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Fire safety engineering — Procedures and requirements for verification and validation of calculation methods —

Part 1:
General

Ingénierie de la sécurité incendie — Procédures et exigences pour la vérification et la validation des méthodes de calcul —

Partie 1: Généralités

Reference number
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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 procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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Any trade name used in this document is information given for the convenience of users and does not constitute an endorsement.

For an explanation on the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the WTO principles in the Technical Barriers to Trade (TBT) see the following URL: Foreword - Supplementary information

The committee responsible for this document is ISO/TC 92, *Fire safety*, Subcommittee SC 4, *Fire safety engineering*.

This document cancels and replaces ISO 16730:2008, which has been technically revised. The original title *Fire safety engineering — Assessment, verification and validation of calculation methods* has been replaced by *Fire safety engineering — Procedures and requirements for verification and validation of calculation methods — Part 1: General*.

Introduction

The objective of fire safety engineering is to assist in the achievement of an acceptable predicted level of fire safety. Part of this work involves the use of calculation methods to

— predict the course of events potentially occurring in case of a fire or as a consequence of a fire, and

— evaluate the ability of fire protection measures to mitigate the adverse effects of a fire on people, property, the environment and other objectives.

The main principles necessary for establishing credibility of these calculation methods are verification and validation. This International Standard addresses the procedures for verification and validation of calculation methods for fire safety engineering in general.

Potential users of calculation methods and those who are asked to accept the results need to be assured that the calculation methods provide sufficiently accurate predictions of the course and consequences of the fire for the specific application planned. To provide this assurance, the calculation methods chosen need to be verified for mathematical accuracy and validated for capability to reproduce the phenomena. A rigorous verification and validation process is a key element of quality assurance.

There is no fixed requirement of accuracy that is applicable to all calculation methods. The accuracy level depends on the purposes for which a calculation method is to be used. Not all calculation methods need to demonstrate high accuracy as long as the error, uncertainty and limits of applicability of the calculation methods are known.

This International Standard focuses on the predictive accuracy of calculation methods. However, other factors such as ease of use, relevance, completeness and status of development play an important role in assessing the most appropriate method to use for a particular application. The assessment of the suitability of a calculation method for a special purpose within the field of fire safety engineering is supported by the use of quality assurance methodology for the proof of the requirements being fulfilled. Guidance for establishing metrics for measuring the attributes of the relevant quality characteristics is outlined in brief in this International Standard.

This International Standard contains elements that are intended, in part or in whole, to be used by

a) developers of calculation methods (individuals or organizations who perform development activities, including requirement analysis, design and testing of components) – to document the usefulness of a particular calculation method, perhaps for specific applications. Part of the calculation method development includes identification of precision and limits of applicability, and independent testing,

b) developers of calculation methods (individuals or organizations who maintain computer models, supply computer models and for those who evaluate computer model quality as part of quality assurance and quality control) – to document the software development process to assure users that appropriate development techniques are followed to ensure quality of the application tools,

c) users of calculation methods (individuals or organizations who use calculation methods to perform an analysis) - to assure themselves that they are using an appropriate method for a particular application and that it provides adequate accuracy,

d) developers of performance codes and standards - to determine whether a calculation method is appropriate for a given application,

e) approving bodies/officials (individuals or organizations who review or approve the use of assessment methods and tools) - to ensure that the calculation methods submitted show clearly that the calculation method is used within its applicability limits and has an acceptable level of accuracy, and

f) educators - to demonstrate the application and acceptability of calculation methods being taught.

Users of this International Standard should be appropriately qualified and competent in the fields of fire safety engineering and risk assessment. It is important that users understand the parameters within which specific methodologies may be used.

General principles are described in ISO 23932, which provides a performance-based methodology for engineers to assess the level of fire safety for new or existing built environments. Fire safety is evaluated through an engineered approach based on the quantification of the behaviour of fire and based on knowledge of the consequences of such behaviour on life safety, property and the environment. ISO 23932 provides the process (necessary steps) and essential elements to design a robust performance-based fire safety programme.

ISO 23932 is supported by a set of fire safety engineering International Standards available on the methods and data needed for the steps in a fire safety engineering design summarized in ISO 23932:2009, Clause 4 and shown in Figure 1 (taken from ISO 23932:2009, Clause 4). This set of International Standards is referred to as the *Global fire safety engineering analysis and information system*. This global approach and system of standards provides an awareness of the interrelationships between fire evaluations when using the set of fire safety engineering International Standards. The set includes ISO 16733-1[1)], ISO 16732-1, ISO 16734, ISO 16735, ISO 16736, ISO 16737, ISO/TS 24679, ISO 16730-1, ISO 29761[2)], ISO/TS 13447, and other supporting technical reports that provide examples of and guidance on the application of these standards.

Each International Standard supporting the global fire safety engineering analysis and information system includes language in the introduction to tie the standard to the steps in the fire safety engineering design process outlined in ISO 23932. ISO 23932 requires that calculation methods used in scenario-based evaluations of trial designs (ISO 23932:2009, Clause 11) be verified and validated. Pursuant to the requirements of ISO 23932, this International Standard provides the procedures and requirements for the verification and validation of fire calculation methods. This step in the fire safety engineering process is shown as a highlighted box in Figure 1 below and described in ISO 23932.

1) To be published.

2) To be published.

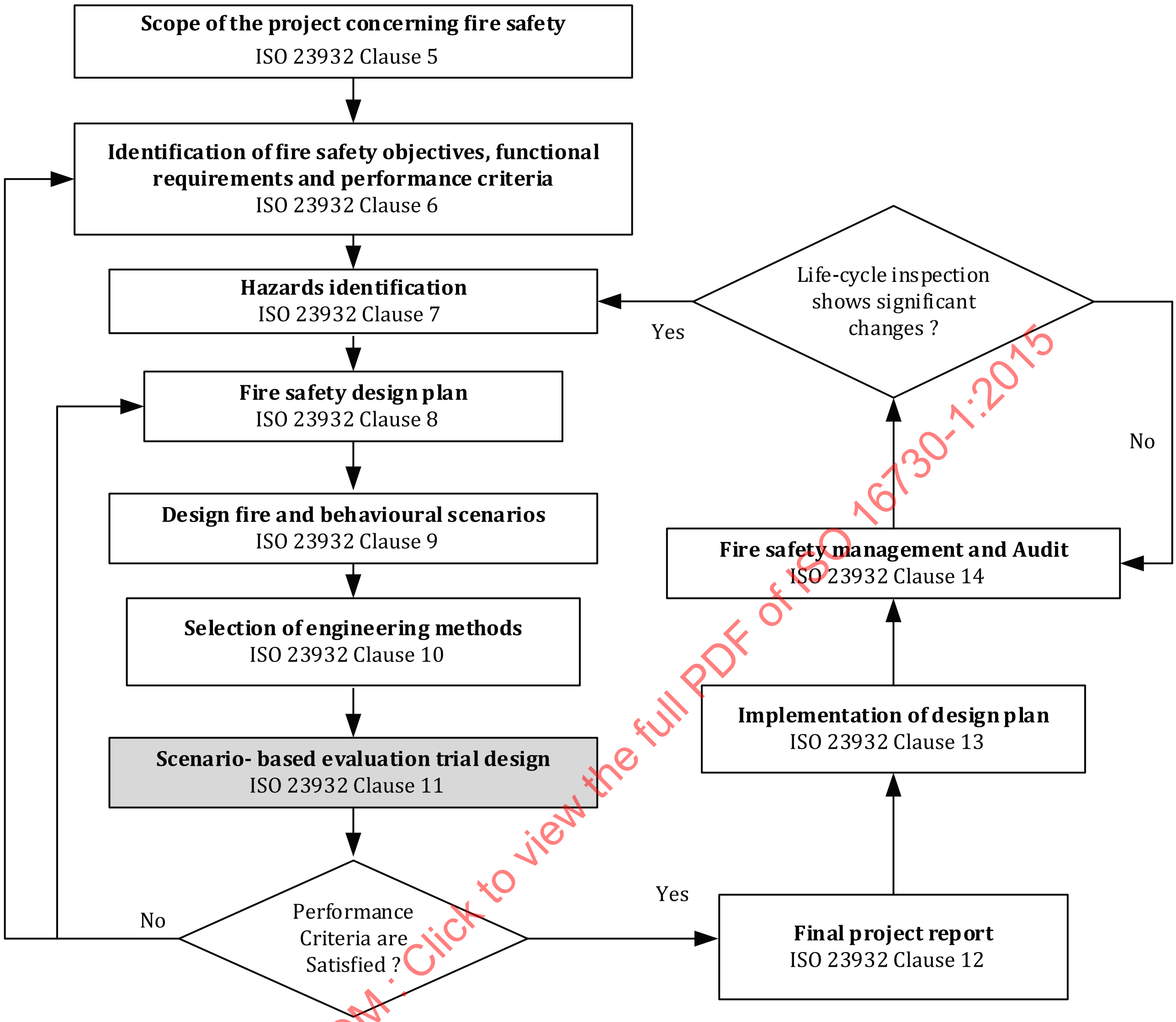


Figure 1 — Flow chart illustrating the fire safety engineering design process (from ISO 23932:2009)

Fire safety engineering — Procedures and requirements for verification and validation of calculation methods —

Part 1: General

1 Scope

This International Standard establishes a framework for the verification and validation of all types of calculation methods used as tools for fire safety engineering by specifying specific procedures and requirements for the purpose. It does not address specific fire models, but it is applicable to analytical models, algebraic correlations and complex numerical models, which are addressed as calculation methods in the context of this International Standard.

This International Standard includes

— a process to determine that the relevant equations and calculation methods are implemented correctly (verification) and that the calculation method being considered is an accurate representation of the real world (validation),

— requirements for documentation to demonstrate the adequacy of the scientific and technical basis of a calculation method,

— requirements for data against which a calculation method's predicted results are checked, and

— guidance on use of this International Standard by developers and/or users of calculation methods, and by those assessing the results obtained by using calculation methods.

2 Normative references

The following documents, in whole or in part, are normatively referenced in this document and are indispensable for its application. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 23932, *Fire safety engineering — General principles*

ISO 13943, *Fire safety — Vocabulary*

ISO/IEC 25000, *Systems and software engineering — Systems and software Quality Requirements and Evaluation (SQuaRE) — Guide to SQuaRE*

ISO/IEC 25010:2011, *Systems and software engineering — Systems and software Quality Requirements and Evaluation (SQuaRE) — System and software quality models*

ISO/IEC 25040:2011, *Systems and software engineering — Systems and software Quality Requirements and Evaluation (SQuaRE) — Evaluation process*

3 Terms and definitions

For the purposes of this document, the terms and definitions given in ISO 13943 and the following apply.

3.1
accuracy
degree of exactness actually possessed by an approximation, measurement, etc.

Note 1 to entry: Accuracy includes *error* (3.9) and *uncertainty* (3.23).

3.2
calculation method
mathematical procedure used to predict fire-related phenomena

Note 1 to entry: Calculation methods may address the behaviour of people as well as objects or fire; may be probabilistic as well as deterministic; and may be algebraic formulae as well as complex computer models.

