



Standard Guide for Evaluating the Predictive Capability of Deterministic Fire Models¹

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1. Scope

1.1 This guide provides a methodology for evaluating the predictive capabilities of a fire model for a specific use. The intent is to cover the whole range of deterministic numerical models which might be used in evaluating the effects of fires in and on structures.

1.2 The methodology is presented in terms of four areas of evaluation:

1.2.1 Defining the model and scenarios for which the evaluation is to be conducted,

1.2.2 Verifying the appropriateness of the theoretical basis and assumptions used in the model,

1.2.3 Verifying the mathematical and numerical robustness of the model, and

1.2.4 Quantifying the uncertainty and accuracy of the model results in predicting of the course of events in similar fire scenarios.

1.3 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

1.4 This fire standard cannot be used to provide quantitative measures.

2. Referenced Documents

2.1 ASTM Standards:²

E176 Terminology of Fire Standards

E603 Guide for Room Fire Experiments

E1591 Guide for Obtaining Data for Deterministic Fire Models

2.2 International Standards Organization Standards:³

ISO/IEC Guide 98 (2008) Uncertainty of measurement – Part 3: Guide to the expression of uncertainty in measurement

ISO 13943 (2008) Fire safety – Vocabulary

ISO 16730 (2008) Fire safety engineering – Assessment, verification and validation of calculation methods

3. Terminology

3.1 *Definitions:* For definitions of terms used in this guide and associated with fire issues, refer to terminology contained in Terminology E176 and ISO 13943. In case of conflict, the definitions given in Terminology E176 shall prevail.

3.2 Definitions of Terms Specific to This Standard:

3.2.1 *model evaluation*—the process of quantifying the accuracy of chosen results from a model when applied for a specific use.

3.2.2 *model validation*—the process of determining the degree to which a calculation method is an accurate representation of the real world from the perspective of the intended uses of the calculation method.

3.2.2.1 *Discussion*—The fundamental strategy of validation is the identification and quantification of error and uncertainty in the conceptual and computational models with respect to intended uses.

3.2.3 *model verification*—the process of determining that the implementation of a calculation method accurately represents the developer's conceptual description of the calculation method and the solution to the calculation method.

3.2.3.1 *Discussion*—The fundamental strategy of verification of computational models is the identification and quantification of error in the computational model and its solution.

3.2.4 The precision of a model refers to the deterministic capability of a model and its repeatability.

3.2.5 The accuracy refers to how well the model replicates the evolution of an actual fire.

4. Summary of Guide

4.1 A recommended process for evaluating the predictive capability of fire models is described. This process includes a brief description of the model and the scenarios for which evaluation is sought. Then, methodologies for conducting an analysis to quantify the sensitivity of model predictions to various uncertain factors are presented, and several alternatives

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² For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

³ Available from American National Standards Institute, 11 West 42nd Street, 13th Floor, New York, NY 10036.

for evaluating the accuracy of the predictions of the model are provided. Historically, numerical accuracy has been concerned with time step size and errors. A more complete evaluation must include spatial discretization. Finally, guidance is given concerning the relevant documentation required to summarize the evaluation process.

5. Significance and Use

5.1 The process of model evaluation is critical to establishing both the acceptable uses and limitations of fire models. It is not possible to evaluate a model in total; instead, this guide is intended to provide a methodology for evaluating the predictive capabilities for a specific use. Validation for one application or scenario does not imply validation for different scenarios. Several alternatives are provided for performing the evaluation process including: comparison of predictions against standard fire tests, full-scale fire experiments, field experience, published literature, or previously evaluated models.

5.2 The use of fire models currently extends beyond the fire research laboratory and into the engineering, fire service and legal communities. Sufficient evaluation of fire models is necessary to ensure that those using the models can judge the adequacy of the scientific and technical basis for the models, select models appropriate for a desired use, and understand the level of confidence which can be placed on the results predicted by the models. Adequate evaluation will help prevent the unintentional misuse of fire models.

5.3 This guide is intended to be used in conjunction with other guides under development by Committee E05. It is intended for use by:

5.3.1 *Model Developers*—To document the usefulness of a particular calculation method perhaps for specific applications. Part of model development includes identification of precision and limits of applicability, and independent testing.

5.3.2 *Model Users*—To assure themselves that they are using an appropriate model for an application and that it provides adequate accuracy.

5.3.3 *Developers of Model Performance Codes*—To be sure that they are incorporating valid calculation procedures into codes.

5.3.4 *Approving Officials*—To ensure that the results of calculations using mathematical models stating conformance to this guide, cited in a submission, show clearly that the model is used within its applicable limits and has an acceptable level of accuracy.

5.3.5 *Educators*—To demonstrate the application and acceptability of calculation methods being taught.

