
Fire safety engineering —

Part 3:

**Assessment and verification of mathematical
fire models**

Ingénierie de la sécurité contre l'incendie —

Partie 3: Évaluation et vérification des modèles mathématiques



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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The main task of ISO technical committees is to prepare International Standards, but in exceptional circumstances a technical committee may propose the publication of a Technical Report of one of the following types:

- type 1, when the required support cannot be obtained for the publication of an International Standard, despite repeated efforts;
- type 2, when the subject is still under technical development or where for any other reason there is the future but not immediate possibility of an agreement on an International Standard;
- type 3, when a technical committee has collected data of a different kind from that which is normally published as an International Standard ("state of the art", for example).

Technical Reports of types 1 and 2 are subject to review within three years of publication, to decide whether they can be transformed into International Standards. Technical Reports of type 3 do not necessarily have to be reviewed until the data they provide are considered to be no longer valid or useful.

ISO/TR 13387-3, which is a Technical Report of type 2, was prepared by Technical Committee ISO/TC 92, *Fire safety*, Subcommittee SC 4, *Fire safety engineering*.

It is one of eight parts which outlines important aspects which need to be considered in making a fundamental approach to the provision of fire safety in buildings. The approach ignores any constraints which might apply as a consequence of regulations or codes; following the approach will not, therefore, necessarily mean compliance with national regulations.

ISO/TR 13387 consists of the following parts, under the general title *Fire safety engineering*:

- *Part 1: Application of fire performance concepts to design objectives*
- *Part 2: Design fire scenarios and design fires*
- *Part 3: Assessment and verification of mathematical fire models*
- *Part 4: Initiation and development of fire and generation of fire effluents*
- *Part 5: Movement of fire effluents*
- *Part 6: Structural response and fire spread beyond the enclosure of origin*
- *Part 7: Detection, activation and suppression*
- *Part 8: Life safety — Occupant behaviour, location and condition*

Annex A of this part of ISO/TR 13387 is for information only.

Introduction

ISO/TR 13387 describes a systematic engineering approach to addressing fire safety in buildings. Other parts of the Technical Report address fire spread, smoke movement, fire detection and suppression, and life safety. The objective of fire safety engineering is to assist in the creation of buildings which have an acceptable predicted level of fire safety. Part of this work involves the use of mathematical models to predict the course of events of potential fires in those buildings. Part 3, which addresses the assessment and verification of mathematical models for fire prediction, applies to mathematical fire models in general and not just to those that are part of the ISO fire safety engineering framework. Although the current focus of the document is on fire in buildings, it may also be used to assess fire models that concern other fires, such as outdoor fires and transportation fires.

Totally deterministic and totally probabilistic approaches to fire safety engineering are used today. Mathematical fire models are usually deterministic but sometimes contain probabilistic elements.

When combined, mathematical descriptions of physical phenomena and people movement can be programmed to create complex computer codes that estimate the expected course of a fire based on given input parameters. Mathematical fire models have progressed to the point of providing good predictions for some parameters of fire behaviour. However, input data is not always available, and many factors that affect the course of a fire, such as the position of doors or the location of people, are probabilistic in nature and cannot be determined from physics. These data and probabilistic factors require engineering judgement. For more detailed discussion of deterministic and probabilistic approaches to fire safety engineering the reader should refer to part 1 of ISO/TR 13387. The assessment and verification of probabilistic elements or totally probabilistic approaches are not addressed in this part of ISO/TR 13387.

Potential users of deterministic fire models and those who are asked to accept the results need to be assured that the models will provide sufficiently accurate predictions of the course of a fire for the specific application planned. To provide this assurance, the model(s) being considered should be verified for physical representation and mathematical accuracy. Verification involves checking that the theoretical basis and assumptions used in the model are appropriate, that the model contains no serious mathematical errors, and that it has been shown, by comparison with experimental data, to provide predictions of the course of events in similar fire situations with a known accuracy. It is understood that such comparisons cannot encompass every possible application of interest to the user. However, they should be representative of a range of similar applications. The fact that a model provides accurate predictions for one fire situation is not an absolute guarantee that it provides accurate predictions in a similar situation.

Concern for the accuracy of fire model predictions has been expressed by the international community of fire protection engineers and fire modelers themselves since the early models were published. The International Council for Building Research Studies and Documentation (CIB), Commission W14, Fire, recognized the need to expand international discussion on the use, application and limitations of fire models. The ISO task group that developed this ISO document used the ASTM standard guide^[1] as a reference text, and has outlined a format for collecting and making available experimental data on fire development and smoke spread in buildings. In addition, the methodology embodied in ISO 9000 for quality assurance of software should be followed.

Included in this document are:

- a) guidance on the documentation necessary to assess the adequacy of the scientific and technical basis of a model;
- b) a general methodology to check a model for errors and test it against experimental data;
- c) guidance on assessing the numerical accuracy and stability of the numerical algorithms of a model;
- d) guidance on assessing the uncertainty of experimental measurements against which a model's predicted results may be checked;
- e) guidance on the use of sensitivity analysis to ensure the most appropriate use of a model.

This document focuses on the predictive accuracy of mathematical fire models. However, other factors such as ease of use, relevance, completeness and status of development play an important role in the assessment of the use of the most appropriate model for a particular application.

Fire safety engineering —

Part 3:

Assessment and verification of mathematical fire models

1 Scope

This part of ISO/TR 13387 provides guidance on procedures for assessing and verifying the accuracy and applicability of deterministic mathematical fire models used as tools for fire safety engineering. It does not address specific fire models. It is not a step-by-step procedure, but does describe techniques for detecting errors and finding limitations in a calculation model. This part of ISO/TR 13387 does not address the assessment and verification of totally probabilistic approaches to fire safety calculations, or the probabilistic elements that may be combined with deterministic calculations.

