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Numerical modeling of the coupled feedback between pool fires and their environment

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Numerical modeling of the coupled feedback between pool fires and their environment

Abstract

Computational fluid dynamics (CFD) is often used within performance based fire safety engineering and its use has increased as available computational power has increased. However, there is still a need to improve CFD modeling to push it beyond its current usage limitations. Of course such steps must be accompanied by quality assurance by means of validation and verification. In this thesis three key problems were identified within performance based design; prediction of the mass loss rate that interact with the environment dynamically, understanding of fires in enclosures equipped with mechanical ventilation as well as taking the built environment, such as building materials, building geometry and various technical installations, into account when designing a fire scenario. In the presented work Fire Dynamics Simulator (FDS) was chosen as a modeling framework which could be expanded upon if needed to be able to perform predictions of the presented problems. A validation of FDS was done against experimental data obtained using the novel, non-intrusive technique ps-LIDAR. The built in HVAC (heating, ventilation, and air conditioning) model in FDS was validated against a series of full-scale fires using mechanical ventilation. A new pool fire sub-model, which takes reduction in oxygen concentration and external radiative heat flux into account when predicating the mass loss rate, was formulated, implemented in FDS and then verified and validated. The verified and validated models and sub-models were applied on two engineering problems; predicting fire growth related to building characteristics and predicting performance of measures against smoke spread in ventilation systems.

Key words

Fire safety engineering, computational fluid dynamics, CFD, mechanical ventilation, HVAC, design fires, numerical experiment

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Jonathan Wahlqvist

Lund, June 2018

Summary

Use of computational fluid dynamics (CFD) software packages within performance based fire safety engineering has been increasing substantially over the last decade as available computational power has increased. Meanwhile, in performance based fire safety engineering there are several key problems that are still considered too challenging for most CFD models to accurately predict and are therefore simplified. But in order to improve CFD modeling beyond its current limitations, the ability to predict more challenging problems has to be progressed, but at the same time also be quality assured by means of validation and verification.

In this thesis three key problems were identified within performance based design. Firstly, a very common problem in any fire scenario is predicting the mass loss rate and the resulting heat release rate. Modeling of dynamic fires that interact with the environment dynamically are very much needed in engineering applications since two situations rarely are the same.

Secondly, understanding of fires in enclosures equipped with mechanical ventilation is needed to be able to predict the dynamic interaction between a fire and mechanical ventilation, as well as being able to predict smoke spread through duct networks.

Thirdly, most often the built environment, such as building materials, building geometry and various technical installations, is not taken into account when designing a fire scenario, even though it might affect the behavior and consequences of the fire.

The work presented in this thesis aims to provide more knowledge and tools that can be applied to the presented problems with a focus on quality assurance and practical engineering applicability.

In order to do so Fire Dynamics Simulator (FDS) was chosen as a modeling framework which could be expanded upon to meet all application requirements. FDS is generally considered well validated, but an additional validation exercise was performed against experimental data obtained using the novel, non-intrusive laser technique called ps-LIDAR as a way of demonstrating current and future needs for more detailed experimental data as computer models gets more advanced. The

validation exercise was considered a success overall, but the ps-LIDAR technique showed some limitation due to sensitivity to particles in the air and fire plume. However, detailed 2D-planes of temperature measurements was presented and compared which shows great potential of the technique.

To be able to do predict the behavior of ventilation systems, the built in HVAC (heating, ventilation, and air conditioning) model in FDS was validated against a series of full-scale fire experiments consisting of one to three sealed, interconnected compartments with mechanical ventilation attached. The response of the ventilation system, quantified by volume flow and pressure, was reproduced by FDS using data collected without a fire present (e.g. wall materials, loss factors in ventilation system components) in combination with a prescribed fire source.

As the current pyrolysis models in FDS was not suitable for the purpose, a new pool fire sub-model was formulated and implemented into FDS. This sub-model takes reduction in oxygen concentration and external radiative heat flux into account when predicating the mass loss rate. The sub-model was verified through several verification tests specifically designed to ensure a correct implementation, as well as validated against two test series with various scenarios spanning multiple oxygen concentration and external radiative heat flux levels.

The verified and validated models and sub-models were applied on two engineering problems; predicting fire growth related to building characteristics and predicting performance of measures against smoke spread in ventilation systems. This was done by using so called numerical experiments in part due to traditional experiments being cost prohibitive, but also to demonstrate the benefit of the verification and validation work previously performed.

The thesis concludes that the work carried out accomplished what it was set out to do; increased knowledge and provided verified and validated tools that can be used in scenarios where there is a strong interaction between pool fires and the built environment. However, there are still many neighboring research areas that needs to be explored further and used to build upon the presented work.

Populärvetenskaplig sammanfattning

Bränder är vanligt förekommande i samhället och orsakar årligen många dödsfall och stora ekonomiska skador. I ett försök att minska antalet bränder, samt konsekvenserna av när en brand faktiskt inträffar, används ofta så kallad funktionsbaserad design när en ny byggnad planeras eller en äldre byggnad renoveras. Funktionsbaserad design innebär att man med hjälp modeller, antingen handberäkningar eller datorprogram, gör beräkningar för att säkerställa att byggnadens utformning är godtagbar vad gäller brandsäkerhet och utrymning.

Inom funktionsbaserad design är användandet av datorprogram för numerisk strömningsmekanik (CFD) väldigt vanligt och har ökat väsentligt det senaste årtiondet i takt med att tillgänglig datorberäkningskraft har ökat. CFD-program kan lösa ekvationer som förutspår fluiders (som till exempel vatten, luft) rörelse, till exempel hur brandgaser och rök sprids från ett utrymme till ett annat. De innehåller ofta också ytterligare modeller för att förutspå andra fysikaliska fenomen, till exempel flamspridning över en soffa eller värmeledning in i en vägg. Men då dessa program är extremt komplicerade, både att utveckla men även att använda, så krävs det att dessa program ständigt testas så att de fungerar så som det var tänkt. Det är även nödvändigt att dessa program ständigt utvecklas för att klara av nya, mer komplicerade problem och med kan leverera resultat med högre precision.

I denna avhandling identifierades tre problem inom funktionsbaserad design som ofta ger problem vid funktionsbaserad design på grund av deras komplexitet. Det första var att kunna förutspå storleken av en brand och hur den utvecklar sig över tid. Ofta tvingas ingenjörer använda sig utav värden från tabeller eller experiment då det är väldigt svårt att tillförlitligt förutspå hur en brand beter sig i ett givet utrymme, då samma brand mycket väl kan bete sig annorlunda i ett annat utrymme.

Det andra problemet som identifierades var avsaknaden av kunskap och beräkningsverktyg för att kunna förutspå hur bränder i slutna utrymmen som är utrustade med mekanisk ventilation beter sig. Detta är viktigt för att kunna förutspå samverkan mellan en brand och mekanisk ventilation för att till exempel kunna förutsäga rökspridning genom kanaler från ett rum till ett annat. Detta kan vara av stor betydelse i till exempel kärnkraftverk där känslig utrustning kan bli förstörd och ha väldigt stora konsekvenser. Ett annat viktigt tillämpningsområde är hotell och flerfamiljshus där rökspridning kan ske till intet ont anande personer som sover.

Det tredje problemet som identifierades är det faktum att den byggda miljön, såsom byggnadsmaterial, byggnadsgeometri och olika tekniska installationer, ofta inte beaktas vid utformning av brandscenarier som används vid funktionsbaserad design. Men i takt med att vi använder oss utav mer icke-traditionell arkitektur och nya byggnadsmaterial, till exempel mer isolerande eller brännbara material, så kommer vi behöva beräkningsverktyg som tar hänsyn till detta.