5.4 This guide is not meant to describe an acceptance testing procedure.

5.5 The emphasis of this guide is numerical models of fire evolution.

5.5.1 The precision of a model refers to the deterministic capability of a model and its repeatability.

5.5.2 The accuracy of a model refers to how well the model replicates the evolution of an actual fire.

6. General Methodology

6.1 The methodology is presented in terms of four areas of evaluation:

6.1.1 Defining the model and scenarios for which the evaluation is to be conducted,

6.1.2 Assessing the appropriateness of the theoretical basis and assumptions used in the model,

6.1.3 Assessing the mathematical and numerical robustness of the model, and

6.1.4 Quantifying the uncertainty and accuracy of the model results in predicting the course of events in similar fire scenarios.

6.1.5 This general methodology is also consistent with the methodology presented in **ISO 16730**, Fire safety engineering – Assessment, verification and validation of calculation methods, which is a potentially useful resource which can be used with ASTM E1355.

6.2 Model and Scenario Documentation:

6.2.1 *Model Documentation*—Sufficient documentation of calculation models, including computer software, is absolutely necessary to assess the adequacy of the scientific and technical basis of the models, and the accuracy of computational procedures. Also, adequate documentation will help prevent the unintentional misuse of fire models. Guidance on the documentation of computer-based fire models is provided in Section 7.

6.2.2 *Scenario Documentation*—Provide a complete description of the scenarios or phenomena of interest in the evaluation to facilitate appropriate application of the model, to aid in developing realistic inputs for the model, and to develop criteria for judging the results of the evaluation. Details applicable to evaluation of the predictive capability of fire models are provided in 7.2.

6.3 *Theoretical Basis and Assumptions in the Model*—An independent review of the underlying physics and chemistry inherent in a model ensures appropriate application of submodels which have been combined to produce the overall model. Details applicable to evaluation of the predictive capability of fire models are provided in Section 8.

6.4 *Mathematical and Numerical Robustness*—The computer implementation of the model should be checked to ensure such implementation matches the stated documentation. Details applicable to evaluation of the predictive capability of fire models are provided in Section 9. Along with 6.3, this constitutes verification of the model.

6.5 Quantifying the Uncertainty and Accuracy of the Model:

6.5.1 *Model Uncertainty*—Even deterministic models rely on inputs often based on experimental measurements, empirical correlations, or estimates made by engineering judgment. Uncertainties in the model inputs can lead to corresponding uncertainties in the model outputs. Sensitivity analysis is used to quantify these uncertainties in the model outputs based upon known or estimated uncertainties in model inputs. Guidance for obtaining input data for fire models is provided by Guide **E1591**. Details of sensitivity analysis applicable to evaluation of the predictive capability of fire models are provided in Section 10.

6.5.2 Experimental Uncertainty—In general, the result of measurement is only the result of an approximation or estimate of the specific quantity subject to measurement, and thus the result is complete only when accompanied by a quantitative statement of uncertainty. Guidance for conducting full-scale compartment tests is provided by Guide E603. Guidance for determining the uncertainty in measurements is provided in the ISO Guide to the Expression of Uncertainty in Measurement.

6.5.3 Model Evaluation—Obtaining accurate estimates of fire behavior using predictive fire models involves insuring correct model inputs appropriate to the scenarios to be modeled, correct selection of a model appropriate to the scenarios to be modeled, correct calculations by the model chosen, and correct interpretation of the results of the model calculation. Evaluation of a specific scenario with different levels of knowledge of the expected results of the calculation addresses these multiple sources of potential error. Details applicable to evaluation of the predictive capability of fire models are provided in Section 11.

7. Model and Scenario Definition

7.1 Model Documentation—Provides details of the model evaluated in sufficient detail such that the user of the evaluation could independently repeat the evaluation. The following information should be provided:

7.1.1 Program Identification:

7.1.1.1 Provide the name of the program or model, a descriptive title, and any information necessary to define the version uniquely.

7.1.1.2 Define the basic processing tasks performed, and describe the methods and procedures employed. A schematic display of the flow of the calculations is useful.

7.1.1.3 Identify the computer(s) on which the program has been executed successfully and any required peripherals, including memory requirements and tapes.

7.1.1.4 Identify the programming languages and versions in use.

7.1.1.5 Identify the software operating system and versions in use, including library routines.

7.1.1.6 Describe any relationships to other models.

7.1.1.7 Describe the history of the model's development and the names and addresses of the individual(s) and organizations(s) responsible.

7.1.1.8 Provide instructions for obtaining more detailed information about the model from the individual(s) responsible for maintenance of the model.

7.1.2 References—List the publications and other reference materials directly related to the fire model or software.

7.1.3 Problem or Function Identification:

7.1.3.1 Define the fire problem modeled or function performed by the program, for example, calculation of fire growth, smoke spread, people movement, etc.

7.1.3.2 Describe the total fire problem environment. General block or flow diagrams may be included here.

7.1.3.3 Include any desirable background information, such as feasibility studies or justification statements.

7.1.4 Theoretical Foundation:

7.1.4.1 Describe the theoretical basis of the phenomenon and the physical laws on which the model is based.

7.1.4.2 Present the governing equations and the mathematical model employed.

7.1.4.3 Identify the major assumptions on which the fire model is based and any simplifying assumptions.

7.1.4.4 Provide results of any independent review of the theoretical basis of the model. This guide recommends a review by one or more recognized experts fully conversant with the chemistry and physics of fire phenomena but not involved with the production of the model.

