V&V METHODOLOGY COMPARISSONS: AIAA G-077(1998), ASME V&V 20 (2009), ASTM E1355-05a(2005), NEA/CSNI/R(2007), and NRC CSAU(1988)

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Abstract

The AIAA, ASME, NRC, NEA and NIST approaches to V&V are reviewed with emphasis on common elements and discussion of differences in intent. The AIAA, ASME, and NEA standards and guidelines apply specifically to CFD. The NIST standard as applicable to fire modeling using the Fire Dynamics Simulation (FDS) large eddy simulation CFD code as adopted by the USNRC is reviewed. The CSAU methodology was developed for reactor system simulations during anticipated transients and hypothetical accidents. CSAU is well established in the US nuclear safety community for providing best estimate simulation outcomes, with quantified uncertainties for prescribed confidence intervals.

1. Introduction

The complexity of simulations continues to escalate as computational resources allow more comprehensive modeling of physics. Nuclear reactor simulation must be carried forward with assurance of quality in simulation outcomes. Formalisms to insure defendable, accurate and well circumscribed simulation outcomes were developed for NRC to support movement to best estimate plus uncertainty approaches to modeling of emergency core cooling systems (ECCS) in 1988. Those methods define Code Scaling, Applicability and Uncertainty (CSAU) and remain in use, but many other methods have been developed since their introduction. CSAU was developed primarily for application to the main reactor system simulation codes of that time, RELAP5, TRAC, and variants.

There is need for V&V methodology that is applicable to modern CFD codes and other multi-physics simulation platforms. Simulation outcomes used to define risk to the public must be accompanied by defendable uncertainties within a confidence interval. This is a review of currently available methods to accomplish these goals. The review will supply a basis for adoption of best practices, or perhaps adoption of a menu of approaches to achieve a high quality simulation that will survive expert scrutiny, and adversarial scrutiny. A flexible V&V architecture may also provide for scaling the degree of effort invested in V&V with the impact of the simulation outcome on public safety.

Increasingly, performance based assessment or more specifically probabilistic risk assessment (PRA) is central to reactor safety evaluation. A large number of simulations and assumptions enter a PRA, including the reactor safety transient simulations, fire progression simulations, human performance models, external threat models and equipment performance and reliability models. A balanced approach to establishing the quality of the inputs to the PRA is required to insure the quality of the PRA prediction. Certainly the elements of the PRA that appear to contribute most to risk should have V&V applied to assure the models and assumptions are accurate to defined limits, and defendable. CFD and other similar simulation tools are used to establish consequences for the range of initiating circumstances posed in the PRA. V&V of the CFD simulations is needed to define accuracy of integral PRA outcomes.

2. A Comparison of the Key Elements in the V&V Process

The definitions used in the standards and guidelines reviewed here are not uniform, so we must concisely define terms to make this comparison tractable, using ASME V&V 20 as the lead. We first review the V&V methods and then examine common elements and contrasting features of the methods.

2.1 ASME V&V 20[1]

The ASME process for V&V is shown in figure 1. To begin the process, ASME V&V 20 emphasizes the need to define the system to be modeled, with initial and boundary conditions prescribed, and the specific target parameters to be qualified with uncertainties also defined. With the reality of interest and parameters to be quantified defined, the assumptions and models of concepts required to undertake the simulation can be identified, moving down the right leg of figure 1. The models of concepts are some combination of conservation laws and constituitive models, implemented in a numerical solution scheme. Numerical solutions involve a grid approximation of the continuum, and a method to represent the mathematics in the conceptual model on that grid. The process of assuring the mathematics of the conceptual model is properly represented in the numerical solution coding is verification. Assuring the correct conceptual model is selected for the simulation of interest is qualification for the AIAA, and we adopt that definition here.

Experiments provide data that may be compared with simulation outcomes. The ASME suggests that legacy experiments be selected, or new experiments be conducted to support the V&V process, with the reality of interest and simulation informing the design and selection of these experiments. Experiments are often reduced in complexity and scale relative to the reality of interest, and may only challenge some limited portion of the simulation. The process of comparing simulation outcomes to experimental data is validation. ASME has standard 19.1[2] for quantifying the uncertainty in experimental data. The total uncertainty included in a direct comparison of simulation outcomes with experimental data, $U_{val.}$, includes uncertainty in the selected conceptual models, the uncertainty in the numerical approach, the uncertainty in outcomes attributed to the uncertainty in simulation inputs, and the uncertainty in the experimental data. This process is shown in figure 1.

