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Short communication

The international FORUM of fire research directors: A position paper on verification and validation of numerical fire models

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Abstract

The international FORUM of Fire research directors periodically takes positions on issues dealing with the direction and implementation of fire research with the potential for significant impact on safety and/or global practices, standards and test methods. This short communication represents the FORUM's position on the validation of numerical fire models. These models are increasingly being used on the fire protection engineering community, and have the potential for a significant impact with the increasing acceptance of performance based fire codes. The FORUM position is to require verification and validation of these models. Activities should include; code verification to identify and reduce coding errors, calculation verification to establish appropriate model usage, and model validation to provide a quantitative assessment of the predictive capabilities of a model. Peer-reviewed documentation of these activities should be published in the open literature. The importance of verification of models for fire phenomenon, and an overview of these activities, are discussed.

Keywords: Fire modeling; Verification; Validation; Uncertainty

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1. Introduction and background

Numerical simulation of fire environments using computational models has become increasingly widespread in fire research and fire safety engineering. The ability to accurately predict fire behavior using these models is of high utility for hazard assessment, investigations and performance-based design. Accordingly, the FORUM position supports the development of accurate models, using material property data as input, as the appropriate long-term goal of the fire research community [1].

In general, accurate numerical fire models must represent many nonlinear, coupled phenomena over a broad range of length and time scales. Physics-based fire computer codes typically include an order of magnitude more (>10) degrees of freedom than codes commonly employed for engineering mechanics. Models with varying degrees of development and maturity are being increasingly employed to provide predictions of fire growth, fire spread and fire suppression. These models may invoke the use of algebraic relations, zone, and computational fluid dynamics based techniques. The credibility of the results from these models has not been generally established. Guidance has been developed for evaluating model capabilities [2,3] and for determining uses and limitations [4], however, time and resources often prohibit such exhaustive prescriptive approaches from being employed by each analyst. The complexity and non-linearities inherent in fire modeling yields a significant potential for results which can be explained by the analyst as reasonable, but are sufficiently in error as to lead to incorrect conclusions by a decision maker.

The FORUM position is to require verification and validation of fire models as needed to establish known levels of confidence in model predictions. The benefit of this activity includes (1) improved quality of predictions over a broader range of applications, (2) improved confidence by decision makers as needed to encourage acceptance of model results, and (3) continual advancement of the state of knowledge. It is acknowledged that these activities require additional effort on the part of the developer and the user. This effort is a necessary and useful long-term investment to allow fire safety engineering to progress from a test-based field to a knowledge and simulation-based field of practice. In some cases, a graded approach can be employed where the level of rigor is increased based on the end use of the results [5].

2. The essential features of verification and validation

Verification and validation are two independent processes. Verification can be simply defined as "solving the equations right," and validation as "solving the right equations." Verification deals solely with computational science and mathematics, while validation deals with physical phenomena. The theory and processes of verification and validation are well established and documented [6,7] and will, therefore, not be repeated in detail. The main features, and the corresponding position of the FORUM, will be highlighted and discussed in terms of their relevance to fire research and engineering.

It is necessary to verify both codes and calculations to assure that the equations have been programmed correctly and that they are being solved correctly in a given calculation. Codes cannot be validated. Only specific models, which are created by the analyst and executed by the code, can be validated. Validation is performed for the "intended uses of the model". The validity of a model is therefore restricted by model formulation and model parameters inherent in the code as well as the input parameters and conditions specified by the user. Use of the model with confidence would, therefore, be limited to the class of applications for which it was validated; use for any other purpose would require additional validation. Furthermore, any changes to the model, or use of the model with significantly different inputs, require additional validation.

Verification and validation must be conducted in the following sequence: (1) verification of computer codes, (2) verification of calculations and (3) validation of models. These activities should all be performed within the range of the parameter space of the intended use.

2.1. Code verification

The primary purpose of this step is to establish that correct solutions to the equations *can* be obtained. Successful verification implies no coding errors and the use of sound, robust numerical methods. Code verification can be performed via comparison of the computed solution with exact, analytical solutions (which is limited to simple problems) or more recently through the used of the "method of manufactured solutions" [8]. In this technique, a source term and boundary conditions are determined analytically for a known function which is in turn compared to code results with the use of the specified source term and boundary conditions as code input. Code verification should exercise all parts of the code for the range of values expected for general use. This generally requires access to source code, and *it is the FORUM position that code verification be performed, and documented, by the code developer.* Discovering coding errors should not be left to the analyst, although a feedback mechanism should exist to allow analyst observations to be provided to the developer in case such errors are encountered. The analyst should have access to verification documentation to ensure that the capabilities and features to be used have been verified.