7.1.5 Mathematical Foundation:

7.1.5.1 Describe the mathematical techniques, procedures, and computational algorithms employed to obtain numerical solutions.

7.1.5.2 Provide references to the algorithms and numerical techniques.

7.1.5.3 Present the mathematical equations in conventional terminology and show how they are implemented in the code.

7.1.5.4 Discuss the precision of the results obtained by important algorithms and any known dependence on the particular computer facility.

7.1.5.5 For iterative solutions, discuss the use and interpretation of convergence tests, and recommend a range of values for convergence criteria. For probabilistic solutions, discuss the precision of the results having a statistical variance.

7.1.5.6 Identify the limitations of the model based on the algorithms and numerical techniques.

7.1.5.7 Provide results of any analyses that have been performed on the mathematical and numerical robustness of the model. Analytical tests, code checking, and numerical tests are among the analyses listed in this guide that are appropriate for this purpose.

7.1.6 Program Description:

7.1.6.1 Describe the program.

7.1.6.2 List any auxiliary programs or external data files required for utilization of this program.

7.1.6.3 Describe the function of each major option available for solving various problems, pay special attention to the effects of combinations of options.

7.1.6.4 Describe alternate paths that may be dynamically selected by the program from tests on calculated results.

7.1.6.5 Describe the relationship between input and output items for programs that reformat information.

7.1.6.6 Describe the method and technical basis for decisions in programs that perform logical operations.

7.1.6.7 Describe the basis for the operations that occur in the program.

7.1.6.8 Identify the source language(s).

7.1.6.9 Include a flowchart showing the overall program structure and logic, and detailed flowcharts, where appropriate. The subprogram names should be included on these charts.

7.1.6.10 Pinpoint any known areas of dependency on the local computer installation support facilities.

7.1.6.11 Include a detailed narrative and graphical description of the programming techniques used in writing the program, that is, calling sequence, overlay structure, test plan, common usage, etc.

7.1.6.12 Provide a source listing, or make sure it is readily available.

7.1.6.13 Use comments within the program. The liberal use of comments is a key to understandable programs. An alternative is a commentary keyed to the executable statements of the program.

7.1.7 Restrictions and Limitations:

7.1.7.1 List hardware and software restrictions.

7.1.7.2 Provide data ranges and capacities.

7.1.7.3 Describe the program behavior when restrictions are violated, and describe recovery procedures.

7.1.7.4 If accuracy characteristics are significant, describe them in detail.

7.1.7.5 Provide information and cautions on the degree and level of care to be taken in selecting input and running the model.

7.1.7.6 Provide both general and specific limitations of the fire model for specific applications.

7.1.8 Input Data:

7.1.8.1 Describe the source of input information, for example, handbooks, journals, research reports, standard tests, experiments, etc.

7.1.8.2 Provide the default values or the general conventions governing those values.

7.1.8.3 Identify the limits on input based on stability, accuracy, and practicality, as well as their resulting limitations to output.

7.1.8.4 When property values are defined within the program, list the properties and the assigned values.

7.1.8.5 Identify the procedures that should be used or were used to obtain property and other input data.

7.1.8.6 Provide information on the dominant variables in the models.

7.1.9 Output Information:

7.1.9.1 Describe the program output.

7.1.9.2 Relate the edited output to input options.

7.1.9.3 Relate the output to appropriate equations.

7.1.9.4 Describe any normalization of results and list associated dimensional units.

7.1.9.5 Identify any special forms of output, for example, graphics display and plots.

7.1.10 List of Variables:

7.1.10.1 List the program and subprogram variables and parameters. The list should include their use and purpose within the program, as well as in its inputs and results. Identify them as local or global variables; that is, do they apply within the module, or are they common to two or more modules of the system?

7.1.10.2 Define all meaningful symbols and arrays used in the routine. Refer to the mathematical or technical notations and terms used in the technical document. Provide units, where applicable. Describe the nominal and initial values of parameters (for example, a computational zero, step sizes, and convergence factors), along with their ranges. Discuss how they affect the computational process.

7.2 Scenarios for which the Model has been Evaluated—Provides details on the range of parameters for which the evaluation has been conducted. Sufficient information should be included such that the user of the evaluation could indepen-

dently repeat the evaluation. At a minimum, the following information should be provided:

7.2.1 A description of the scenarios or phenomena of interest,

7.2.2 A list of quantities predicted by the model for which evaluation is sought, and

7.2.3 The degree of accuracy required for each quantity.

8. Theoretical Basis for the Model

8.1 The theoretical basis of the model should be subjected to a peer review by one or more recognized experts fully conversant with the chemistry and physics of fire phenomena but not involved with the production of the model. Publication of the theoretical basis of the model in a peer-reviewed journal article may be sufficient to fulfill this review. This review should include:

8.1.1 An assessment of the completeness of the documentation particularly with regard to the assumptions and approximations.