Arbetet som presenteras i denna avhandling syftar till att ge mer kunskap och beräkningsverktyg som kan tillämpas på de presenterade problemen med fokus på kvalitetssäkring och praktisk tillämpbarhet.

Table of contents

1 Introduction

Use of computational fluid dynamics (CFD) software packages within performance based fire safety engineering has been increasing substantially over the last decade as available computational power has increased. CFD can be applied to solve the motion of almost any fluid flow and is often used for complex problems and scenarios where simpler models and hand calculations would most likely fail to deliver credible results. Due to the complex nature of CFD modeling tools an important part in the CFD process is quality assurance by means of validation and verification. Validation is done to assure that the formulated model is correctly implemented in the software, while verification is done to assure that the implemented model is able to predict the physics or behavior for which it was developed. This part of the CFD process ensures that the models can be used for performance based fire safety engineering with confidence that the end results are accurate enough to assess safety properly.

However, in performance based design there are several key problems that are still considered too challenging for most CFD models to accurately predict and are therefore simplified by using e.g. standard values or non-transient calculations. But in order to improve CFD modeling beyond its current limitations, the ability to predict more challenging problems has to be pushed, tested and evaluated. A first step to in doing so is to identify common and specific key problems:

Firstly, a very common problem in any fire scenario is predicting the mass loss rate and the resulting heat release rate. Computational simulations using a prescribed fuel mass loss rate, so called a posteriori simulations, have been shown to give good agreement with experimental results (Audouin, et al., 2011a; Gutiérrez-Montes et al., 2009, Hurley & Munguia, 2009; Ma & Quintiere, 2003; McGrattan et al., 20014a; van Hees et al., 2011; Wahlqvist & van Hees, 2016), but this data is not very often available for a specific scenario or application. When instead using a non-prescribed fuel mass loss rate the accuracy is often not as high, as demonstrated in the round robin study of the Dalmarnock fire test 1 (Rein et al., 2009). Detailed pyrolysis models are available in most computational fluid dynamics software packages, but due to their complexity and computational requirements they are rarely used outside of research applications. However, fires that interact with the environment dynamically are still very much needed in engineering applications since two situations rarely are the same. Therefore, it can be argued that a simple and robust pyrolysis model which takes the environmental interaction into account is needed.

A second key problem for performance based fire safety engineering is fires in enclosures equipped with mechanical ventilation. This is especially true in modern multi-family homes and process and power industries, such as the nuclear industry, since fire and smoke spread within the ventilation system pose a significant threat to occupants and equipment in case of a fire. A ventilation system can also influence the fire behavior, e.g. by supplying oxygen or affect the pressure (Audouin et al., 2011b, 2013), which has to be taken into account. This is especially true in modern buildings that are increasingly air-tight, due to energy requirements, which puts more stress on the ventilation system. Therefore, robust tools are needed to be able to understand and predict the dynamic interaction between a fire and mechanical ventilation, as well as being able to predict smoke spread through duct networks.

A third key problem, which is tightly interconnected with the previous two, is the fact that most often the built environment, such as building materials, building geometry and various technical installations, is not taken into account when designing a fire scenario in the case of performance based design. E.g., the Swedish National Board of Housing, Building and Planning (Boverket in Swedish) recommends different fire growth rates depending on the type of activity in a building (Boverket, 2011), but several key characteristics of the fire compartment are never taken into account. Will a heavily insulated building behave the same as a steel sheet building or does the radiative feedback increase the fire growth and maximum heat release rate? Does a smaller room behave different from a big room? How much does the amount of openings to the fire room (both normal openings and those caused by evacuating people, as in doors being opened) affect the development of a fire? A model to predict the consequence of such variables would be of high value within the performance based fire safety engineering field.

The work presented in this thesis aims to provide more knowledge and tools that can be applied to the presented problems with a focus on quality assurance and practical engineering applicability.

1.1. Background

Although the problems described in the introduction are general problems, there are specific environments were the consequences of an uncontained fire might be far more devastating than others. One such environment is nuclear power plants.

Fire at nuclear power plants is still a significant contributor to the overall risk (Röwekamp et al., 2000) as the fire occurrence is in the order of 10^{-2}/reactor year (Werner et al., 2009). CFD modeling tools can be used to evaluate the consequences of fire events, but to be able to ensure the quality of any modeling software output, verification and validation work must be performed and evaluated, especially when applied to nuclear power plants and similar facilities where a fire could cause extensive damage. Significant validation work has been done within the field (Hill et al., 2007; Stroup & Lindeman, 2013), but there is still a need for further validation for a wide selection of fire phenomena. This is turn creates a large need for experimental data that can be used for validation purposes.

To meet the specific needs for nuclear power plants, both regarding experimental data and well suited modeling tools, the PRISME (PRISME is the French acronym for "Fire Propagation in Elementary Multi-Room Scenarios") fire research program was conducted in an international framework between 2006 and 2011. The PRISME project was initiated by IRSN under the sponsorship of OECD/AEN and was largely carried out in the specially-designed DIVA facilities located at the GALAXIE site in Cadarache (France). Within this program various fire test scenarios were carried out with the specific needs for nuclear fire safety in mind. The three major research areas addressed by the PRISME project were:

- Propagation of heat and smoke from the fire room to adjacent rooms.
- Impact of heat and smoke on safety–critical systems (such as cable malfunction).
- Impact of the ventilation network on limiting heat and smoke propagation.

In all, five experimental campaigns consisting of more than 35 large-scale fire tests were carried out using the DIVA facility. These tests were carried out using two different main fuel types; liquid pools and cables. Both were considered highly relevant as transformers generally contain flammable liquids that could leak and ignite, and electrical cables are used through all parts of a nuclear power plant for various purposes.

In parallel to the tests, PRISME partners evaluated the capability of various fire computer models to simulate fire scenarios based on the PRISME data results. A number of benchmark exercises were conducted with the aim do validation and to further advance the predictive capabilities of the involved computer models. These benchmark exercises were also used to identify lacking features or under-performing sub-models to help developers further improve their model. After validation was successfully performed, the goal was that the modeling tools could be applied for simulating other fire propagation scenarios in various room configurations with a good degree of confidence.

While the PRISME project (OECD, 2011) was focused on environments representative of nuclear power plants, there are many other areas that face similar problems and challenges and which would benefit from an increase in knowledge of fire development in confined and ventilated large-scale compartments. One such area is multi-residential buildings that often use complex ventilation systems spanning several fire cells. This is especially true in Sweden where the fire code is performance based, stating that satisfactory protection against the spread of fire gases may be obtained by:

> *Allowing fire gases to enter the ventilation system but designing the system in such a way that the spread of fire gases between fire compartments is prevented or considerably impeded depending on the design and the nature of the premises. (Boverket, 2011)*

To meet these standards in a cost effective manner many times custom solutions are designed aided by computer or hand calculations. Quite often the calculation procedure is as follows: hand calculations or a two-zone model like CFAST (Forney et al., 2008) are used to calculate the fire induced flow. Then, this output is used in a HVAC-software, such as PFS (Jensen, 2007). This method will not present a transient solution, but a "worst case" steady state solution. This makes it very hard or even impossible to determine the damage caused by smoke spread. As an alternative, a CFD model capable of predicting the interaction between the fire source and built environment could be used to simulate the fire, predict the pressure created by the fire in the compartment and consequently the smoke spread via the ventilation system. This is almost identical to the needs of a computer model as specified in the PRISME project for nuclear power plants.

