

# Numerical experiments - a research method in fire science

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# Numerical experiments

## a research method in fire science

Licentiate thesis

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Nils Johansson

Lund, December 2013

# Summary

Experiments are and have always been a natural part of fire science. It is hard to derive relationships from theory in fire science due to the complex nature of fire and flames. Full-scale and small-scale experiments have been used with great success during the twentieth century and our understanding of fire chemistry and fire dynamics have progressed considerably during this time. This has also paved the way for fire safety engineering. But, there are shortcomings and difficulties with conducting fire experiments.

Firstly, fire experiments in full-scale are costly and time consuming. This means that it can be hard to conduct a large enough test series in order to find correlations between different variables. Also, full-scale compartment fire experiments can only be performed at a few locations in the world, which means that the number of research groups in this area is limited.

Secondly, it is hard to control important variables in a full-scale fire experiment. This means that a number of tests are needed in order to get an overview of the random variation in the experiment. Additionally, the variability in the experiment related to the lack of control can make it impossible to distinguish how different variables affect each other.

During the last decades computer models that can be used to simulate fires and smoke spread have developed rapidly. Some of these models have been shown to give predictions of some compartment fire properties within the bounds of measurement uncertainty of performed experiments. Consequently, numerical experiments emerge as a possible complement to traditional compartment fire experiments.

In this thesis, numerical experiments are explored as a research method and put into the context of traditional compartment fire experiments. Both pros and cons of numerical experiments compared to traditional compartment fire experiments and prerequisites for numerical experiments are presented and summarised in the thesis. Numerical experiments are a promising method in fire science research. However, it is currently not considered satisfying to solely use a numerical experiment to find a correlation for a certain fire phenomena without checking the correlation with data from some traditional experiments.

There is no experimental method that can be recommended for use for all types of research tasks in fire science. It is intuitive that traditional experiments should be used when important variables can be controlled and the resources are available, but that is not always the case. The different experimental methods should not be regarded as competitive but as complementary, and a combination of traditional and numerical experimental methods are in many cases appropriate in order to analysis a certain fire phenomena. Consequently, it is believed that numerical experiments will play an important roll in the future of fire science, and in order to keep a high quality of numerical experiments it is believed to be important that the fire science community recognizes fire models as a tool for experiments in fire science.

# Sammanfattning (in Swedish)

Experiment är och har alltid varit en naturlig del av forskningen om bränder och brandskydd. Det är svårt att härleda samband om bränder från teori på grund av fenomenets komplexitet. Fullskaliga och småskaliga brandtekniska experiment har använts med stor framgång under nittonhundratalet och förståelsen av brandkemi och branddynamik har ökat betydligt. Det har också banat väg för möjligheter till analytisk brandteknisk dimensionering av byggnader. Det finns dock svårigheter och problem med att genomföra brandtekniska experiment.

Brandtekniska experiment i full skala är kostsamma och tidskrävande. Det är därför svårt att genomföra en tillräckligt stor testserie för att finna korrelationer mellan olika variabler. Dessutom kan fullskaliga experiment av rumsbränder endast utföras på ett fåtal platser i världen, vilket innebär att antalet forskargrupper inom detta område är begränsat.

Det är dessutom svårt att kontrollera alla viktiga variabler i ett fullskaligt brandtekniskt experiment och för att få en överblick över den slumpmässiga variationen i ett experiment måste experimentet upprepas. Om det finns variabler som inte är möjliga att kontrollera i ett experiment kan variationen göra det omöjligt att urskilja hur olika variabler påverkar resultatet.

Datormodeller för att simulera bränder och brandgasspridning har utvecklats mycket under de senaste decennierna. Vissa av dessa datormodeller har visats kunna prediktera egenskaper för rumsbränder inom gränserna för mätosäkerheterna vid utförda experiment.

I denna avhandling utforskas numeriska experiment som en metod för brandteknisk forskning inom samma områden som traditionella brandtekniska experiment. För- och nackdelar med numeriska experiment jämfört med traditionella experiment samt förutsättningar för numeriska experiment presenteras och sammanfattas i avhandlingen. Numeriska experiment är en lovande metod för brandteknisk forskning. För närvarande anses det dock inte tillfredsställande att enbart använda numeriska experiment för att finna en korrelation för ett visst fenomen utan att kontrollera korrelationen med data från vissa traditionella experiment.

Det finns ingen experimentell metod som kan rekommenderas för alla typer av brandtekniska experiment. Det är intuitivt att traditionella experiment bör användas när viktiga variabler kan kontrolleras och när resurser finns tillgängliga, men det är inte alltid fallet. De olika experimentella metoderna som finns tillgängliga bör inte betraktas som konkurrerande, utan snarare som kompletterande. Det är i många fall lämpligt att kombinera traditionella och numeriska experimentella metoder för att analysera ett visst brandtekniskt fenomen. Detta innebär att numeriska experiment förmodligen kommer att spela en viktig roll i framtida brandteknisk forskning och för att numeriska experiment ska hålla en hög kvalitet är det viktigt att det erkänns som ett verktyg för brandteknisk forskning.

# Table of contents

**1 Introduction ..... 1**
**1.1 Numerical experiments ..... 2**
**1.2 Papers included in the thesis ..... 3**
**1.3 Research process ..... 4**
1.3.1 Problem identification ..... 5
1.3.2 Problem solution ..... 6
1.3.3 Evaluation ..... 6
**1.4 Research questions ..... 7**
**1.5 Method ..... 7**
**1.6 Limitations ..... 8**
**1.7 The author's experience of experimental work ..... 8**

**2 Accuracy, validity and uncertainty ..... 11**
**2.1 Accuracy ..... 11**
2.1.1 Precision ..... 12
2.1.2 Trueness ..... 12
**2.2 Validity ..... 13**
**2.3 Experimental uncertainty ..... 13**

**3 Traditional fire experiments ..... 15**
**3.1 Problems with traditional fire experiments ..... 15**
3.1.1 Full-scale experiments ..... 15
3.1.2 Small-scale experiments ..... 16
**3.2 Accuracy in fire experiments ..... 17**
3.2.1 Heat release rate ..... 17
3.2.2 Temperature ..... 18

**4 Numerical experiments ..... 21**
**4.1 Examples of numerical experiments in fire science ..... 21**
**4.2 Accuracy in numerical experiments ..... 22**
**4.3 Model evaluation ..... 23**

**5 Advantages and challenges ..... 27**

**5.1 Advantages of numerical experiments ..... 27**
5.1.1 Resource efficient ..... 27
5.1.2 Possibilities to test hypothesis ..... 30
5.1.3 Level of control of the experiment ..... 30
5.1.4 Measurements ..... 32
**5.2 Challenges with numerical experiments ..... 32**
5.2.1 Description of the fire phenomena ..... 32
5.2.2 Experienced user ..... 33
5.2.3 Accuracy of fire models ..... 33
**6 Prerequisites for numerical experiments ..... 35**
**7 Conclusions ..... 39**
**7.1 Pros and cons of numerical experiments ..... 39**
**7.2 Numerical experiments as a substitute for traditional experiments ..... 40**
**7.3 Future research ..... 41**
7.3.1 User uncertainty ..... 41
7.3.2 Accurate fire models and new areas ..... 42
**References ..... 43**

# 1 Introduction

It is hard to derive relationships from theory in fire science due to the complex and casual behaviour of fires and flames. Therefore, it has been necessary to perform fire experiments in order to get an understanding of some fire phenomena. As an example, there is a range of empirical correlations, derived with the help of experiments that gives some explanation of different fire phenomena. These experiments have been conducted in a variety of ways, e.g. in limited-scale were only some single variables have been studied, in small-scale or in full-scale.

The cone calorimeter [1] is an example of a limited-scale experiment where the reaction to fire of a material subjected to a heat flux is studied. Another example is the small-scale furnace according to SP Fire 119 [2], which can be used to study how a material reacts to different heating conditions [3]. These types of experiments are performed in a controlled environment in order to study a relationship between a few variables. Everything except the variables of interest is kept constant and by changing the variables the correlation between them can be studied. Limited-scale experiments can be used to investigate relationships on a fundamental level in fire science, e.g. critical heat flux for a certain material. However, results from these experiments are not sufficient in order to understand and evaluate fire development and smoke spread in single- and multiple-room compartments.

Small-scale experiments can be used to scale down a realistic fire situation to an appropriate size with the help of scaling laws. With a small-scale experimental setup it is possible to conduct the experiments in a more controlled environment (i.e. in a fire laboratory). Ideally, everything except the variable of interest can be kept constant and by varying it can the effect of the variable on the experiment be analysed. Some compromises are necessary in the small-scale experiments because it is not possible to fulfil the scaling laws for all the mechanisms of importance in fire science [4].

The most realistic experiment is of course in full-scale. It is possible to conducted full-scale experiments of multi-room compartments or even entire buildings in some indoor fire laboratories in the world (e.g. at SP in Sweden,

Underwriters Laboratories and FM Global in USA), but it is hard to control important variables as the experimental setup increases in size. Even if variables are controlled it can still be hard to reproduce fire experiments [5] due to the complex combustion phenomena present in fires. Also, it might not be possible to conduct the experiment in an indoor laboratory environment due to economical reasons or lack of laboratory space and equipment to handle a large experimental setup. In such a situation the alternative can be to move the experiment outdoors. Although, in that case it can be even more problematic to control important variables, e.g. wind speed and wind direction can be hard to control and measure sufficiently accurate.