8.1.2 An assessment of whether there is sufficient scientific evidence in the open scientific literature to justify the approaches and assumptions being used.

8.1.3 An assessment of the accuracy and applicability of the empirical or reference data used for constants and default values in the context of the model.

8.1.4 The set of equations that is being solved; in cases for which closure equations are needed (not included in 8.1.3) the assumption and implication of such choices.

9. Mathematical and Numerical Robustness

9.1 Analyses which can be performed include:

9.1.1 *Analytical Tests*—If the program is to be applied to a situation for which there is a known mathematical solution, analytical testing is a powerful way of testing the correct functioning of a model. However, there are relatively few situations (especially for complex scenarios) for which analytical solutions are known. Analytic tests for submodels should be performed. For example, it is possible to provide a closed-form solution for heat loss through a partition; the model should be able to do this calculation.

9.1.2 *Code Checking*—The code can be verified on a structural basis preferably by a third party either totally manually or by using code checking programs to detect irregularities and inconsistencies within the computer code. A process of code checking can increase the level of confidence in the program's ability to process the data to the program correctly, but it cannot give any indication of the likely adequacy or accuracy of the program in use.

9.1.3 *Numerical Tests*—Mathematical models are usually expressed in the form of differential or integral equations. The models are in general very complex, and analytical solutions are hard or even impossible to find. Numerical techniques are needed for finding approximate solutions. These numerical techniques can be a source of error in the predicted results. Numerical tests include an investigation of the magnitude of the residuals from the solution of the system of equations employed in the model as an indicator of numerical accuracy and of the reduction in residuals as an indicator of numerical convergence. Algebraic equations should be subject to error

tests (uncertainty), ordinary differential equations to time step errors, and partial differential equations to grid discretization analysis. This would include check of residual error of the solution, the stability of output variables, a global check on conservation of appropriate quantities, the effect of boundary conditions, and that there is grid and time step convergence. Finally, it is necessary to check that the requirements for consistency and stability are met.

9.1.4 Many fire problems involve the interaction of different physical processes, such as the chemical or thermal processes and the mechanical response. Time scales associated with the processes may be substantially different, which easily causes numerical difficulties. Such problems are called stiff. Some numerical methods have difficulty with stiff problems since they slavishly follow the rapid changes even when they are less important than the general trend in the solution. Special algorithms have been devised for solving stiff problems.⁴

9.1.5 Numerical accuracy of predictive fire models has been considered in the literature.⁵

10. Model Sensitivity

10.1 Fire growth models are typically based on a system of ordinary differential equations of the form

$$\frac{dz}{d\tau} = f(z, p, \tau) \quad z(\tau = 0) = z_0 \quad (1)$$

where:

z ($z_1, z_2, \dots, z_m$) = the solution vector for the system of equations (for example, mass, temperature, or volume)
 p ($p_1, p_2, \dots, p_n$) = a vector of input parameters (for example, room area, room height, heat release rate), and
 τ = time.

The solutions to these equations are, in general, not known explicitly and must be determined numerically. To study the sensitivity of such a set of equations, the partial derivatives of an output z_j with respect to an input p_i (for $j = 1, \dots, m$ and $i = 1, \dots, n$) should be examined.

10.2 A sensitivity analysis of a model is a study of how changes in model parameters affect the results generated by the model. Model predictions may be sensitive to uncertainties in input data, to the level of rigor employed in modeling the relevant physics and chemistry, and to the accuracy of numerical treatments. The purpose of conducting a sensitivity analysis is to assess the extent to which uncertainty in model inputs is manifested to become uncertainty in the results of interest from the model. This information can be used to:

10.2.1 Determine the dominant variables in the models,

10.2.2 Define the acceptable range of values for each input variable,

10.2.3 Quantify the sensitivity of output variables to variations in input data, and

10.2.4 Inform and caution any potential users about the degree and level of care to be taken in selecting input and running the model.

10.3 Inputs to models consist of:

10.3.1 *Scenario Specific Data*—Such as the geometry of the domain, the environmental conditions, and specifics of the fire description.

10.3.2 *Property Data*—Such as thermal conductivity, density, and heat capacity, and

10.3.3 *Numerical Constants*—Such as turbulence model constants, entrainment coefficients, and orifice constants.

10.4 Conducting a sensitivity analysis of a fire model is not a simple task. Many models require extensive input data and generate predictions for multiple output variables over an extended period of time.

10.4.1 Time and cost become critical factors in determining the extent and degree of an analysis. A practical problem to be faced when designing a sensitivity analysis experiment, is that the number of model runs required will rapidly increase with the number of input parameters and number of independent variables considered. Hence a full factorial experiment may be prohibitive in terms of man hours expended for the return gained.

10.4.2 In many cases partial factorial experiments will be adequate for the purpose of obtaining information on the effect of varying the input parameters and consequential interactions considered important. In this case, third and higher order interactions may often be ignored.