3.3
calibration
⟨of a model⟩ process of adjusting modelling parameters in a computational model for the purpose of improving agreement with experimental data

3.4
computer model
computerized model
operational computer program that implements a conceptual model

3.5
conceptual model
description composed of all the information, mathematical modelling data and mathematical equations that describe the (physical) system or process of interest

3.6
default value
standard setting or state to be taken by the program if no alternate setting or state is initiated by the system or the user

3.7
deterministic model
calculation method that uses science-based mathematical expressions to produce the same result each time the method is exercised with the same set of input data values

3.8
engineering judgement
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

3.9
error
recognizable deficiency in any phase or activity of calculation that is not due to lack of knowledge

3.10
fire model
representation of a system or process related to fire development, including fire dynamics and fire impacts

3.11
mathematical model
sets of equations that describe the behaviour of a physical system

3.12
measure
variable to which a value is assigned as the result of measurement

3.13
measurement
set of operations having the object of determining a value of a measure

3.14
metric
measure, quantitative or qualitative, of relative achievement of a desired quality characteristic

3.15
modelling
process of construction or modification of a model

3.16
numerical model
numerical representation of a physical (fire) model

3.17
physical model
model that attempts to reproduce fire phenomena in a simplified physical situation. (e.g. scale models)

3.18
probabilistic model
model that treats phenomena as a series of sequential events or states, with mathematical rules to govern the transition from one event to another (e.g. from ignition to established burning) and probabilities assigned to each transfer point

3.19
precision
error in the implementation and solution of calculation method to accurately represents the developer's conceptual description of the calculation method

3.20
sensitivity analysis
<calculation method> study of how changes in specific parameters affect the results generated by the calculation method

3.21
simulation
exercise or use of a calculation method

3.22
simulation model
model that treats the dynamic relationships that are assumed to exist in the real situation as a series of elementary operations on the appropriate variables

3.23
uncertainty
potential deficiency in any phase or activity of the modelling process that is due to lack of knowledge

3.24
validation
process of determining the degree to which a calculation method is an accurate representation of the real world from the perspective of the intended uses of the calculation method

3.25
verification
process of determining that a calculation method implementation accurately represents the developer's conceptual description of the calculation method and the solution to the calculation method

Note 1 to entry: The fundamental strategy of verification of computational models is the identification and quantification of error in the computational model and its solution.

4 Documentation

4.1 General

The technical documentation should be sufficiently detailed so that all calculation results can be reproduced within the stated accuracy by an appropriately qualified independent individual or group. Sufficient documentation of calculation methods, including computer software, is essential to assess the adequacy of the scientific and technical basis of the calculation methods, and the accuracy of computational procedures. In addition, adequate documentation can assist to prevent the unintentional misuse of calculation methods. Reports on any verification and validation of a specific calculation method should become part of the documentation. The validity of a calculation method includes comparing results to data from real fire incidents, or from statistical surveys, tests and experiments, and shall be stated by applying quality assurance methodology. These methodology give a measure or a set of measures that shall be compared to previously defined criteria to demonstrate whether agreed quality requirements have been met.

Documentation shall include

— technical documentation that explains the scientific basis of the calculation method, see 4.2, and

— a user's manual, in the case of a computer program, see 4.3.

The necessary requirements for technical documentation and a user's manual are described in 4.2 and 4.3. 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 calculation method.

4.2 Technical documentation

4.2.1 General

Technical documentation is needed to assess the scientific basis of the calculation method. The provision of technical documentation of a calculation method is a task to be done by model developers. Technical documentation must describe thoroughly the calculation method and its basis, demonstrate its ability to perform adequately and provide users with the information they need to apply the calculation method correctly. In cases where calculations make use of algebraic formulae derived from experimental results by regression or when analytical solutions are applied, the user shall rely on relevant documentation from standards or similar material like scientific literature. When standards are developed that contain calculation methods to be used for fire safety engineering, the source(s) for the calculation methods to be used together with technical documentation as described in 4.2.2 to 4.2.4 shall be given, where applicable.

4.2.2 Description of the calculation method

The description of the calculation method shall include complete details on

a) purpose:

   1) define the problem solved or function performed;

   2) describe the results of the calculation method;

   3) include any feasibility studies and justification statements,

b) theory:

   1) describe the underlying conceptual model (governing phenomena), if applicable;

2) describe the theoretical basis of the phenomena and physical laws on which the calculation method is based, if applicable,

c) implementation of theory, if applicable:

1) present the governing equations;

2) describe the mathematical techniques, procedures, and computational algorithms employed and provide references to them;

3) identify all the assumptions embedded in the logic; take into account limitations on the input parameters that are caused by the range of applicability of the calculation method;

4) discuss the precision (error) of the results obtained by important algorithms, and, in the case of computer models, any dependence on particular computer capabilities;

5) describe results of the sensitivity analyses, and

d) input:

1) describe the input required;

2) provide information on the source of the data required;

3) for computer models, list any auxiliary programs or external data files required;

4) provide information on the source, contents and use of data libraries for computer models.

4.2.3 Description of the verification and validation of the calculation method

The verification and validation of the calculation method must be completely described, with details on

a) the results of any efforts to evaluate the predictive capabilities of the calculation method in accordance with Clause 5; this should be presented in a quantitative manner,

b) references to reviews, analytical tests, comparison tests, experimental validation, and code checking already performed; if, in case of computer models, the verification of the calculation method is based on beta testing, the documentation should include a profile of those involved in the testing (e.g. whether they were involved to any degree in the development of the calculation method or whether they were naive users; whether they were given any extra instruction that would not be available to the intended users of the final product, etc.), and

c) the extent to which the calculation method meets this International Standard.

The technical documents shall be collected in one document, such as a manual, as far as computer models are concerned. Whenever explicit algebraic formulae are used to solve a fire safety engineering problem, relevant technical documentation may be cited from sources as indicated above.

Quality assurance methods shall be used to determine the suitability of the software for its intended purposes. This process is further defined in 5.6. It is supported by definition and use of relevant quality assurance methods to arrive at a measure or a set of (derived) measures that allow scaling of the quality of a calculation method and consider whether a calculation method is accurate enough to meet the requirements of the intended user. [See, for example, the concept on internal and external metrics and on quality in use from the ISO/IEC series of Software Quality Requirements and Evaluation (SquaRE)]. For further information see the ISO/IEC 25000-series (and following) documents. The purpose of a calculation method's evaluation, in general, is to compare the quality of a calculation method against quality requirements that express user needs, or even to select a calculation method by comparing different calculation methods.

4.2.4 Worked examples

The technical documentation shall include at least one (or more) worked example(s). Worked examples may be required both for explicit algebraic formulae and for mathematical models. The latter is addressed in 4.3.9. The purpose of a worked example is to demonstrate what the required input data are and their limitations, and the range of applicability of the result(s) of the calculation method being considered. Examples for required input data and their intended range or limitations within which the calculation has been validated are, for example, geometry, material properties and boundary conditions. The range of applicability and accuracy of the calculation method shall be clearly stated in the documentation.

NOTE Significant errors in safety decisions and fire protection measures implemented will result from the use of the calculation method outside the range of stated scenarios determined through the validation process (see 5.3 for requirements to identify the range of applicability established by a validation process).

Standards on calculation methods shall include worked example(s) in an informative annex. By specifying the required components of a worked example in a standard on calculation methods (e.g. ISO 16734 to ISO 16737) guidance is therefore given on how to apply the standard correctly, together with the information given in the standard itself about requirements on limitations and input parameters. Examples taken from real world problems may be: (development of) temperature of a steel member; a fire insult to a cable in a nuclear power plant. As there are examples available in the open literature, the requirement of worked examples in an informative annex to a standard on calculation methods may also be met by reference to, for example, textbooks that include such examples.

4.3 User's manual

4.3.1 General

A user's manual is required only in cases where computer models are used. The user's manual for a computer model should enable users 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 should be included in the user's manual or be provided separately. There should be sufficient information to install the program on a computer. All forms of documentation should include the name and sufficient information to define the specific version of the calculation method and identify the organization responsible for maintenance of the calculation method and for providing further assistance.

For computer models, the user's manual must provide all the information necessary for a user to apply a computer model correctly. The items it should include are listed in 4.3.2 to 4.3.10.

4.3.2 Program description

The program description is

a) a self-contained description of the model,

b) a description of the basic processing tasks performed, and the calculation methods and procedures employed (a flow chart can be useful), and

c) a description of the types of skills required to execute typical runs.

4.3.3 Installation and operating instructions

The installation and operating instructions

a) identify the minimum hardware configuration required,

b) identify the computer(s) on which the program has been executed successfully,

c) identify the programming languages and software operating systems and version in use,

d) provide instructions for installing the program,

e) provide the typical personnel time and setup time to perform a typical run, and

f) provide information necessary to estimate the computer execution time on applicable computer systems for typical applications.

4.3.4 Program considerations

The program considerations

a) describe the functions of each major option available for solving various problems with guidance for choosing these options,

b) identify the limits of applicability (e.g. the range of scenarios over which the underlying theory is known or believed to be valid or the range of input data over which the calculation method was tested), and

c) list the restrictions and/or limitations of the software, including appropriate data ranges and the program's behaviour when the ranges are exceeded, where this information should be derived from and be consistent with that contained in the technical documentation.

4.3.5 Input data description

The input data description

a) name and describe each input variable, its dimensional units, the default value (if any) and the source (if not widely available),

b) describe any special input techniques,

c) identify limits on input based on stability, accuracy and practicality of the data and the applicability of the model, as well as their resulting limitations to output,

d) describe any default variables and the process for setting those variables to user-defined values, and,

e) if handling of consecutive cases is possible, explain the conditions of data retention or reinitialization from case to case.

4.3.6 External data files

The external data files

a) describe the contents and organization of any external data files, and

b) provide references to any auxiliary programs that create, modify or edit these files.

4.3.7 System control requirements

The system control requirements

a) detail the procedure required to set up and run the program,

b) list the operating system control commands,

c) list the program's prompts, with the ranges of appropriate responses, and,

d) if possible to do so, describe how to halt the program during execution, how to resume or exit, and the status of the files and data after the interruption.

4.3.8 Output information

The output information

a) describe the program output and any graphics display and plot routines, and,

b) where appropriate, provide instructions to judge whether the program has converged to a good solution.

4.3.9 Sample problems/worked examples

The sample problems/worked examples provide sample data files with associated outputs to allow the user to verify the correct operation of the program. These sample problems should exercise a large portion of the available programmed options. (See, for comparison, 4.2.4.)

4.3.10 Error handling

The error handling

a) list error messages that can be generated by the program,

b) provide a list of instructions for appropriate actions when error messages occur,

c) describe the program's behaviour when restrictions are violated, and

d) describe recovery procedures.

5 Methodology

5.1 General

Verification and validation of a calculation method are the processes of determining the degree to which a calculation method is an accurate representation of the real world from the perspective of the intended uses of the calculation method (validation) and the degree to which a calculation method implementation accurately represents the developer's conceptual description of the calculation method and the solution to the calculation method (verification). Verification is the process of determining whether the equations are being solved correctly, presuming that the correct equations are being utilized. Validation is to ensure that the results meet what is expected in the real world.

In Figure 2 the phases of modelling and simulation are presented in a very general manner, and the role of verification and validation in these processes is shown as applied to computer fire models.

