. The expense of this scheme may motivate the use of additional synchronized acquisition systems to enable simultaneous acquisition of all data. In some experiments (especially those with unstable separated flow regions), the experiment may tend to one state on one day and a different state later. These effects should be avoided.

Experiments of any type normally focus on reporting the experimental outputs (termed System Response Quantities, or SRQs). In validation experiments, the output may constitute a minor part of the experimental effort, while emphasis is placed on measuring experimental inputs such as boundary conditions and inflow. In fact, measuring some SRQs may compromise other aspects of a validation experiment by introducing obstructive probes or using measurements of unknown uncertainty.

It is difficult to specify exactly which data are required for a CFD validation experiment to define the model inputs, since this may vary from one case to another. The broadest statement that can be made is that one must measure all information required by the modeler as input to the model. In a typical low-speed wind tunnel experiment, this will include the inflow velocity. However, for a natural convection experiment, the modeler may prefer the pressure change across the test section to the inflow. Even the modeler's choice in turbulence model may impact the necessary inflow information (e.g. a $k - \epsilon$ model requires the mean velocity, turbulence kinetic energy and dissipation rate while a Reynolds stress model may require all of the Reynolds stresses). Clearly, it is not possible to design and execute a quality validation experiment without the involvement of modelers.

5 VALIDATION EXPERIMENT FEATURES

Two fundamental types of information must be captured in a validation experiment: information on input data and information on output data for a potential mathematical model. Stated differently, the focus of a validation experiment is information needed for the model, not information needed to understand the physics occurring in the experiment. These two fundamental types of information can be separated into six independent attributes described in the subsections below. For a much more detailed description of these attributes, the reader may consult [12].

5.1 Experimental Facility

This attribute requires information concerned with the functional operation and design of the facility and its operating procedures. The attribute gathers information on (a) how a facility works, (b) how flow conditions are controlled, (c) how the flow is conditioned ahead of the test section, and (d) how it was operated for the validation experiment being assessed.

One of the most important features of the facility to enable high-fidelity modeling of the flow in the test section is the flow conditioning upstream of the test section. Details of the flow, turbulence, and temperature conditioning system should be provided. This information should include the types of screens and honeycomb used and their spacing, the three-dimensional geometry of the contraction section (including any wall irregularities) and hardware for mounting probes.

5.2 Analog Instrumentation and Signal Processing

This attribute refers to all of the important sensors used in the experiment, including transducers, all of the analog acquisition and recording equipment, as well as all data reduction and analog and digital signal processing. In many cases, signal conditioning is performed in the same package as the sensor, which does not remove the need for a description of the signal conditioning. This is particularly important if filtering of the analog output signal from the sensor is performed within the instrument (before being digitally sampled or recorded) and when time-varying quantities are measured.

The information provided for this attribute will be used to interpret the quality, accuracy, and usability of the experimental data. Without this information about the instrumentation and signal processing, it may be impossible to understand, or the CFD analyst may misinterpret the measurement reported results. For example, lack of information dealing with the time correlation of two signals measured with different sensors may not allow a useful interpretation of the two measurements. Also, lack of information about the analog or digital time averaging of a sensor output in the experiment will not allow a CFD analyst to apply an analogous time filter to the simulation outputs. An additional reason for requiring this information is that new information may come to light about the temporal or spatial resolution of a certain measurement technique. This new information may alter the interpretation of the performance of the measurement technique.

In optical measurements, lenses and optical filters fall under signal processing. This information may be used to better understand subtle aspects of the data that might go unnoticed to the experimentalist and uncertainty sources of which the experimentalist may be unaware. For example, when using particle-imaging velocimetry (PIV), the optical features and the related assumptions in a measurement directly impact the measurement uncertainty in a manner that is a current research topic [13].

Any and all digital processing of the data, including assumptions made in the processing, must also be reported. This could range from subtraction of an offset in a pressure measurement to time averaging, to application of a median filter to signal processing in the frequency domain. Each digital operation should be described in detail. Ideally, the code used to perform the digital processing should be made available.

5.3 Boundary and Initial Conditions

Obtaining boundary condition (BC) and initial condition (IC) data is critically important because these data are directly used as inputs to the CFD simulation of the experiment and can often impact the system response. If the CFD simulation defines the computational domain as the test section, then the inflow and wall boundary conditions must be provided by the experimentalist and reported as part of the experiment. Special care to repeat experimental conditions is required if all measurements are not obtained simultaneously with the measurement of the SRQs of interest. Any lack of repeatability should be quantified. If the inflow conditions vary as a function of run time of the facility, then the inflow conditions should be given as a function of time.