An alternative or complement to laboratory experiments is the use of numerical experiments where all variables are controlled and a phenomenon can be studied and analysed. In a numerical experiment a fire model, like CFAST [6] or FDS [7] is used. Models include interpretations and approximations of the real world but can be used in order to understand some physical reality [8]. This means that even though the models only provide a representation of the real world they can be very helpful or as stated by Box and Draper [9], "Essentially, all models are wrong, but some are useful" (p. 424).

Numerical experiments are considered to be a promising method for research in fire science, even though there are both advantages and problems compared with small- and full-scale experiments. In this thesis numerical experiments are explored as a research method in the same context as other experimental methods currently used in fire science research.

## 1.1 Numerical experiments

Both experiments and observations can be used to collect data and test hypotheses. Different ways of collecting data will lead to different types of relationships. A passive observation involves an investigation of a pre-existing state without attempting to influence it. Collecting data by observing a system and then trying to extract interesting information afterwards is common in research [10], but it is not an experiment.

An experiment is something more than just an observation and collection of data. In an experiment the state of the system is changed and the result of that change in the system is measured and analysed in order to generate information that is relevant to the research question (see Figure 1).

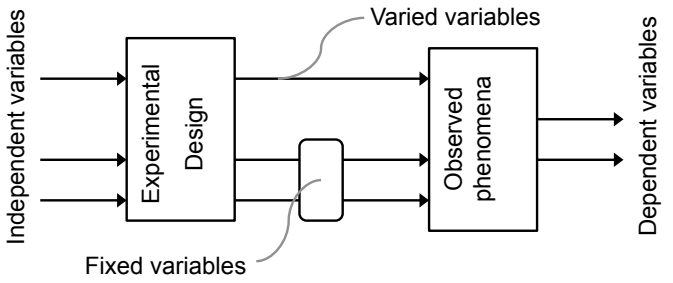


**Figure 1: Illustration of an experiment (recreated from Höst et al [11]).**

The term numerical experiment has been used in other scientific fields, like metrology [12], for quite some time and lately there are also examples of the term being used in fire science [13–15]. However, there is, to the knowledge of the author, no established definition or description of numerical experiment in field of fire science. Therefore, the following definition of numerical experiments is applied in this thesis:

*A numerical experiment is an experimental study with a numerical model.*

The term experimental study refers to the description of experiments given in Figure 1, i.e. a systematic manipulation of a system in order to address a certain research question. This distinguishes numerical experiments from simulations that are e.g. used for building design; the purpose of the latter is normally to demonstrate the performance of a building with regard to some selected fires and not to explain how the system works.

Physical experiments that have traditionally been used to study compartment fires are referred to as traditional experiments in this thesis. These traditional experiments can be conducted in small- or full-scale.

## 1.2 Papers included in the thesis

Four papers are included as appendices to support the discussion and reasoning in this thesis. Paper I and III has been accepted for publication in two different international scientific journals. Paper II has been submitted to Fire Technology and paper IV has been submitted to Fire and Materials.

I. Johansson N, Wahlqvist J, van Hees P (2012) Detection of a Typical Arson Fire Scenario - Comparison Between Experiments and Simulations. Journal of Fire Protection Engineering 22:23-44.

II. Johansson N, Svensson S, van Hees P (2013) A Study of Reproducibility of a Full-scale Multi-Room Compartment Fire. Submitted to Fire Technology.
III. Johansson N, van Hees P (2012) A correlation for predicting smoke layer temperature in a room adjacent to a room involved in a pre-flashover fire. Fire and Materials DOI: 10.1002/fam.2172 (published online).
IV. Johansson N, Wahlqvist J, van Hees P (2013) Numerical Experiments in Fire Science - A Study of Ceiling Jets. Submitted to Fire and Materials.

All four papers are original research papers. Paper IV is an expansion of a paper [16] presented at the 13th International Conference and Exhibition on Fire Science and Engineering (Interflam 2013). The author's contributions to the four papers are presented in Table 1.

**Table 1: The author's contribution to the appended papers.**

| Paper | Contribution |
|---|---|
| I | The author planned and performed the full- and small-scale experiments together with one co-author. A co-author performed the simulations. The author performed the analysis and wrote the majority of the paper. The author contributed to 2/3 of the paper. |
| II | The author performed the analysis of the data and wrote the paper. The author contributed to more than 3/4 of the paper. |
| III | The author planned and performed the numerical experiments. The author conducted the statistical analysis and wrote the majority of the paper. In total the author contributed to more than 3/4 of the paper. |
| IV | The author planned the numerical experiments and derived the simplified ceiling jet theory. A co-author performed the simulations, but the author conducted the statistical analysis and wrote the paper. The author contributed to 3/4 of the paper. |

## 1.3 Research process

The research process consists of three parts and is illustrated in Figure 2. The process of identifying research questions consists of the two first parts, which are the dark grey in Figure 2. These research questions are the starting point of this thesis, which constitutes the light grey part of Figure 2.

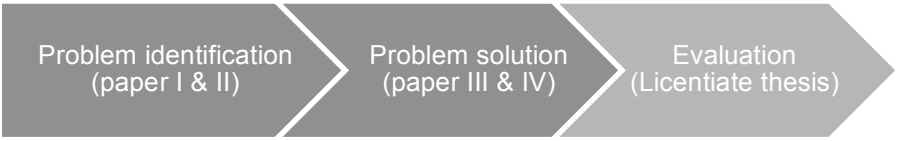


**Figure 2: Process of research.**

The research process is explained, with the support of the papers included in the thesis, in the following sections.

### 1.3.1 Problem identification

Paper I and II are part of the problem identification of the research process (see Figure 2). In paper I, exterior arson fires and how they can be detected are studied with small-scale laboratory experiments along with a full-scale outdoor experiment. Simulations with FDS were used to recreate the small-scale and full-scale experiments in the paper. There was a good agreement between the experimental and simulated results in the small-scale. But, the weather conditions and especially wind speed and wind direction could not be controlled and did have a large influence on the full-scale experiment; consequently, it was hard to analyse it.

Paper II contains a study of the reproducibility of four different ventilation scenarios in a multi-room compartment connected to a stairwell. The paper shows the variation between forty fire tests. In the paper combined uncertainties, which includes the random error in the measurements and an estimated systematic uncertainty in the thermocouple measurements, are presented. It was not possible to find the cause of the variation but it was probably due to different weather parameters and other unknown influencing variables that could not be controlled in the tests.

The problem identified from the studies in paper I and II is that it can be hard to control variables of importance in full-scale fire experiments. Another issue identified is that it is hard to study the random variation and the dependencies between variables in full-scale experiments because they are rigorous and costly and sometimes only single experiments can be performed with one or no repetition.

An alternative to small-scale and full-scale fire experiments could be numerical experiments, which were used as research method in paper III and IV.

### 1.3.2 Problem solution

A setup with two compartments connected with an opening was studied by means of numerical experiments in paper III. The heat release rate, size of the compartments and opening size varied in the approximately 100 FDS simulations conducted. A correlation for the smoke layer temperature in the compartment adjacent to the fire room was derived with a multiple linear regression analysis. A minor validation study of the derived correlation was conducted in the paper. The result from the comparison with experiments was encouraging, even though the number of data points was few.

All the variables of interest were controlled in the numerical experiment and this created an opportunity to study how a predefined set of variables influences the smoke layer temperatures in an adjacent room. It is not likely that it would have been possible to perform the same amount of traditional full-scale experiments in a fire laboratory.

The same type of approach was used in paper IV, but in order to study ceiling jets. A total of 90 FDS simulations were carried out in order to gather data. The data collected from the numerical experiment were the temperature and gas velocities under a smooth unobstructed and unconfined ceiling. The heat release rate, room height and ceiling surface properties were varied in the simulations.

Paper IV had two purposes. Firstly, to explore numerical experiments as a research method in fire science and demonstrate how numerical experiments can be used as a complement to traditional fire experiments. Secondly an evaluation of previously derived correlations for ceiling jet temperatures and velocities by Alpert [17] was performed.

### 1.3.3 Evaluation

In Paper III and IV a rather promising method was used as a complement to traditional experiments. However, there are both advantages and disadvantages compared with small- and full-scale experiments. Paper IV contains a minor evaluation of numerical experiments. But except this there has not, to the knowledge of the author, been any thoroughly evaluation of using numerical experiments in fire science research. This means that there is an obvious gap of knowledge in this area, consequently there is a need to explore numerical experiments as a research method in fire science and it is performed in this thesis. This evaluation is based on two research questions.

## 1.4 Research questions

The last part of Figure 2, i.e. the evaluation of the proposed solution, is conducted by studying two research questions. The purpose of the first question is to distinguish advantages and challenges with numerical experiments compared to small- and real-scale fires. The first question is formulated as follows:

1) *What are the pros and cons of numerical experiments compared to traditional compartment fire experiments?*

This first research question leads up to the question: "Can numerical experiments be used as a substitute for traditional compartment fire experiments?" This is rather diffuse question and is therefore specified as the following in the second research question in this thesis:

2) *When can numerical experiments be considered as a substitute for traditional compartment fire experiments?*

In order to be able to address these questions it is necessary to give a brief description of some fundamental terms (chapter 2) and to highlight some problems with traditional compartment fire experiments (chapter 3). Furthermore, the use and accuracy of numerical experiments in fire science need to be discussed (chapter 4). Finally the research questions are discussed in chapter 5 and chapter 6 and addressed more explicitly in chapter 7.