Uncertainties are due to limitations in knowledge, and often can be well defined by probability distributions. Errors are defined as mistakes not caused by limitations in knowledge. Errors may also be introduced with the selection of conceptual models, assumptions, boundary conditions, geometry and numerical approach to solution. Errors may also occur in the acquisition and reporting of data. The errors are also included in the comparison of the simulation outcomes with experimental data, and are different from uncertainties in that error distributions are more difficult to define.

If individual uncertainties contributing to the simulation outcome are quantified, and their impact propagated through to the simulation outcome using one of several available methods, then the total expected uncertainty in the simulation outcome can be known. Similarly, the uncertainty in the data can be known. If the total expected sum of uncertainties exceeds the comparison defect between data and simulation outcomes, then all may be well. If the sum of uncertainties is less than the comparison defect, then there are errors or omissions. ASME uses the term error to represent the difference between the simulation outcomes and the experiment data. We will use the definition of error as mistakes not caused by limitations in knowledge, as introduced in the previous paragraph and as adopted by AIAA. The defect between the simulation outcome and the data will be due to uncertainty, which can be formally quantified, and perhaps may include errors.

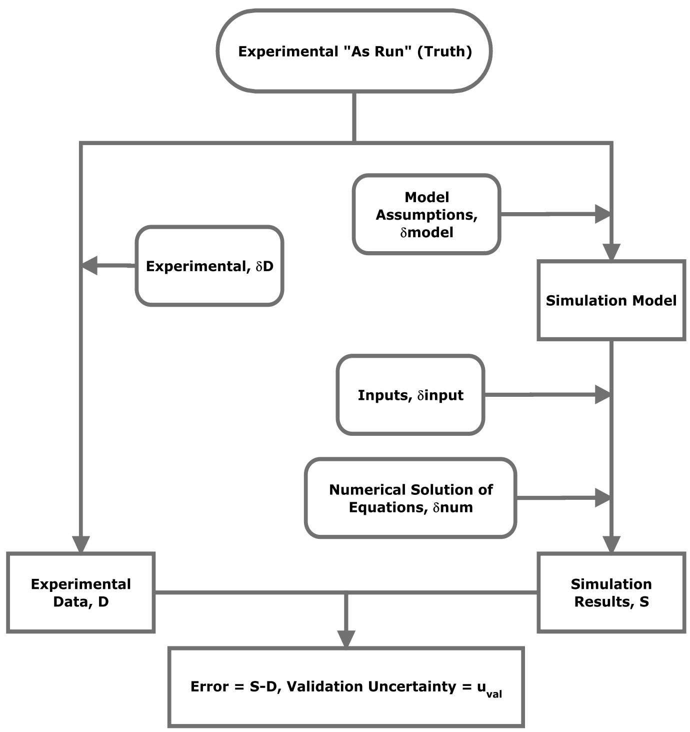

Figure 1 ASME V&V 20 Process

2.2 AIAA-G077-1998[3,4] method

The AIAA V&V method is similar to the ASME approach in Verification. Distinction is made between the conceptual model and the computational model and numerical solution. The AIAA process diagram offered in figure 2 shows verification including comparison of computation outcomes with exact solutions and benchmark solutions. Some include these activities under Validation. The AIAA offers a more structured approach to selection and construction of experiments to generate data for validation, as shown in figure 3. AIAA offers four tiers of experiments, starting with unit problems that address one or two physical processes in a very simple geometry and ending with the complete system experiment with complexity close to the real world system. Unit problem experiments can produce high resolution data for validation of a specific model in the simulation. Complete system experiments offer limited opportunity for acquisition of detailed data on a specific phenomenon.

The AIAA also encourages the experiment development be supported and coordinated with the simulation development. AIAA cautions against using data from experiments to calibrate the simulation. Calibration is the use of data to adjust variables, constants and models in the simulation. Calibration, properly executed, can support model development, or method development, but it is not validation. Calibration can introduce compensating errors when improperly executed.