Knowing what information is required by the CFD analyst for the outflow boundary conditions can be problematic. If the streamwise component of the flow velocity over the entire outflow plane is downstream, then the typical outflow boundary condition imposed by the analyst is to set the streamwise derivative of all dependent variables in the PDEs to zero or to set the downstream pressure. To assess whether this modeling assumption is justified, the experimentalist would be required to measure at least some of the flow quantities at the exit of the test section. If reverse flow exists at the exit of the test section, i.e., flow is in the upstream direction, then the information required from the experimentalist is significantly increased. For example, the experimentalist would need to better characterize the spatial and temporal distribution of flow at the exit of the test section or provide detailed geometric information about the mounting structure holding any test article in position and possibly the geometric features of the facility downstream of the test section so that the analyst could move the outflow boundary aft of the test section.

5.4 Fluid and Material Properties

Properties of the fluid are required inputs to any simulation of a fluid system. For a simulation that includes the energy equation, the experimentalist must also report the dependence of all fluid properties on temperature and pressure. To provide this information, the composition of the working fluid must be precisely reported. For instance, the simple case of air, it is necessary to report the fluid properties at the condition upstream of the test section. This would include pressure, temperature, relative humidity, and possibly air composition for an expected unusual composition. For a water tunnel, information would be required about the amount of dissolved air, any bubbles, particles, contaminants, or salt in the water.

For CFD simulations that would include heat transfer through the walls of the test article or through the walls of the test section, the experiment should document the thermal transport properties of each of the walls. This would include information such as thermal conductivity and thermal emissivity, including spatial variation of these quantities.

5.5 Test Conditions

This attribute is similar to the Boundary and Initial Conditions attribute, but here the emphasis is on reporting detailed temporal variation of conditions during an experiment or series of experiments. For a long-running experiment, the room conditions can change during the experiment either because of changes in atmospheric conditions or recirculation of heated or cooled air in the room. In addition, there could be changes in conditions at the exit of a facility, such as a wind tunnel that exhausts outdoors. For these types of facilities, environmental monitoring equipment should be used that automatically logs all pertinent environmental variables. Records from these logs should be reported in the documentation of the experiment.

5.6 Measurement of System Responses

This attribute deals with the measurement of system responses during the execution of the experiment that could be compared to the output of a CFD simulation. These quantities can be the dependent variables in the Partial Differential Equations (PDEs) being solved in the simulation of the experiment, any derived quantities such as forces or surface heat flux, or any other quantities of interest. This attribute stresses two aspects of measurement of system responses: (a) spatial and temporal coverage of SRQs and (b) the number and variety of SRQs measured. Spatial and temporal coverage refers to the range of spatial dimensionality and time scales over which SRQs are measured. The range of spatial dimensionality can vary from measurements (a) at a point in space; (b) along a line (for example, on a line spanning 360 degrees along the surface of a sphere); (c) in a 2-D plane in space (for example, in a streamwise plane near a model geometry of interest); and (d) in a 3-D volume in space. In general, it becomes more difficult and time-consuming to obtain measurements over an increasing spatial domain. Some experimental techniques, however, are able to inherently obtain measurements over a plane in space, such as particle image velocimetry (PIV). For certain types of SRQs, it is also important to measure over a large range of time scales or frequency.

The number and variety of SRQs measured refers to not only the wide range of dependent variables that can be used in the formulation of the PDEs in the mathematical model, but also to the wide range of physical quantities that can be experimentally measured. From a CFD perspective, this wide range of simulation output quantities is obtained by the post-processing of dependent variables such as computing derivatives, functionals, and combinations of these quantities. For example, in a wind tunnel experiment the experimentalist can measure surface pressure and surface shear stress, forces and moments on an independently attached portion of the test article and the total body forces and moments exerted by the fluid on the test article. Stated differently, the experimentalist can measure this range of quantities, some of which are integrated by nature.

The ability to measure and predict this wide range of SRQs is an important aspect of the general concept of Measurement of System Responses. From a model validation perspective, it is extremely valuable for the experimentalist to measure a number of quantities over a wide range of physical phenomena. In this way the model validation can better assess if the mathematical model is getting the correct answer for the correct physical modeling reasons over the entire range. One method of resolving the general difficulty of measuring and predicting this range of quantities was given by [3]. They constructed a spectrum of SRQs based on whether the quantity is a derivative or an integral of a dependent variable in the PDEs. For example, an integral of pressure and fluid velocity, such as lift and draft on an object, is (in general) easier to predict and measure than the pressure and velocity of the fluid in the vicinity of the object. Similarly, predicting and measuring fluid velocity is easier than predicting and measuring the derivatives of fluid velocity components, such as local heat flux and shear stress. Once again, communication between the modeler and experimentalist is essential in choosing SRQs that are relevant and broad enough to ensure rigorous validation.

