TECHNICAL REPORT

ISO/TR 13387-3

First edition
1999-10-15

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

Reference number
ISO/TR 13387-3:1999(E)

Contents

International Organization for Standardization
Case postale 56 • CH-1211 Genève 20 • Switzerland
Internet iso@iso.ch

Printed in Switzerland

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 Technical Reports of type 3 do not necessarily have to be reviewed until the data they provide are considered to be no longer valid or useful.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:

a) 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.

b) 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 over-simplifies 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 evolutes.

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.