Figure 4 shows the AIAA V&V activities, and offers an alternative dimension to the V&V process. Figure 4 is adopted from the Society for Computer Simulation (SCS)[5] and the definition of terms used in the AIAA guide is consistent with the SCS framework. The AIAA recommends the conceptual model be composed of all the information and mathematical equations that describe the physical system or process of interest. The conceptual model is produced from analysis and observation of the physical system. Figure 4 shows the activity of analysis converts the physical reality to conceptual models, and this is part of the development effort represented by dotted lines. Assurance that the conceptual models represent the physical reality is called code qualification.

The transformation of the conceptual models to a code is programming. Assuring the code performance represents the conceptual models is verification. The activity of predicting behavior of an experiment using the code is simulation. The assurance that the simulation outcomes are consistent with data from the experiment is validation. The depiction of activities in figure 4 is helpful to differentiating the simulation development activities from the V&V activities.

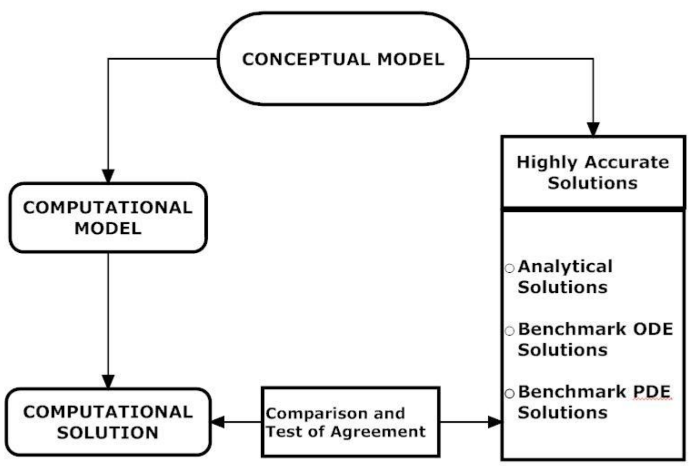

Figure 2: AIAA Verification Process

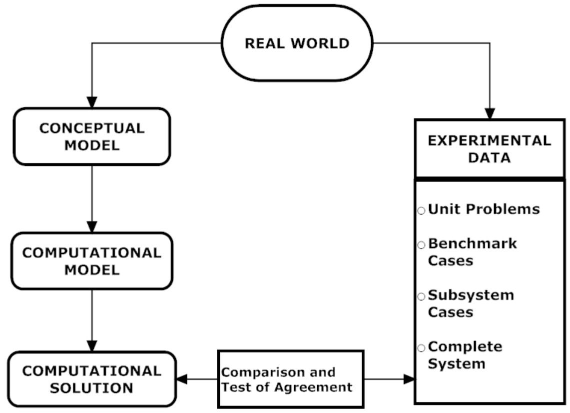

Figure 3 AIAA Validation Process

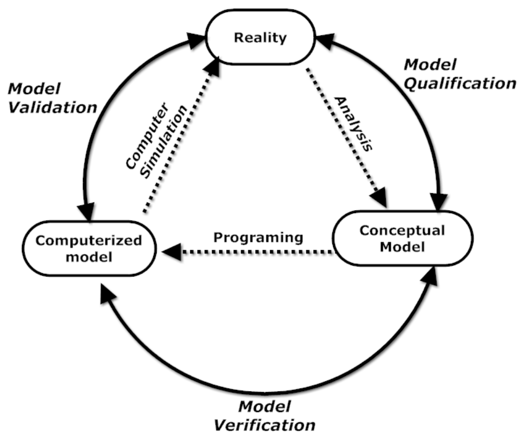

Figure 4 AIAA V&V Phases

2.3 ASTM V&V[6] Process

The ASTM V&V approach is for computational models in general, but we have reviewed the application of the ASTM technique to fire modeling in Nuclear Power Plants, as adopted by the NRC in NUREG-1824[7]. The ASTM V&V methodology is represented in figure 5 as a chain of steps that contain verification and/or validation elements. The ASTM approach, as implemented for NRC, took mature fire modeling programs and validated them for use in situations of interest to nuclear power plants. One of the programs examined was the Fire Dynamics Simulator (FDS). FDS is a finite difference Large Eddy Simulation (LES) CFD code with special provisions for fire modeling. The FDS was mature and had been compared to other fire data, so the process of validation using data representative of nuclear power plants was not conducted in parallel with the initial code development and verification. The specific parameters to be simulated were broadly defined as all parameters measured in the experiments used for validation. This approach is intended to establish the suitability of the FDS code for predicting specific parameters in certain situations found in nuclear installations.