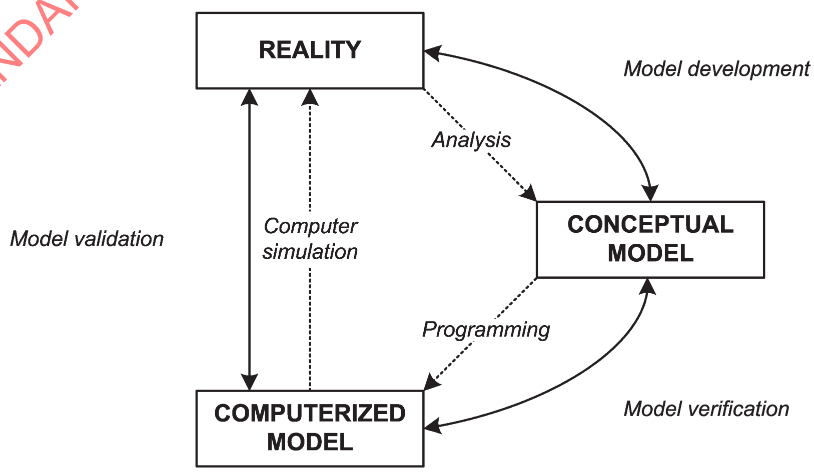


Figure 2 — Example: Phases of development of computer(ized) models

The conceptual model is produced by analysing the real world (sometimes physical system) and is composed of mathematical modelling data and equations that describe the physical system (Navier-Stokes equations, conservation of energy and mass, and additional physical models such as turbulence models, human behaviour aspects, structural behaviour, risk, etc.). Verification deals with the relationship between conceptual model and computerized model, while validation deals with the relationship between computerized model and reality.

Figure 3 expands on Figure 2 and presents the information in the form of a flowchart for general application, illustrating the potential use of algebraic formulae where deemed appropriate.

The procedure starts with (required knowledge of) tests and experiments or surveys to describe what is going on in the real world. From the perception of real world behaviour, a conceptual model is developed as a detailed (verbal) description of the process(es) considered, which is further developed into a (set of) mathematical relationships. From these a solution (or solutions) can be determined by breaking them down line-by-line from a highly sophisticated level to a less sophisticated level, and by applying approximations to such a degree that the problem may be solved with both sufficient accuracy and an acceptable solution effort (e.g. in time and computer performance).

The theoretical basis of the calculation method of a computer model should be reviewed by one or more experts who are fully conversant with the basic science of fire phenomena and computational techniques, but who are not involved with the development of the model. This review should include an assessment of the completeness of the documentation, particularly with regard to the numerical approximations. The reviewer should be able to judge whether there is sufficient scientific evidence in the open scientific literature to justify the approaches 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 calculation method and intended use. This is especially relevant as the data used for numerical constants may have specific values for specific scenarios. Practical upper and lower limits to variables used as input data should be defined clearly to restrict application to a proven range of applicability.

Between the steps of breaking down to a system that can be handled, the processes of verification and validation must be carried out in order to permanently check the solution system for possible sources of error. Due to the complexity of mathematical formulations of fire-related phenomena, the example in Figure 3 shows details that are not needed for the assessment of (empirical) calculation methods, i.e. algebraic formula, which are also covered in this document, and which are shown in a bypass box.

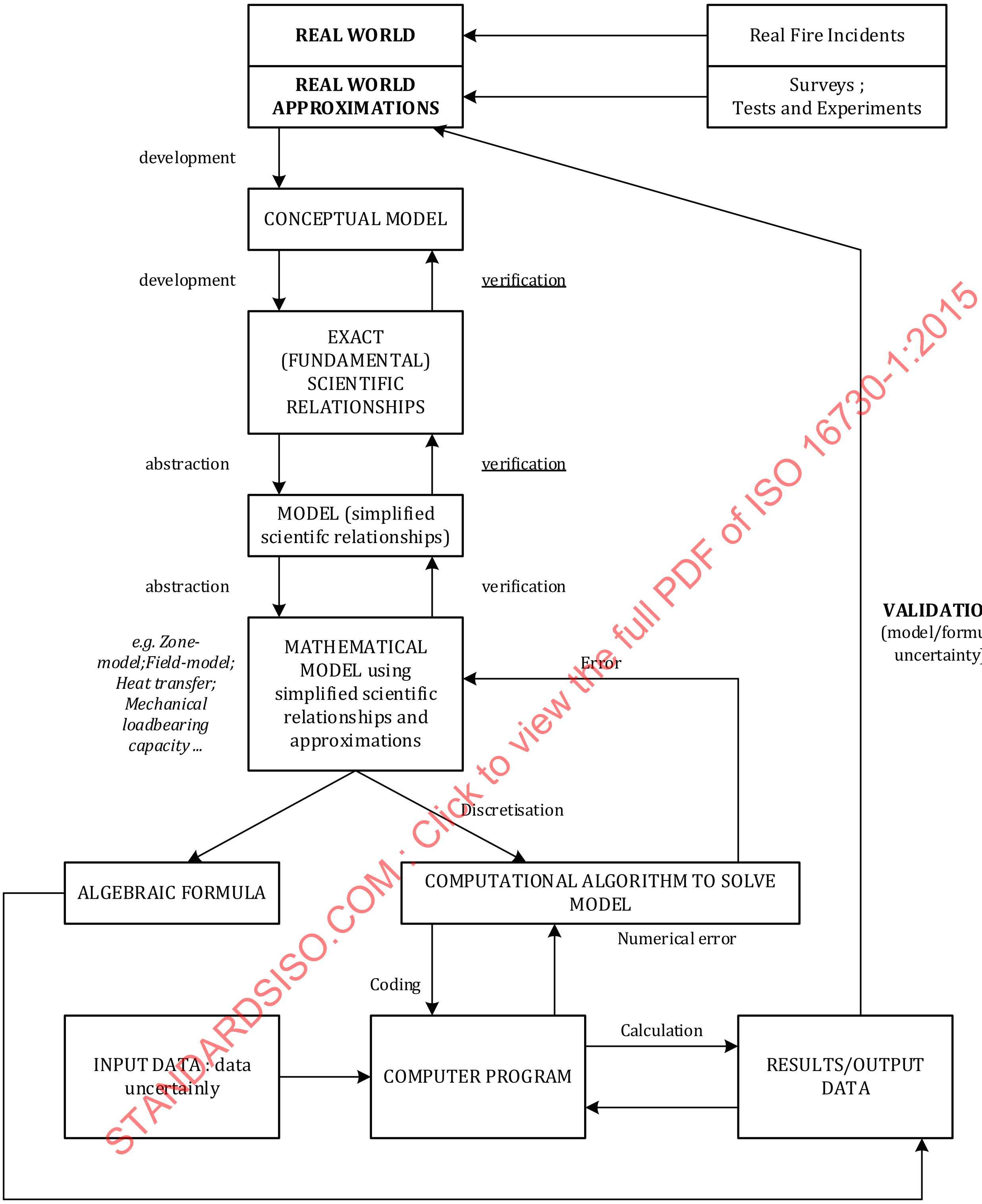


Figure 3 — Flowchart representation of model validation and verification

The methodology is not restricted to fire spread and similar problems, but is also to be applied to the validation and verification of calculation methods for behaviour and movement of people, to structural behaviour and to risk assessment (risk = probability of occurrence × consequence, see ISO 16732-1).

5.2 Verification

Verification is the process of determining that the implementation of a calculation method accurately represents the developer's conceptual description of the calculation method and the solution to the calculation method. This does not imply that the governing equations are appropriate, only that the equations are being implemented and solved correctly, and that the implementation accurately represents the developer's conceptual description of the calculation method and the solution to the calculation method.

The aim of the verification process is then to check the code correctness and to assess the control of the numerical error, which can be divided into three categories: round off, truncation and discretization error. Round off error occurs because computers represent real numbers using a finite number of digits. Truncation error occurs when a continuous process is replaced by a finite one. This can happen, for example, when an infinite series is truncated after a finite number of terms or when an iteration is terminated after a convergence criterion has been satisfied. Discretization error occurs when a continuous process such as a derivative is approximated by a discrete analogue such as a divided difference. A verification of a computational method should include an analysis and discussions of the methods used and the inherent limitations in the particular choices which have been made.

5.2.1 Code checking

The program code can be checked on a structural basis either manually or by using code checking programs to detect irregularities and inconsistencies within the computer code, which also applies to code revisions. Ensuring that the techniques and methodologies used to check the code, together with any deficiencies found, are clearly identified and recorded, increases the level of confidence in the program's ability to process the data reliably, but it cannot give any indication of the likely adequacy or accuracy of the program in use. It is not necessarily the case that an error renders a program unusable, but documentation of these "bugs" prevents use in the affected regimes.

5.2.2 Temporal and spatial discretization

Mathematical models are usually expressed in the form of differential or integral equations. The models are in general complex, and analytical solutions are often difficult 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. Discretization is done both in time and space (grid).

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, the discrete model is required to mimic the properties and the behaviour of the continuous model. This means that the discrete solution should 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. Stability means that the error terms do not increase as the program proceeds.

The formal order of error in both spatial and temporal discretization should be explained and discussed. It may not be possible to be exhaustive, but an analysis must be done as part of the process of verifying the implementation of the equations into discrete numerical form.

Many problems related to fire involve the interaction of different physical processes, such as chemical or thermal processes and the mechanical response. Time and space scales associated with the processes may be substantially different, which causes numerical difficulties. Consequently, in solving differential equations some care must be exercised when choosing the time and space steps, to ensure stability (especially with respect to the time step for transient computations) and a sufficient convergence of the computation. Some numerical techniques can be used in order to dynamically monitor discretization parameters to meet stability and accuracy requirements (e.g. as far as the spatial discretization is concerned, a posteriori error estimation coupled to dynamic meshing refinement). Making use of such methods is recommended, especially for the time stability issue for nonlinear problems, as encountered in zone models. In this case, the code documentation should extensively explain how this has been accomplished, and numerical experiments addressing the validity of the used algorithm should be presented. This does not prevent the user from performing, for a particular computation, a study of time and space convergence; this task should be accomplished systematically and the choice of the discretization parameters is left to the user.

5.2.3 Iterative convergence and consistency tests

It is important to check that the implementation of the conceptual model into a computer program is done correctly. For this purpose, the following procedures should be executed, when applicable:

a) check the residual error criteria;

b) check for the stability of output variables;

c) apply global checks on conservation of appropriate quantities;

d) to the extent possible, compare against analytic solutions;

e) compare against more accurate solutions obtained by more complete models that are known to be verified and validated;

f) check the effects of artificial boundary conditions for open flow problems.

5.2.4 Review of the numerical treatment of models

A critical part of the verification of a model is to ensure that the equations and methods as stated in the documentation describing the approach have been implemented as intended. This includes an evaluation of the documentation, implementation of the equations in the computer code, and an analysis of the discretization and numerical methods used.

5.3 Validation

5.3.1 General

This section provides procedures to determine the calculation method's accuracy for a range of applications. A rigorous validation procedure is needed to set the range of applicability of the calculation method, and to determine the accuracy of the calculation method in the acceptable range. This is true for any kind of calculation method covered by this standard. Correlations are valid predictive tools, and are to be validated in the same manner as computer models using similar methods.

Generally, closed form solutions do not exist for whole fire problems, even for the simplest cases. That is, there are no closed-form solutions to this type of problem. However, it is possible to do two kinds of checking. The first type is that by which individual algorithms are validated against experimental work. The second consists of simple experiments, e.g. conduction and radiation, for which the results are asymptotic, and provide analytical solutions for some part of the phenomena. For example, for a simple, single-compartment test case with no fire, temperatures should equilibrate asymptotically to a single value. A model should be able to replicate this behaviour. Finally, it is possible to compute solutions to situations for which there are analytic answers, though these might not occur naturally.

The discrepancy between a comparison of an algebraic equation or computer model with an experiment is due to the degree of uncertainty to which a calculation method is an accurate representation of the real world from the perspective of the intended uses of the calculation method (validation), and the error in the developer's conceptual description of the calculation method and the solution to the calculation method (verification).