10.4.3 For sensitivity analysis of models with large numbers of parameters, efficient methods are available to conduct the analysis with a manageable number of individual model simulations.⁶ For highly non-linear fire models, the method of choice is most often Latin hypercube sampling:

10.4.3.1 *Latin Hypercube Sampling*—The possible range for input parameter is divided into N intervals of equal probability. For each input parameter, one value is randomly chosen within each of the N intervals. From the resulting N possibilities for each input parameter, one value is randomly selected. This set of values is used for the first simulation. The preceding is repeated N times to generate N sets of parameters for N total model simulations. Software is available which can calculate parameter values for a Latin Hypercube sampling.⁷

10.5 Several methods of sensitivity analysis have been applied to fire models.⁸ The one chosen for use will be

⁶ Clemson, B., Yongming, T., Pyne, J., and Unal, R., "Efficient Methods for Sensitivity Analysis," *Systems Dynamics Review*, Vol 11, No. 1 (Spring 1995), 31–49.

⁷ Iman, R. L. and Shortencarier, A. FORTRAN 77 Program and User's Guide for the Generation of Latin Hypercube and Random Samples for Use with Computer Models. NUREG/CR-3624, SAND83-2365, Sandia National Laboratories, Albuquerque, New Mexico (1984).

⁸ Davies, A. D., "Some Tools for Fire Model Validation," *Fire Technology*, Vol 23, No. 2, May 1987, pp. 95–114; Khoudja, N., "Procedures for Quantitative Sensitivity and Performance Validation Studies of a Deterministic Fire Safety Model," *NBS-GCR-88-544*, U.S. Department of Commerce, National Bureau of Standards, 1988; and Peacock, R. D., Davis, S., and Lee, B. T., "An Experimental Data Set for the Accuracy Assessment of Room Fire Models," *NBSIR 88-3752*, U.S. Department of Commerce, National Bureau of Standards, 1988.

⁴ Petzold, L. R., *A Description of DASSL: A Differential/Algebraic System Solver*, Technical Report 8637, Sandia National Laboratories, 1982.

⁵ Mitler, H. E., "Mathematical Modeling of Enclosure Fires, Numerical Approaches to Combustion Modeling," ed. Oran, E. S. and Boris, J. P., *Progress in Astronautics and Aeronautics* 135, pp. 711–753, American Institute of Aeronautics and Astronautics, Washington, 1991, and Forney, G. P. and Moss, W. F., "Analyzing and Exploiting the Numerical Characteristics of Zone Fire Models," *Fire Science and Technology*, 14: 49–60, 1994.

dependent upon the resources available and the model being analyzed. Two common methods of analysis follow:

10.5.1 Global Methods—Produce sensitivity measures which are averaged over the entire range of input parameters. Global methods require knowledge of the probability density functions of the input parameters, which in the case of fire models, is generally unknown.

10.5.2 Local Methods—Produce sensitivity measures for a particular set of input parameters and must be repeated for a range of input parameters to obtain information on the overall model performance. Finite difference methods can be applied without modifying a model's equation set, but require careful selection of input parameters to obtain good estimates. Direct methods supplement the equation set solved by a model with sensitivity equations derived from the equation set solved by the model.⁹ The sensitivity equations are then solved in conjunction with the model's system of equations to obtain the sensitivities. Direct methods must be incorporated into the design of a fire model and are not often available for already existing fire models. There are several classes of local methods which are of interest. Using the nomenclature of equation (1), these are outlined below.

10.5.2.1 Finite difference methods provide estimates of sensitivity functions by approximating the partial derivatives of an output z_i with respect to an input p_j as finite differences:

$$\frac{\partial z_j}{\partial p_m} = \frac{z_j(p_1, p_2, \dots, p_m + \Delta p_m, \dots, p_k) - z_j(p_1, p_2, \dots, p_m, \dots, p_k)}{\Delta p_m} \quad (2)$$

$$j = 1, 2, \dots, n, \quad m = 1, 2, \dots, k$$

This method is easy and straightforward to implement. However, as with any finite difference method, the choice of Δp_m is pivotal in obtaining good estimates. To determine the $n \cdot k$ first-order sensitivity equations requires $k + 1$ runs of the model. These may be run simultaneously as a larger system or in parallel.

10.5.2.2 Direct methods derive the sensitivity differential equations from the model's system of ordinary differential equations:

$$\frac{d}{dt} \frac{\partial z_j}{\partial p_m} = \frac{\partial f_j}{\partial p_m} + \sum_i \frac{\partial f_j}{\partial z_i} \frac{\partial z_i}{\partial p_m} \quad j = 1, 2, \dots, n, \quad m = 1, 2, \dots, k \quad (3)$$

These equations are then solved in conjunction with the model's system of differential equations to obtain the sensitivities. To compute the $n \times k$ first-order sensitivities requires 1 model run. These may be incorporated directly into the model and solved as a single, coupled set of $n + (n \cdot k)$ differential equations¹⁰ or decoupled solving the model equations and the sensitivity equations iteratively using the model's solution and an appropriate interpolation scheme.¹¹

10.5.3 Response Surface Method—An appropriate vector of functions is fit to a selected set of model runs. The resulting

metamodel is then assumed to behave in the same manner as the model. By appropriate choice of functions, the resulting metamodel is simpler and easier to analyze than the actual model. The equations are then solved to perform a sensitivity analysis on the metamodel. The Jacobian of the metamodel solution represents the sensitivity equations.