Both of the mentioned usage areas share very similar problems, and hopefully similar solutions in the form of capable, well validated modeling software. There are also many other applications where an increase in knowledge and improved computational tools could be utilized to improve fire safety in general, which should be the end goal.

The nuclear power industry identifies both cables and liquids as a potential main fuel source. However, cable fires can be very complex and can change drastically based on the cable bunching, orientation, configuration, internal heating due to resistance and classification. They are also highly heterogeneous with several layers made out of different materials. Pool fires are generally considered less complex, e.g.

they are homogenous, and it was believed that to reduce the complexity of an already complex set of problems, focusing on pool fires instead of cable fires or other solid fuels was appropriate. Liquid fuels still behave similar to solid fuels as the pyrolysis rate will be very much dependent on the surrounding conditions, and if using liquid fuels successfully to solve the general problems that were presented, it was likely that future research could use the results and implement more general pyrolysis models as those fields progressed. Also, one potential big upside to using a less complex fuel source would likely be that any existing or newly implemented sub-model would be less sensitive to user error, which hopefully would make usage in applied engineering more encouraging.

One could argue that liquid pool fires are not a common issue in a residential setting. However, as previously stated liquid fuels still behave similar to solid fuels as the pyrolysis rate will be very much dependent on the surrounding conditions, and in performance based fire safety engineering when using design fires the actual fuel is rarely specified as long as the combustion products and oxygen consumption is representative. In the long term it is highly desirable to predict pyrolysis of combustible items in an actual living room or shopping mall, but until that point is reached we need to improve in steps.

1.2. Research objectives

Based on the introduction and background it was clear that there was a need for CFD tools which could be used for doing general smoke spread between compartments, predict the response of any mechanical ventilation system attached to these compartments and predict the mass loss rate by taking environmental interaction into account. In short, predict the coupled feedback between fires and their environment.

Based on the listed requirements, five research objectives were formulated:

- Evaluate a CFD modeling framework to ensure that it can accurately predict thermally-driven flow, with an emphasis on smoke and heat transport from fires.
- Validate, and if necessary improve or develop, a CFD sub-model that can predict the behavior of a ventilation system connected to one or several enclosures, both with and without any fire present.
- Validate, and if necessary improve or develop, a CFD pool fire sub-model that is capable of dynamic interaction with the surrounding environment in a feedback loop and that is robust (not overly sensitive to grid-size) and require relatively small amount of input data from the user.

- Validate the CFD model for predicting dynamic fire behavior caused by environmental interaction, including mechanical ventilation system response.
- Apply the CFD model to typical engineering problems and key issues raised in the introduction and background to demonstrate practical usefulness and obtain novel knowledge.

A large focus was the verification and validation efforts to make sure that quality assurance was in place for applied engineering, where prediction, rather than validation, is of primary interest.

2 Publications

Thesis papers

This thesis is based on five papers that have been accepted for publication in different international peer-reviewed scientific journals.

Paper I	Kaldvee, B., Wahlqvist, J., Jonsson, M., Brackmann, C., Andersson, B., van Hees, P., Bood, J. and Aldén, M. (2013) Room-Fire Characterization Using Highly Range-Resolved Picosecond ps-LIDAR Diagnostics and CFD Simulations, Combustion Science and Technology, Volume 183, Issue 5, pp. 749-765. DOI: 10.1080/00102202.2012.750310
Paper II	Wahlqvist, J. and Van Hees, P. (2013) Validation of FDS for large-scale well-confined mechanically ventilated fire scenarios with emphasis on predicting ventilation system behaviour, Fire Safety Journal, Volume 62, pp.102-114, DOI: 10.1016/j.firesaf.2013.07.007
Paper III	Wahlqvist, J. and Van Hees, P. (2016) Implementation and validation of an environmental feedback fire model based on oxygen depletion and radiative feedback in FDS, Fire Safety Journal, Volume 85, pp. 35-49, DOI: 10.1016/j.firesaf.2016.08.003
Paper IV	Wahlqvist, J. and Van Hees, P. (2016) Influence of the built environment on design fires, Case Studies in Fire Safety, Volume 5, pp. 20-33, DOI: 10.1016/j.csfs.2015.12.001
Paper V	Wahlqvist, J. and Van Hees, P. (2016) Evaluating methods for preventing smoke spread through ventilation systems using Fire Dynamics Simulator, Fire and Materials, DOI: 10.1002/fam.2404

The author's contributions to each paper is specified in Table 1.

Paper	Author's contribution
I	The author conducted and wrote the parts that concerned the fire experiments, as well as performing and writing the parts about fire modeling. Other contributors performed the ps-LIDAR measurements, wrote the remaining parts of the paper as well as providing comments to the parts that concerned the fire experiments.
II	The author performed all simulations and wrote the whole paper, comments were provided by the author´s main supervisor.
III	The author implemented the proposed model, performed all simulations, analyzed the data and wrote the whole paper. Comments were provided by the author´s main supervisor.
IV	The author performed all simulations, analyzed the data and wrote the whole paper. Comments were provided by the author´s main supervisor.
V	The author performed all simulations, analyzed the data and wrote the whole paper. Comments were provided by the author´s main supervisor.

Table 1 Specification of the author's contribution to the five papers.

Related publications

Publications that are not included in the thesis, but published by the author during his time as a Ph.D. student, are presented below.

Peer-reviewed papers

Johansson, N., Wahlqvist, J. and van Hees, P. (2012) Detection of a Typical Arson Fire Scenario - Comparison Between Experiments and Simulations, Journal of Fire Protection Engineering 22(1), pp. 23-44, DOI: 10.1177/ 1042391511431508.

Johansson, N., Wahlqvist, J. and van Hees, P. (2014) Numerical Experiments in Fire Science - A Study of Ceiling Jets, Fire and Materials, DOI: 10.1002/ fam.2253.

Non peer-reviewed international conference papers

van Hees, P., Johansson, N., Wahlqvist, J. and Magnusson, T. (2011) Validation and development of different calculations methods and software packages for fire safety assessment in Swedish nuclear power plants, 21st International Conference on Structural Mechanics in Reactor Technology (SMiRT 21) - 12th International Pre-Conference Seminar on "FIRE SAFETY IN NUCLEAR POWER PLANTS AND INSTALLATIONS"

Wahlqvist, J. and van Hees, P. (2012) Predicting smoke spread from mechanically ventilated compartments using FDS, taking into account the importance of leakage, SFPE Conference 2012, Hong Kong

Wahlqvist, J., Hellebuyck, D., van Hees, P., Magnusson, T. and Jörud, F. (2013) Recent fire research related to Swedish nuclear power plants and European spallation source, 22nd International Conference on Structural Mechanics in Reactor Technology (SMiRT 22) - 13th International Pre-Conference Seminar on "FIRE SAFETY IN NUCLEAR POWER PLANTS AND INSTALLATIONS"

Johansson, N., Wahlqvist, J. and van Hees, P. (2013) Simple ceiling jet correlation derived from numerical experiments, 13th International Interflam Conference, London, England, pp. 61-72

Wahlqvist, J., Runefors, M. and van Hees, P. (2016) A study on radiation screens – a comparison between experiments and different numerical models, 14th International Interflam Conference

Runefors, M., Anderson, J., Wahlqvist, J., Huang, C. and Husted, B. (2016) A Comparison of Radiative Heat Transfer Models in FireFoam and FDS, 14th International Interflam Conference

Non peer-reviewed international conference posters

Wahlqvist, J. and van Hees, P. (2011) Quantifying differences between computational results and measurements in the case of a large-scale well-confined ventilated fire scenario using FDS and ANSYS-CFX, IAFSS 2011 poster 10th International Symposium on Fire Safety Science