2 Normative references

The following normative documents contain provisions which, through reference in this text, constitute provisions of this part of ISO/TR 13387. For dated references, subsequent amendments to, or revisions of, any of these publications do not apply. However, parties to agreements based on this part of ISO/TR 13387 are encouraged to investigate the possibility of applying the most recent additions of the normative documents indicated below. For undated references, the latest addition of the normative document referred to applies. Members of ISO and IEC maintain registers of currently valid international standards.

ISO/TR 13387-1, *Fire safety engineering — Part 1: Application of fire performance concepts to design objectives*.

ISO/TR 13387-2, *Fire safety engineering — Part 2: Design fire scenarios and design fires*.

ISO/TR 13387-4, *Fire safety engineering — Part 4: Initiation and development of fire and generation of fire effluents*.

ISO/TR 13387-5, *Fire safety engineering — Part 5: Movement of fire effluents*.

ISO/TR 13387-6, *Fire safety engineering — Part 6: Structural response and fire spread beyond the enclosure of origin*.

ISO/TR 13387-7, *Fire safety engineering — Part 7: Detection, activation and suppression*.

ISO/TR 13387-8, *Fire safety engineering — Part 8: Life safety — Occupant behaviour, location and condition*.

ISO 13943, *Fire safety — Vocabulary*.

3 Terms and definitions

For the purposes of this part of ISO/TR 13387, the terms and definitions given in ISO 13943, ISO/TR 13387-1 and the following apply.

3.1 engineering judgement

the process exercised by a professional who is qualified by way of education, experience and recognized skills to complement, supplement, accept or reject elements of a quantitative analysis

3.2 verification (as applied to mathematical fire models)

the process of checking a mathematical fire model for correct physical representation and mathematical accuracy for a specific application or range of applications

The process involves checking the theoretical basis, the appropriateness of the assumptions used in the model, that the model contains no unacceptable mathematical errors and that the model has been shown, by comparison with experimental data, to provide predictions of the course of events in similar fire situations with a known accuracy.

3.3 validation (as applied to fire calculation models)

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

4 Symbols and abbreviated terms

k	coverage symbol
s_i	standard deviation
U	expanded uncertainty
u_c	combined standard uncertainty
u_i	standard uncertainty
u_j	uncertainty component in category B (see 9.1)
v_i	number of degrees of freedom

5 Potential users and their needs

This part of ISO/TR 13387 is intended for use by:

- 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.
- Model users — to assure themselves that they are using an appropriate model for an application and that it provides adequate accuracy. Mathematical models will be used mostly by professional engineers for fire safety design of buildings, fire hazard and risk analysis of new products, fire investigation and litigation. In litigation involving corporations from different countries, an ISO standard for assessment and verification of calculation methods is likely to form the basis for acceptance of those methods. This identification process should be undertaken by a team of stakeholders including the building owner, the architect and all design engineers (including a fire safety engineer), the building manager, the building inspector or other approval authority and a fire service representative.

- c) Developers of model performance codes — to provide a means to detect invalid calculation procedures and avoid incorporating them into codes. Performance codes under development in a number of countries are likely to be models for fire codes in developing countries.
- d) Approving officials — to ensure that the results of calculations using mathematical models stating conformance to this part of ISO/TR 13387, cited in a submission, show clearly that the model is used within its applicability limits and has an acceptable level of accuracy.
- e) Educators — to demonstrate the application and acceptability of calculation methods being taught.

The importance of each clause of this part of ISO/TR 13387 will depend on the user. For example, model developers should be particularly interested in clause 6, Documentation, clause 8, Numerical accuracy, and clause 10, Sensitivity analysis. Whereas users, developers of model performance codes and approval officials will be more interested in clause 6, Documentation, clause 7, General methodology, clause 10, Sensitivity analysis, and clause 11, Reference fire tests.

6 Documentation

6.1 General

ASTM has published a standard guide for evaluating the predictive capability of fire models^[1], and a number of papers have been published on the subject^{[2],[3],[4],[5],[6],[7],[8]}. Annex A contains a review of the ASTM standard, a survey of fire models, and reviews of five of those publications.

The technical documentation should be sufficiently detailed that all calculation results can be reproduced within the stated accuracy by an independent engineer experienced in mathematics, numerical analysis and computer programming, but without using the described computer programme.

Sufficient documentation of calculation models, including computer software, is essential 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. Reports on any assessment and verification of a specific model should become part of the documentation. The ASTM guide for documenting computer software for fire models^[9] is the primary source for information contained in this clause.

Documentation of computer models should include technical documentation and a user's manual. The technical documentation, often in the form of a scientific or engineering journal publication, is needed to assess the scientific basis of the model. A user's manual should enable the user to understand the model application and methodology, reproduce the computer operating environment and the results of sample problems included in the manual, modify data inputs, and run the program for specified ranges of parameters and extreme cases. The manual should be concise enough to serve as a reference document for the preparation of input data and the interpretation of results. Installation, maintenance and programming documentation may be included in the user's manual or be provided separately. There should be sufficient information to install the programme on a computer. All forms of documentation should include the name and sufficient information to define the specific version of the model and identify the organization responsible for maintenance of the model and for providing further assistance.

The following subclauses describe the suggested contents of technical documentation and a user's manual. The list is quite lengthy, but is not intended to exclude other forms of information that can assist the user in assessing the applicability and usability of the model.

6.2 Technical documents

Technical documentation should:

- a) define the fire problem modelled, or the function performed by the model;
- b) include any feasibility studies and justification statements;
- c) describe the theoretical basis of the phenomena and the physical laws on which the model is based;

- d) present the governing equations;
- e) identify the major assumptions and limits of applicability;
- f) describe the mathematical techniques, procedures and computational algorithms employed and provide references for them;
- g) discuss the precision of the results obtained by important algorithms, and any dependence on particular computer capabilities;
- h) list any auxiliary programmes or external data files required;
- i) provide information on the source, contents and use of data libraries;
- j) provide the results of any efforts to evaluate the predictive capabilities of the model;
- k) provide references to reviews, analytical tests, comparison tests, experimental validation and code checking already performed;
- l) indicate the extent to which the model meets this part of ISO/TR 13387.