6 IMPORTANCE OF MEASUREMENT UNCERTAINTY

In order to determine the uncertainty of a model, one must propagate the uncertainty of the model inputs through the model. In order to make a meaningful comparison between the model results and the experiment, one must also have uncertainties on the SRQs. These requirements make intrusive measurements that can generate errors that are very difficult to estimate a poor choice, even when an experimentalist suspects (but cannot demonstrate) that the intrusive measurement is superior to an alternative with known uncertainty. Cutting-edge unobtrusive optical measurements, such as Particle Image Velocimetry (PIV) for fluid velocities or Planar Laser Induced Florence (PLIF) for temperature, often significantly extend measurement capability, but nearly as often have unknown uncertainty.

Going further, it is crucial that validation experiments report uncertainty that is an accurate estimate of the experimental error, rather than the result of blind adherence to an uncertainty or QA procedure. It is the author's experience that the largest uncertainty in an experiment is one of which the experimentalist is unaware [14]. However, one may easily propagate elemental instrument uncertainties through to the final result without risk of criticism and without considering the unknown uncertainties. One excellent example comes from PIV measurements. While the velocity uncertainty of measurements made with PIV has recently made excellent progress [13, 15, 16], the ability to accurately know the origin of the measurement domain remains a major issue. This spatial error is often not considered when performing uncertainty analysis on PIV measurements, yet in the presence of large gradients, it can lead to very large velocity errors.

7 IMPORTANCE OF DISSEMINATION

The requirements of validation experiments come at a cost. It is therefore crucial to maximize the benefit of the validation experiment by retaining the input and output information in a manner that is easily accessible to the numerical analyst. This has proven difficult in the past, but many efforts are underway to retain validation experiment information. These efforts vary widely in terms of accessibility and the level of data retained. Some examples will now be briefly described.

7.1 Validation Journal Articles

This is a new idea with the first such article currently in press [17]. Along with a mostly typical journal article that describes the experiment and the data, the journal will make available all of the measurements of the experimental inputs and outputs on their website. This method has features that are very attractive to academics, as the validation studies result in a publications that should garner citations.

7.2 ERCOFTAC

The European Research Community on Flow, Turbulence and Combustion (ERCOFTAC) maintains an online database of CFD validation data. The data are organized according to flow regimes, making it simple to see whether data for a given problem are currently available. The ERCOFTAC currently uses a review process to ensure that the required data are made available. The review criteria are similar to, but somewhat different from those advocated here. Data sets that have met the ERCOFTAC criteria are available only to ERCOFTAC members. Data sets that have not been so reviewed are in the public domain.

7.3 NE-KAMS

One effort to retain and disseminate validation data (as well as other knowledge connected to Validation and Verification) that is specific to the nuclear energy community is the Knowledge Base for Advanced Modeling and Simulation (NE-KAMS). The objective of this consortium effort is to establish a comprehensive and web-accessible knowledge base to provide V&V and UQ resources for modeling and simulation for nuclear reactor design, analysis and licensing. The knowledge base will serve as an important resource for technical exchange that will enable credible computational models and simulations for application to nuclear power. NE-KAMS will serve as a valuable resource for the nuclear industry, academia, the national laboratories, the U.S. Nuclear Regulatory Commission (NRC), and the public, and will help ensure the safe, economical and reliable operation of existing and future nuclear reactors. This ongoing effort is currently not available online.

8 BENEFITS OF VALIDATION EXPERIMENTS TO THE EXPERIMENTALIST

Some experimentalists bristle at the idea of their work should be a service to numerical modelers who compete with them for funding and relevance in some organizations. We would like to point out some side benefits to the experimentalist of CFD validation experiments that may not be immediately apparent.

First, we note that funding agencies are increasingly reluctant to fund expensive experiments. Done correctly, the return on investment for validation experiments is very high, since it enables further exploration of the problem of interest through CFD. Therefore, the value proposition of a validation experiment can be stronger than other experiments.

Additionally, validation experiments often call for returning to canonical flows with state-of-the-art diagnostics, which are much more powerful than the instruments used in the classical measurements. University students performing these measurements have the rare experience of immersion in canonical flows that were previously the domain of researchers from the 1960s to 1980s.

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