Wahlqvist, J., Kaldvee, B., Jonsson, M., Brackmann, C., Andersson, B., van Hees, P., Bood, J. and Aldén, M. (2011) Experimental results for validation of CFD codes - Evaluation of alternative measurement techniques for room fire experiments, IAFSS 2011 poster 10th International Symposium on Fire Safety Science

Arias, S., Nilsson, D., Ronchi, E. and Wahlqvist, J. (2017) Use of omnidirectional treadmill in virtual reality evacuation experiments, IAFSS 2017 poster 12th International Symposium on Fire Safety Science

Scientific reports (non peer-reviewed)

van Hees, P. and Wahlqvist, J (2011) Swedish PRISME project – Part 1 – Overview and Summary of Tests and Results, Department of Fire Safety Engineering, Lund University, Sweden, Report 3154

van Hees, P. and Johansson, N., Wahlqvist, J (2011) Swedish PRISME project – Part 2 – Use of test results from PRISME for practical applications in Sweden, Department of Fire Safety Engineering, Lund University, Sweden, Report 3155

van Hees, P. and Wahlqvist, J (2011) Swedish PRISME project – Part 3 – Results and use of overall benchmark exercises in PRISME, Department of Fire Safety Engineering, Lund University, Sweden, Report 3156

van Hees, P. and Wahlqvist, J (2011) Swedish PRISME project – Part 4 – Results of benchmark exercises at LTH, Department of Fire Safety Engineering, Lund University, Sweden, Report 3157

van Hees, P. and Wahlqvist, J (2011) Swedish PRISME project – Part 5 – Results and use of benchmark exercises from other partners in PRISME, Department of Fire Safety Engineering, Lund University, Sweden, Report 3158

Wahlqvist, J., Andres, B., Bhargava, A., Livkiss, K., Wilkens, K., Johansson, N., van Hees, P., Carlstein, F. and Magnusson, T. (2014) Experimental study on enclosed fires with various interconnections between compartments, Department of Fire Safety Engineering, Lund University, Sweden, Report 3176

van Hees, P., Wahlqvist, J., Hostikka, S., Sikanen, T., Husted, B., Magnusson, T. and Jörud, F. (2014) Prediction and validation of pool fire development in enclosures by means of CFD Models for risk assessment of nuclear power plants (Poolfire) – Final Report, Department of Fire Safety Engineering, Lund University, Sweden, Report 3183

3 Research process

A well-defined research process had to be formulated to ensure that each presented objective was successfully addressed. As quality assurance is a significant concern due to the complex nature of CFD models, as well as the fact that the application is aimed to be applied engineering, an iterative process was needed to ensure that the end result was acceptably accurate. Based on the set objectives, the following flow-chart (Figure 1) was created and used throughout the process:

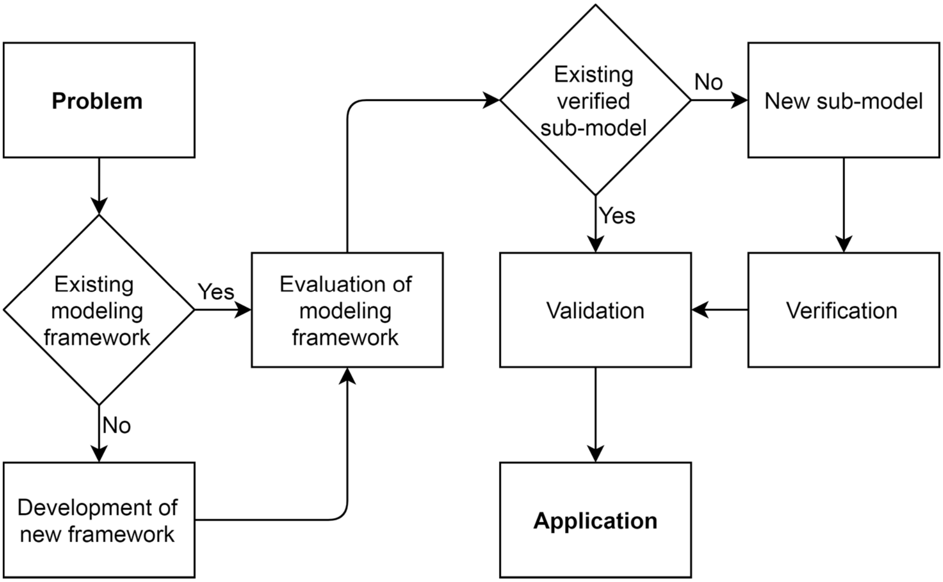


Figure 1 Illustration of the research process used.

The following sections describe each step of the process more in detail, as well outlining the findings.

3.1 Problem

If the main problem is not very well defined or contains several key aspects, this step might require the problem to be divided into smaller problems to ensure that transparency and quality assurance is properly in place for each part that comes together to solve the bigger problem.

Condensing the problem formulation, it was clear that what was needed was a modeling tool that could predict smoke and heat transport from fires, as well as predicting the coupled feedback between pool fires and their environment. In this case the environment included any built structure or system that could affect the mass loss rate of a pool fire.

3.2 Modeling framework

Using an existing modelling framework suitable for solving some, or in the best case, all of the identified problems would be highly beneficial as it potentially could enable large time savings. Not only will it cut down on the development time, but also the needed verification and validation work that has to be done for any new model.

In this case a highly suitable candidate was found; namely Fire Dynamics Simulator (FDS) (McGrattan et al., 2014b). FDS is a computational fluid dynamics (CFD) model made specifically for fire-driven fluid flow. The model numerically solves a large eddy simulation (LES) form of the Navier-Stokes equations appropriate for low-speed, thermally-driven flow, with an emphasis on smoke and heat transport from fires.

FDS was used as it was easily available, well documented, largely accepted within the fire community and open source, enabling modifications to the code base if needed. FDS also had well documented verification (McGrattan et al., 2013) and validation (Hill et al., 2007; McGrattan et al., 2014a; Stroup & Lindeman, 2013) work done which was highly valued. Chapter 6.1 contains more information regarding FDS.

3.3 Evaluation of modeling framework

Once the problem was formulated, it was necessary to identify any sub-model or models that were needed, existing or not. As FDS have several built-in sub-models, the initial work was to map out the capabilities of FDS.

It was found that a new sub-model recently was implemented by the developers of FDS that could simulate heating, venting and cooling (HVAC) systems (Floyd, 2011; McGrattan et al., 2014b). This type of sub-model could be highly useful to predict the interaction between a fire and ventilation system which was needed, however it was not fully validated for the intended purpose. This meant that verification and validation work had to be performed in order to be certain that the sub-model was of use for the earlier mentioned objectives. As the validation work was carried out, this existing sub-model was shown to perform as needed. Chapter 6.2 contains more information regarding the HVAC sub-model in FDS.

The second sub-model that was identified to be needed was a pyrolysis model that would react and interact with any current conditions surrounding the fire. While FDS have several built-in more or less complex pyrolysis sub-models, none of the existing ones were found to be suitable for the application in mind, largely due to grid-dependent results (specifically at "coarser" cell sizes) but also due to the amount of data and input needed by an end-user (Sikanen & Hostikka, 2017). As such a suitable existing sub-model had to be either implemented or a new sub-model had to be developed and then implemented.

3.4 New sub-model/models

If a required sub-model did not exist, or an existing model did not pass the validation stage, a new model would have to be developed, or at the very least strongly characterized as support for future development. The model would first have to be theoretically formulated and then implemented into the chosen framework, which in turn would require quality assurance in the form of verification.