6.3 User's manual

The user's manual should:

- a) include a self-contained description of the programme;
- b) describe the basic processing tasks performed, and the methods and procedures employed (a flow chart can be useful);
- c) identify the computer(s) on which the programme can be executed, and any peripherals required;
- d) provide instructions for installing the programme;
- e) identify the programming languages and software operating systems and versions in use;
- f) describe the source of input information and any special input techniques;
- g) describe the handling of cases in which only minor differences are introduced between runs;
- h) provide the default values or the general conventions governing them;
- i) list any property values defined within the programme;
- j) describe the contents and organization of any external data files;
- k) list the operating-system control commands;
- l) describe the programme output and any graphics display and plot routines;
- m) provide information to enable the user to estimate the execution time on applicable computer systems for typical applications;
- n) provide sample data files with associated outputs to allow the user to verify the correct operation of the programme;
- o) list instructions for appropriate actions when error messages occur;
- p) provide instructions on judging whether the programme has converged to a good solution where appropriate.

7 General methodology

7.1 General

In this part of ISO/TR 13387 the term "model" encompasses all the physical, mathematical and numerical assumptions and approximations that are employed to describe a particular fire process, movement of effluents, building or occupant response, and fire detection, activation or suppression system, including those boundary conditions that are necessary for its application to a particular scenario. This document is written on the assumption that the model is implemented as a programme on a digital computer. In order to check that such a computer model can satisfactorily represent physical reality, a process of verification is necessary to test the adequacy of a model's theoretical basis and implementation. Such a process requires that the computer code be fully documented to permit independent review of the theoretical assumptions and mathematical techniques used in the model. Whenever possible, the source code should be a part of the evaluation, but it is recognized that when commercial software is used the source code is often not available.

A verification methodology can be designed to reveal inappropriate methods or erroneous assumptions that can arise from any of the following sources:

- a) the use of inappropriate algorithms or wrong physics to describe the fire processes and sub-processes that are being modelled,
- b) the use of incorrect or unsubstantiated constants or default values;
- c) the omission of (sub)-processes in describing the development of a fire (this is essentially that the model oversimplifies the phenomena which it is attempting to represent);
- d) the use of inappropriate numerical algorithms to solve the equation set(s) that result from the application of algorithms to describe the (sub)-processes;
- e) errors in the computer code.

The techniques for detecting errors in a model can be classified as:

- a) review of the theoretical basis of the model;
- b) code checking;
- c) analytical tests;
- d) inter-model comparison;
- e) empirical validation.

7.2 Review of the theoretical basis of the model

The theoretical basis of the model should be reviewed by one or more experts fully conversant with the chemistry and physics of fire phenomena but not involved with the production of the model. This review should include an assessment of the completeness of the documentation, particularly with regard to the assumptions and approximations. Reviewers should judge whether there is sufficient scientific evidence in the open scientific literature to justify the approaches and assumptions being used. Data used for constants and default values in the code should also be assessed for accuracy and applicability in the context of the model.

7.3 Analytical tests

If the programme 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.

7.4 Comparison with other programmes

The predictions of one model (that under "test") are compared with those from other models supplied with identical data. If these other programmes have themselves undergone validation, they can serve as benchmarks against which the programme under test can be judged. If used with care and judgement, inter-model comparisons can reveal areas where programmes are inadequate.

7.5 Empirical verification

The comparison of the predictions of a model with data gathered experimentally is the primary way users feel confident in a model's predictive capability. When a phenomenon is not well or fully understood, empirical verification provides a way of testing that its representation in the model (programme) is adequate for the intended use of the programme. Programme predictions should be made without reference to the experimental data to be used for the comparison. Of course, this restriction does not include required input data that may have been obtained by bench-scale tests. Uncertainties in the measurements should be accounted for in a systematic and logical manner. No attempt to adjust a fit between the measurements and the predictions should be made.

Comparison of model predictions with experimental data requires:

- a) a thorough understanding of the sources of uncertainty in the experiments performed;
- b) quantification of these sources of uncertainty;
- c) sensitivity analysis to assess the effect of the uncertainty on the predictions;
- d) data/programme comparison techniques to account for such uncertainty.

Most published work on the comparison of model predictions with experimental data is qualitative, i.e. reported as "satisfactory", "good" or "reasonable". Beard^{[2],[3]} provides some guidance on quantification.

7.6 Code checking

The code can be checked on a structural basis, preferably by a third party either totally manually or by using code-checking programmes, to detect irregularities and inconsistencies within the computer code. Ensuring that the techniques and methodologies used to check the code, together with any deficiencies found, are clearly identified and recorded will increase the level of confidence in the programme's ability to process the data reliably, but it cannot give any indication of the likely adequacy or accuracy of the programme in use.

Table 1 summarizes the errors and shortcomings that the above techniques can detect.

Table 1 — Techniques for detecting model errors and shortcomings

Techniques	Incorrect algorithms	Incorrect constants	Missing processes	Inappropriate numerical techniques	Coding errors
Theoretical review	X	X	X	X	
Analytical tests			X		X
Comparison with reference programmes	X	X	X		
Experimental verification		X	X		X
Code checking					X

8 Numerical accuracy

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. In a numerical method, the continuous mathematical model is discretized, i.e. approximated by a discrete numerical model. The discretization errors are discussed below.

A continuous mathematical model can be discretized in many different ways, resulting in as many different discrete models. To achieve a good approximation of the solution of the continuous models, we require the discrete model to mimic the properties and the behaviour of the continuous model. This means that we want our discrete solution to converge to the solution (when it exists) of the continuous problem, when the discretization parameters (time step, space mesh, etc.) decrease. This is achieved when the requirements for consistency and stability are met. Consistency means that the discrete model approximates the continuous model well in the sense of some measure, i.e. a norm. The choice of the norm depends on the specific problem. The stability means that the error terms do not increase as the programme proceeds.