2.2. Calculation verification

In this step, the numerical accuracy of a particular calculation, which employs a code to generate a model for a specific scenario, is determined and documented. The specification of input parameters is critical for all models. Numerical models that use a discretized form of the equations to obtain a solution (generally using a computational grid) also require careful definition of boundary conditions and consideration of grid refinement. Since numerical fire models only provide resolved (i.e. discrete forms of the exact equation) solutions for a limited range of physics, they will not in general provide convergence to the exact answer with increasing discretization. Grid (or discretization) sensitivities must, therefore, be determined and documented. This feature is particularly important for large-eddy simulation type codes in which grid resolution and spatial filtering are intertwined. It is essential to estimate the accuracy of the computed solution, i.e., to put error bars on the computed results. Calculation verification is highly dependent on the specific scenario and, therefore, must be performed by the analyst. Sufficient detail should be provided in the documentation to allow future analysts, when faced with a similar problem, to use or at least compare results with the outcome of previous calculation verification activities.

2.3. Model validation

Validation is the process of determining the degree of agreement between model predictions and real world events for one or more results of interest. The goal of validation is to quantify confidence in the predictive capability of the model. Therefore, validation assesses agreement between model output and experimental data, as determined by an appropriate metric. The comparison must include the uncertainty estimates from both verification calculations as well as experimental measurements. For example, results of verification calculations may illustrate the need for materials characterization experiments to reduce uncertainties.

Validation experiments are the standard against which the model outputs are compared. As such, they include some unique requirements. Collaboration between experimenters and modelers is essential for validation experiments. A shared understanding of the goals and conditions of the experiment is necessary. Pretest analyses should be conducted to help support experimental design. A clear understanding of the nature, resolution, and expected uncertainty of the experimental measurements that comprise the boundary and initial conditions, as well as a clear definition of the validation metric, is required. In selecting the validation metric, the primary considerations should be the desired end use of the model in conjunction with what type of data are available from the experiment. Accuracy and precision are of the utmost importance, and both should be determined through uncertainty quantification including repeated experiments. Guidance on the selection of experimental and simulation metrics (such as consideration of parameters, treatment of temporal and spatial variations) for comparison is available in the literature [9]. Field measurements are often used for visual comparison, but fall short of validation due to a lack of quantitative comparison of multi-dimensional model results and experimental data. Due to compensating errors, good agreement between prediction and experiment does not imply comprehensive confidence in all aspects of the model. Therefore, it is advisable to perform validation activities that address individual phenomenology before conducting integral level validation to address a complex scenario. Final calculations for comparison should be performed with careful consideration of the initial and boundary conditions, but without a priori knowledge of the results. In some cases, it is acknowledged that data are sparse and boundary conditions cannot be fully characterized. The extent to which these uncertainties affect the confidence in the model should be quantified by appropriate consideration of experimental uncertainties and model sensitivities.

Because many problems show significant sensitivity to physical, numerical and model parameters, it is often easy to adjust the prediction of computer models to match measurements. Calibration of the model to agree with known test results does not constitute validation. *It is the FORUM position that adjustments should not be made to models or model constants to improve agreement between model predictions and data. Only after a compelling body of data has been obtained, and/or a clear physical explanation has been provided, should model changes* (*subject to software quality guidelines* [10]) *be implemented.*

Validation is application specific, i.e. models that provide results within acceptable levels of confidence for one application may not provide them for another. It is ultimately the responsibility of the analyst to perform or cite model validation results to ensure the achievable level of confidence is appropriate for the application of interest. *The FORUM position is to encourage baseline model validation for the intended application space of the code by the code developers such as to provide the user an indication of the predictive capability of models that can be employed for similar applications.* The specific cases and validation metrics will vary according to the intended use of the code.

Data from model validation experiments and validation exercises must be carefully documented to benefit future users. Otherwise, each user must repeat the validation exercise for each application, in a manner similar to a test-based approach, and the knowledge base will not progress.

3. Forum position

The FORUM cite the need for known levels of confidence in fire models used in fire protection engineering. Since the necessary procedures are now sufficiently well-defined to be employed in practice, the FORUM position is to require verification and validation to include:

- Code verification by the developer to identify and reduce coding errors.
- Calculation verification including characterization of discretization (normally grid) and input parameter dependence to establish appropriate model usage.
- Model validation in the parameter space of interest, based on an established metric and employing high-quality experimental data, to provide a quantitative assessment of the predictive capabilities of a model.
- Documentation of validation studies, following established guidelines, in the open literature with sufficient rigor and detail to be used as a basis for increased confidence in future analyses.

The principal barrier to verification and validation is the additional effort and cost required by the developer and analyst. Although this cost is recognized and acknowledged by the FORUM, efforts of appropriate rigor are clearly necessary to improve acceptance of model results by decision makers and to progressively advance the state of knowledge.

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