It was concluded in the framework step that a new model for pool fire pyrolysis was needed. A literature study was initially made in search of a suitable model to implement, but no previously presented model fully met all criteria set out by the objectives. Therefore, a new simplified pool fire model was formulated, by using parts from previous work combined into one model, well suited for the needs. This model was then implemented into FDS. Chapter 4.3 further details the simplified pool fire model and chapter 6.3 describes the implementation in FDS.

3.5 Verification

Any developed model or sub model needs to go through thorough verification to ensure that the formulated model is implemented correctly in the code. This is especially true when using computational fluid dynamics codes due to their complex nature. This step is often overlooked since generally only the developer of the model is able to influence the outcome; most end-users are mainly concerned with the theoretical formulation and validation since they set the limits for application.

One new sub-model was implemented and needed to go through the verification step; the simplified pool fire model. Several different verifications tests were designed to make sure that the implemented model behaved as intended, all of which the model passed. The process of verification and the test cases used are described more in detail in chapter 7.

3.6 Validation

Any model or sub-model, either existing or new, has to be validated for the intended purpose. This step determines if the proposed model is able to predict the physics or behavior for which it was developed. Without validation it would be unsuitable to later apply these models in any applied engineering, which in turn would lead to one of the objectives being unfulfilled. This process and the validation cases used are described more in detail in chapter 8.

The validation process was divided into three major parts; validation of smoke and heat transport in FDS, validation of ventilation sub-model in FDS and validation of the simplified pool fire model implemented in FDS.

3.7 Application

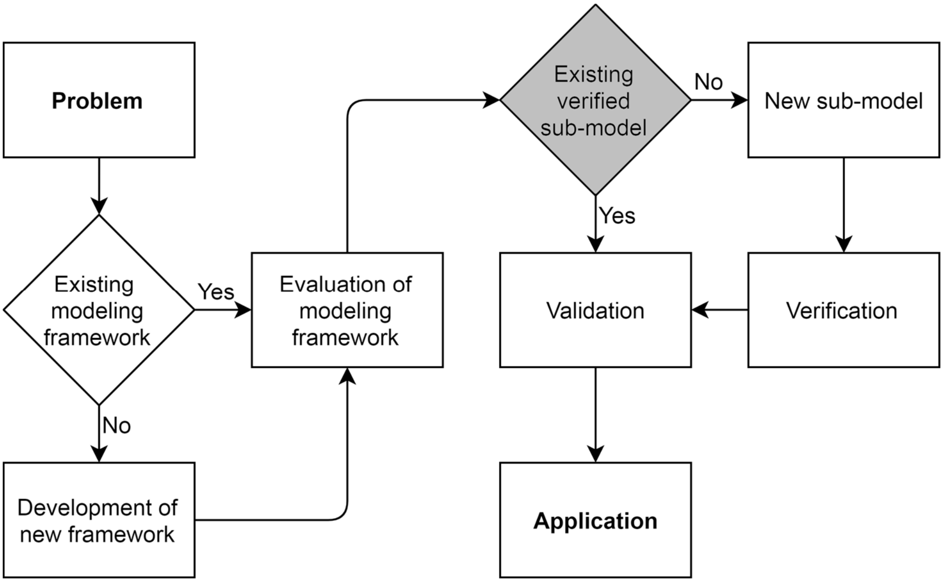
The final, and perhaps most important, step in the process was to use the validated model from previous steps and apply it to the initial problem and demonstrate its feasibility for users. This step was important as it provides societal value as practicing engineers can use the available tools to improve or to demonstrate fire safety in general.

Two engineering applications were performed; firstly, *predicting fire growth related to building characteristics*, where different design fires were exposed to different environments to see how they were influenced by taking re-radiation and oxygen depletion into account. This application is demonstrated in chapter 9.2.

Secondly, *predicting performance of measures against smoke spread in ventilation systems*, where a methodology for evaluating smoke spread in ventilation systems was shown, as well as showcasing several typical counter-measures for smoke spread in ventilation systems and their relative performance levels. This application is demonstrated in chapter 9.3.

Both of these applications were made using so called numerical experiments (Johansson et al., 2014), which meant that no actual experiments were performed to validate the findings. Instead, the results were thought credible due to the previous verification and validation work performed, where it was shown that the model could predict similar scenarios with satisfactory accuracy. This is exactly how most applied engineering is performed, which was the final objective.

4 Pool fire modeling



As stated in the introduction, the mass loss rate, and the resulting heat release rate, is one of the key issues in predicting the fire dynamics of a compartment fire. Detailed pyrolysis models are available in most computational fluid dynamics software packages, but due to their complexity and computational requirements they are rarely used outside of research applications. The reason for this is twofold; firstly, advanced pyrolysis models require a lot of detailed input data and are generally very complex; secondly, traditional pyrolysis models can be very sensitive to the user choice of cell size. This is largely due to the flame not being well resolved with a coarser grid, which in turn affects the radiative feedback given back to the fuel which in turn affects the mass loss rate. An example of this using a 1 m x 1 m open atmosphere fire source, where the only change between cases is the grid size, can be seen in Figure 2 (Paper III, Wahlqvist & van Hees, 2016) where the radiative heat flux feedback to the fuel surface is greatly affected by the choice of cell size in FDS. A similar trend was shown by Sikanen and Hostikka (2016).

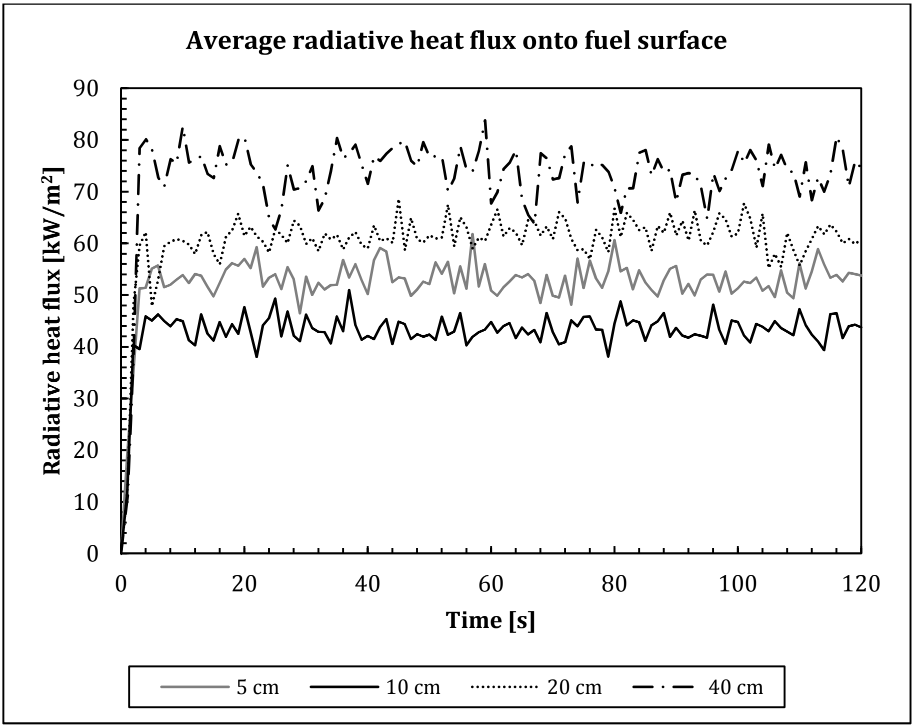


Figure 2 Measured average radiative heat flux onto the fuel surface of a 1x1 meter burner using different cell sizes in FDS (Wahlqvist & van Hees, 2016).

However, fires that interact with the environment are still very much needed in engineering applications; therefore, it can be argued that a simple and robust model for doing so is certainly needed.