Often the continuous mathematical model is a set of partial differential equations (PDEs). After semi-discretization in space, a set of non-linear or linear ordinary differential equations (ODEs) is obtained. Higher-order differential equations can be transformed to systems of first-order equations, and we will consider in the following only first-order equations. The full discrete model is created by discretizing the ODEs in the time space (usually by a finite-difference method or finite-element method). The resulting set of non-linear or linear algebraic equations is, in turn, solved using appropriate numerical methods (Gauss, Newton, etc.).

Many fire problems involve the interaction of different processes, such as the chemical or thermal processes and the mechanical response. The time scales associated with these 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.

Discretization can also result in a stiff discrete model: for example when heat conduction equations (a continuous model described with PDEs) are first semi-discretized in space and a stiff ODE is obtained. In this case, the stiffness of the semi-discrete model increases when the spatial discretization parameter (mesh) decreases.

A stiff discrete problem may also arise even though the original continuous problem was not stiff. In non-linear cases, the behaviour and then the stiffness of the model can change all the time as the solution evolves.

Stability must be considered in the analysis and performance of temporal (transient) algorithms to prove the convergence of the solution algorithm. An algorithm for which stability imposes a restriction on the size of the time step is called "conditionally stable". An algorithm for which there is no time step restriction imposed by stability is called "unconditionally stable". Stable integration gives decaying solutions (e.g. the analytical solutions of the continuous-problem ODEs). Unstable methods can give quickly unbounded and oscillating numerical solutions for some sizes of time step. It is important to realize that the numerical model can be unstable even when the continuous model is stable. There are, however, cases in which the original continuous model is unstable, and then accurate solutions cannot be expected by any numerical method. Conversely, unconditionally stable algorithms may lead to stable numerical models even when the conditions are unstable. This means that unconditionally stable algorithms may fail to take account of rapidly increasing phenomena such as the fire itself.

Time integration of the ODEs can generally be carried out using two different types of numerical quadrature algorithm: explicit or implicit. In the explicit method, the new values of the solutions are given explicitly in terms of the old values. This is sometimes called time marching, and a typical example is the forward Euler algorithm. In the case of the implicit method, the new values depend on the old and the new ones. Examples of implicit methods are backward Euler, Cranck-Nicolson and the midpoint family method. Explicit methods are conditionally stable. All the implicit methods are unconditionally stable in the linear case.

Integration of stiff systems of ODEs using inadequate algorithms like the unstable or conditionally stable methods may result in unbounded solutions and therefore considerable errors. The stability of the integration, i.e. of the approximate solution, is determined by the more rapidly varying solution, even after the solution has effectively died away. This is a generic problem of stiff equations, and we are forced to follow variation in the solution on the shortest time scale to maintain stability of the integration, even though accuracy requirements allow a much larger size of (time) step. A way out of the problem is to use implicit methods.

In non-linear problems, the stability regions of the solution all evolve with the solution itself, and the conditions of stability may change. For example, the unconditional stability of the implicit trapezoidal (Crank-Nicolson) integration scheme is not carried over to the non-linear regime. Methods like those of the generalized midpoint family exist which may also preserve unconditional stability in the non-linear regime.

In addition to the discretization errors, one has also to consider the machine errors caused by the finite accuracy of computer's floating-point presentation of numbers. This may raise problems when calculating derivatives with small discretization steps. Round-off error of a difference quotient can lead to catastrophic cancellation, i.e. the error due to subtraction of nearly equal numbers. There may also be a problem when the magnitude of variables varies by orders of magnitude. In a good algorithm, the variables are scaled to be of the same order of magnitude if possible.

Because the numerical convergence depends both on the original mathematical model and the method of discretization, no general method exists for checking the consistency and stability in every case. Confidence in the numerical method may be increased by checking the rate of convergence by repeating the calculations with various discretization steps. If the error according to a relevant norm decreases with decreasing step size, the method is consistent. Yet, this does not guarantee the solution found to be a correct one.

In the case of field models, it is important to examine the sensitivity of the solution to grid refinement. This can be an expensive task. Refining a grid by a factor of two in each coordinate direction will increase computational cost roughly by a factor of eight and so it is often necessary to strike a compromise between cost and accuracy. Most general-purpose computer fluid-dynamics packages provide diagnostic information on the progress of residual errors for each of the equations solved. However, it is important to be satisfied that the overall mass and energy balances for the whole domain are within acceptable bounds. Compartment mass outflows must balance mass inflows, and heat lost into the structure taken together with heat lost from the compartment through its opening must balance that generated by the fire.

It is important to ensure that the solution is "well behaved". This might include inspection, for example, to ensure that it is free from spurious oscillations, that the characteristics of the fire source, especially its buoyancy flux and flame length, are correctly simulated, and that predicted downstream temperatures away from the areas of chemical reaction are less than those at the source. If problems of this nature do occur, then consideration should be given to reducing the grid spacing and/or time step.

There will be occasions when the computer simulation using field modelling may suggest unexpected behaviour. If a physical simulation were to produce something unexpected, the engineer would exert his ingenuity to explain what has been observed or what has been measured and relate it to the practical problem at hand. However, with a numerical simulation such an eventuality is more disturbing since it can have two explanations: either it is genuine and would have been observed in a physical simulation, or it is some sort of misleading numerical artifact.

The possibility of the latter cannot be completely discounted with such complex numerical simulations as those involved in computer fluid dynamics (CFD). It is therefore essential to "shadow" the numerical solution, where possible, with known simple calculation methods.

Some examples of the consideration of numerical problems in fire simulation models can be found in the paper by Mitterl^[10]. A discussion of the principles involved in CFD when applied to fire can be found in reference [11], and of the problems associated with numerical approximation in reference [12].