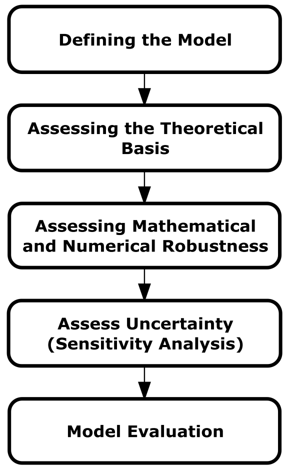

Figure 5: ASTM V&V Process

2.4 CSAU (1988)[8]

The NRC developed an approach to V&V of reactor safety codes in concert with introducing the ECCS acceptance rules that allow use of best estimate simulation outcomes when uncertainties are quantified within acceptable confidence intervals. The CSAU process that NRC developed will be considered here as a V&V process, and is shown in figure 6.

The CSAU process starts with clear definition of the reality to be simulated, the initial conditions, the boundary conditions and specific target simulation outcomes. CSAU also requires that the code be well documented and fixed throughout the process. CSAU departs from the AIAA and ASME methods in the degree of formalism associated with the qualification of the conceptual models. The code qualification begins with construction of a Phenomena Identification and Ranking Table (PIRT) using an analytical hierarchy process from decision theory. A panel of experts is required for this effort, along with a facilitator, and the outcome is a prioritized ranking of phenomena as appropriate to the reality to be simulated. This list is compared with the conceptual models in the code and the suitability of each model to the simulation demands assessed. Highly ranked phenomena in the PIRT for which conceptual models are not well developed, and for which data are not found well suited to the defined simulation challenge may require new experiments.

CSAU tests sensitivities and propagates uncertainties using well established methods such as Monte-Carlo and Latin Hypercube. There is a nodalization refinement convergence evaluation, and there are four contributions to uncertainty identified. One uncertainty is the output uncertainty associated with input uncertainties from experiments, in conjunction with associated sensitivities of outcomes to input variation. The second is associated with the experiment data uncertainty. The third uncertainty is associated with the scale of the experiments relative to the scale of the real system of interest, and the fourth is the uncertainty in outputs associated with the uncertainty in inputs required for the real system simulation of interest.