This International Standard specifies two procedures, either of which can be followed by a party conducting a validation. These are the "blind" and "open" validation procedures. In the blind procedure, the party conducting the validation is only knowledgeable of the initial and boundary conditions of the experiment that are needed to exercise the calculation methods being validated, including any parameter (e.g. heat release rate) for which the predictive capability of the model is not being tested. The party does not have any access to the experimental measurements of the output(s) of the calculation method that is being validated. In the open procedure, the party is knowledgeable of the initial and boundary conditions of the experiment, as well as the measurements of the output parameters of the calculation method being validated before the calculation method is exercised. There are other definitions used in the literature on the subject such as "a priori", "a posteriori", "total blind" and "semi-blind". This International Standard adopts and uses only two terms, "blind" and "open," as defined above, which cover the range conditions that will be encountered in the validation process.

There are several pros and cons of these two validation processes.[20] It is up to the interested party to determine which process best meets their needs. The user of this International Standard will comply with its requirements by following either the open or blind validation procedure.

The procedure that should be used in either the open or blind validation process is described in 5.3.2 and 5.3.3.

In all cases, validation should define comparison metrics, then the nature of the values to be compared should be selected. A model validated for total heat release rate doesn't mean that the model is validated for other parameters. Several interacting model behaviours can lead to an agreement with the total heat release curve, but with an incorrect consideration of the burning items that produce this heat release.

A zone model mainly solves the global mass and energy balances per layer. The first step in the validation process for such models would be to check the heat release and mass loss rates, then comparisons for values related to each layer, such as layer interface, temperature and composition, can be made.

For a computational fluid dynamics (CFD) model, global and local validations of energy, mass, mass per species and movement quantities have to be validated. A complete validation of the model will require global data such as total mass lost or heat release rate (HRR), and local data such air velocities, local gas composition and local temperatures.

5.3.2 Open validation procedure

There are no requirements for an audit in the open validation procedure. The procedure that should be followed in the open validation process is presented below:

a) the party conducting the validation has or is given access to the initial and boundary conditions of the experiments, as well as the measurements of the output parameters being predicted by their calculation method before the calculation methods are exercised;

b) the boundary conditions and input values to be used for the calculation methods should be established and documented before the calculation methods are exercised;

c) in no case should the calculation methods be re-exercised varying the boundary conditions of the experiments used as input values, except as part of an uncertainty analysis in a risk assessment where the effect of uncertainty in experimental data is examined.

5.3.3 Blind validation procedure

The blind validation procedure requires an audit to confirm that the procedures specified in this section are followed. The audit may be conducted either according to requirements established by the organization performing the validation, or more formally according to ISO 19011 and ISO/IEC 17021-1 as "first" or "second party" audits, or "third party audit and certification." The audit policies and procedures in the ISO 9000 family of standards are summarized in (informative) Annex A. The user of this International Standard meets the requirements by either following an audit programme designed by the user, or one that is in accordance with the requirements and guidance in the ISO 9000 family of standards.

The procedure for the blind validation process is as follows:

a) the party conducting the validation should only be knowledgeable of the initial and boundary conditions of the experiment that are needed to exercise the calculation methods being validated.

The party should not have any access to the experimental measurements of the output(s) of the calculation method that is (are) being validated;

b) the blind validation process can only be used when new validation experiments are to be conducted, or when validation experiments not available to the public and the party conducting the validation exist;

c) the specification of the experiments used for the validation process, including initial and boundary conditions, should be sufficiently detailed such that analysts of the calculation methods have all the necessary input data;

d) depending on the objective of the validation, certain parameters such as heat release rate may be used in the validation exercise as a boundary condition and input to the calculation method. These parameters should be identified as such in the validation exercise;

e) the party conducting the validation should be provided the experimental measurements of the output(s) of the calculation that is being validated after the calculation method has been exercised and the results have been provided to the auditor;

f) the experiments which produce the results used for validation of the calculation method may be conducted either before or after the calculation methods have been exercised;

g) in some cases, the initial and boundary conditions of the experiments provided to the party conducting the validation have to be modified after the experiments have been conducted to reflect the actual conditions of the experiments. In such cases, the revised boundary conditions should be provided to the party conducting the validation for a re-exercise of the calculation methods if the calculations were conducted before the experiments;

h) in all cases, there should be agreement on the boundary conditions and inputs used for the calculation methods before the final exercise of the calculation methods and prior to the release of the experimental measurements of the output(s) of the calculation that is being validated;

i) in no case can the calculation method be re-exercised once the experimental measurements of the output(s) of the calculation that is being validated are released;

j) the results of the calculation method being validated should be provided to an auditor before the experimental measurements of the output(s) of the calculation are released;

k) the party conducting the validation should develop a specific validation procedure that complies with this International Standard. The procedure should be approved by the auditor before the validation process is initiated.

5.3.4 Reporting of validation

The results of the open and blind validation process should be documented to include the following:

a) a description of the experiments and the measurements, including uncertainty in the measurements (see Annex B);

b) input data used for the calculation methods;

c) comparison of outputs of the calculation method with experimental data using established metrics in quantitative terms;

d) a tabulation of the discrepancies using the established metrics in quantitative terms;

NOTE The discrepancy is due to the error in and uncertainty of the calculation method.

e) the boundary and initial conditions of the experiments and therefore the resulting fire scenario(s) for which the validation is applicable.

5.3.5 Specific considerations in comparison of predictions with data

Since the results from algebraic formula are mostly single value predictions, the same considerations apply for these as for single value predictions from computer models. Single value predictions shall be checked against (experimental, survey) data, whenever these are available for the considered problem and if these were produced with an equivalent set of initial and boundary conditions.

For comparison of time value prediction with data, Annex C describes two methods to quantify the similarities and differences of two curves such as, for example, the time history of the upper layer temperature for a model prediction and an experiment. One method works by treating the curves as infinite dimensional vectors and then using vector analysis to describe the differences. This analysis provides a quantitative method of validating fire models and quantifying the uncertainty in experimental data. The second method, called the normalized Euclidean distance, considers the differences between computational results and measurements during the entire fire duration. This metric provides information on the global errors and gives a comprehensive overview of code capabilities.

Annex C describes the two methods and illustrates their applications.

5.4 Review of the theoretical and experimental basis of probabilistic models

The equations employed in a probabilistic model, typically as part of a risk assessment, are normally those that define risk in terms of a probabilistic function on a space defined by scenarios and those used to derive needed probabilities from other, more readily available probabilities. The review of the correctness of the equations should answer the following questions:

a) Does the model use only well-defined probability variables and parameters?

Probabilistic modelling and risk assessment typically use experiential databases or engineering judgement to produce probability variables and parameters. Evidence of accuracy of single-value variable or parameter estimates is obtained by comparing the estimates to alternative estimates computed in the same manner from independent data. For example, judgement values obtained from one group of experts can be compared to judgement values obtained from a second group of experts. In such a case, special attention should be paid to the characteristics of experts that are considered most likely to influence the judgements. Also, experientially-based probabilities (for example, ignition probabilities) can be verified by comparison to like probabilities based on experience from a different place or a different period of time.

Output variables of a risk assessment are typically based on probabilities and consequences, where the latter are derived from a deterministic model. The deterministic model predictions can be validated in the manner described elsewhere in this document. The combined calculation of risk, either for the whole calculation or for subsystem cases or other portions, can be validated by comparison with actual loss experience. Where the probability values are experientially based, the loss experience used for validation should be taken from the same places and times as were used to set the probability values.

b) Do the probability variables, parameters and calculations follow the laws of probabilities (e.g. probabilities must fall between 0 and 1)?

c) Are all formulae employing conditional probabilities complete? For example, $P(A) = [P(A \text{ given } B) \times P(B)] + [P(A \text{ given not } B) \times P(\text{not } B)]$. If the second part of the expression is omitted, an explicit case must be made that either $P(\text{not } B)$ or, more often, $P(A \text{ given not } B)$ is zero or approximately zero.

d) Is risk defined by an explicit expression linking the measure of risk to probabilities and consequences of scenarios? If not, is there an underlying expression?

e) Does the expression defining risk in terms of scenarios capture all possible scenarios? If not, does the calculation comprehensively address the impact of the omitted scenarios on the calculation?

f) Are the uncertainties associated with the probabilistic variables and parameters explicitly addressed in the calculation? Are both random uncertainties and sources of systematic bias considered and addressed?

g) If any equations are simplified from the complete forms, have they been compared for accuracy with their complete counterparts?

5.5 Sensitivity analysis

A sensitivity analysis of a calculation method is a study of how changes in specific parameters affect the results generated by the calculation method. Predictions may be sensitive to uncertainties in input data, to the level of rigor employed in modelling the relevant physics and chemistry, and to the use of inadequate numerical treatments. A well designed and executed sensitivity analysis serves to

a) identify the dominant variables in the calculation methods,

b) define the acceptable range of values for each input variable,

c) demonstrate the sensitivity of output variables to variations in input data (at this step, a metric needs to be established to evaluate the sensitivity of the model),

d) inform and caution any potential users about the degree and level of care to be taken in selecting input and running the model, and

e) provide insights as to which parameters should be monitored in large scale experiments.

Conducting a sensitivity analysis of a complex fire model is an arduous task. Many models require extensive input data and generate predictions for numerous output variables over a period of simulated time. The technique chosen for use is dependent on the objectives of the study, the required results, the resources available and the complexity of the model being analysed. Methods available for conducting sensitivity analysis are presented in Annex D.

5.6 Quality assurance

Evaluation of computer programs to determine they are adequate for the intended purpose is essential. Certification may be used to establish the adequacy of the computer programs. The quality of such programs can be assessed by applying quality assurance models. These make use of procedures that lead to an evaluation of both "external quality", which is important for the end-user, and "internal quality", which is important for the proper functioning of the program. Software quality attributes are categorised into eight characteristics (functional suitability, performance efficiency, compatibility, usability, reliability, security, maintainability and portability), which are further subdivided into sub-characteristics (see Figure 4). For each characteristic and sub-characteristic, the quality of the software should be determined by a set of measured internal attributes. The characteristics and sub-characteristics should be measured externally by the extent to which the capability is provided by the system containing the software. An essential element of quality assurance for fire safety calculation methods is determining the suitability and accuracy of the methods (functional suitability).

Strict quality control requirements are necessary for the validation of fire calculation methods because of their rudimentary stages of development and expanding application in fire safety engineering. Fire development is a complex phenomenon, covers a very broad range of scenarios and includes many factors that can influence its development. One of the most critical elements for quality assurance of a fire calculation method is the determination and identification of the range of validation and therefore applicability, i.e. what are the specific fire scenarios for which the calculation method has been validated? An adequate validation procedure, as discussed in 5.3, for determining the accuracy of the calculation method for suitable metrics and for establishing the range of applicability, is key to quality assurance. The use of the correct accuracy of fire calculation methods to determine the safety factors needed in the broader context of fire safety engineering applications, as required by ISO 23932, is the ultimate goal for ensuring quality decision making for fire safety.