9 Measurement uncertainty of data

9.1 General

Much of this clause is taken from NIST Technical Note 1297, "Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results", by Taylor and Kuyatt^[13].

This clause is provided to assist experimenters in expressing the uncertainty of their measurements, and model users in judging the usefulness of experimental data when making an empirical verification of the model. Not all published experimental data will include information on the uncertainty of the data.

In general, the result of a measurement is only 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.

The uncertainty of the result of a measurement generally consists of several components which, in the approach used by the International Council on Weights and Measures, may be grouped into two categories according to the method used to estimate their numerical values:

- Category A: those which are evaluated by statistical methods;
- Category B: those which are evaluated by other means.

Uncertainty is commonly divided into two components: random and systematic. Each component that contributes to the uncertainty of a measurement is represented by an estimated standard deviation termed "standard uncertainty", with a suggested symbol u_i , and equal to the positive square root of the estimated variance u_i^2 . An uncertainty component in category A can be represented by a statistically estimated standard deviation s_i (equal to the positive square root of the statistically estimated variance s_i^2) and the associated number of degrees of freedom ν_i . For such a component, the standard uncertainty $u_i = s_i$. In a similar manner, an uncertainty component in category B is represented by a quantity u_j which may be considered an approximation to the corresponding standard deviation; it is equal to the positive square root of u_j^2 , which may be considered an approximation to the corresponding variance and which is obtained from an assumed probability distribution based on all the available information. Since the quantity u_j^2 is treated like a variance and u_j like a standard deviation, for such a component the standard uncertainty is simply u_j .

9.2 Category A determination of standard uncertainty

A category A determination of standard uncertainty may be based on any valid statistical method for treating data. An example is calculating the standard deviation of the mean of a series of independent observations using the method of least squares to fit a curve to data in order to estimate the parameters of the curve and their standard deviations. This part of ISO/TR 13387 does not attempt to give detailed statistical techniques for carrying out statistical determinations (see references [13], [14], [15] and [16]).

9.3 Category B determination of standard uncertainty

A category B determination of uncertainty is usually based on scientific judgement using all the relevant information available, which may include:

- a) previous measurement data;
- b) experience with, or general knowledge of, the behaviour and properties of relevant materials and instruments;
- c) manufacturer's specifications;
- d) data provided in calibration and other reports, and uncertainties assigned to reference data taken from handbooks.

Because the reliability of determination of components of uncertainty depends on the quality of information available, it is recommended that all parameters upon which the measurement depends be varied to the fullest extent practicable so that the determinations are based as much as possible on observed data. Whenever feasible, the use of empirical models of the measurement process founded on long-term quantitative data, and the use of check standards and control charts that can indicate that a measurement process is under statistical control, should be part of the effort to obtain reliable determinations of components of uncertainty.

9.4 Combined standard uncertainty

The combined standard uncertainty of a measured result, suggested symbol u_c , is taken to represent the estimated standard deviation of the result. It is obtained by combining the individual standard uncertainties u_i , whether arising from a category A or a category B determination, using the usual method for combining standard deviations. This method is often called the "law of propagation of uncertainty" or the "root-sum-of-squares" method. Combined standard uncertainty u_c is a widely used measure of uncertainty.

9.5 Expanded uncertainty

Although the combined standard uncertainty u_c is used to express the uncertainty of many measurement results, what is often required is a measure that defines the interval about the measurement result y with which the value of the measurement Y can be confidently asserted to lie. This measure is termed "expanded uncertainty", suggested symbol U , and is obtained by multiplying $u_c(y)$ by a coverage factor, suggested symbol k . Thus $U = k \times U(y)$ and it can be confidently asserted that $y - U \leq Y \leq y + U$, which is commonly written as $Y = y \pm U$.

In general, the coverage factor k is chosen at the desired level of confidence. Typically, k is in the range 2 to 3. When the normal distribution applies and u_c has negligible uncertainty, $k = 2$ defines an interval having a level of confidence of approximately 95 %, and $k = 3$ defines a level of confidence greater than 99 %. Current international practice is to use the value $k = 2$.

9.6 Reporting uncertainty

To report measurement uncertainty, report U together with the coverage factor k used to obtain it, or report u_c . When reporting a measurement result and its uncertainty, include the following information in the report itself or by referring to a published document:

- A list of all components of standard uncertainty, together with their degrees of freedom where appropriate, and the resulting value of u_c . The components should be identified according to the method used to estimate their numerical values (statistical or other means).
- A detailed description of how each component of standard uncertainty was determined.

10 Sensitivity analysis

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 rigour employed in modelling the relevant physics and chemistry, and to use of inadequate numerical treatments. A well designed and executed sensitivity analysis serves to:

- a) identify the dominant variables in the models;
- b) define the acceptable range of values for each input variable;
- c) demonstrate the sensitivity of output variables to variations in input data;
- d) inform and caution any potential users about the degree and level of care to be taken in selecting inputs and running the model;
- e) provide insights as to which parameters should be monitored in large-scale fire experiments.

Conducting a sensitivity analysis of a complex fire model is not a simple task (see references [17] and [18]). 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.

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.

The selection of parameters to be investigated will be aided by the knowledge and familiarity of the investigator with fire dynamics in single-compartment, multi-compartment and complex spaces.

A distinction must also be made between parameters which are internal and those which are external to the model. The former provide an insight on how well the physics and the mathematics utilized in the model reflect real fire behaviour and should be subject to verification. In some types of model, internal parameters may be open to

manipulation by the user. In particular, for CFD field models the numerical factors such as relaxation, numerical grid and number of iterations are internal parameters.

External parameters are those which the user can manipulate as inputs. They can be partitioned as follows:

- geometrical: fire enclosure's basic dimensions, openings, vents and connecting adjacent spaces;
- fire scenario: derived from a knowledge of the heats of combustion and mass loss rate of fuel or from large- or small-scale rate of heat release (calorimetric) measurements and the distribution of fuels;
- thermophysical: the thermophysical properties of the enclosure's boundaries can influence the growth and development of fire, hence properties such as conductivity, specific heat, density and emissivity of floors, walls and ceilings are necessary inputs.