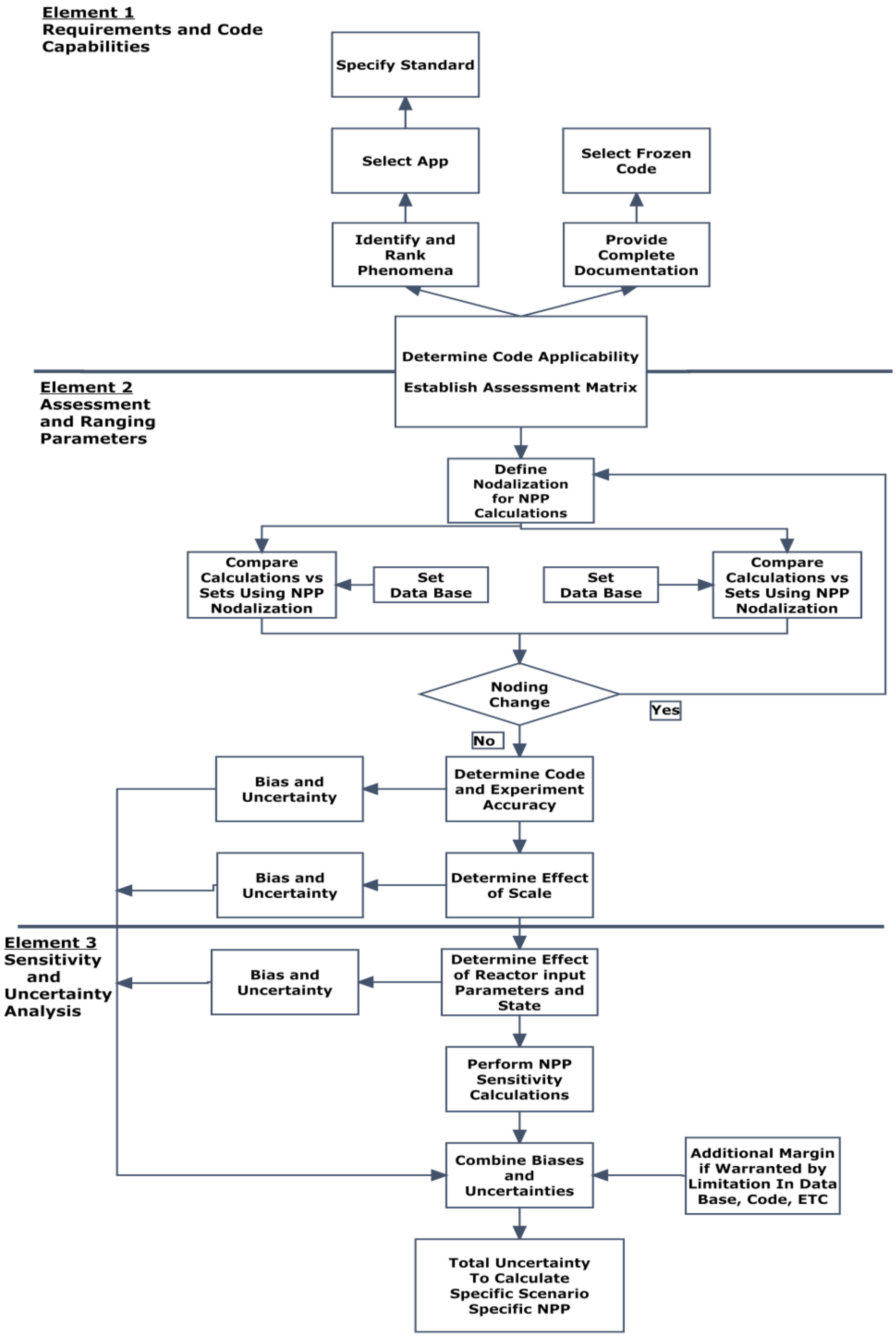

Figure 6: CSAU Process

2.5 NEA/CSNI/R (2007)[9]

The NEA Committee on the Safety of Nuclear Installations issued Best Practice Guidelines for the use of CFD in Nuclear Reactor Safety Applications in 2007. The guidelines include a V&V approach, and offer a broad overview of current CFD competencies, available benchmark data with past simulation efforts, and suggestions for CFD use in Reactor Safety Applications.

The V&V method embedded in NEA Guidelines begins with definition of the reality for simulation, and identification of target parameters for prediction. This is followed by construction of a PIRT, using an approach similar to that in the CSAU method. The NEA offers specific advice on how to select a panel of experts to insure maximum return from the PIRT development investment.

The NEA guidelines suggest the CFD code be selected after the PIRT development, with attention to the code applicability to the reality of interest. Criteria for model selection for turbulence are offered, and criteria for special modeling challenges associated with, as examples, reactor containment condensation, fire analysis, and natural convection are provided.

The NEA adopts a distinction between error and uncertainty like that of the AIAA. They also use an error hierarchy, with machine round-off errors at the bottom, proceeding up to iteration errors, then to discretization errors, and finally up to errors in the conceptual models. Approaches to quantify these errors are provided in the NEA best practices. They also suggest monitoring global balances across the computational domain to detect integral mass, momentum and energy errors.

Uncertainties are treated following approaches similar to the other methods, but NEA suggests use of the ASME PTC 19.1 for treatment of experimental data uncertainties. The NEA does not offer a specific V&V process structure. They do offer a three page check-list of activities required for a best practice calculation. They also suggest that a Quality Assurance (QA) plan be implemented for the development of code, simulation inputs and related experiments. The QA plan includes the code V&V examined here, as well as other formalized documentation, review and checking activities.