4.1 Pool fire model requirements

In many applied cases it is assumed that solid objects are combusted, e.g. a couch, electrical cables or commodity on pallets. However, these types of fuels are considered relatively complex and computationally expensive to model since they often consist of multiple materials, deform, shrink, collapse and char which all require complex models and detailed user input data. This means that a simpler approach is desirable for it to be practically applicable and robust in fire safety engineering applications.

Liquids are often used to study fire behavior in compartments (Melis & Audouin, 2008; Pretrel & Audouin, 2010; Pretrel & Audouin, 2011; Gutiérrez-Montes et al.,

2009) as they are generally less complex than solid fuels due to being homogeneous and not changing shape by being contained in a vessel to form a pool fire. However, both solid and liquid fuels do still share similar pyrolysis processes, i.e. the mass loss rate is correlated to the net heat flux into the fuel, which is not the case for most gaseous fuel sources that also might be used in an experimental environment. This means that both solid and liquid fuels react to their environment, such as radiative feedback and lowered oxygen levels, in similar qualitative fashion.

The pyrolysis rate from a pool fire is determined through a heat balance of the pool. A general pool fire heat balance was presented by Hamins et al. (1994) in which all general heat fluxes are represented (recreated in Figure 3). However, the source of the heat fluxes is not defined as it is assumed that it is based on free atmosphere burning. Convective and radiative heat fluxes are supplied by the flame itself, but can also come from other sources, "external sources". External sources are plentiful in the built environment, such as hot walls, ceilings, hot gas layers and natural or mechanical ventilation. The contribution from external sources would for example likely be the difference between a highly insulated building and a steel sheet building, in which the highly insulated building would produce higher temperatures, increase the radiative feedback to the pool, which would increase the mass loss rate, all in a feedback loop. These mechanisms are of key interest to the presented problems.

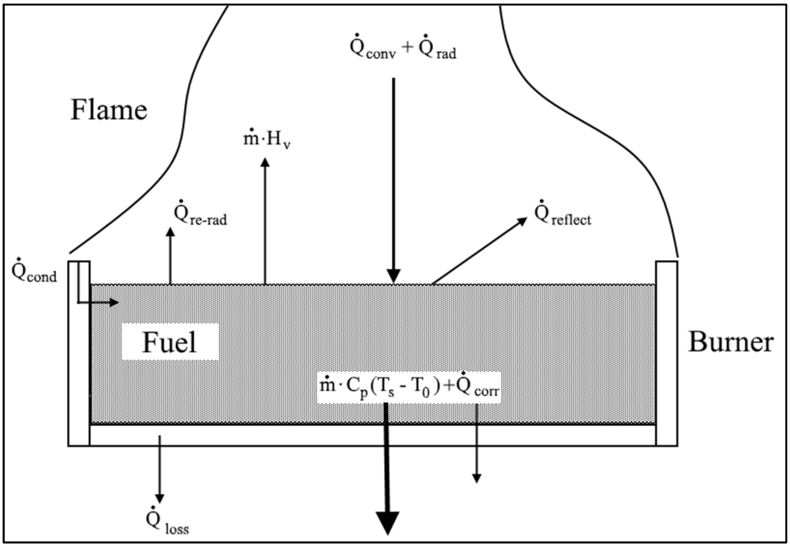


Figure 3 Heat balance for a typical pool fire. Recreated from Hamins et al. (1994).

4.2 Literature review

Pool fires have been researched extensively, and one of the more practical modeling approaches was developed by Babrauskas (1983). He showed that the mass loss rate in an open-atmosphere could be estimated with a simple correlation that only requires the knowledge of certain fuel properties which can be experimentally determined. It is based on a simple heat balance of the pool fire taking into account mainly the effect of radiation. However, this model does not offer any type of feedback loop with the environment as only the diameter of the pool fire changes the mass loss rate for a specific fuel.

Another empirical model correlation was formulated by Peatross and Beyler (Peatross & Beyler, 1997). This model relates the mass loss rate against oxygen concentration measured at the flame base for large-scale fire compartments. However, all of the experimental data used when formulating the model was obtained in conditions for which external heat fluxes were very minor and that term was hence not considered. This means that the only feedback the model will react to is the oxygen volume fraction, and it will neglect radiative heat flux caused by high gas and wall temperatures. Related theoretical work was done by Melis and Audouin (2008), which used a well-stirred reactor approach and showed good agreement with the linear correlation of Peatross and Beyler, but the same limitations applied to this approach regarding external radiative heat flux. Quintiere and Rangwala (2004) presented theoretical work focusing on flame extinction which included a term for external radiative heat flux. But in this work only small scale experiments were compared to the presented model and no general conclusions regarding applicability on full scale fires was presented.

Utiskul (2006) presented a theoretical model that is based on the mass loss rate in an open-atmosphere and feedback due to vitiated air as well as hot gas and wall temperatures. It was shown that the model could predict the mass loss of small-scale heptane pool fires, but since radiative heat flux feedback from the flames to the fuel was ignored this theory was found to be unsuitable for use with large-scale fires. This was also later shown by Nasr et al. (2010).

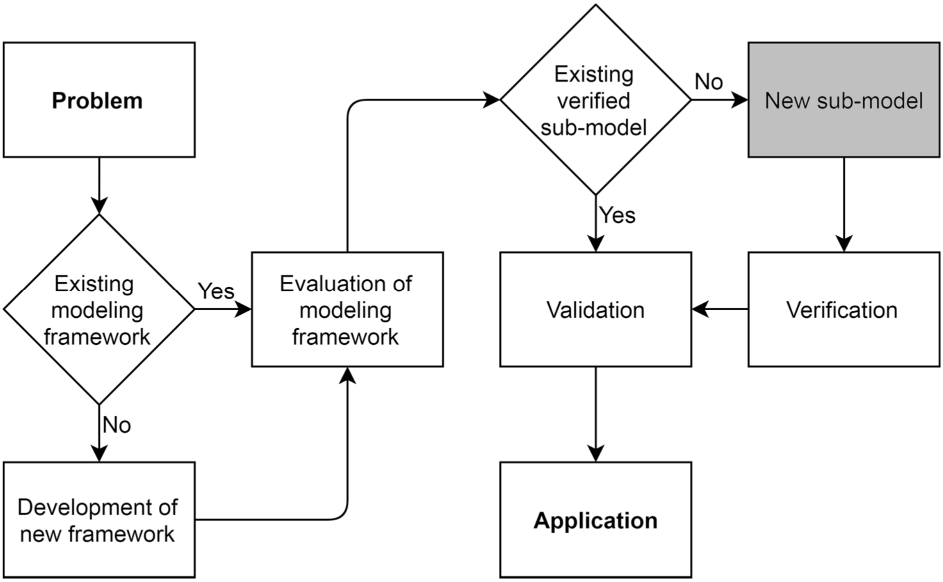
A few studies have added models for taking into account radiative heat flux, one of which was performed by Tewarson et al. (1981). This study focused on determining the convective and radiant heat fluxes by using a steady-state heat balance equation at the fuel surface with a radiation correction for the Spalding number. Further work on how to estimate the flame heat feedback to the fuel surface was also done by Orloff and de Ris (1982), who illustrated the application of Froude modelling principles to the development of a homogeneous fire radiation model. The convective heat transfer from the flame to the fuel surface was determined according to the stagnant film layer theory, which gives its variation with the mass transfer at the pyrolyzing surface. Klassen et al. (1992) developed an equation of radiative transfer to account for the effects of fluctuations on the heat feedback. In this work an experimental study was also performed to obtain measurements of radiative heat feedback in a 30 cm diameter, heavily sooted, toluene pool fire. This work was further developed by Hamins et al. (1994, 1999) who formulated a global model to predict the mass burning flux for pool fires. Total radiation to the pool surface was given according to Siegel and Howell (1981), and the convective heat transfer was determined using the stagnant film layer model (Orloff & de Ris, 1982).

