



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.

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 The output from this document should not be used for regulatory purposes or the basis for regulations.

2. Referenced Documents

2.1 *ASTM Standards:*

E 176 Terminology of Fire Standards²

E 603 Guide for Room Fire Experiments²

E 1472 Guide for Documenting Computer Software for Fire Models²

E 1591 Guide for Data for Fire Models²

2.2 *International Standards Organization Standards:*
Guide to the Expression of Uncertainty in Measurement³

3. Terminology

3.1 *Definitions Specific to This Guide:*

¹ This guide is under the jurisdiction of ASTM Committee E-5 on Fire Standards and is the direct responsibility of Subcommittee E05.39 on Fire Modeling.

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² *Annual Book of ASTM Standards*, Vol 04.07.

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

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

3.1.2 *model validation*—the process of determining the correctness of the assumptions and governing equations implemented in a model when applied to the entire class of problems addressed by the model.

3.1.3 *model verification*—the process of determining the correctness of the solution of a system of governing equations in a model. With this definition, verification does not imply the solution of the correct set of governing equations, only that the given set of equations is solved correctly.

3.2 For additional definitions of terms used in this guide refer to Terminology E 176.

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 for evaluating the accuracy of the predictions of the model are provided. 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 E-5. It is intended for use by:

5.3.1 *Model Developers/Marketers*—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 a 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 primary emphasis of this guide is on zone models of compartment fires. However, other types of mathematical models need similar evaluations of their predictive capabilities.

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.

6.2 *Model and Scenario Definition:*

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 Guide E 1472. Details applicable to evaluation of the predictive capability of fire models are provided in 7.1.

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 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.

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 judgement. 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 E 1591. 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 an 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 E 603. 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*—Provide the following information:

7.1.1 The name and version of the model,

7.1.2 The name of the model developer(s),

7.1.3 A list of relevant publications,

7.1.4 A statement of the stated uses, limitations, and results of the model,

7.1.5 The type of model (zone, field, etc.),

7.1.6 A statement of the modeling rigor, including:

7.1.6.1 The assumptions inherent in the model and the governing equations included in the model formulation, and

7.1.6.2 The numerics employed to solve the equations and the method by which individual solutions are coupled.

7.1.7 Additional assumptions of the model as they relate to the stated uses or other potential uses,

7.1.8 The input data required to run the model, and

7.1.9 Property data that are defined with the computer program or were assumed in the model development.

7.2 *Scenarios for Which Evaluation is Sought*—Provide the following information:

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 reviewed 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. 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 Empirical or reference data used for constants and default values in the code should also be assessed for accuracy and applicability in the context of the model.

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.

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.

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.

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 Astronautics 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.