## 1.5 Method

The research questions are addressed by using an exploratory approach [11, 18] i.e. seeking insight into how numerical experiments can be used as an experimental method in fire science research. This is done with a comparative study where numerical experiments are compared to traditional compartment fire experiments. The comparison proceeds from a description of the terms accuracy, validity and uncertainty of traditional and numerical experiments. The four appended papers constitute the main material used for this comparative study.

## 1.6 Limitations

This thesis is limited to numerical experiments that are used to study compartment fires. This thesis has a fire researcher focus and experimental methods for research purpose, which means that this work does not deal with standardized fire testing methods.

## 1.7 The author's experience of experimental work

This thesis deals with experimental work in fire science. A short description of the experimental activities conducted by the author is presented here in order to give the reader an idea of the author's background and experience of experimental activities.

Two experimental test series are included in paper I. The author planned and organised a full-scale outdoor experiment and a small-scale experiment. In the full-scale experiment a typical exterior arson scenario was studied on an actual building. Detection times for a smoke detector placed in a small attic and a linear heat cable were studied. In the small-scale experiment a propane burner was used to study the detection time of a linear heat detection cable under rather controlled conditions.

A more comprehensive experimental test series was conducted to study smoke entrainment into an attic space through openings for natural ventilation [19]. These experiments were also planned and to a large extent performed by the author. In this case a small-scale experiment in a laboratory was followed up with a full-scale experiment. In the small-scale experiment temperature measurements with thermocouples and obscuration measurements with a white light system in the small attic space were performed. In the full-scale experiments temperatures on the façade and in the attic were measured with thermocouples. Three different types of linear detection cables and four smoke detectors were used in order to compare detection times.

A study of forty fire tests is presented in paper II. The tests were performed during a five-year period as a part of an undergraduate course in Fire Dynamics (VBRF10) at Lund University. The author performed the analysis of the data from the tests.

An intumescent system intended for cavities was studied in two other experiments [3]. The intumescent material was first studied in a Cone

Calorimeter [1]. This experimental test series was planned and performed by the author. The intumescent system was then studied in a scale furnace [2] at SP Fire Technology. These experimental tests were primarily planned by the author but performed by the staff at SP Fire Technology. The author performed the analysis of both experiments.

# 2 Accuracy, validity and uncertainty

In order to be able to address the two research questions, presented in section 1.4, a short overview of accuracy, validity and uncertainty is given. In this chapter these terms are presented and explained.

## 2.1 Accuracy

Accuracy is defined as the closeness of agreement between a measured value and the true value [20]. Here, this is explained with the help of the terms precision and trueness. The relationship between precision trueness and accuracy is illustrated in Figure 3.

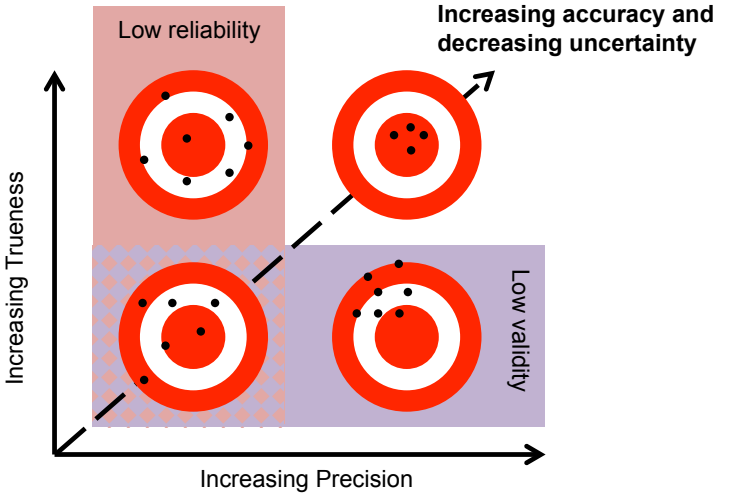


**Figure 3: Relation between precision, trueness and accuracy. The relation to the terms reliability and validity is also presented. The picture is inspired by [21].**

The centre of each circle in Figure 3 corresponds to the "true value" of the variable that is measured and the black dots are the observations. The precision

increases as the scatter of the measurement is smaller and the trueness increases when the average prediction is closer to the centre. The accuracy will increase with increasing trueness and precision.

### 2.1.1 Precision

Precision, or reliability, is the closeness of agreement between replicated measurements on the same or similar objects under the same specified conditions [20]. In Figure 3 the precision of measurement is pictured as the scatter of measurement points, or in other terms as a random error. It is not possible to account for the random error but more measurements will generally give a better estimate of the expected value.

Precision is related to both reproducibility and repeatability. Repeatability of measurement results is the representation of the agreement (variation) between the different results that are carried out under the same conditions. When the variation between measurements is smaller than a certain limit the measurements can be said to be repeatable. Reproducibility is the agreement of results under changed conditions of measurement, e.g. different location, environmental conditions or human resources. If repeatability is tested the same measurement procedure, observer, instruments and location must be used. The repetition must also take place over a short period of time. When these conditions change between measurements it is possible to test the reproducibility. Both the repeatability and the reproducibility can be expressed in terms of the dispersion characteristics of the results [22]. This means that reproducibility and repeatability are ways to describe the precision of measurements.

Since precision is based on the distribution of random error and not the true value, there is no systematic error in the precision. A description of uncertainty is often used to indicate the precision of a measurement. [21]

### 2.1.2 Trueness

The measurement trueness is the closeness of agreement between the average value of an infinite number of replicated measurements and an accepted true value [20, 21]. The trueness can also be described as the total systematic error, i.e. the difference between the average value of the large series of measurements and the accepted true value.

Repeating measurements will not reduce the systematic error because the same influence affects each of the measurements. It is difficult to account for systematic errors and it is only possible to make corrections with a correction

factor when the magnitude and direction of the bias is unknown [23], and the correction only leads to an estimate of the measurand which means there is an uncertainty associated with this imperfect correction [24]. Andersson [10] mentions calibration of instruments, knowledge of background effects and standardized procedures as examples of some actions to take in order to reduce systematic errors. Nevertheless, it is still very hard to determine the "true value" of a measured property and some degree of error must generally be accepted.

## 2.2 Validity

Accuracy as described above is related to validity, but there is a difference. Accuracy refers to the distance to the centre of each circle in Figure 3 from each observation, i.e. the actual amount of error, while validity refers to whether an experiment really do measure what it is supposed to measure [18, 25]. Thus, measurement can be accurate but invalid, but not valid and inaccurate.

Validity can be divided into internal and external validity. External validity refers to what extent the findings could be generalised outside the experimental setup. The internal validity refers to the extent on which cause and effect relations can be established [26]. Small-scale experiments, where the different variables that affect the system can be controlled, are usually needed in order to establish the internal validity. External validity is studied in experiments in a real environment. Therefore, it is hard to conduct an experiment with high internal and external validity at the same time, because when the internal validity is high the external validity is sacrificed and vice versa.

The term validation is often used for the process of comparing models with experimental data.

## 2.3 Experimental uncertainty

The uncertainty of measurements provides a range of values in which the true value is claimed to lie. Both random and systematic errors should be addressed when determining uncertainty and the uncertainty is considered to be a suitable way of expressing accuracy in experimental results. As illustrated in Figure 3, an increasing trueness and precision of a measurement will yield in an increased accuracy and decreased uncertainty [21]. Only repeating the experiment will not address the total uncertainty, it will decrease the influence

of random errors (i.e. increase precision) but not the influence of systematic error. To do the latter it is necessary to have knowledge about possible error in the equipment (e.g. thermocouple measurements).

There are many possible sources of uncertainty in measurements; the following and more are mentioned by JCGM [24], similar sources of error are also mentioned by Beard [27].

- Incomplete definition of the measurand.
- Non-representing sampling – the sample measured may not represent the defined measurand.
- Personal bias in reading analogue instruments.
- Inadequate knowledge of the effects of environmental conditions on the measurement or imperfect measurement of environmental conditions.

Uncertainty that is computed based on statistical analysis of a series of observations is called a type A uncertainty. An assessment of uncertainty can also be based on scientific judgment, experience and available data and is then called a type B uncertainty [24].

Experimental uncertainty is commonly presented with a so-called combined expanded uncertainty. The combined uncertainty, $u_c$, is the quadrature of different components of uncertainty [28] (i and j) according to equation 1. The two components can be the measurement uncertainty and the model input uncertainty in an experiment.

$$u_c = \sqrt{u_i^2 + u_j^2} \qquad \text{Equation 1}$$

The combined uncertainty will probably give a better representation of the total uncertainty than for example only using one part [29]. But, this can lead to some double counting, which will give a higher and more conservative estimate of the uncertainty [28]. The expanded uncertainty is a bound in which the measurement falls with a certain confidence level. In most cases a confidence level of 95% is used.

# 3 Traditional fire experiments

A large amount of compartment fire experiments have been performed during the last fifty years and the results of many of them have been published in research reports and in peer-reviewed journals. In this chapter the problems and accuracy of such traditional fire experiments are discussed.