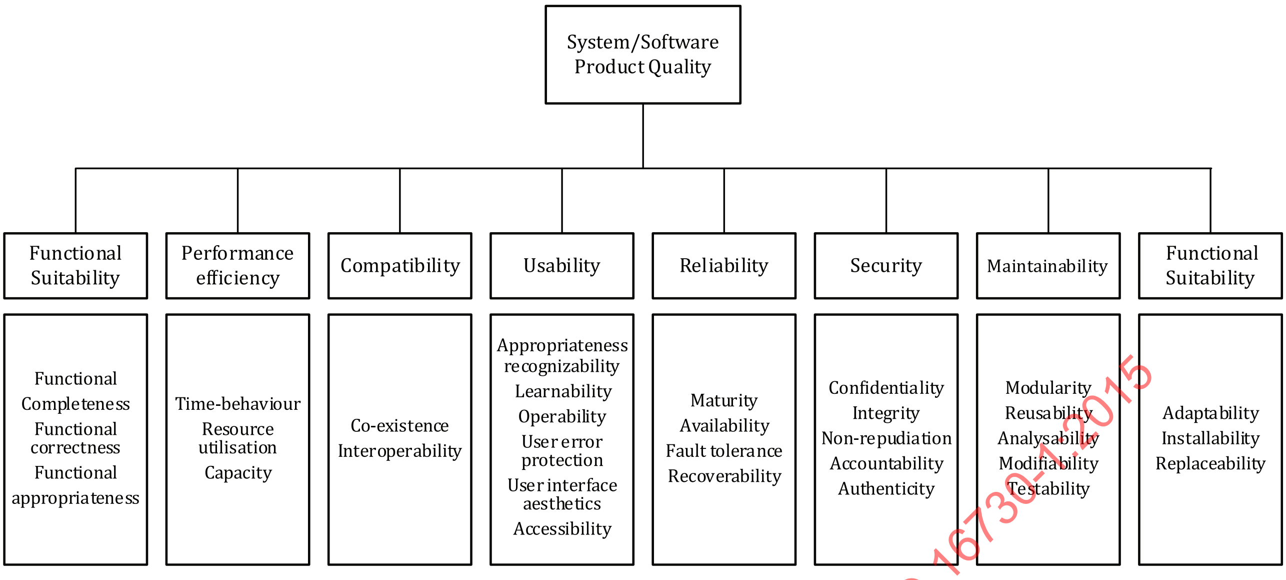


Figure 4 — Quality model for external and internal quality, describing characteristics and sub-characteristics

For the assessment or evaluation of the quality of a calculation method, the procedures as outlined in the ISO/IEC 25000-series based on ISO/IEC 25010:2011 and ISO/IEC 25040:2011 apply. A short abridged version of the procedure is found in (informative) Annex E.

6 Requirements for reference data to validate a calculation method

6.1 General requirements

Reference data to validate a calculation method can be obtained from experiments, surveys on multiple similar or single well-documented fire events, or other validated calculation methods, as appropriate to the parameters and other quantities to be validated.

Data used to define, set or estimate a quantity in a calculation method cannot be used to validate that quantity. Independent data must be used for validation.

Differences between a calculation-method quantity and data used to validate that quantity can be due to errors in the quantity or errors in the data.

To support conclusions about the validity of the calculation method, the validation exercise must assess the magnitude and nature of errors in the reference data and assess the impact of those errors on the differences between quantities and data. Therefore, the completeness, quality, precision and bias of the reference data must be characterized before it can be used for validation.

For *experimental data*, the repeatability and reproducibility of the test procedure that is the source of the data must be assessed. Precision and bias characterizations of the reference data can be obtained from available precision and bias characterizations of the apparatus or measurement device that is the source of the data.

For *(statistical) survey data*, the representativeness of the survey design and achieved sample must be assessed. Uncertainty due to sample size must also be ascertained.

For *forensic analysis data*, it has to be stated how these data were collected.

For *data from other validated calculation methods*, the evidence from the validation of those methods, together with characterization of its precision, bias, and sources and magnitudes of error are required.

An assessment is needed of the correspondence between the conditions of reference data collection and the conditions assumed by the calculation method. This includes initial and boundary conditions. For example, if experiments provide reference data on evacuation performance of a population composed exclusively of young, healthy adults, then that data do not suffice to validate a calculation method applied to a more mixed population.

It is necessary to validate the whole calculation method and separately to validate its subsystems and sub-models. Appropriate data must be identified and acquired for each of these levels of validation.

An assessment is necessary of any reduction, conversion, or interpretation procedure applied to raw data in order to produce reference data suitable for use in validation. For example, if raw survey data are available only for selected high-rise office buildings in a single city, then its applicability to other types of buildings of other heights in other cities in other countries is uncertain, and this imperfect match must be noted and assessed.

An assessment is necessary of the independence of the reference data generation and review from the development of the calculation method.

Full validation of a calculation method requires assessment of the full range of outputs for a full range of cases and conditions. Reference data are needed to support as complete an assessment as possible, and any limitations on the range of outputs and cases assessed must be explicitly noted, if possible in the form of limitations on applications of the calculation method for which validation has been successfully completed. For example, if experimental data are available only for ceiling temperatures, then calculation method predictions of temperatures elsewhere in a room have not been directly validated.

6.2 Specific requirements for validation data

The first step is to compare predictions of the model or analytical technique with appropriate data. As outlined in the introduction to this International Standard, it must be clear that, whereas the model is a realization of a theoretical concept, experimental data are a representation of the real world. In this context it is important to ensure that appropriate models and input data represent the experiment being used. Both representations have limitations and inherent errors, and appropriate statements of the uncertainties in both must be included in a comparison. Correctness in the sense of validation is that the model yields appropriate answers for input data representing the scenarios under consideration. The process of validation includes a statement of the range of validity of the input data.

The data comprise, in general

— insuring the completeness of environmental data (e.g. temperature gradients in buildings or temperature differences between the building interior and the outside, wind effects), and

— using correct property data; if constants are used, a sensitivity analysis must show their influence on the outputs; if constants are used instead of, for example, temperature dependent variables, the outcome of this approximation (cf. above) must be evaluated for the range of applicability of the model or calculation method.

For data taken from the literature the sources shall be referenced. Examples of literature are handbooks, standards, journals, research reports. Where peer reviewed literature data are not available, these data shall be checked against evidence.

The same principles apply, independent of the degree of sophistication of the representation of real world phenomena by either calculation methods or models. These may be used to predict the course of a fire in a building or evacuation processes, or both, while human behavioural aspects may also influence the results and should be evaluated based on the same principles. On data for deterministic fire models see, for example, ASTM E 1591–00.[3]

Annex A
(informative)

Guidance on audits in ISO 9000 family of standards

A.1 Scope

This annex summarizes the policies and guidance contained in the ISO 9000 family of standards for audit programmes.

A.2 Informative references

The references ISO 9000:2005[77], ISO 19011:2011[78] and ISO/IEC 17021-1:2015[79] are given in the Bibliography.

A.3 Summary of audit policies, definitions and guidance

ISO 19011:2011 specifies the requirements for audits in a quality management system. Audits are used to determine the extent to which the quality management system requirements are fulfilled. First-party audits are conducted by, or on behalf of, the organization itself for internal purposes and can form the basis for an organization's self-declaration of conformity. Second-party audits are conducted by customers of the organization or by other persons on behalf of the customer. Third-party audits are conducted by external independent organizations. Such organizations, usually accredited, provide certification or registration of conformity with requirements such as those of ISO 9001:2011.

ISO 19011:2011 provides guidance on audits of management systems. The principles on which auditing is based are discussed. These principles help the user to understand the essential nature of auditing and they are important in understanding the guidance set forth in ISO 19011:2011. Guidance on establishing and managing an audit programme, establishing the audit programme objectives, and coordinating auditing activities is also provided; as well as guidance relating to the competence and evaluation of management system auditors and audit teams. Specific application of the guidance in ISO 19011:2011 for different disciplines, including safety management systems, is provided in an annex.

ISO/IEC 17021 sets out the requirements for third party certification of management systems and is based in part on the guidelines contained in ISO 19011. ISO/IEC 17021 also includes the requirements for management system certification audits. ISO 19011 provides guidance for all users, including small and medium-sized organizations, and concentrates on what are commonly termed "internal audits" (first party) and "audits conducted by customers on their suppliers" (second party). The requirements for third party certification audits are contained in ISO/IEC 17021.

Annex B
(informative)

Uncertainty

B.1 Measurement uncertainty of data

B.1.1 General

Much of B.1 is taken from Taylor and Kuyatt[1].

B.1 has been 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 validation of the model. Not all published experimental data include information on the uncertainty of the data.

In general, the result of measurement is only the result of an approximation or estimate of the specific quantity subject to measurement, and thus the result is complete only when accompanied by a quantitative statement of uncertainty. 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:

— Type A: those which are evaluated by statistical methods;

— Type 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_{i2}, 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_{j2}, 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_{j2} is treated like a variance and u_j like a standard deviation, for such a component the standard uncertainty is simply u_j.

B.1.2 Type A evaluation of standard uncertainty

A Type A evaluation 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 annex does not attempt to give detailed statistical techniques for carrying out statistical evaluations. See[9-12] for comparison.

B.1.3 Type B evaluation of standard uncertainty

A Type B evaluation 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 property of relevant materials and instruments,

c) manufacturer's specifications, and

d) data provided in calibration and other reports and, uncertainties assigned to reference data taken from handbooks.

Because the reliability of evaluation 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 evaluations 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 carts that can indicate that a measurement process is under statistical control, should be part of the effort to obtain reliable evaluations of components of uncertainty.

B.1.4 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 Type A or a Type B evaluation, 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.

B.1.5 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 $U = kU(y)$ 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 $k = 2$, which 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 $k = 2$.

B.1.6 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 refer 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 evaluated.

Annex C
(informative)

Example validation methods

C.1 General

The key to validation of fire models is the ability to quantify the difference between model predictions and experimental measurements or between two model predictions or two experimental data sets. These techniques are seen to be of use in comparing models and experiments, comparing models to one another, and comparing model predictions with sensor data for use in fire detection and prediction in real-time systems.

C.2 Functional analysis method

The first validation method described in this annex uses a mathematical technique known as functional analysis. Functional analysis is a generalization of linear algebra, analysis and geometry. It is a field of study that arose around 1900 from the work of Hilbert and others. Functional analysis is becoming of increasing importance in a number of fields, including theoretical physics, economics and engineering, to answer questions on differential equations, numerical methods, approximation theory and applied mathematical techniques. Problems are described in vector notation and appropriate operations on these vectors can be defined to allow quantitative analysis of the properties of the underlying physical system. The primary vector operations of interest are the norm, a measure of the length of a vector, and inner product, a measure of the angle between two vectors.

To obtain an overall comparison of two curves, this single point comparison can be extended to multiple points. Each of these curves can be represented as a multi-dimensional vector, with each point in time defining an additional dimension. Using such a vector notation, a direct extension of the simple comparisons of maximums is the norm of the difference of the vectors of experimental and model data.

The concept of a norm provides a definition of the length of a vector. The distance between two vectors is simply the length of the vector resulting from the difference of two vectors. The symbolic representation is written as $\left\|\vec{x}\right\|$ where $\vec{x}$ is the notation for the n-dimensional vector $(x_1, x_2, ..., x_{n\text{-}1}, x_n)$.