3. Composite Comparison

All the methods require the reality simulated be well defined at the start. All methods except the ASTM ask that the outcome to be predicted also be identified, with uncertainty and confidence intervals established. The methods have some differences due in part to the designed purpose of the method. The NEA and AIAA have some elements of phenomena identification and conceptual model selection in the V&V process. The CSAU and ASME presume the conceptual models and code are fixed at the start of the V&V process. CSAU presumes the code is mature and verified, so that only grid convergence tests are required once it is established the conceptual models are appropriate to the reality to be simulated.

The ASTM approach to code assessment is used in some organizations, such as the DOE and NRC, to establish if a code should be placed in a “toolbox”. Once a code is accepted to the toolbox it may be used for a certain class of evaluations. Additional V&V may be required for each specific analysis done using that tool. In some cases the DOE toolbox users must also be “qualified” to use the tool.

Using the three activities or phases defined in figure 4 from AIAA and SCS, a comparison of the V&V approaches is offered in table 1. The tasks involved in the verification process are not ubiquitous across the investigated methodologies. Various levels of guidance are provided for task execution. Table 2 displays tasks associated with each verification methodology. The method of manufactured solutions (MMS) is a general procedure for generating exact analytic solutions capable of exercising relevant features of a code. Richardson Extrapolation (RE) is one method for obtaining an error estimate as a grid is refined.

Table 1 Comparison of Approaches to V&V

	Model Qualification	Model Verification	Model Validation
AIAA	Conceptual Model is developed through observation and analysis of physical system.	Only correctness of mathematic approached used in the computational model is examined.	The degree of accuracy of the computation model as representation of reality is determined in the validation. Determine if necessary physics is included
ASME	Does not address this.	Verifies code solves math equations. Estimates numerical accuracy of a specific calculation.	Determine errors due to all assumptions and the cumulative effect of the associated uncertainties.
ASTM	Requires a peer review of the physical models.	Code checking and tests of numerical robustness of the model.	Validation is how well the model represents test data.
NEA	Experts create PIRT to prioritize models required for simulation.	Suggest use of several methods to test code fidelity to conceptual models. Also advocate use of a QA code management approach.	Comprehensive assessment of model and data uncertainty used to define total simulation uncertainty.
CSAU	Experts create PIRT to prioritize models and data required for simulation.	Assumes a mature documented code with reliable numerical approach. Nodalization is examined converged outcomes.	Conceptual model quality evaluation includes comparison to test data. Validation compares simulation to integral test data.

Table 2 Comparison of Methods used for Verification

		Code Verification			Solution Verification
	Code Checking	Code-to-Code	Exact Analytic Comparison	Grid Refinement Studies
AIAA	X		X	RE
ASME	X	X	MMS	RE
ASTM	X		X	X
CSAU				X
NEA	QA	X	X	X

ASME assumes that prior to code verification efforts, the code has been checked for coding errors. ASME states that code verification assesses code correctness and specifically involves error evaluation for a known solution. In contrast solution verification involves error estimation. The ASME “model” verification processes purely compares mathematical and computational outcomes. The AIAA's model verification strategy is to identify and quantify error in the computational model and solution. Code checking is noted as a potential source of error reduction. It is implied that this task should be performed. AIAA's solution verification process is concerned with insufficient discretization convergence, the lack of iterative convergence, and associated errors. Code checking is one of three main objectives in the ASTM model verification process. Analytic solutions, if attainable, should be compared to computational solutions. The last step in the ASTM model verification process is the estimation of the magnitude of residuals as a numerical accuracy indication and the reduction of the residuals as a convergence indicator.

CSAU assumes that a mature and documented code is being investigated, so coding errors are not addressed. It further assumes that what ASME calls code verification has been performed. CSAU model verification is concerned only with solution convergence and error estimation.