Another modeling approach based on the energy balance at the fuel surface and on the stagnant film layer theory was derived by Nasr et al. (2010). This model was added to a CFD code in order to enable prediction of the mass loss rate of a hydrogenated tetra propylene (TPH) pool fire in a confined, mechanically ventilated compartment scenario PRISME program (OECD, 2011). This model was validated against experimental measurements and showed good agreement for the prediction of the transient heat release rate of a fire compartment (Pretrel & Such, 2005; Pretrel et al., 2005). However, air vitiation effect on the fuel mass loss rate was not investigated in this study.

Concerning the complete coupling between the liquid/solid and gas phases, only a few computational fluid dynamics (CFD) studies have been carried out in which the burning rates were satisfactory reproduced in the wide range from small to large pool sizes (Novozhilov & Koseki, 2004; Snegirev, 2004). The main reason is due to the difficulties in the prediction of the radiative and convective heat fluxes emitted by a turbulent flame and received by the pool surface. More recent work made by Sikanen and Hostikka (2016) which takes in-depth radiation as well as the conduction in the liquid into account have shown good agreement with experimental data (Sikanen & Hostikka, 2017), but this work was conducted in parallel with the work performed in this thesis and was thus not a feasible model to consider. The model also requires relatively small grid cells to predict converging results of the radiative and convective heat fluxes to the pool surface (Sikanen & Hostikka, 2016) which might not be practically feasible in applied engineering.

The literature review reveals that there are several models available but there is no complete model that addresses all requirements. There is also a lack of validation attempts and data when high external radiative heat fluxes are present, as well as oxygen depletion in large-scale environments. The models also vary in complexity, but based on the objectives a simpler model is preferred, assuming it can accurately predict the behavior of the intended applications.

4.3 New sub-model – simplified environmental feedback model



Based on the presented previous work by other researchers, a simple model, appropriate for applied engineering use, was formulated. The model was divided into two main parts; mass loss rate changes due to oxygen depletion and mass loss rate changes due to external radiative heat flux. Since the application was intended to be large-scale fires, no additional convection model was included as the radiation heat would be dominant in most cases (Mudan & Croce, 1988; Joulain, 1998; Joulain, 1996; Howell & Erturk, 2001).

The presented model requires a "base line" mass loss rate collected in a free burning environment or from data derived from correlations as derived by Babrauskas (1983). The "base line" mass loss rate is then modified by taking into account the environmental feedback.

4.3.1 Oxygen depletion

When a fire is enclosed the supply of oxygen might be finite or supplied at a lower rate than the consumption of the current fire size. In such a case the oxygen volume fraction will decrease over time thus affecting the combustion process in several ways. A lot of work has been done to investigate the properties of flames in oxygen depleted environments (Utiskul, 2006; Tewarson et al., 1981, Santo & Tamini, 1981; Santo & Delachatsios, 1984; Andrews et al., 2000; Utiskul et al., 2005; Beaulieu & Dembsey, 2007), and as mentioned in the literature review Peatross and Beyler correlated a range of experiments to determine a linear dependency between the oxygen fraction close to the flame base and the normalized mass loss rate compared to a free burning value (Peatross & Beyler, 1997). The correlation provides fuel mass loss rate against oxygen concentration measured at the flame base for large-scale fire compartments. The data was taken for several different tests with different fuels. The resulting empirical correlation can be seen in Equation 1:

$$\dot{m}''_{O_2} = \dot{m}''_{\infty} \cdot (0.1 \cdot O_2[\%] - 1.1) \quad \text{Equation 1}$$

Where $\dot{m}''_{O_2}$ is the predicted mass loss is rate, $\dot{m}''_{\infty}$ is the steady-state free burning value of a specific fire source and $O_2[\%]$ is the oxygen volume percentage close to the flame base. The oxygen volume fraction at the flame base is used as a substitute to describe the change of radiative heat flux feedback to the fuel caused by cooling of the flame, changed absorption coefficient in the flame, extension of the flame or detachment of the flame from the pool surface. The reduction in radiative heat flux feedback in turn results in lowered mass loss rate.

Since simulating the decrease in radiative feedback from the flame can be very challenging, using the oxygen fraction at the flame base can potentially represent this behavior in a simplified model. This does however require that the combustion process and consumption of oxygen is relatively well predicted globally.

4.3.2 External radiative heat flux

In cases where the temperature of the fire room walls and smoke layer does heat up enough to re-radiate any significant amount of energy to the fire source, such as sealed compartments or well insulated compartments, this re-radiation can amount to a significant portion of the total mass loss rate and in some cases even be the dominating contributor. This has been seen in cases where the flame detaches from the fuel source and combusts close to openings instead of near the fuel source (Audouin et al., 1997). Since the latter often coincide with low oxygen levels it is important to address this phenomenon in in a simplified pyrolysis model. Since the aim of the model is to be relatively simple, a very basic approach has been taken. The net radiative heat flux to the fire source that does not originate from the flame, as in radiation from heated walls and smoke layer, is divided by the heat of vaporization of the fuel will result in a linear addition of mass loss rate, see Equation 2. The outgoing term is approximated to be directly determined by the boiling temperature of the fuel (Spalding, 1952). If the outgoing radiative heat flux is larger than the incoming this term is disregarded.

$$\dot{m}''_{rad} = \max\left(0, \frac{\dot{q}''_{rad.in,external} - \dot{q}''_{rad.out,fuel}}{\Delta h_{v,fuel}}\right) \quad \text{Equation 2}$$

Where $\dot{m}''_{rad}$ is the extra mass loss rate [kg/s] due to radiation, $\dot{q}''_{rad.in,external}$ is the radiative feedback [kW/m^2] from anything except the flame in the enclosure, such as the walls, ceiling or smoke layer, $\dot{q}''_{rad.out,fuel}$ is the outgoing radiate heat flux [kW/m^2] based on the boiling temperature of the fuel and $\Delta h_{v,fuel}$ is the heat of vaporization [kJ/kg] of the fuel.

4.3.3 Combined effects

Combining Equation 1 and Equation 2 yields the following equation:

$$\dot{m}''_{tot} = \dot{m}''_{O_2} + \dot{m}''_{rad} \quad \text{Equation 3}$$

The total mass loss rate is then proportional to the oxygen volume fraction close to the fuel base and the radiation from external sources; the complex radiation from the flame is altogether ignored in the formulation (although indirectly included due to the user being forced to specify the free burning mass loss rate value). This general formulation is similar to the one presented by Utiskul et al. (2005) and Quintiere and Rangwala (2004) but differ in the way how each term is obtained.

4.3.4 Limitations

As the proposed model is relatively simple there are some inherent limitations. Firstly, the influence of external heat flux is limited to radiation and ignores any additional convective heat flux. The radiation term is often the dominant one in large scale pool fires (Koseki, H., 2002) which makes this a reasonable assumption, as separating different sources of convective heat transfer would be very difficult but necessary to take this effect into account. If significant natural or forced flows are expected across the fuel surface this model is not applicable.

The model also does not take any fluid movement or heat transfer within and from the fuel into account. This means that the growth phase can never be modeled but has to be approximated by the user. Consumption of fuel does also not change any characteristics of the fire, so a phenomenon such as boil-over where a large portion of fuel vaporizes very quickly is not possible to predict.