11. Model Evaluation

11.1 A model should be assessed for a specific use in terms of its quantitative ability to predict outcomes such as:

11.1.1 Fire growth and spread (as typified by temperature, smoke, gas concentrations, etc.),

11.1.2 Rate of flame spread, fire resistance, etc.,

11.1.3 Fire hazard (as typified by available egress time, tenability etc.),

11.1.4 Response of active and passive fire protection or,

11.1.5 Some other property.

11.2 Model evaluation addresses multiple sources of potential error in the design and use of predictive fire models, including insuring correct model inputs appropriate to the scenarios to be modeled, correct selection of a model appropriate to the scenarios to be modeled, correct calculations by the model chosen, and correct interpretation of the results of the model calculation. Evaluation of a specific scenario with different levels of knowledge of the expected results of the calculation addresses these multiple sources of potential error. It is understood that only one or more of these levels of evaluation may be included in a particular model evaluation.

11.2.1 Blind Calculation—The model user is provided with a basic description of the scenario to be modeled. For this application, the problem description is not exact; the model user is responsible for developing appropriate model inputs from the problem description, including additional details of the geometry, material properties, and fire description, as appropriate. Additional details necessary to simulate the scenario with a specific model are left to the judgement of the model user. In addition to illustrating the comparability of models in actual end-use conditions, this will test the ability of those who use the model to develop appropriate input data for the models.

11.2.2 Specified Calculation—The model user is provided with a complete detailed description of model inputs, including geometry, material properties, and fire description. As a follow-on to the blind calculation, this test provides a more careful comparison of the underlying physics in the models with a more completely specified scenario.

11.2.3 Open Calculation—The model user is provided with the most complete information about the scenario, including geometry, material properties, fire description, and the results of experimental tests or benchmark model runs which were used in the evaluation of the blind or specified calculations of the scenario. Deficiencies in available input (used for the blind calculation) should become most apparent with comparison of the open and blind calculation.

11.2.4 Problem Description and Model Inputs—Different models may require substantially different details in the problem description for each of the three levels outlined above. For example, some models may require precise details of geometry, while other for models, a simple compartment volume may

⁹ Wierzbicki, A., *Models and Sensitivity of Control Systems*, Wiley and Sons, New York, 1984.

¹⁰ Dickinson, R. P. and Gelinas, R. J., "Sensitivity Analysis of Ordinary Differential Equation Systems—A Direct Method," *Journal of Comp. Physics*, Vol 21, 123–143 (1976).

¹¹ Dunker, A. M., "The Decoupled Direct Method for Calculating Sensitivity Coefficients in Chemical Kinetics," *J. Chem. Phys.*, 81 (5), pp. 2385–2393, 1984.

suffice. For some models, a detailed description of the fire in terms of heat release rate, pyrolysis rate, and species production rates are necessary inputs. For other models, these may be calculated outputs. For each of the three levels of evaluation, an appropriate problem description sufficient to allow the problem to be simulated is necessary.

11.3 A model may be evaluated employing one or more of the following tools:

11.3.1 *Comparison with Standard Tests:*

11.3.1.1 Guidance for conducting the tests is provided by the relevant test method. Generally test conditions are well defined and focus on one or more specific output variables.

11.3.1.2 Model predictions can be tested against test output variables. This approach may be particularly useful for evaluating models designed to predict quantities such as fire resistance, flame-spread rates, etc.

11.3.1.3 Where data are available, model predictions should be viewed in light of the uncertainty in test/experimental data as compared to the uncertainty in the model results that arise due to uncertainty in the model inputs.

11.3.2 *Comparison with Full-Scale Tests Conducted Specifically for the Chosen Evaluation:*

11.3.2.1 Guidance for conducting full-scale compartment tests is provided by Guide E603.

11.3.2.2 The simulations are to be designed to duplicate, as well as possible, the salient features of the scenarios for which evaluation is sought. Data shall contain sufficient detail (for example, initial conditions, time scales, and so forth) to establish correspondence between predicted and measured quantities.

11.3.2.3 The predictive capabilities can be assessed by comparing predicted values and measured values of important quantities, by comparing key events in the fire, and by comparing key behavioral traits predicted by the model and measured during the simulation.

11.3.2.4 Where data are available, model predictions should be viewed in light of the variability of the full-scale test results and model sensitivity.

11.3.3 *Comparison with Previously Published Full-Scale Tests Data:*

11.3.3.1 Care should be taken to ensure the test closely simulated the scenario for which evaluation is sought. For example, input data to the model prediction should reflect the actual test conditions and some data normalization may be required to ensure the accuracy of the comparisons.