## 3.1 Problems with traditional fire experiments

In this section the discussion of traditional experimental methods that was initiated in section 1.3.1 is resumed. The discussion is primarily based on the experiments that are presented in paper I and II.

### 3.1.1 Full-scale experiments

Full-scale experiments are used in both paper I and II. In paper I it is concluded that the wind speed and wind direction had a great affect on the experimental results, and these variables could not be controlled in the experiment. Little could be concluded about the relationship between the measured variable and the independent variables; thus, it can be argued that the internal validity was not satisfying. Exterior arson fires have previously been found to be a common cause for severe school fires in Sweden [30] and the experiments in paper I were considered to represent this type of fire where weather conditions can have a large influence on the fire development and fire spread. Consequently, the external validity of the experiment for this particular building can be considered to be reasonable.

In paper II a study of the reproducibility of four different ventilation scenarios in a multi-room compartment was conducted. The results of the paper were primarily the size of the variation between the different tests. The result was very dependent on the experimental setup, thus the external validity was poor. However, it gives an idea of the possible variation in this type of experimental setup. It was not possible to distinguish what variable or variables that caused the variation between the individual tests and in that sense the internal validity cannot be considered to be good.

The experiments in paper I and II could have been conducted more carefully and rigorously but to a higher cost. The papers are considered to illustrate a problem of controlling important variables when conducting traditional full-scale fire experiments. An alternative to these experiments could have been to use small-scale experiments where it could be possible to have a higher degree of control of the experiment.

### 3.1.2 Small-scale experiments

Turbulence and combustion phenomena are inherent in small-scale experiments [4]; consequently, a small-scale compartment fire experiment can capture the dynamics of an enclosure fire [31]. The scaling laws that can be used to study fire phenomena are related to governing differential conservation equations, and by introducing normalising parameters the dimensionless groups can be identified [32]. However, the number of dimensionless groups are too many to allow for complete scaling, e.g. heat transfer through radiation, convection and conduction to materials cannot be persevered at the same time. This means that some parameters need to be sacrificed, e.g. radiation when smoke movement from smaller fires are studied or convection when large fires are studied [31]. Therefore, when using scaling it is necessary to be aware of the dominant dimensionless groups and how the effects of not accounting for some parameters affect the results and if that is acceptable. Froude scaling, i.e. when the Froude number is kept constant, is effective in order to study smoke movement [4]. The Reynolds number is ignored in Froude scaling, but it is still necessary to ensure that the flow is turbulent.

Even though it is not possible to preserve all terms simultaneously, scaling has several advantages. The fire behaves as it does in the real world, i.e. combustion takes place, soot forms and species emerges. For some specific fire phenomena, like studies of smoke layer temperatures, the most important variables can be preserved and in such cases scaling becomes a very powerful tool in fire science research [31]. Another advantage of scaling is that it requires fewer resources compared to full-scale experiments. A smaller size of the experimental setup is also believed to allow for a better overview and control of the experiment.

There are several examples when scaling has been used for fire investigation and fire research purposes. For example was scaling used in the investigation of the Kings Cross fire [33] and the discotheque fire in Gothenburg [34], scaling has also been shown to be a valuable tool in studies of tunnel fire dynamics [35]. Quintiere [4] gives a range of examples when scaling has been used to find empirical correlations for different fire phenomena.

Small-scale experiments were conducted in paper I. The experiment was conducted under well-controlled conditions due to the small-scale and this was a prerequisite for the analysis that followed. Scaling in the regard of using scaling laws was not used, since the purpose was not to create a setup with correct proportions, but to gather data to do comparison with simulations. In the full-scale experiment (see section 3.1.1) presented in the same paper it was not possible to get the same consistency between experiment and simulation and this illustrates the advantage of small-scale experiments. The internal validity of the small-scale experiment was considered as high because of the high control of the experiment. On the other hand the full-scale experiment was considered to reflect reality and an authentic situation, even though many factors that could not be controlled influenced it.

## 3.2 Accuracy in fire experiments

As previously described in chapter 2, there is a relation between accuracy and uncertainty. It is highlighted in paper II that it is difficult to find well-documented fire experiments. There are many publications on large-scale experiments. But, many of them do not provide a sufficient description of the experimental uncertainty [36] or are too complex in order to estimate an uncertainty based on engineering judgment. However, fortunately there are exceptions and some well-documented experiments have been published.

In this section a compilation of expanded measurement uncertainties of heat release rate and temperature measurements is presented in order to get an idea of the accuracy of these quantities in compartment fire experiments. The experimental uncertainty will vary between different setups due to many issues, e.g. due to differences in the type of instrumentation and the experimental setup [36], but the uncertainties stated in the next paragraphs are believed to give an indication of the order of magnitude of measurement uncertainties.

### 3.2.1 Heat release rate

Heat release rate is generally considered to be the most important variable in fire modelling [37]; therefore, it is of course of great value to have a good estimate of the experimental uncertainty when measuring heat release rates. The uncertainty of heat release measurements will vary with both the size of the heat released and the experimental conditions.

The heat release rates in fire experiments are usually estimated with the oxygen calorimetry [38]. Oxygen calorimetry involves several independent

measurements with different equipment, like oxygen analyser, carbon dioxide analyser, thermocouples and bi-directional probes [28]. Each one of these measurements is connected to some degree of uncertainty that will add up to a combined uncertainty. Uncertainties in heat release measurements reported in some literature are presented in Table 2.

**Table 2: Example of estimated expanded uncertainties in heat release measurement.**

| Description | Expanded uncertainty | Ref. |
|---|---|---|
| A natural gas burner with heat release rates ranging from 0.05 to 2.70 MW was placed under the 6m by 6 m hood | ±11% (>400 kW) | [28] |
| A study of four sets of fire experiments in full-scale compartments where the oxygen depletion method was used. | ± 15-20% | [36] |
| Room/corner test with 150 kW and 1 MW fire. | ±11% (150 kW)<br>±7% (1 MW) | [38] |
| SBI with 35 and 50 kW fire. | ±13% (35 kW)<br>±10% (50 kW) | [38] |

The values of uncertainty in Table 2 should not be compared with each other, because the experimental setups are not comparable and the magnitudes of heat release rate as well as the depth of analysis vary. The major sources of uncertainty that are mentioned in the studies in Table 2 are the oxygen concentration measurements, mass flow measurements and heat of combustion factor [38].

An alternative to oxygen calorimetry is to use the fuel mass loss or mass flow to estimate the heat release rate. Mass flow rate measurements have typically low uncertainty, but the heat of combustion and combustion efficiency are needed to calculate the heat release rate and little is known about the combustion efficiency inside a compartment [29], which means that the uncertainties can be large. In the study by NRC mass loss rate was used to estimate the heat release rate in two sets of third party fire experiments and the uncertainties was estimated to 15 and 25% [29, 36], which is in the same magnitude as the uncertainty when using the oxygen depletion method for similar types of fires (see Table 2).

### 3.2.2 Temperature

The most common way to measure gas temperatures in fire experiments is with bare bead thermocouples. Temperature measurements with bare bead

thermocouples can have significant systematic errors [39]. Errors can arise due to damaged insulation, corrosion, radiative exchange effects, aging of the thermocouple and the accuracy of the data logger. Pitts et al [39] found that the absolute error in thermocouple measurements due to the radiative environment in the lower layer could be as high as 75% and about 7% in the upper layer. However, thermocouple measurements in a sooty hot upper layer might not need to be corrected for radiative exchange effects since it is in a nearly optical thick environment [29].

According to Pitts et al [39] it should be possible to correct for radiative exchange effects by expressing it as a type A uncertainty. But in most cases it is not possible to measure the important properties, e.g. radiative environment and gas velocity. Therefore, it is more reasonable to use error propagation based on estimates and uncertainty ranges (type B uncertainty) of the various properties. This approach was used in the NRC study [29].

NRC presented a combined expanded uncertainty, $U_E$, for bare bead thermocouples in the hot upper layer. The expanded uncertainty consists of measurement errors due to radiative exchange, inherent uncertainty associated with bare bead thermocouples and the error associated with the use of an aspirated thermocouple.

**Table 3: Expanded uncertainty for bare bead thermocouples in the upper layer [29].**

| Gas temperature (°C) | $U_E$ (°C) |
|---|---|
| 0 | 3 |
| 60 | 6 |
| 120 | 8 |
| 150 | 8 |
| 300 | 15 |
| 500 | 20 |
| 800 | 32 |

According to Table 3 the expanded uncertainty can be 2-2.5% of the gas temperature expressed in Kelvin for pre-flashover fires and 2.6-3% for the hotter (>500°C, i.e. >773 K) post-flashover fires. These are interpreted as estimates of the systematic error and the random error should also be accounted for in order to get an estimate of the total uncertainty.

In a study within the PRISME project [40], the relative expanded experimental uncertainty for gas temperature was judged to be 10%. Furthermore, in paper II the expanded uncertainty of the measured temperature rise covered ±5-33% around the mean, depending on place of measurement and studied scenario.

This variation gives a feeling for the random error that can be expected in multi-room compartment fire experiments.