For this example, the comparison of peak values is called the sup norm, or a norm based on maximum absolute values. To extend the sup norm, all of the data can also be represented by a vector of values measured at each time point, $\vec{E}$. The model predictions at the same time points can be represented by a vector, $\vec{m}$. The distance between these two vectors is the norm of the difference of the vectors, or $\left\|\vec{E}-\vec{m}\right\|$. It is convenient to normalize this as a relative difference to the experimental data as

$$\frac{\left\|\vec{E}-\vec{m}\right\|}{\left\|\vec{E}\right\|} \qquad (1)$$

The difference vector is calculated just as it was for the simple example by comparing the maximums of the two curves, taking the difference between the experiment and model at each time point. Initially, the Euclidean norm is most intuitive for computing length

$$\left\|\vec{x}\right\| = \sqrt{\sum_{i=1}^{n} x_i^2} \ . \qquad (2)$$

As discussed later, other geometries can also be useful for real-time comparisons. For the example in Figure C.1, the distance between the two vectors, $\left\|\vec{E}-\vec{m}\right\|$, is 14,1 and the relative difference is 0,056.

For these simple curves, the comparison of peak values provides a good measure of the overall agreement, nearly identical to the overall comparison from Formula (1) since the two curves were chosen to differ only at the peak. For more complex curves, the comparison of maxima may not be as good an indicator. Several examples are presented later in this annex.

While the difference, $\left\|\vec{E}-\vec{m}\right\|$, and the relative difference, $\left\|\vec{E}-\vec{m}\right\| / \left\|\vec{E}\right\|$, provide measures of the difference between experimental data and model predictions, other calculations provide useful information on the source of the difference. When comparing vectors, there are basically two geometric components to consider: a difference in length between the two vectors and the (non-zero) angle between the two vectors. The inner product, $\left\langle \vec{x}, \vec{y} \right\rangle$ of two vectors is the product of the length of the two vectors and the cosine of the angle between them, or

$$\left\langle \vec{x}, \vec{y} \right\rangle = \left\|\vec{x}\right\| \left\|\vec{y}\right\| \cos\left(\angle\left(\vec{x}, \vec{y}\right)\right) \tag{3}$$

or

$$\cos\left(\angle\left(\vec{x}, \vec{y}\right)\right) = \frac{\left\langle \vec{x}, \vec{y} \right\rangle}{\left\|\vec{x}\right\| \left\|\vec{y}\right\|} \tag{4}$$

Choosing the inner product to be the standard dot product gives results consistent with typical Euclidean geometric perception

$$\left\langle \vec{x}, \vec{y} \right\rangle = \sum_{i=1}^{n} x_i y_i \tag{5}$$

For this example, $\cos\left(\angle\left(\vec{x}, \vec{y}\right)\right) = 0{,}99$. Visually, this angle between the two vectors represents a measure of how well the shapes of the two vectors match. As the cosine of the angle approaches unity, the overall shape of the curves becomes identical.

In general, an inner product is simply a function that takes two vectors and returns a number. The number can be either real or complex – for our purposes, only real inner products are considered. The following axioms provide a sufficient definition of the inner product and norm to have the necessary properties to perform vector calculations.[13]

	Inner product	**Norm**
I	$\left\langle \vec{x}, \vec{x} \right\rangle \geq 0$	$\left\|\vec{x}\right\| \geq 0$
II	$\left\langle \vec{x}, \vec{x} \right\rangle = 0 \Leftrightarrow \vec{x} = 0$	$\left\|\vec{x}\right\| = 0 \Leftrightarrow \vec{x} = 0$
III	$\left\langle \alpha\, \vec{x}, \vec{y} \right\rangle = \alpha \left\langle \vec{x}, \vec{y} \right\rangle$	$\left\|\alpha\, \vec{x}\right\| = \left\|\alpha\right\| \left\|\vec{x}\right\|$
IV	$\left\langle \vec{x}+\vec{y}, \vec{z} \right\rangle = \left\langle \vec{x}, \vec{z} \right\rangle + \left\langle \vec{y}, \vec{z} \right\rangle$	$\left\|\vec{x}+\vec{y}\right\| \leq \left\|\vec{x}\right\| + \left\|\vec{y}\right\|$
V	$\left\langle \vec{x}, \vec{y} \right\rangle = \overline{\left\langle \vec{y}, \vec{x} \right\rangle}$	

These axioms provide appropriate rules to define the inner product and norm for other geometries in addition to Euclidean space. Three additional definitions, Hellinger, secant and a hybrid of Euclidean and secant, are considered. For consistency, the norm can be defined in terms of the inner product. This ensures that appropriate, consistent definitions for the norm and inner product are used in calculations. Since the angle between a vector and itself is by definition zero, it follows from Formula (3) that

$$\langle \vec{x}, \vec{x} \rangle = \|\vec{x}\|^2 \text{ or } \|\vec{x}\| = \sqrt{\langle \vec{x}, \vec{x} \rangle} \quad (6)$$

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

$$\langle x(t), y(t) \rangle = \int_0^T x'(t)\, y'(t)\, dt \quad (7)$$

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

$$\langle \vec{x}, \vec{y} \rangle = \frac{\sum_{i=1}^{n} (x_i - x_{i-1})(y_i - y_{i-1})}{t_i - t_{i-1}} \quad (8)$$

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

$$\langle x(t), y(t) \rangle = \int_{pT}^{T} \frac{(x(t) - x(t - pT))(y(t) - y(t - pT))}{(pT)^2} dt \quad (9)$$

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

$$\langle \vec{x}, \vec{y} \rangle = \frac{\sum_{i=1,s}^{n} (x_i - x_{i-s})(y_i - y_{i-s})}{t_i - t_{i-s}} \quad (10)$$

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

$$\langle \vec{x}, \vec{y} \rangle = \frac{1}{n} \sum_{i=1}^{n} x_i y_i + \frac{1}{n-s} \frac{\sum_{i=1,s}^{n} (x_i - x_{i-s})(y_i - y_{i-s})}{t_i - t_{i-s}} \quad (11)$$

The weighting factors equalize the contribution of the Euclidean inner product and the secant inner product to the combination.

Figure C.2 shows a simple example of data compared with three model predictions. Model 1 is simply the experimental data multiplied by 0.9. Model 2 has the same peak value as model 1, but with the peak shifted −25 s. Model 3 has the same peak as Model 1 and Model 2, but with a 20 s plateau centred around the peak of the experimental data. The comparison only of maxima would show that all three models are identical with a relative difference of 0.1. Clearly this comparison fails to capture the differences between the three models. Table C.1 shows the relative difference and cosine between the vectors of experimental data and model predictions for the three models using other definitions for the inner product and norm.

All the metrics rank the models in the same order, with Model 1 closest to the experimental data, followed by Models 2 and 3. The rank order matches a visual interpretation of the comparisons. Model 1 is clearly the best, with the same functional form and a peak timed correctly but slightly lower than the experimental data. Conversely, Model 2, with its peak so offset from the experiment, appears the worst. Although Model 3 does not have the correct type of peak (an elongated plateau rather than a sharp peak), it does have the right general form; changing to match the experiment.

The relative difference for Model 1 is the same for all of the metrics as it should be. By choice, the vector form of Model 1, $\vec{m}$, is simply $\vec{m} = 0.9\vec{E}$. Thus, the relative difference, $\left\|\vec{E} - \vec{m}\right\| / \left\|\vec{E}\right\|$, regardless of the definition of the norm is just $\left\|\vec{E} - 0.9\vec{E}\right\| / \left\|\vec{E}\right\|$ or 0.1. Similarly, the cosine of the angle between Model 1 and the experiment is 1.0 for all of the comparisons.

While both the Euclidean relative difference and cosine have the appropriate ranking for all of the models, the cosine does not provide much differentiation between the model predictions. The Hellinger and secant values provide a wider range since they specifically compare the functional forms of the experiment and models.

As an example, a comparison of the model CFAST with five different real-scale fire tests is shown in Table C.2, using this technique. They consist of

a) a single-room test using upholstered furniture as the burning item was selected for its well-characterized and realistic fire source in a simple single-room geometry,[14]

b) a single-room fire test using furniture as the fire source[15] provided a test similar to the first test with a more realistic fire source,

c) a three room configuration; the data cited is an average of a series of 11 replicate tests with simple steady-state gas burner fires,

d) a series of tests conducted in a multiple room configuration with more complex gas burner fires than the previous data set,[16] and

e) a series of full-scale experiments conducted to evaluate zoned smoke control systems with and without stairwell pressurization.[17]

Test e) was conducted in an eight-story hotel with multiple rooms on each floor and a stairwell connecting to all floors. A selection of data from these same tests is used in this annex to provide examples of equivalent comparisons quantified using the norm and inner product. Details of the geometry, experimental measurements and model predictions are available.[18] Table C.1 presents the hybrid relative difference norm, Formula 1, and cosine of the angle between the vectors of experimental data and model predictions for a selection of the data from these five tests. To better understand these quantified comparisons, Figure C.3 shows what the experimental data and model predictions for one of the variables included in Table C.2.

Figure C.3 shows a comparison of upper layer temperatures for a single room test. In this test, two measurement positions were available from the experimental data. The predicted temperatures show obvious similarities to the measured values. Peak values occur at similar times with comparable rise and fall for both measurement positions. For both positions, peak temperatures are higher than the model predictions, with one position somewhat higher than the other position. Both the relative difference norm and cosine reflect these trends. The relative difference norm is somewhat higher for one of the experimental positions (0.36 versus 0.31) reflecting the higher temperature at this measurement position. With the shapes of all the curves similar, the cosine shows similar values for both curves (0.93 and 0.95).

For the experiments and models examined, the techniques provide the ability to quantify the comparison magnitude and functional form consistent with visual examination of the comparisons.

Table C.1 — Comparison of "fictional" experimental data with three model predictions using several different inner product definitions

Geometry	Model	Relative difference	Cosine
Euclidean	1	0,10	1,00
	2	0,40	0,92
	3	0,20	0,98
Hellinger	1	0,10	1,00
	2	0,94	0,58
	3	0,74	0,77
Secant	1	0,10	1,00
	2	0,92	0,58
	3	0,66	0,83
Hybrid	1	0,10	1,00
	2	0,64	0,78
	3	0,43	0,91

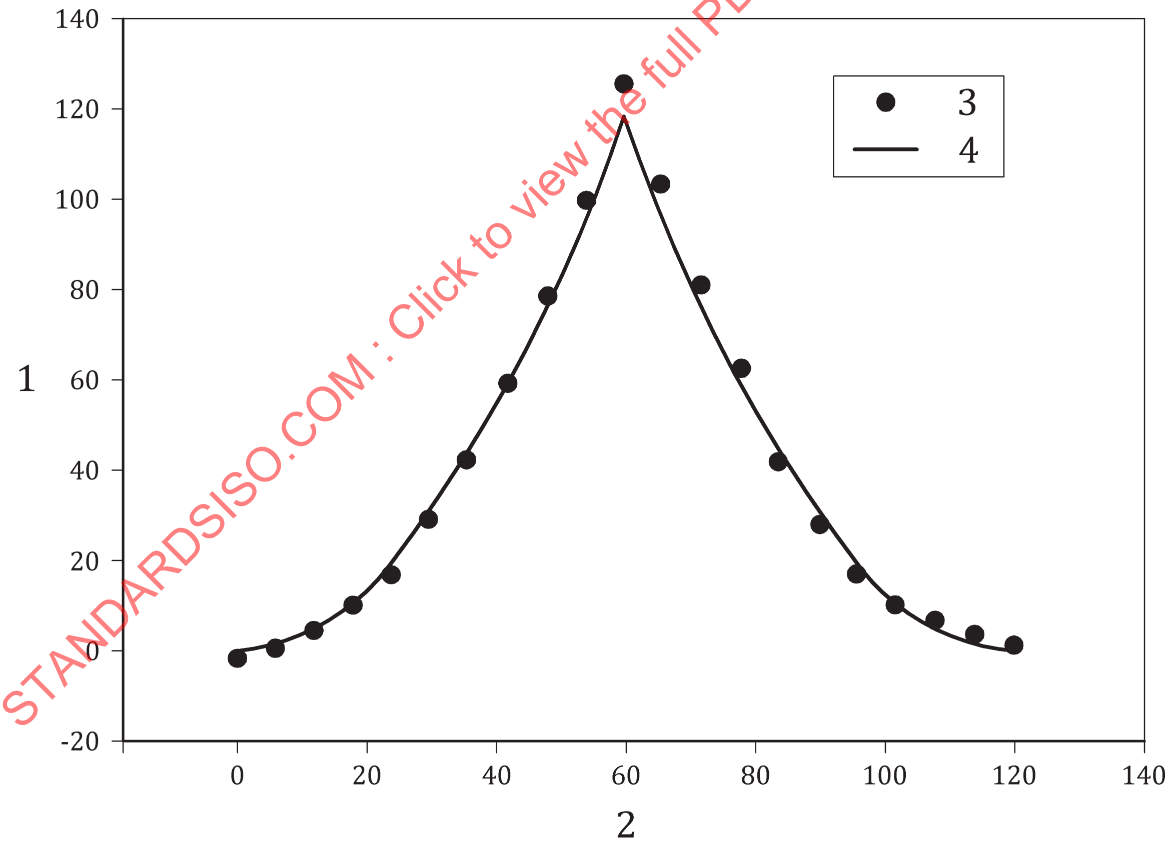
Table C.2 — Comparison of experimental measurements and model predictions for several tests