11.3.3.2 Although key measurements may or may not have been taken, the predictive capabilities can often be assessed by comparing predicted values and measured values of important variables, by comparing key events in the fire, and by comparing key behavioral traits predicted by the model and measured during the simulation.

11.3.3.3 Where data are available, model predictions should be viewed in light of the variability of the full-scale test results and model sensitivity.

11.3.4 *Comparison with Documented Fire Experience:*

11.3.4.1 Statistical data on fire experience must be judged for reliability.

11.3.4.2 Model predictions can be compared with eyewitness accounts of real fires.

11.3.4.3 Model predictions can be compared with known behavior of materials in fires (for example, melting temperatures of materials).

11.3.4.4 Model predictions can be compared with observed post-fire conditions such as known behavior of materials in fires (for example, melting temperatures of materials), extent of fire spread, tenability, etc.

11.3.5 *Comparison with Proven Benchmark Models:*

11.3.5.1 Care should be taken to ensure that the *benchmark* model has been evaluated for the scenarios of interest.

11.3.5.2 The predictive capabilities can be assessed by comparing the predicted values of important quantities, by comparing key events in the fire predicted by both models, and by comparing key behavioral traits predicted by both models.

11.3.5.3 Where data are available, model predictions should be viewed in light of the variability of the sensitivity of both model predictions.

11.3.6 *Quantifying Model Evaluation*—The necessary and perceived level of agreement for any predicted quantity is dependent upon the typical use of the quantity in the context of the specific use being evaluated, the nature of the comparison, and the context of the comparison in relation to other comparisons being made.

11.3.7 For single-point comparisons such as time to critical events or peak values, the results of the comparison may be expressed as an absolute difference (*model value—reference value*), relative difference (*model value—reference value*)/*reference value*, or other comparison as appropriate.

11.3.8 For comparison of two timed-based curves, appropriate quantitative comparisons depend upon the characteristics of the curves:

11.3.8.1 For steady-state or nearly steady state comparisons, the comparison may be expressed as an average absolute difference or average relative difference.

11.3.8.2 *For Other Than Steady-State:*

(a) The comparison may be expressed in terms of a range of the calculated absolute difference or relative difference, and

(b) The comparison may be expressed by comparing a time-integrated value of the quantity of interest.

(c) The concept of a norm provides a definition of the length of a vector. The distance between two vectors is simply the length of the vector resulting from the difference of two vectors. The symbolic representation is written as $\|\vec{x}\|$ where $\vec{x}$ is the notation for the n -dimensional vector $(x_1, x_2, \dots, x_{n-1}, x_n)$. All of the data can be represented by a vector of values measured at each time point, $\vec{E}$. The model predictions at the same time points can be represented by a vector $\vec{m}$. The distance between these two vectors is the norm of the difference of the vectors, or $\|\vec{E} - \vec{m}\|$. The Euclidean norm is most intuitive for computing this length:

$$\|\vec{x}\| = \sqrt{\sum_i x_i^2} \quad (4)$$

The inner product, $\langle \vec{x}, \vec{y} \rangle$, of two vectors is the product of the length of the two vectors and the cosine of the angle between them, or

$$\langle \vec{x}, \vec{y} \rangle = \|\vec{x}\| \cdot \|\vec{y}\| \cos(\angle(\vec{x}, \vec{y})) \quad (5)$$

or

$$\cos(\angle(\vec{x}, \vec{y})) = \frac{\langle \vec{x}, \vec{y} \rangle}{\|\vec{x}\| \cdot \|\vec{y}\|} \quad (6)$$

which is the difference in the shape of the two curves. Choosing the inner product to be the standard dot product gives results consistent with typical Euclidean interpretation:

$$\langle \vec{x}, \vec{y} \rangle = \sum x_i y_i \quad (7)$$

The Hellinger inner product for functions x such that $x(0)=0$ is defined based on the first derivative of the function:

$$\langle \vec{x}, \vec{y} \rangle = \int_0^T x'(t) y'(t) dt \quad (8)$$

For discrete vectors, this can be approximated with first differences as:

$$\langle \vec{x}, \vec{y} \rangle = \frac{\sum_{i=1}^N (x_i - x_{i-1})(y_i - y_{i-1})}{t_i - t_{i-1}} \quad (9)$$

Based on the first derivative or tangents to the curves, the Hellinger inner product and norm provide a sensitive measure of the comparison of the shape of two vectors. A variation of the Hellinger inner product can be defined based on the secant rather than tangent as:

$$\langle \vec{x}, \vec{y} \rangle = \int_{pT}^T \frac{(x(t) - x(t - pT)) \cdot (y(t) - y(t - pT))}{(pT)^2} dt \quad (10)$$

where $0 < p < 0.5$ defines the length of the secant. The limit of the secant inner product as $p \rightarrow 0$ is the Hellinger integral. For discrete vectors, this can be approximated analogous to the Hellinger geometry:

$$\langle \vec{x}, \vec{y} \rangle = \frac{\sum_{i=s}^N (x_i - x_{i-s})(y_i - y_{i-s})}{t_i - t_{i-s}} \quad (11)$$