In a two-zone model the smoke layer height is given by the definition of the hot and cold zone. In an experiment this interface is not as distinct and it is not entirely clear how to define the height of the smoke layer. The smoke layer height can be estimated visually, with smoke density meters, pressure profiles or with the help of temperature profiles. The latter is called the two-zone reduction method [41] and has been applied in several validation exercises. NRC [36] gives as estimate (type B uncertainty) of the uncertainty connected to the smoke layer height measurements with the help of the two-layer reduction method and temperature measurements. In the six experimental series studied by NRC the relative expanded measurement uncertainty for the smoke layer depth range from 6% to 35% and from 4% to 25% for the smoke layer temperature rise. The uncertainty was due to errors in temperature measurement and estimated measurement location, e.g. location of the thermocouple and the distance between thermocouples. The uncertainty will increase with increasing distance between measurements, i.e. a sparsely equipped experiment will be associated with a larger uncertainty.

In the NRC report [36] the measurement uncertainty is combined with an estimate of the model input uncertainty. When studying model input uncertainty it is investigated how uncertainties propagate in a certain model, something that is important when comparing model predictions with experimental values. The magnitude of the model input uncertainty could be high; thus, it is important to take into account. In the NRC study the expanded model input uncertainty was estimated to be 2% for the smoke layer depth and ranges from 10 to 17%, depending on experimental series, for the smoke layer temperature rise. This means that the relative combined uncertainty, calculated with equation 1, ranges from 6% to 35% for the smoke layer depth and from 11% to 30% for the smoke layer temperature rise.

In one of the tests studied by NRC the difference in the calculated layer depth was compared for four pairs of repeated tests differed about 1% on average. This was considered to be a negligible contribution to the overall uncertainty and it shows that the total uncertainty, due to both systematic and random errors, can be much larger than purely shown by repetitions.

# 4 Numerical experiments

In this chapter numerical experiments are discussed with the background of chapter 2, paper III and paper IV. Numerical experiments have previously been used in other research disciplines as for example when studying climate [12]. However, this review of numerical experiments is focused on the application to fires in compartments. Also, a brief description of model evaluation is given in this chapter in order to illustrate how fire models, which are used for numerical experiments, can be evaluated.

## 4.1 Examples of numerical experiments in fire science

Chow and Zou [14] used the term numerical experiments when using FDS to derive an empirical correlation for doorway flows. Chow and Zou first compared results from the computer model with existing experimental data and then used FDS to find a value for the constant, $k$, in the in the well known expression for mass flow through an opening, $\dot{m} = k \cdot A_0\sqrt{H_o}$, first recognized by Kawagoe [42].

Tilley et al [43] studied whether FDS simulations could be used in numerical experiments by studying the agreement with experimental data from two different small-scale setups, a tunnel and an atria. Tilley et al [43] described that the main advantage of numerical experiments is that it is possible to study the effect of a significant amount of different parameters by varying them. Tilley et al [43] found that the CFD model gave good predictions with regard to the small-scale experiments and a study of the effect of varying different parameters with the help of numerical experiments could be conducted within in a similar configuration as the small-scale experiments. Tilley et al followed up the first study with a study of car parks [13] with numerical experiments in order to create a simple analytical formula for the critical ventilation velocity and backlayering distance in car park fires. Tilley et al used the data from the numerical experiments to retrieve a simple analytical expression for large closed car parks with flat ceiling. Data from some full-scale car park experiments were used to confirm the derived expression for the studied configuration. The

presented formulas were seen to provide a reasonable estimate for the smoke backlayering distance for given extraction flow rate and fire source [13].

As described previously, numerical experiments were used in paper III. The aim of paper III was to present a correlation for predicting gas temperature in a room adjacent to a room involved in a pre-flashover fire. An association connected to the Swedish nuclear power plant industry (NBSG), which had a desire to develop an easy to use method that could be used in fire risk analyses, first raised the need for such correlation. It was not considered possible to develop such a method with empirical data from traditional experiments due to the lack of resources in terms of laboratory space and time. Instead FDS was used to gather enough empirical data to be able to conduct a multiple regression analysis. Several parameters were varied and finally included as independent variables in the correlation presented in paper III. The method was similar to what Tilley et al [13, 43] used. However, it was not considered necessary to validate the computer model for the application before the generation of data in paper III, because the previous validation [29] was considered to be sufficient. Even so, the correlation found with the regression analysis was compared with some results from traditional full-scale experiments in order to get an understanding of the external validity.

In paper IV a similar approach was used but the main objective was not to derive a correlation, instead it was to demonstrate how numerical experiments could be used in fire science research. Ceiling jets under an unobstructed ceiling were used in the study because the setup was rather simple and because there are existing correlations that the result could be compared to. A simplified ceiling jet theory and some assumptions was used in order to derive an expression for the ceiling jet temperature. This expression included some unknown constants that could be found with the help of a regression analysis on the data from the numerical experiments.

## 4.2 Accuracy in numerical experiments

Error in models is not defined in the same manner as in experiments. Error in experiments was previously explained with the help of Figure 3 as a random or systematic difference from a “true value”. This definition is not possible to use with regard to numerical models because the “true value” is not known [44]. In experiments error and uncertainty are linked together but in computational simulations error and uncertainty are kept apart. AIAA [45] gives the following definitions of uncertainty and error in computational simulations:

- Uncertainty is defined as: "A potential deficiency in any phase or activity of the modelling process that is due to the lack of knowledge."
- Error is defined as: "A recognizable deficiency in any phase or activity of modelling and simulation that is not due to lack of knowledge."

The difference between the two definitions is in relationship to knowledge. Uncertainty arises when there is a potential for a lack of knowledge, this means that some deficiencies may or may not exist. Model uncertainties will arise as physical and mathematical assumptions and approximation of the real world are made in different types of models used in fire science [29]. This type of uncertainty is difficult to quantify [29] and the difficulty increases with the model complexity.

The assumptions and simplifications that are necessary to perform the calculations will contribute to uncertainties being introduced in the output and it is not easy to determine how the individual assumptions and simplifications will contribute to the uncertainty in the output. The level of uncertainty will of course also depend on the situation.

Resources, assumptions and decisions made by the user add to the uncertainties in the calculations, e.g. the estimate of the heat release rate, which of course will influence the uncertainty in the output. Van Hees [44] raises the issue that the user of a model can contribute to an overall uncertainty. This uncertainty would of course also be desirable to quantify when performing numerical experiments. Such user uncertainties could be studied by using blind or a priori simulations of predefined scenarios [46]. This type of uncertainty should however be distinguished from model uncertainties, but it is important that it is recognized when conducting numerical experiments.

## 4.3 Model evaluation

In a survey of fire models conducted in 2003 it was concluded that there were roughly 50 different zone models and around 20 field models available for fire modelling [47]. The number models have most likely increased since then. No attempt is made in this thesis to give an overview of different models that could be used for numerical experiments. Nor is it within the scope of the thesis to describe how well validated or verified the different fire models are. However, it is not possible to discuss numerical experiments without commenting verification and validation of the numerical models used. Verification is a process were model implementation is checked [45] and it has two aspects, the

verification of the code and of the calculation. Experiments are not used in the verification assessment process, instead the programming, iterative consistency, convergence etc. are examined [44]. But, in validation experiments are crucial because it is a process where the accuracy of the model with regard to the real world is determined. This is done by identifying and quantifying error and uncertainty by comparing experimental data and data from simulations. In such exercises it is important to acknowledge that the experimental data contains errors and uncertainties (see section 3.2) that must be considered when doing the comparison.

Many fire models will give a time dependent output and the difference between some measurements and model results cannot be expected to be constant. The difference will change with time when studying some transient phenomena as illustrated in Figure 4 and the difference will also differ between different situations (scenarios) [5]. This complicates comparisons between measurements and models, but a simplified approach, which has been used by e.g. NRC [29], is to compare maximum values.

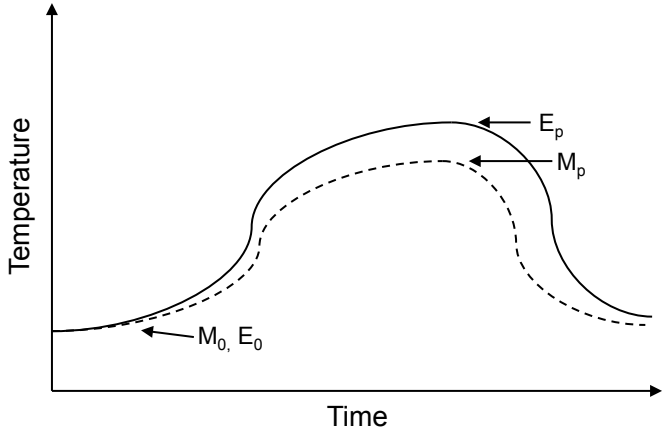


**Figure 4: The difference between measurement (black line) and model prediction (dotted line) can be time dependent, in the illustrated case the differences varies with time (figure inspired by [36]).**

The ASTM guide: "Standard Guide for Evaluating the Predicative Capability of Deterministic Fire Models" [48] describes the steps in the evaluation process of a given model. NRC [29] applied this approach in an evaluation of fire models. In the NRC evaluation the relative difference between model

predictions and experimental measurements was studied. This difference, $\varepsilon$, is computed with the following expression:

$$\varepsilon = \frac{\Delta M - \Delta E}{\Delta E} = \frac{(M_p - M_0) - (E_p - E_0)}{(E_p - E_0)} \qquad \text{Equation 2}$$

Where $\Delta M$ is the difference between the peak value of the model prediction and the baseline and $\Delta E$ is the difference between the peak value of the experimental measurement and the baseline. This relative difference is compared to a combined experimental uncertainty, which included the model input uncertainty and experimental measurement uncertainty. The concept of comparing simulations with experimental uncertainty can be discussed in similar terms as in section 2.1 and Figure 3.