Test type	Position / compartment	Relative difference	Cosine	Relative difference	Cosine	Relative difference	Cosine
Temperature and position		**Upper layer temperature**		**Lower layer temperature**		**Interface position**	
Single-room furniture tests	1	0,31	0,95	0,47	0,92	1,38	-0,60
	2	0,36	0,93	0,63	0,78	0,63	0,78
Three-room tests with corridor	1	0,25	0,97	–	–	–	–
	2	0,26	0,99	–	–	–	–
	3	0,26	0,98	–	–	–	–
Four-room tests with corridor	1	0,51	0,93	0,33	0,95	2,26	0,06
	2	0,54	0,91	0,52	0,87	–	–
	3	0,36	0,97	0,78	0,86	–	–
	4	0,20	0,98	–	–	–	–
Multiple-story building	1	0,28	0,97	–	–	–	–
	2	0,27	0,96	–	–	–	–
	7	2,99	0,20	–	–	–	–
Gas concentration		**Oxygen**		**Carbon monoxide**		**Carbon dioxide**	
Single-room furniture tests	1	0,48	0,90	0,93	0,66	0,69	0,93
Four-room tests with corridor	1	0,85	0,53	1,05	0,61	1,16	0,63
	2	0,93	0,39	1,02	0,57	0,90	0,63
Multiple-story building	2	0,74	0,68	0,72	0,90	0,87	0,93
HRR, pressure and vent flow		**Heat rate release**		**Pressure**		**Vent flow**	

NOTE When data for the comparison was not available, the entry is noted with –.

Table C.2 *(continued)*

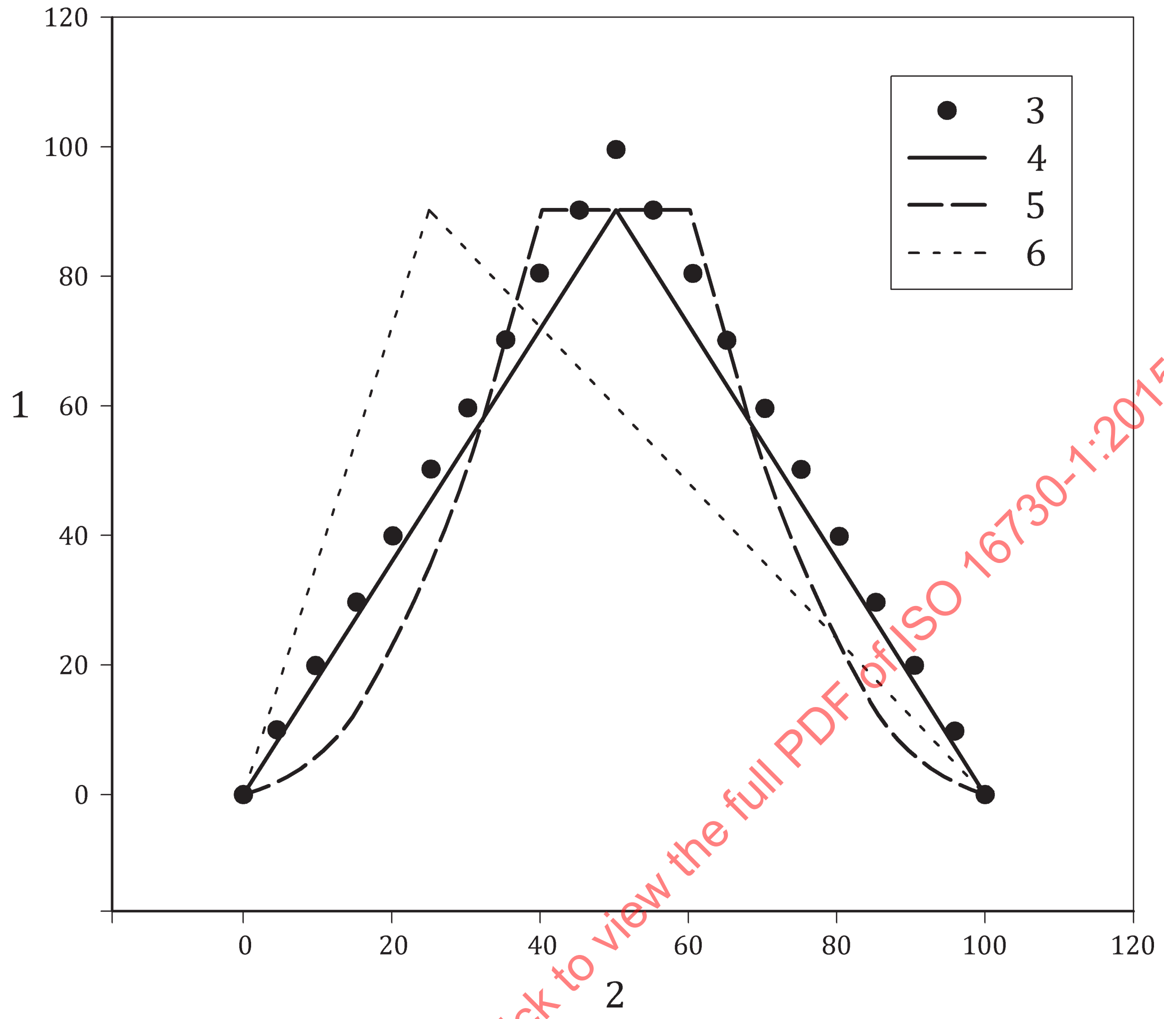
Test type	Position / compartment	Relative difference	Cosine	Relative difference	Cosine	Relative difference	Cosine
Temperature and position		**Upper layer temperature**		**Lower layer temperature**		**Interface position**	
Single-room furniture tests		0,19	0,98	–	–	0,61	0,79
Single-room tests with wall burning		0,21	0,98	1,31	0,80	–	–
Three-room tests with corridor	1	0,43	0,98	0,15	0,99	0,14	0,99
	2	–	–	0,68	0,98	0,20	0,98
Four-room tests with corridor		–	–	6,57	0,74	–	–
Multiple-story building	1	–	–	1,12	-0,41	–	–
NOTE When data for the comparison was not available, the entry is noted with –.							



Key

1 measurement
2 time
3 experiment
4 model

Figure C.1 — Simple example of experimental data compared with a model prediction



Key

1 measurement

2 time

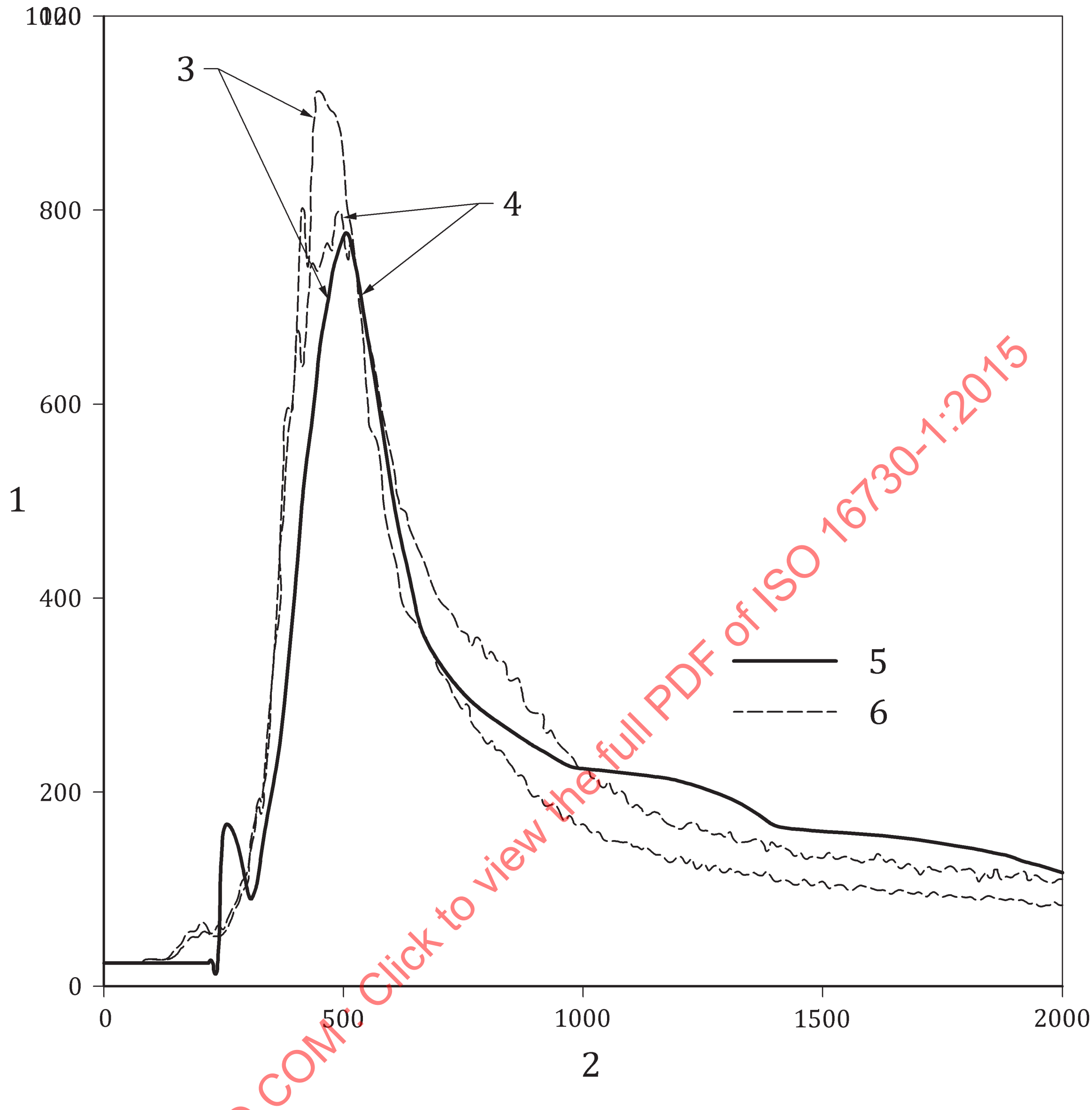
3 col 6 vs col 7

4 col 6 vs col 9

5 col 6 vs col 11

6 col 6 vs col 13

Figure C.2 — Three possible model predictions for an example of experimental data



