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An American National Standard

Standard Guide for
Evaluating the Predictive Capability of Deterministic Fire Models[1]

This standard is issued under the fixed designation E1355; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

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 guide assumes understanding of the use and limitations of the model under analysis as detailed in Guide E1895.

1.5 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
E1472 Guide for Documenting Computer Software for Fire Models
E1591 Guide for Obtaining Data for Deterministic Fire Models
E1895 Guide for Determining Uses and Limitations of Deterministic Fire Models

2.2 *International Standards Organization Standards:*
Guide to the Expression of Uncertainty in Measurement [3]

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

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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.

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. 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 assumes understanding of the use and limitations of the model under analysis as detailed in E1895.

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

5.4.1 *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.

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

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

5.4.4 *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.

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

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

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

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

5.6.2 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.

6.2 *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 E1472. Guidance on the use and limitations of deterministic fire models and on required knowledge is provided in Guide E1895. 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 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. At a minimum, the following information should be provided:

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, that is the general basis in terms of finite element control volume, Lagrangian, 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. This should include what empirical information is included and the uncertainty inherent in the choice. An example in zone modeling would be the plume equation, and in a CFD model it might be the free slip/no slip boundary conditions.

7.2 *Scenarios for which the Model has been Evalutated*—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 independently repeat the evalutation. 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

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

where:

$z\ (z_1, z_2, \ldots, z_m)$ = the solution vector for the system of equations (for example, mass, temperature, or volume)

$p\ (p_1, p_2, \ldots, p_n)$ = 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, . . ., m and I = 1, . . ., 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 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

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[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.

[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.