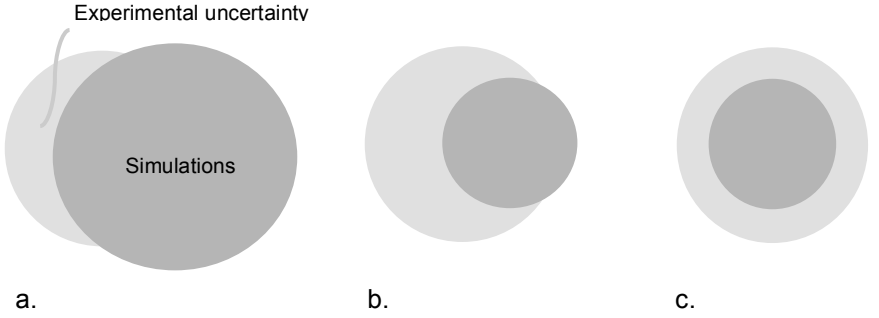


**Figure 5: Comparing experimental uncertainty and model uncertainty.**

The circles in Figure 5a illustrate the case where the scatter of the simulations (dark grey circle) is larger than the uncertainty of the experiment (light grey). The circles in Figure 5b illustrate a smaller difference in $\varepsilon$ between simulations, but the model uncertainty still falls outside the uncertainty of the experiment. The circles in Figure 5c illustrate the case where the simulations fall within some combined experimental uncertainty. The circles can be related to the concept of accuracy presented in Figure 3. Figure 5a has low trueness and low precision, Figure 5b has high precision but low trueness and Figure 5c has high trueness and high precision.

In the model evaluation performed by NRC five different fire-modelling tools were evaluated for some possible fire scenarios in nuclear facilities. An assessment of the different models accuracy in predicting transport of heat and combustion products in compartments was made in the study. The models

capability of predicting fire growth or fire spread was not studied. A total of 13 output quantities from the models were chosen for the evaluation. The results from the evaluation are presented in the final report [29] in a matrix with a simple colour system, in order to indicate to what degree a certain model predicted a certain output quantity. "Green" indicated that the model predicted a particular parameter with the accuracy comparable with the experimental uncertainty and "Yellow" indicated that the predictions were clearly outside the bounds of uncertainty. For instance, the smoke layer temperature was labelled as "Green" for FDS, while predictions of smoke concentration was labelled as "Yellow". This means that FDS can predict smoke layer temperatures for multi-room compartments with an acceptable accuracy, in regard to experimental uncertainties, while predictions of smoke concentration can be questionable.

# 5 Advantages and challenges

The studies presented in section 4.1 illustrate that numerical models can be used in a manner that can be regarded as an experiment according to the previous depiction of experiments in section 1.1. In all four studies mentioned in section 4.1 a system (car park or compartment) has been described in a numerical model, the state of the system has been changed and the consequence of that change was measured and analysed (as illustrated in Figure 1). But there are of course advantages and challenges when using numerical experiments. The following advantages and challenges have been identified based on the author's experience of the traditional and numerical experiments that are presented in paper I-IV. Some of the points discussed in this chapter are also raised in paper IV, however the discussion here is more extensive.

## 5.1 Advantages of numerical experiments

The main advantages with numerical experiments are discussed and motivated in the following four sections.

### 5.1.1 Resource efficient

Numerical experiments are considered to be much less expensive compared to full-scale experiments. Numerical experiments can be conducted on a personal computer or a computer cluster with free software while traditional experiments need to be conducted in a laboratory and a range of measurement equipment that needs calibration is necessary. Tens or even hundreds of numerical experiments can be run at the same time if the computer power is available while one traditional experiment usually is carried out at the time and after each experiment the experimental setup needs to be reset. The less resource demanding numerical experiments create opportunities for more researchers and research groups to contribute to an increased knowledge of fire science and its phenomena.

Small-scale experiments are more resource efficient compared to full-scale experiments, but still not as cost effective as numerical experiments and as

mentioned in section 3.1.2 it is in most cases not possible to conduct a complete scaling, consequently errors can be introduced in small-scale experiments, due to the lack of possibility to scale all terms simultaneously.

Numerical experiments can be used as a complement to traditional experiments (see Figure 6). If the data from the numerical experiment is ignored it is possible that the actual dependence of the dependent variable would be considered to be linear, but the numerical experiment in Figure 6 reveals that there is a logarithmical relation. This might not be possible to distinguish with traditional experiments only, if the resources are limited and only four experiments (dots in Figure 6) can be performed but at least the double amount is needed to see the type of dependence between the variables.

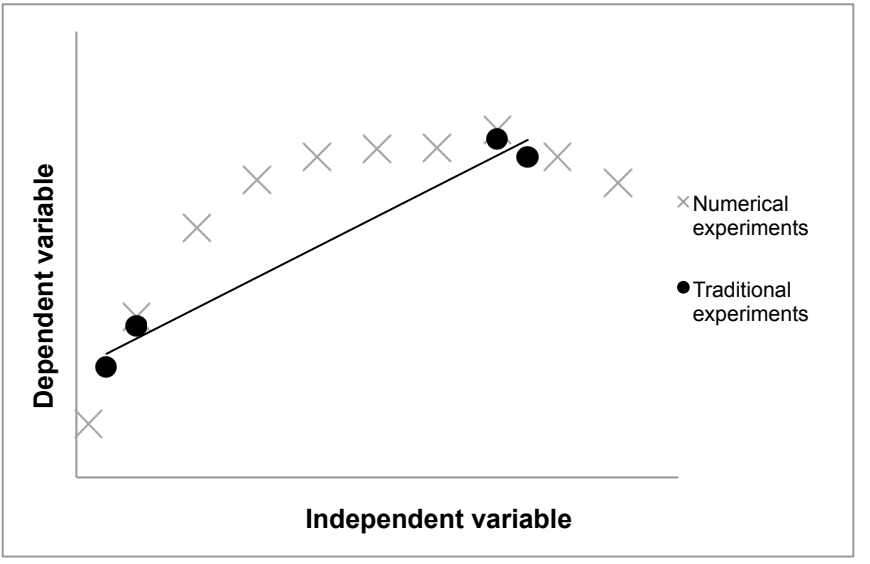


**Figure 6: Example of how numerical experiments can complement traditional experiments in order to study the dependency of an independent variable.**

A problem with Figure 6 is that it can be argued whether the numerical experiments do not give a satisfying prediction for values of the independent variable in between the dots. In that case a single supplementary traditional experiment for the independent variable in between the dots should be enough to support the relationship found with the numerical experiment.

It is also possible to use numerical experiments to study a problem in a larger scale than what is possible with traditional experiments. This was done in the study of the discotheque fire in Gothenburg in 1998 [34]. In this study, SP

Fire Technology conducted small-scale experiments in a laboratory and later used a CFD model to study the problem in the full-scale to confirm the results from the small-scale experiments. It was not possible to conduct a full-scale experiment but the combination of modelling and small-scale experiments gave a credible explanation for how and where the fire started. So, a numerical experiment can be used to extrapolate or confirm some relationship found in a small-scale or smaller experimental setup as illustrated in Figure 7.

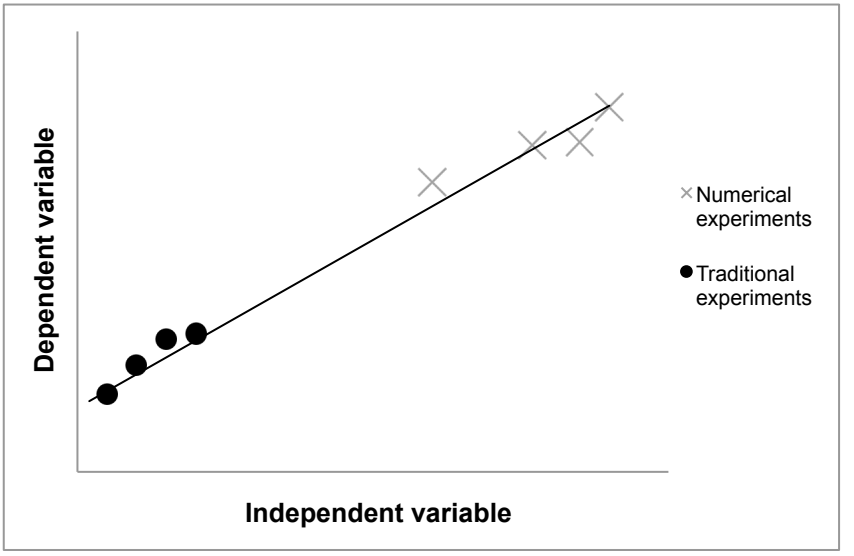


**Figure 7: Example of how numerical experiments can complement traditional experiments to extrapolate results from a smaller experimental setup.**

It is of course crucial to take care when using a fire model to study a phenomenon in a larger scale or domain as demonstrated in Figure 7, because there is a obvious risk that the study will be outside the limits of the fire model. For instance, Figure 7 could be complemented with a single traditional experiment in same range as the numerical experiments, thus confirming the linear trend. In this way are small- or reduced-scale experiments used together with numerical experiments to form a hypothesis that can be confirmed with a few full-scale experiments.