When $s=1$, the secant definition is equivalent to the discrete Hellinger inner product. Depending on the value of p or s , the secant inner product and norm provide a level of smoothing of the data and thus better measures large-scale differences between vectors. For experimental data with inherent small-scale noise or model predictions with numerical instabilities, the secant provides a filter to compare the overall functional form of the curves without the underlying noise. Finally, a hybrid of the Euclidean and secant inner product provides a balance between the rank ordering of the Euclidean norm and the functional form comparison of the secant. From the axioms above, the sum of two inner products is also an inner product. For this paper, we will consider a simple weighted sum of the Euclidean inner product and secant inner product, or

$$\langle \vec{x}, \vec{y} \rangle = \frac{1}{n} \sum_{i=1}^N x_i y_i + \frac{1}{n-s} \sum_{i=s}^n \frac{(x_i - x_{i-s})(y_i - y_{i-s})}{(t_i - t_{i-s})} \quad (12)$$

While both the Euclidean relative difference and cosine have the appropriate ranking for all models, the cosine does not

provide much differentiation between the model predictions. The Hellinger and secant values provide a wider range since they specifically compare the functional forms of the experiment and models. The hybrid form combines the best features of these two. Values of the hybrid norm less than 0.3 and the hybrid shape factor greater than 0.9 satisfy the criteria that the two curves are in agreement.

12. Evaluation Report

12.1 The evaluation report is intended to provide sufficient detail such that the user of the evaluation could independently repeat the evaluation. At a minimum, the following information should be provided:

12.1.1 Date of the evaluation report,

12.1.2 Person or organization responsible for the evaluation,

12.1.3 Specific reference information for the evaluation report. References to model documentation, reports of experimental measurements, sensitivity analysis reports, and additional evaluation reports are appropriate,

12.1.4 Description of the model and scenarios for which evaluation is sought as outlined in 7.1 and 7.2,

12.1.5 Description of the theoretical basis for the model as outlined in Section 8,

12.1.6 Description of the mathematical and numerical robustness of the model as outlined in Section 9,

12.1.7 Details of the sensitivity analysis conducted as outlined in Section 10,

12.1.8 Details of the analysis of the predictive capabilities of the model conducted as outlined in Section 11, and

12.1.9 Known limitations for the use of the evaluation for other fire scenarios.

13. Guidance for Model Users Who are not Responsible for Maintenance of the Model

13.1 If the model(s) do not fit the user's requirements, then the user must determine the feasibility of appropriately modifying the model.

13.2 It is strongly recommended that any modification to the code of a fire model be made in collaboration with the model developer. Modifications must be well documented.

13.3 The new code should be extensively validated for the application of interest. Evaluations of the unmodified model do not suffice as evaluation of a modified model.

13.4 The use of other fire science tools, such as small and large scale fire tests; or a different type of model may be more appropriate than modification of an existing model.

14. Guidance for the Authority Having Jurisdiction

14.1 Often an individual or entity is responsible for the regulatory review and acceptance of an engineering assessment involving the use of fire models.

14.2 To assist in the review process, submittal of specific information can be requested of the model user.

14.3 The reviewer should request a copy of the model documentation and information on the predictive capability of the model and check that documentation and information against this guide.

14.4 As part of their review of an analysis based on a model, the reviewer can ask for evidence of the model user's fitness to

use the model for analysis, including the model user's experience, education, and credentials that may demonstrate the user's knowledgeable and responsible use of the fire model. Such experience should include experience with fire models in general and experience with the specific model used in the application of interest.

15. Keywords

15.1 evaluation; fire model; sensitivity; validation

APPENDIX

(Nonmandatory Information)

X1. COMMENTARY

X1.1 Introduction—This commentary has been prepared to provide the user of the guide with background information on its development and use.

X1.2 History of the Guide:

X1.2.1 When Subcommittee E05.39 on Fire Modeling was formed in 1985, one of its mandates, as formulated in response to the results of a survey of Committee E05 members, was to develop guidelines for the validation of fire models. This work has been subsumed by E05.33 Fire Safety Engineering.

X1.2.2 It has been recognized that the use of fire models extended beyond the fire research laboratory and into the engineering community. Reliance on model predictions in engineering applications is warranted only if the model has been validated for that application, but there was no accepted validation standard available at the time.

X1.2.3 Fire modelers had conducted validation exercises on their models and the Center for Fire Research of the National Institute of Standards and Technology was developing general procedures for model validation. This guide was developed to summarize the state-of-the-art in model validation into a single document of the use of either the modeler or the user of the model.

X1.2.4 Sensitivity, mathematical robustness, and a method for mathematical quantification of models are now made explicit in this guide.

X1.2.5 In 2011, two of the guides referenced in this document – ASTM E1472 and ASTM E1895 – were withdrawn. Material from those two withdrawn guides was added to this document as necessary to make this document complete.

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