NEA suggests the use of all available methods to test code fidelity to models. NEA advocates use of a QA code management approach to reduce coding errors. It also states that manufactured solutions are incapable of aiding in verification of coding of complex algebraic expressions (wall heat transfer functions, reaction rates, etc.) and that often code developers are only capable of verifying these expressions. However, on a less rigorous level these models can be contrasted against derived physical models. This is the only methodology that does not assume all users of the code are equally experienced, but NEA provides no guidance as to quantifying user induced error.

Validation approaches for the four V&V methods are contrasted in table 3. AIAA recommends the building block approach for validation assessment. This approach indentifies uncertainty in experimental data, and compares this with the simulation outcome. NEA proposes a method similar to the AIAA for the validation process, with experiment data uncertainty quantified using ASME 19.1, and offers more detail regarding quantification of uncertainty contributions from the modeling side, including use of input sensitivity coefficients and Monte Carlo techniques. The ASME validation assessment also includes uncertainty from the model derived from the Monte Carlo or the Sensitivity method. The sensitivity coefficient method is used locally for input uncertainty propagation, and neglects non-linear effects.

Table 3 Comparison of Methods used for Validation

	The building block approach	Sensitivity coefficient	Monte Carlo	Others
AIAA	X			
ASME		X	X	X
ASTM	X			
CSAU	X		X	X
NEA	X	X	X	

Monte Carlo is a global method that can be used to capture nonlinear behavior in the parameter space. ASME includes experiment data uncertainty in the validation as derived from the ASME standard 19.1. ASTM validation, as implemented by NRC for FDS modeling, is accomplished by comparing the computation model to standard tests, full scale tests, proven benchmark tests, and documented fire experience. This approach is similar to AIAA's building block approach. As for CSAU, the Monte Carlo method and Latin Hypercube method are suggested for uncertainty propagation from inputs to outcomes.

4. Conclusions and Perspective

The use of peer review, as suggested in the ASTM method for assuring the theoretical basis is correct, and as implemented in NEA and CSAU to develop a PIRT often has a broader impact than just assuring the correct models are in the simulation. The panel of experts used in developing the PIRT also provides a political base should outcomes be contested later. In the case of NRC CFD applications, the process of adjudication ultimately may decide the acceptance of a simulation outcome.

Code verification establishes that the code accurately solves the mathematical model incorporated in the code. Solution verification estimates the numerical accuracy of a particular calculation. It is assumed that code verification is successfully performed prior to the solution verification process. Grid refinement studies are critical to the solution verification process. However, grid refinement offers only an estimate of the error associated with discretization. In the case of using a CFD code in a predictive role, errors in the representation of geometry, boundary condition or initial condition cannot be discovered using these approaches. Input checking must be used, along with judgment and experience. Input for a complicated simulation may be quite large, with many portions of the input generated using tools like an automated grid generator, perhaps accepting files from a computer aided design program to establish geometry, and a graphical user interface. All these tools offer opportunities to introduce errors to the input.

Modern quality assurance programs have successfully reduced errors and faults in complicated manufacturing environments, and these methods could be adapted to CFD use in critical applications. The NEA best practices document advocates use of QA methods as an umbrella over the V&V activities outlined here, but the methods were not detailed or tailored to CFD simulation. Several quality assurance approaches specific to software development exist, but are not treated further here.

Experience with large complicated codes such as RELAP5 and TRAC indicates that continued use of a code for a family of applications, in conjunction with a user group actively reporting problems and suggesting enhancements, can lead to continuous improvement of a code if the information is properly managed. This approach to collecting data from the field to guide improvement is part of modern quality assurance methods in manufacturing industries, and could be formalized in CFD development. Most of the major CFD vendors offer venues for such information exchange, either in user groups and/or in conferences. The source code for many of the commercial CFD products is not available to users, so the code custodians must implement appropriate changes. An open source code can benefit from user feedback and from constant code checking and development. However, configuration control and a well designed process for acceptance of developer contributions are required.

NRC has established precedent with the CSAU method for calculation V&V of the nuclear reactor transient simulation codes TRAC and RELAP5. A second precedent is now established with the V&V assessment of FDS by NRC for fire hazard analysis using the ASTM approach. We have examined CSAU and the ASTM approaches to V&V, as well as the methods for V&V suggested by NEA and ASME. It may be that strengths and weaknesses of each V&V approach will come clear as CFD matures.

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