11 Reference fire tests

Fire tests used for making comparisons with mathematical fire model predictions should be carefully planned, executed and documented. ASTM, BSI and NORDTEST provide guidance for running large fire tests^{[19],[20],[21]}.

To be useful to the model user, fire test data should be readily accessible. An example of a collection of reference experimental fire tests for comparison with the predictions of calculation fire models is contained in the Fire Data Management System (FDMS) being developed by the National Institute of Standards and Technology in the USA^[22]. FDMS is a computer database for organizing and presenting fire data obtained from bench-scale and real-scale tests as well as fire simulation programmes. Data in the data base have not been examined for accuracy. Users must refer to the documentation provided by the test laboratory for detailed information on experimental procedures and the precision of the instrumentation used.

Available fire test values are stored in a common format, and are readily available to computer models, plotting programmes and report generators. All file formats and programme functionality provided in the current version of FDMS will be supported in later versions along with appropriate user-recommended additions.

FDMS provides a database format for test values generated from a variety of sources within the fire community. A sample of what is available be accessed through the internet, providing all participants with immediate access to new results. The access address is "candela.cfr.nist.gov". The FDMS concept is not limited by computer platforms, computer languages or data inflexibilities. FDMS provides a user interface that is independent of the computer platform.

A programmer's reference guide^[23] provides details of the FDMS internal file formats, including database files and import/export formats. These formats are detailed to assist model developers in accessing test data in FDMS and in verifying that all data required by their models is available.

The technical documentation^[24] is intended to present the current design plan for the physical files in FDMS. Initially, the clauses in this document should be read in a sequential manner in order to follow the development of the physical design. After an initial review, the document should serve as a technical reference. Some knowledge and experience with computer databases and database concepts is assumed throughout the technical reference documentation.

Currently, FDMS contains data from 125 fire tests ranging from room fire tests to larger simulations of multi-room fires, including all those listed in "Data for Room Fire Model Comparisons"^[25]. Tests include:

- a) single room with furniture;
- b) single room with furniture and wall burning;
- c) three rooms including corridor;
- d) four rooms including corridor;
- e) multi-storey building;

- f) room corner tests;
- g) cone calorimeter tests.

The data base, which contains data from laboratories in a number of countries including Finland, Norway, Sweden, and the USA, is continually being expanded as more data becomes available.

Users of FDMS may search the whole catalogue, by test method, laboratory, type (bench-scale or full-scale), sponsor, product tested, the measurements taken or any combination of the above. Once the selection of a particular test has been made, an export programme creates an ASCII file for transfer to the user.

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Annex A (informative)

Literature review

NOTE The reviews of documents contained in this annex are provided to guide the reader on the contents of some of the referenced documents. The list is not intended to be comprehensive.

A.1 List of reviewed documents

A.1.1 ASTM E 1355-97, *Standard Guide for Evaluating the Predictive Capability of Deterministic Fire Models*.

A.1.2 BEARD, A., The Limitations of Computer Models. *Fire Safety Journal*, **18**, pp. 375-391, 1992.

A.1.3 BEARD, A., Evaluation of Deterministic Fire Models — Part I: Introduction. *Fire Safety Journal*, **19**, pp. 295-306, 1992.

A.1.4 DAVIES, A.D., Some Tools for Fire Model Validation. *Fire Technology*, **23**, pp. 95-114, 1987.

A.1.5 FRIEDMAN, R., An International Survey of Computer Models for Fire and Smoke. *Journal of Fire Protection Engineering*, **4**, pp. 81-92, 1992.

A.1.6 IMAN, R.L., and HELTON, J.C., An Investigation of Uncertainty and Sensitivity Analysis Techniques for Computer Models. *Risk Analysis*, **8**, pp. 71-90, 1988.

A.1.7 NELSON, H. E., and DEAL, S., Comparing Compartment Fires with Compartment Fire Models, *Fire Safety Science — Proceedings of the Third International Symposium*, ed. by COX, G., and LANGFORD, B., pp. 719-728, Elsevier, New York, 1991.

A.1.8 MAGNUSSON, S.E., FRANTZICH, H., and HARADO, K., Fire Safety Design Based on Calculations-Uncertainty Analysis and Safety Verification, ISSN 1102-8246, ISRN LUTVDG/TVBB-3078-SE, Department of Fire Safety Engineering, Lund University.

A.2 Review of ASTM E 1355-97, *Standard Guide for Evaluating the Predictive Capability of Deterministic Fire Models*

A.2.1 Scope

This guide provides a methodology for evaluating the predictive capabilities of a fire model for a specific use.

A.2.2 Review

A brief description of the model and the scenario for which evaluation is sought are necessary.

A sensitivity analysis should be conducted to determine how changes in model parameters affect the results generated by the model. Model predictions may be sensitive to:

- uncertainties in input data;
- the rigour employed in modelling the relevant physics and chemistry;
- poor numerical treatments.

Two methods for conducting a sensitivity analysis are:

- the partial derivative method: the partial derivative of each of the predicted values is computed and used as a measure of model sensitivity;
- the response surface method: a metamodel is developed as a simpler and more easily analysed model of the fire model; the sensitivity analysis is then conducted on the metamodel.

Several alternatives are provided for evaluating the accuracy of predictions of a model. Comparisons can be made between predictions and the results of:

- standard fire tests;
- full-scale fire experiments;
- field experience;
- published literature or
- previously evaluated models.

The predictive capabilities may be expressed as percent accuracy, although the prediction of key behavioural traits can also be an important measure.

Finally, guidance is given concerning the relevant documentation required to summarise the evaluation process.