Key

1 temperature (°C)

2 time(s)

3 rel.diff. = 0.36, cosine = 0.95

4 rel.diff = 0.31, cosine = 0.93

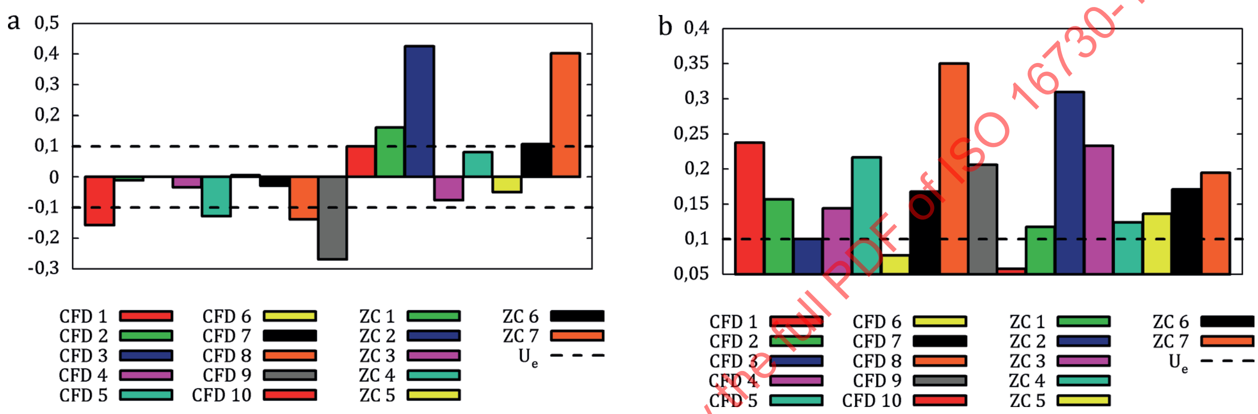
5 model

6 experiment

Figure C.3 — Comparison of upper layer temperature for a single-room test

C.3 Euclidean method

A second example is the collaborative work performed by the PRISME benchmarking group in the framework of an OECD experimental research programme.[21] This numerical study involved 17 participants using 8 fire models (3 CFD or field models and 5 zone models). The definition of the purpose of the validation process is also a critical issue in assessing numerical models. Obviously, the compared quantities and the metrics selected in a validation process directly depend on the intended use. The experiments consisted of a full-scale liquid pool fire in a confined and mechanically ventilated compartment. The calculation was qualified as “open”, therefore, wall and fuel properties were specified as well as the fuel burning rate, the ventilation conditions and test data. For the validation process, six quantities were compared during the whole fire duration: gas temperature, oxygen concentration, wall temperature, total heat flux to a wall, compartment pressure and the ventilation flow rate at the inlet branch. Two metrics were used for quantifying the evaluation of the models. The first metric, also used by the USNRC and EPRI in the validation work of fire models,[22] considers the numerical and experimental results expressed in term of difference between maximum values. This metric considers only instantaneous values and behaves as a measurement of local error. The second metric, called the normalized Euclidean distance, considers the differences between computational results and measurements during the entire fire duration. This metric provides information of the global error and gives a comprehensive overview of code capabilities. The study showed that it is important to consider more than one metric for the validation process of computer codes (Figure C.4 shows an example of results). In this work, the assessment of metric capabilities in the case of a fire in a confined compartment has shown that the time dependent behaviour of a phenomenon was as significant as peak or local values.



(a) Local error of the mean temperature **(b) Global error of the mean temperature**

Figure C.4 — Local (a) and global (b) error of the mean temperature

Annex D
(informative)

Methods for sensitivity analysis

Two basic approaches exist for obtaining sensitivity information:

a) *local methods* produce sensitivity measures for a particular set of input parameters and must be repeated for a range of input parameters to obtain information on the overall model performance.

   Finite difference methods can be applied without modifying a model's equation set, but require careful selection of input parameters to obtain good estimates. Direct methods supplement the equation set solved by a model with sensitivity equations derived from the equation set solved by the model.[6] The sensitivity equations are then solved in conjunction with the model's system of equations to obtain the sensitivities. Direct methods must be incorporated into the design of a fire model and are not often available for already existing fire models.

b) *global methods* produce sensitivity measures which are averaged over the entire range of input parameters.

   Global methods require knowledge of the probability density functions of the input parameters, which in the case of fire models is generally unknown.

Local methods are most easily applied. Global methods are appropriate if the range of input information is known, for example in risk calculations for fire safety engineering.

Even though it is possible to define the sensitivities and establish various methods for their computation, there are still difficulties associated with performing a sensitivity analysis. Iman and Helton[7] note some of the properties of complex computer models that make analysis difficult:

— there are many input and output variables;

— discontinuities may exist in the behaviour of the model;

— correlations may exist among the input variables and the associated marginal probability distributions are often non-normal;

— model predictions are nonlinear, multivariate, time-dependent functions of the input variables;

— the relative importance of individual input variables is a function of time;

— an ideal situation would be to consider the variables in the model, and assess the sensitivity of each input data that may influence global and local values.

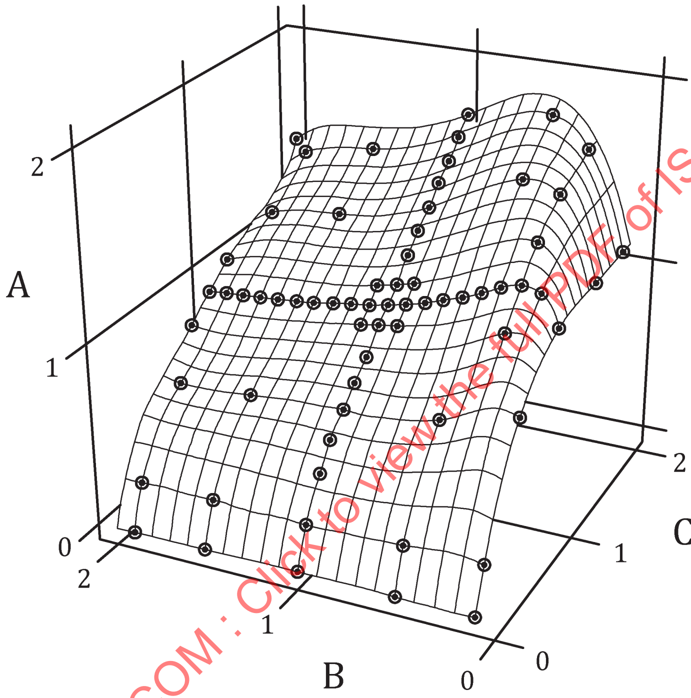
In addition, the sensitivity equations have similar properties. For a given model output and a given model input, there may be regions of time where the model output is sensitive to the input and also regions where the model output is insensitive to the same parameter.

At least two broad questions can be addressed with a sensitivity analysis of a fire model. First, "how sensitive is the model to a specific input?" This is an attempt to gain an overall appreciation of the importance of an input relative to all other inputs. For this question, the range of model inputs could be chosen as broad as possible representing the range of applicability of the model. A subsequent analysis of model outputs for such broad changes would then provide insight into the relative importance of a given input variable on selected outputs. Such an analysis provides an overall picture of model behaviour.

The second question is "how closely must a specific input be specified?" Rather than understanding the overall behaviour of the model, it is an effort to obtain an understanding of the effect on the model outputs of uncertainties in selected inputs. For this question, small perturbations in the inputs could be examined. If a specific scenario is of interest, perturbations of the inputs for this scenario could be examined.

As suggested by Iman and Helton,[7] an average relative difference could thus be used to characterize the model sensitivity for comparing individual inputs and outputs.

Figure D.1 is a response surface for a fire model showing the effect of a changing heat release rate and vent size on the upper layer temperature.[8] It presents the effect of both peak HRR and vent opening (in the fire room) on the peak upper layer temperature. In this figure, actual model calculations are normalized to the base scenario values as indicated by circles overlaid on a surface grid generated by a spline interpolation between the data points. From the surface, it is clear that HRR has more of an effect on the peak temperature than does the vent width. Until the fire becomes oxygen limited, the trends evident in the surface are consistent with expectations – temperature goes up with rising HRR and down with rising vent width. The effects are not, of course, linear with either HRR or vent opening.



Key

A normalized peak temperature

B normalized vent width

C normalized HRR

Figure D.1 — Response surface for a fire model to characterize the model sensitivity for comparing individual inputs and outputs

EXAMPLE Effect of a changing heat release rate and vent size on the upper layer temperature.

McGrattan and Toman[29] published a comparison between numerical and experimental results for a wide set of calculations with complex fire models. Numerical techniques have been developed to establish the sensitivity of complex models, when sampling has to be optimized, i.e. when computational time is critical such that extensive calculations become prohibitively expensive. Many important applications in fire safety engineering are described by computationally expensive model equations, e.g. the Navier-Stokes equations for fluid flows and other transport equations. Most of these computationally expensive systems are strongly nonlinear. Linear approximations as suggested by ISO/IEC Guide 98-3 (hereafter referred to as the GUM)[23] can be applied, but the results may not be trustworthy and hence Monte-Carlo simulations are recommended, e.g. by Supplement 1 to the GUM.[24] Such models have been applied successfully to fire models for sensitivity analysis,[25-27] especially to zone models.[28] However, Monte-Carlo methods are based on a large number of model evaluations and consequently cannot be applied practically. As a result, uncertainty statements in measurements with computationally expensive models are usually either missing or based on crude approximations. Alternative methods to reduce the number of calculation (sampling methods) have been established.

For local assessment, many sampling methods have specific requirements, restrictions or assumptions (inputs must be independent, output quantity can be locally approximated as a polynomial function of the input quantities), which can limit their applicability. To cope with the challenges for sensitivity evaluation involving nonlinear computationally expensive models, two main approaches are currently followed: smart sampling methods and surrogate modelling.

Smart sampling methods such as polynomial chaos (Wiener Chaos expansion)[30-32] and Latin hypercube sampling[33,34] drastically reduce the number of function evaluations and the resulting computational cost required for uncertainty evaluation compared to random sampling.

In surrogate modelling, computationally cheap models replace the computationally expensive models; statistical modelling are then used to account for the unavoidable errors introduced by the surrogate models, smart sampling methods and surrogate modelling. An example is to correlate a CFD model to a zone model, then to study the sensitivity of the zone model. In this case, the sensitivity for inputs that are similar in both models should be coherent.

The estimator used to report sensitivity is also important. Different estimators for the sensitivity of models using the Monte-Carlo method and reduced sampling methods could be used. Techniques used to perform sensitivity analysis are not equivalent in terms of estimator and calculation costs. They all vary in terms of capabilities, limitations and calculation costs. Examples of application are available in references.[28,38,39]The main techniques used are

— Standardized Rank Regression Coefficient (SRRC), a variant of the linear Standardized Regression Coefficient (SRC) variance estimator adapted to nonlinear problems,

— Sobol's indices[35] to estimate the first-order sensitivity indices by the quantity,

— Fourier Amplitude Sensitivity Test (FAST),[36] where multi-dimensional analysis is reduced to a one-dimensional problem in a Fourier space, and

— local polynomial smoothers,[37] where approximation of a model is performed by polynomial approximation around the analysis point.