Figure 6 and Figure 7 and the accompanying discussion illustrate that numerical experiments and traditional experiments are complementary and not competitive, and that a combination of these two methods can yield in convincing arguments for some relationship or conclusion.

### 5.1.2 Possibilities to test hypothesis

Numerical experiments can be used to develop a hypothesis that can be tested with traditional experiments as described in section 5.1.1. But the numerical experiment can also be used to test more challenging theoretical hypotheses than would have been done with traditional experiments. Traditional experiments are more expensive than numerical experiments, which mean that the willingness to risk that the results are poor or hard to interpret due to uncertainties is less. Therefore, having numerical experiments as an option might result in more hypotheses testing in fire science, which in turn can result in great progress in the field.

### 5.1.3 Level of control of the experiment

Experiments are suitable as a tool for providing information only if the experiment is appropriate and disturbing factors are eliminated. If the experiments are based on wrong or deficient knowledge it will lead to the results being faulty. If knowledge is lacking about what the disturbing factors are and how they can be treated or eliminated it could lead to faulty conclusions [49]. Paper I and II illustrates the problem of uncontrolled variables in full-scale experiments and how it creates problems to draw conclusions.

The level of control of the experiment is one of the main advantages of numerical experiments. The experienced model user, who knows how the numerical model works, can have a total control over the numerical experiment. An example is given in Figure 8 and explained in the text below.

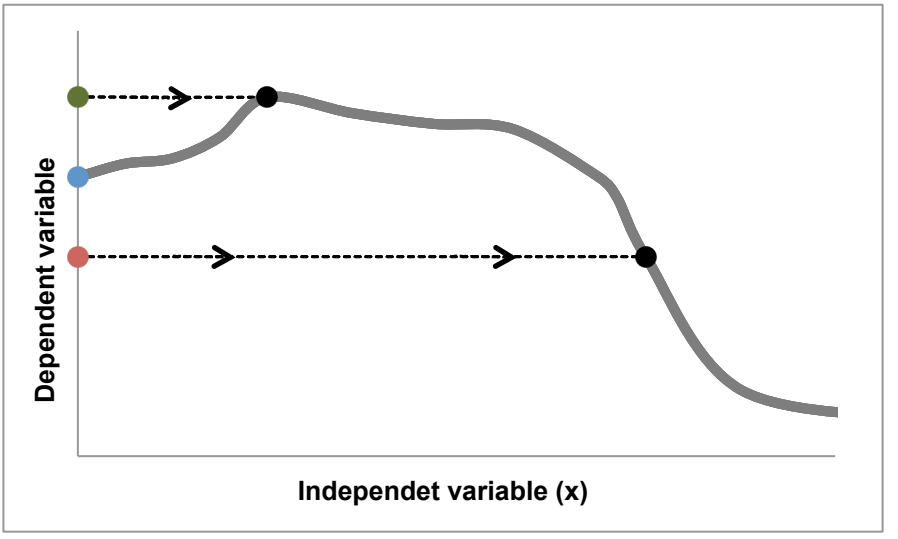


**Figure 8: Example of how an uncontrolled independent variable can affect a dependent variable.**

Figure 8 shows how a measured property (y-axis) in a traditional experiment can be described as a dependence of an independent variable (x-axis). It could be for example how the wind speed affects the temperature in a plume, which was the case in paper I. The three coloured dots in Figure 8 represent possible results from a numerical experiment where no account has been taken to the independent variable. The blue dot is in agreement with the real situation where x=0, i.e. the wind speed is 0 m/s. The green dot gives, for some reason, a higher and the red dot gives, for some reason, a lower prediction than the experiment at x=0. However, the green and red dot corresponds to a measured temperature at a certain value of the independent variable ($x \neq 0$). And if the temperature is measured at one these values of the independent variable it might seem that the green or red dot corresponds to the measured temperature. This is of course not correct because the conditions in the numerical experiment and traditional experiment are not the same. Figure 8 only presents a single independent variable, in reality there will be more uncontrolled independent variables that affect the measurand to different degrees causing a variation between tests. This illustrates that it is necessary to be aware of which variables that needs to be controlled in an experiment.

The random error in traditional experiments can, as presented in section 3.2, be large. In a numerical experiment it is believed that there will be a higher

control of all variables of interest and thus will the independent variable in Figure 8 have a constant value in the numerical model.

### 5.1.4 Measurements

Measurement equipment is a fundamental part of experiments in order to collect data, but the measurement equipment itself can influence the experiment and the measurements. For example, a thermocouple will give the temperature of the thermocouple and not the gas temperature. Another example is measurements with bi-directional probes in an opening that affects the gas flow through that opening [50]. This influence on the experiment is considered to be small compared to the overall measurement uncertainties mentioned in section 3.2, nonetheless it will contribute some error.

In a numerical experiment, there are far greater possibilities to collect data compared to a traditional experiment. If a CFD model like FDS [7] is used, it will be possible to record time dependent information on e.g. temperature or gas concentrations in all cells used in a domain, which could be in millions of different locations. It is impossible to have the same amount of measurements in a traditional experiment. In a numerical experiment it is also possible to record information without adding instrumentation that could influence the experiment, which is still the case in most experiments even though different laser-based measurement techniques [51], which have a lesser influence on the measurements, are being introduced.

## 5.2 Challenges with numerical experiments

The main problems and challenges with numerical experiments are discussed and motivated in the following three sections.

### 5.2.1 Description of the fire phenomena

A model is by definition a simplification of the physical reality that includes some approximations. Quintiere [31] raises several issues with using computer simulation for addressing fire problems. Phenomena like soot formation, fire spread, water droplet breakup and turbulent combustion are things that cannot be addressed adequately with a numerical model according to Quintiere. Traditional small- and full-scale experiments capture these types of phenomena. This causes issues to the external validity and a distinct limitation of numerical experiments conducted with the fire models currently available. For instance, fire spread and fire growth cannot be studied with the current

models [52], currently user defined fires are needed for the models to provide predictions of different output quantities.

Subsequently, there are distinct limitations of numerical experiments, i.e. the fire model used needs to be valid for the studied phenomena. Currently numerical experiments can in general only be applied to study gas temperatures, smoke layer heights, room pressure, oxygen concentration and flame heights in compartments, because it is in these areas that there are models that can be considered validated [29].

### 5.2.2 Experienced user

In any experiment it is necessary that the researcher know his or her equipment, how it should be used, how data can be collected and how it should be interpreted. In a numerical experiment the physics of fires can be interfered with, for instance, different plume model types can be selected in a two-zone model or radiation can be excluded in a CFD model. Such so-called user effect was seen to be of importance in the PRISME project [40]. Also, a model can be misused and applied outside its limitations. This is problematic because the user has been found to be the most critical link in the chain of simulations in previous studies [53, 54]. This in all means that the researcher using numerical experiments needs to have an understanding of both the fire phenomena studied and the model used. Many fire models are easy to obtain and easy to use, this means that they can be used in a careless or incorrect manner. This is problematic, because errors due to misuse can be difficult to discover.

The transparency of the numerical experiment may be poor due to the opportunities for the user to change input parameters, use sub-models etc. A fundamental part of reporting from experiments is that enough information is available so that the experiment can be replicated with similar results [10]. The same should apply for numerical experiments both due to the reason that it should be possible to replicate the experiment and that it is necessary to be able to review how the model has been used and which input parameters and sub-models that have been used by the researcher.

### 5.2.3 Accuracy of fire models

The previously mentioned evaluation of some selected fire models performed by NRC [29] (see section 4.3) illustrates that a couple of models can be used to predict a handful of output quantities within the uncertainty bounds of six experimental series. The predictions of the zone models and CFD model was

labelled “Green” for less than half of the 13 quantities studied, while the hand calculation methods only were labelled “Green” for 1 of the 13 quantities. In retrospect of the NRC study it is evident that numerical experiments of compartment fires are currently limited to studying smoke layer temperatures and smoke layer depths. Only FDS was used in the examples of conducted numerical experiments given in section 4.1. However, it is not a necessity to use a CFD code because more transparent methods like 2-zone models or other calculations methods could be used as long as they are sufficiently accurate for the intended study.

Even though extensive validation of fire models has been conducted, there is a great deal of work left to do [44]. Studies like the one by NRC reveals that there is a limited area where numerical experiments can be applied and outside these limitations should numerical experiments be carried out with great caution.

# 6 Prerequisites for numerical experiments

The description of examples (section 4.1) and the discussion of advantages and challenges (chapter 5) give a base for a discussion on when numerical experiments can be used. There are several things that should be considered before choosing numerical experiments as an experimental procedure. The chart presented in Figure 9 outlines these considerations.