A.3 Review of BEARD, A., The Limitations of Computer Models, *Fire Safety Journal*, 18, pp. 375-391, 1992

A.3.1 Abstract

The limitations of computer models in relation to fire risk are considered in very general terms. The vital importance of the appropriate use of a model and suitable interpretation of results is stressed. Further, the possible capacity of a model to assist in gaining qualitative insights is considered. Some general conclusions are drawn.

A.3.2 Review

Issues which emerge when comparing theory and experiment are:

- a) uncertainty and flexibility associated with experimental results:
 - 1) uncertainty associated with lack of controlled conditions, e.g. uncontrolled ambient conditions,
 - 2) uncertainty and flexibility associated with experimental design, e.g. exact locations of probes,
 - 3) uncertainty associated with error in measurement,
 - 4) uncertainty associated with raw data processing algorithms;
- b) uncertainty and flexibility associated with theoretical predictions:
 - 1) uncertainty associated with conceptual assumptions, e.g. choosing zone vs field modelling,
 - 2) uncertainty and flexibility associated with numerical assumptions, e.g. uncertainty in input parameters, grid sizes.

Sensitivity — As there is often uncertainty in the input parameters required to run a model, there is the need for sensitivity analyses to determine the impact of such uncertainties on predictions.

Deterministic chaos — As a result of the non-linearities inherent in fire problems, there may be a hypersensitive dependence on initial conditions and external disturbances. This could raise fundamental questions about the limits in principle to the repeatability of an experiment.

There is a need for reliable sets of data for different scenarios.

Assessment of models should be carried out by people who have no direct interest in the model.

A.4 Review of BEARD, A., Evaluation of Deterministic Fire Models — Part I: Introduction, *Fire Safety Journal*, 19, pp. 295-306, 1992

A.4.1 Abstract

During 1989 and 1990, a preliminary evaluation of four deterministic fire models was carried out by the University of Edinburgh at the request of the Home Office (London). This paper is the first in a series based on this work and contains material common to the entire study. The models considered were FAST, HAZARD1 (which contains FAST), FIRST and JASMINE.

A.4.2 Review

Comparison between theory and experiment is problematic. Issues include:

- a) uncertainty and flexibility (e.g. location of thermocouples) associated with experimental results;
- b) uncertainty and flexibility (e.g. grid specification) associated with theoretical predictions.

Approach — The four models were tested against three well documented experimental fires exhibiting a range of sizes and complexities:

- a) Foam-slab test: ignition of a slab of polyurethane foam in a room with an open doorway;
- b) House-fire test: ignition of a chair in the lounge of a house;
- c) Department-store test: ignition of a chair and two settees in a large department-store space with doors and windows closed.

Input data for the models were developed on the basis of *a priori* information available to the investigator, i.e. experimental results (e.g. mass loss rate) were not used to determine input data. Further, input parameters were not adjusted to improve agreement between theory and experiment.

Estimating the hazard is complex, as it is difficult to establish criteria for fatality. For the purposes of the study, simple criteria were adopted based on heat flux (temperature), smoke obscuration, carbon monoxide concentration and interface height.

Evaluations are to be described in subsequent papers.

A comparison of a single run of a computer model with a single set of experimental results is in general of limited value.

A mechanism for approval of models for specific applications needs to be established.

A.5 Review of DAVIES, A.D., Some Tools for Fire Model Validation, *Fire Technology*, 23, pp. 95-114, 1987

A.5.1 Abstract

General ideas are offered for describing fire model validity prior to starting product design. Validation of independent test results is part of this phase. Differences between comparable results and graphical methods, and distinctions between random and systematic errors, are discussed.

A.5.2 Review

Model validation has two main purposes: to assess the prototype (research and development) version of a model and to assess the user package. Product design converts the prototype into a user package. The paper addresses prototype validation in which the reduction of uncertainty in principal model outputs is the main goal. Feasibility, soundness and realistic behaviour over the range of interest are also major concerns.

Each model may require some degree of special treatment during validation.

Independent examination is important to reduce concerns about the objectivity of the findings.

Given a limited validation budget, the elements of a resource allocation problem are present.

Validated tests are valuable resources aiding in the study of related models. Important by-products of validated tests include estimates of random and systematic errors for individual sensors, sensor combinations and processed results, and preferred instrumentation and processing configurations.

The number of tests needed is large for two reasons. First, several combinations of the principal variables should be explored over their intended range to test the ability of the model to match test results. Second, each parametric combination should be repeated so that the natural variability of the phenomena can be estimated. Uncertainties in test data limit the precision with which the model can be evaluated.

Understanding the model is important. Look for intermediate results which offer the opportunity to partition the problem into more manageable clauses.

Error means the residual difference between what is observed (test results) and what is predicted (model results). There can be problems from both sources. The intent is to search for the symptoms of a significant error, isolate it, fix it where the cost is not too high, and look for the next one.

Systematic errors are fairly stable over time whereas random errors have a zero mean. Random errors come from experimental features such as instrument noise and turbulence whereas sources of systematic errors include instrument miscalibration and modelling and input data assumptions. (N.B. Actual and measured temperatures may differ significantly due to radiative losses or conduction by wires.)

Graphs are useful in presenting information while avoiding excessive detail. For example, graphs can display the time dependence of the average (of several) test results and corresponding model results, as well as uncertainties in the test results.

Statistical methods, including the use of graphs of the variation in the sample standard deviation with time, can be used to determine whether errors in the test data are significant.

Sensitivity analyses address changes (errors) in an output variable Y , given changes (errors) in input variables X_1, \dots, X_k . The derivative (or ratio of differences) of Y with respect to X_j yields a sensitivity coefficient. Given a range of an input variable, DX_j , the corresponding output error can be computed. Some contributors to overall output error may be ignored because of their relative size. Confidence in a sensitivity analysis can be gained by comparing predicted standard deviations of output variables, given DX_j with observed standard deviations of output variables for the tests.