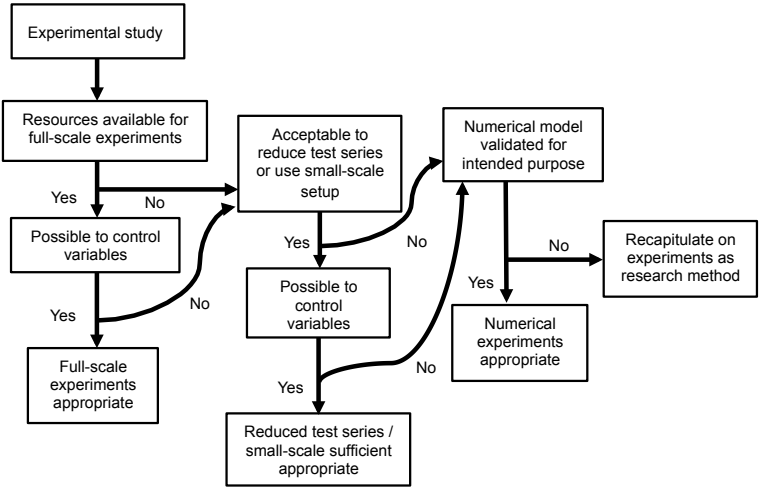


**Figure 9: Chart of considerations.**

The starting point in Figure 9 is in the upper left corner where an experimental study is initiated to explore or explain a certain problem in fire science. Traditional full-scale experiments should first be considered in an experimental study related to compartment fires. There is no reasonable argument not to use traditional experiments if the resources are available for it and if it is possible to control all variables of importance. However, if the resources are lacking or if it is not possible to control all variables that are considered important it is reasonable to turn to small-scale experiments as an alternative. It is acceptable to use the small-scale experiments if all relevant entities can be scaled properly

and it is possible to control important variables. The final result of a study with such small-scale experiments will probably be better than if full-scale experiments, where important variables cannot be controlled, would be used.

If it is not reasonable to use a small-scale setup or if important variables cannot be controlled, numerical experiments can be an alternative. The fundamental condition for going ahead and performing numerical experiments is that the fire model intended is sufficiently accurate for the problem. It is of course the responsibility of the researcher to use a model that is validated for the planned area of study.

Figure 9 might look rather straightforward but it might not be as easy as it seem to determine what approach to use. It is probably evident for a researcher if resources are available for full- or small-scale experiments, but it might not be as evident if it is possible to control important variables or if it is acceptable to use a small-scale setup. Several variables of importance might be unknown, which means that there is a risk of systematic errors.

From Figure 9 it might seem as if numerical experiments are the last choice and a method that will give less good results. But that is not the case, because numerical experiments will be the best choice, if the conditions leading down to the box "Numerical experiment appropriate" in Figure 9 are fulfilled. Nevertheless, there might be exceptions. It may be reasonable to use numerical experiments even though resources for full-scale experiments are available when the numerical experiments are considered to give good enough results for the intended study. This could be much more resource effective.

For the studies presented in paper III and IV the resources for conducting the same amount of full-scale experiments were not available. Reducing the number of experimental tests to any large extent were not possible because a large number of observations were needed in order to perform a satisfying regression analysis. Even performing the same number of observations in small-scale were not considered possible in any of the studies. In the NRC study [29] it was found that FDS could predict compartment fire temperatures in adjacent rooms and ceiling jet temperatures within the experimental uncertainty. Consequently, the only reasonable experimental method for the studies in paper III and IV were numerical experiments.

The general procedure of conducting the numerical experiment should not be different from that of any other experiment. Experimental procedures like for instance described by Anderson [10] including a planning, data collection and analysis and synthesis phases are of course valid for numerical experiments.

Moreover, the same types of procedures for data analysis, like graphical and statistical methods, can be used. As mentioned in paper IV, data from a numerical experiment can be imported into a statistical software package in order to use a regression analysis to derive a correlation. Such an approach can however not be considered to be satisfactory because there can be lack of theoretical understanding, which means that it is hard to claim that such a correlation provides evidence for causation. This also applies for any type of experiment. In paper IV a simple ceiling jet theory was developed and the data from the numerical experiments were used to find some unknown constants in order to derive an expression for the ceiling jet temperature. Thus, the numerical experiments confirmed the theory and the derived correlation has some theoretical basis.

Currently it is not considered possible to use numerical experiments to create a correlation for a certain fire phenomenon without checking that correlation with data from some full-scale or small-scale experiment. There are two reasons for this:

- There can be errors introduced when setting up the numerical experiment that means that even though the model previously is validated for the purpose of the research there can be a misuse of the model that introduced faults.
- The second reason is that there will be a scatter around the regression line that will not be explained with the correlation. This scatter is normally described with the coefficient of determination ($R_2$).

When a correlation is created the error associated with the numerical model and this error in the regression analysis are combined. This combination can result in errors that are difficult to predict in advance. In hindsight of this is it strongly recommended that the final results of a numerical experiment always should be checked against a third independent source of information, which naturally would be data from traditional small- or full-scale experiments.

# 7 Conclusions

Numerical fire models have been used for several decades in fire safety design of buildings. Numerical models have also been used for different research purposes, and as fire models continuously develop they result in more and better opportunities to be used as a tool for conducting experiments.

Using the term numerical experiments and recognizing fire models as a tool for experiments in fire science will possibly lead to that established procedures currently used when planning, performing and analysing traditional experiments also will be applied when performing numerical experiments. The requirements on this research method from the scientific community might also increase when it is acknowledged as experimental work. This will hopefully mean that the quality of numerical experiments will be kept high.

Two research questions are stated in the first chapter of this thesis and they are repeated here for clarity:

1) *What are the pros and cons of numerical experiments compared to traditional compartment fire experiments?*
2) *When can numerical experiments be considered as a substitute for traditional compartment fire experiments?*

These questions have been addressed in the previous chapters but the main conclusions are summarised in 7.1 and 7.2. Some areas of future research have also been identified in the thesis and these are summarised in 7.3.

## 7.1 Pros and cons of numerical experiments

The main advantages with numerical experiments are, with regard to the discussion in the thesis and without any particular order, considered to be the following:

- Lesser resources are required compared to full-scale and small-scale experiments. It is not as costly and time consuming to perform numerical experiments compared to traditional experiments.

- A higher degree of hypotheses testing is possible compared to traditional experiments, which might result in further progresses in fire science.
- A high level of control of the experiment is possible, which means that the influence of uncontrolled variables on the result can be limited and that internal validity can be high.
- Measurements with numerical experiments are convenient and measurement equipment can be used in the model so it does not influence the experiment, which it can do in traditional experiments.

The main challenges or problems of numerical experiments are, without any particular order, considered to be:

- The numerical models might not capture all properties inherent in the fire phenomena of interest, which may result in a low external validity.
- The user of the model needs to have understanding of how the model works. The complexity of the model used can vary and it is of course important that the user understands all relevant parts of the model and that he or she assigns appropriate values of all necessary input parameters. This means that the researcher also needs to have an understanding of the fire phenomena to be able to perform a satisfying numerical experiment. Since many models are easy to obtain it can be problematic if the researcher is not sufficiently qualified.
- Only a couple of models have been validated thoroughly enough to be considered being applicable for numerical experiments. Furthermore, these models only shown to be able to be accurate in predicting a few output quantities e.g. smoke layer temperature and smoke layer depth.

These pros and cons were discussed in more detail in chapter 5.

## 7.2 Numerical experiments as a substitute for traditional experiments

To use a specific experimental method, as a substitute for another is currently not considered to be an option, because the experimental method best suited for the situation should always be used. Traditional full-scale experiments would of course be the ultimate goal for compartment fire experiments. But the two main problems with such experiments, raised in this thesis, are that it

demands a lot of resources and that it is hard to have high degree of control of the experiment.

There is no experimental method that can be recommended for use for all types of research tasks in fire science. In Figure 9 it is illustrated that full-scale experiments should be considered first, followed by small-scale experiments. This is intuitive because if variables can be controlled and the resources are available there is no reason to turn to numerical experiments. But, the experimental methods discussed in this thesis all have their strengths and weaknesses. Traditional experiments and numerical experiments are complementary and not competitive, and a combination of experimental methods could be necessary to analysis a certain phenomena. Consequently, numerical experiments are considered to play a more important roll in fire science in the future. Two examples of how numerical experiments can complement traditional experiments are given in Figure 6 and Figure 7 these are idealised examples but illustrate that a combination of the methods can yield in convincing and resource efficient conclusions.

## 7.3 Future research

Hopefully this thesis will be appreciated for giving directions in the future use of numerical experiments in fire science research. The systematic approach and transparency that have been used in paper III and IV will hopefully serve as an inspiration of how to conduct future numerical experiments in fire science. However, there are several problems with numerical experiments that are considered important to study further. The following two areas are considered to be most important for the future use of numerical experiments in fire science.

### 7.3.1 User uncertainty

The quality of the numerical experiment will depend on the model used but also on the researcher. Different researchers will construct an experiment differently and this is also the case when setting up the experiment in a fire model. It would therefore be appropriate to conduct studies of blind or a priori simulations of predefined scenarios in order to quantify and get an estimate the uncertainty in compartment fire modelling in general and with certain fire models.

### 7.3.2 Accurate fire models and new areas

A prerequisite for numerical experiments is that there are accurate fire models available. In this thesis a NRC study has been used to give a description of some validation work conducted. There are more examples of validation work and van Hees [44] gives some examples. The study by NRC refer to fires in compartments, but there are a range of other areas where numerical experiments could be applied and this could be explored in future research.

More validation work is also needed as current fire models develop and new models and sub-models are presented. There is a tendency to conduct only overall validation of the entire fire model, but it might be also important to conduct sub-validation, e.g. validation of individual sub-models, because errors in individual models can be combined in a model in a way that cannot be determined when only studying the overall validity.

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