A.6 Review of FRIEDMAN, R., An International Survey of Computer Models for Fire And Smoke, *Journal of Fire Protection Engineering*, 4, pp. 81-92, 1992

A.6.1 Abstract

At the request of the Forum for International Cooperation on Fire Research, a worldwide survey was conducted of operational computer programmes relevant to fire protection. A total of 62 programmes, from 10 countries, were identified. These include compartment fire models, fire-sprinkler interaction models and submodels for fire endurance, building evacuation, thermal detector actuation, fire spread on a wall and smoke movement. These are listed, plus 12 additional models, including models from three additional countries. Then a general discussion is provided of the difficulties in achieving an accurate model of a growing fire in an enclosure, and of assessing the accuracy of a given model.

A.6.2 Review

Reasons why a model may not yield results in complete accord with actual fire behaviour are:

- a) idealizations and simplifications on which the model is based deviate significantly from reality;
- b) input parameters supplied to the model are inaccurate;
- c) "default" values of coefficients used internally in the model are incorrect;
- d) the computation process yields a wrong result (due to poor choice of time steps or mesh size or due to mathematical singularities or instabilities);
- e) the experimental measurements are incorrect or non-repeatable.

It is generally risky to apply a model to conditions which are drastically different from those for which the model has been validated.

Usually, it is best to express the accuracy of a model in terms of the percentage deviation of the prediction from the measurements.

An alternative method is proposed for assessing the accuracy of a model. Since what is often required is a simple yes/no answer to a specific question, the concept of the reliability of a yes/no prediction is introduced. A model may be 100 % reliable for certain conditions, but for some conditions it may only be 50 % reliable. For example, for some combinations of input variables a model may give unreliable predictions for a determinable range of each input variable, but otherwise be 100 % reliable.

A.7 Review of IMAN, R.L., and HELTON, J.C., An Investigation of Uncertainty and Sensitivity Analysis Techniques for Computer Models, *Risk Analysis*, 8, pp. 71-90, 1988

A.7.1 Abstract

Many different techniques have been proposed for performing uncertainty and sensitivity analyses on computer models for complex processes. The objective of the present study is to investigate the applicability of three widely used techniques to three computer models having large uncertainties and varying degrees of complexity in order to highlight some of the problem areas that must be addressed in actual applications. The following approaches to uncertainty and sensitivity analysis are considered: (1) response surface methodology based on input determined from a fractional factorial design, (2) Latin hypercube sampling with and without regression analysis and (3) differential analysis. These techniques are investigated with respect to (a) ease of implementation, (b) flexibility, (c) estimation of the cumulative distribution function of the output and (d) adaptability to different methods of sensitivity analysis. With respect to these criteria, the technique using Latin hypercube sampling and regression analysis had the best overall performance. The models used in the investigation are well documented, thus making it possible for researchers to make comparisons of other techniques with the results in this study.

A.7.2 Review

The output of a model, Y , can be expressed as a function $Y=f(X_1, \dots, X_k; t)$ of the independent input variables X_1, \dots, X_k and of time. In fact, there may be several output variables Y_1, Y_2 , etc., calculated by a model.

Uncertainty analysis involves determination of the variation or imprecision in Y that results from the collective variation of X_1, \dots, X_k . The uncertainty associated with Y can be expressed in terms of the estimated cumulative distribution function (cdf) for Y .

Scatter-plots can be a great aid in determining if the model is working as intended. When placed side by side, they may show how several variables jointly influence Y .

Sensitivity analysis involves determination of the change in Y that results from changes in individual model parameters X_1, \dots, X_k . Sensitivity analysis identifies the main contributors to the variation or imprecision in Y .

Sensitivity analysis can be accomplished by:

- ranking normalised coefficients of the input variables X_1, \dots, X_k in a linear regression formula for Y ;
- ranking input variables on the basis of their contributions to the variance of Y or
- computing partial correlation coefficients (these coefficients measure the degree of linear relationship between X_j and Y after adjustment to remove the linear effect of all remaining variables).

When Y is time dependent, the relative importance of the input variables may change with time. This is perhaps best demonstrated graphically.

A response surface replacement for a model is based on selecting sets of specific values of the input variables X_1, \dots, X_k that are used in making $n > k$ runs of the model. The model input and output for the n runs are used to estimate the parameters (coefficients b) of a linear model of the form:

$$Y = b_0 + \sum_j b_j X_j \quad (\text{A.1})$$

The linear model (the fitted response surface) is used as a replacement of the computer model in uncertainty and sensitivity analyses. Selection of the specific values for input variables may be based on a fractional factorial design using two levels (e.g. high and low) to represent each variable. However, if input variables are correlated, appropriate selection of specific values is more complex. Also, models that display discontinuities in Y are usually poorly represented by the response surface method.

The cdf for Y can be estimated using a Monte Carlo simulation with the fitted response surface. A sensitivity analysis can be accomplished by normalising the coefficients b_j .

Latin hypercube sampling (LHS) is a type of Monte Carlo sampling which generates a sample of size n of the input parameters X_1, \dots, X_k . The range of each variable is divided into n intervals on the basis of equal probability. One value is selected at random with respect to the probability density in the interval to form n groupings of the k variables. This set is the Latin hypercube sample. A selection technique is available to ensure that the selection of groupings neither introduces inadvertent correlations nor violates expected correlations among the variables X_1, \dots, X_k .

Due to the probabilistic nature of LHS, uncertainty analysis is simplified as it is possible to estimate the cdf and variance of Y directly.

This is the recommended approach. However, the analysis of a complex system depends on the particular problem under consideration. This makes it difficult to provide a general prescription for performing such an analysis.

Differential analysis is based on a first-order Taylor series expansion (TSE) of Y about some "point" X_{10}, \dots, X_{k0} of "base-case" values for the input variables. This "point" can be formed of the expected values of the input variables, and the TSE would then address small perturbations about this point. The generation of the partial derivatives required in the series can sometimes be done with simple differences schemes.