Thirdly, although the correlation proposed by Peatross & Beyler (1997) does take oxygen enriched environments into account this has not been considered since the intended application did not require it. As such the verification and validation processes did not look into the effects of oxygen enriched environments.

A third limitation, which is closely related to the second, is that the correlation proposed by Peatross and Beyler (1997) is based on consumption of oxygen and production of CO/CO_2 as the main mechanism for reduced heat flux from the flame and resulting reduction of mass loss rate. This implies that suppression agents with similar characteristics as CO/CO_2 might affect the mass loss rate in a similar way, while others may not. As no other mechanism besides oxygen consumption caused by a fire source was of immediate interest to this work this subject was largely left untouched.

5 The built environment

As described in the introduction there can be many factors that can influence the course of a fire. The sheer number of different environments that exist is almost infinite which makes it impossible to perform specific experiments for each given case to ensure that the fire safety level is satisfactory. This directly implies that tools are needed that can use data from a limited set of experiments or material data, be put it into a new environment and then predict the behavior of the new system. In this chapter, several key elements that have been identified to likely influence the development of a fire are discussed.

In most applied engineering cases the fire interacts with the built environment in one way or another. The way that the building is designed, built and maintained can cause drastically different fire scenarios between seemingly similar buildings, and the consequences on occupant safety and building integrity can be significant. Two distinct parts of the built environment that are highly likely to affect the mass loss rate, and hence the heat release rate and fire development, inside a building were identified; namely building materials and ventilation, both natural and mechanical.

5.1 Building materials

Based on the construction materials used in a building, a fire development might be vastly different. The most obvious contribution is whether the materials are combustible or not, but in many types of buildings that are of concern (nuclear power plants, multi-residential buildings) the majority of the construction materials are often concrete or steel, both of which are incombustible at normal enclosure fire temperatures. However, in these cases there are other concerns; heat storage capacity and heat conduction. As a fire develops inside a compartment the walls heat up over time. If the fire is severe enough the wall temperature might get high enough to cause radiative heat flux feedback to the fuel which will increase the mass loss rate. And as buildings typically are more and more insulated due to energy conservation, this effect might increase even more in such cases compared to an older building were the heat gets transported out of the compartment through conduction in the walls. In most codes and regulations this effect is neglected since buildings are not separated into different categories based on their insulating or heat storing ability, and this can lead to underestimation of the fire safety in such buildings since re-radiation effects are not taken into account. By having a pyrolysis model that can predict the re-radiation effects, such as the model suggested in chapter4.3, each building will behave differently based on its building materials.

5.2 Ventilation

Any form of ventilation can have a significant influence on a fire development, as all forms of ventilation can either supply oxygen or be a means for smoke spread, and in many cases both. Ventilation has been divided into two main categories; natural ventilation and mechanical ventilation. This was done since they behave very differently in the presence of a fire and pose different challenges and threats. Another third important factor is building leakage, which is further explained in chapter 5.2.3.

5.2.1 Natural ventilation

Natural ventilation is the process of supplying air to and removing air from an indoor space without using mechanical systems. It refers to the flow of external air to an indoor space as a result of pressure differences arising from natural forces.

There are two types of natural ventilation occurring in buildings: wind driven ventilation and buoyancy-driven ventilation. Wind driven ventilation arises from the different pressures created by wind around a building or structure, and openings being formed on the perimeter which then permit flow through the building. But the most applicable type of natural ventilation for this work is buoyancy-driven ventilation, which occurs as a result of the directional buoyancy force that results from temperature differences. This force will drive air flow through door openings, open windows, ceiling openings and similar orifices. It could also transport air through passive or inactive ventilation systems inside a building.

As mentioned in the previous section, flow can be driven in both ways; it can be a means of spreading hot gases and smoke to other parts of a building, or it can be a means of oxygen supply for a fire. Both of these mechanisms must be taken into account to fully predict the behavior of a fire inside any building.

5.2.2 Mechanical ventilation

Mechanical ventilation refers to any system that uses mechanical means, such as a fan, to move air from one space to another. This includes positive pressure ventilation, exhausts ventilation, and balanced systems that use both supply and exhaust ventilation.

Mechanical ventilation in the context of fire safety is often used for smoke extraction, and in such cases the mechanical ventilation is specifically designed for the purpose. But as mentioned in the introduction and background, the largest concern is often the "normal" mechanical ventilation system. These systems are not designed to run under fire conditions, which make them vulnerable to cause smoke spread which can influence both evacuating occupants or can cause damage to equipment. Smoke spread occurs when the fire generates a flow, pressure or temperature that is beyond the capabilities of the design.

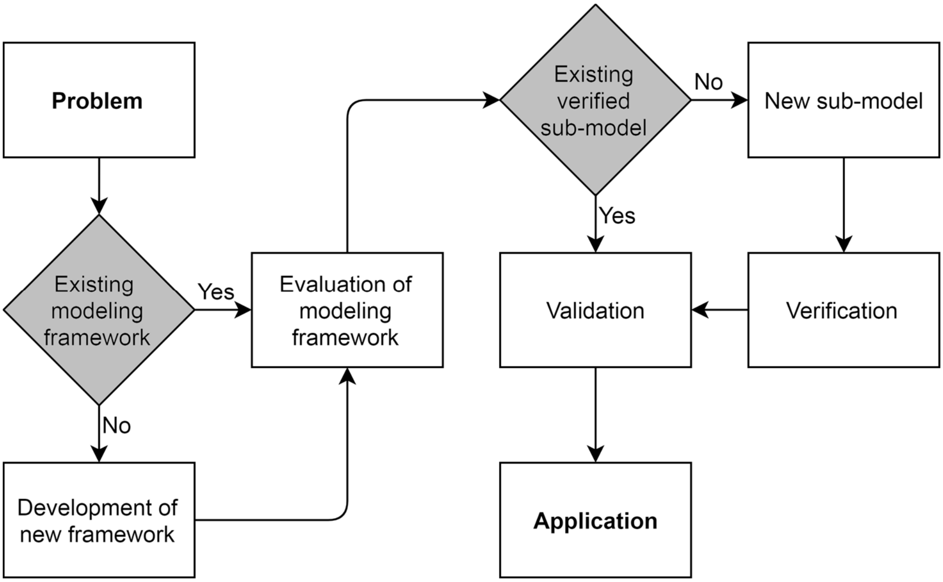
Other than smoke spread, another potentially large issue is the fact that a mechanical ventilation system might actually supply a fire with oxygen beyond what any natural ventilation system could. Most ventilation systems are bound by pressure/flow coupling, as in a certain flow is depending on what upstream pressure is present. Generally, a greater upstream pressure reduces the flow and vice versa. The maximum flow is obtained when no upstream pressure is present and no flow, which is called the stagnation point, is obtained when the maximum upstream pressure is present. Due to the pressure/flow coupling, inlet flows will be reduced or perhaps even reversed, and exhaust flows will be increased with increased room pressure. The opposite is true in the presence of a significant under-pressure, but this is less likely to occur any extended period of time and is most often only seen accompanied by a fire being extinguished.

5.2.3 Leakage

It is highly important to include building leakage when doing ventilation system calculations as air movement through these leaks is to be expected when a pressure difference present. These leaks can e.g. be doorways gaps, cracks in walls, ceilings, windows or facades. The total area of the leakages must be calculated or estimated when calculating the pressure inside a compartment, as this will affect the overall pressure during a fire. The SFPE handbook of fire protection engineering provides a range of values to determine the leakage in buildings (DiNenno et al., 2002), but these vary in the order of 100, which could have significant impact on the ventilation system behavior in a fire. This means that an end-user must be aware what type of building is being dealt with.

Typical leakage areas for walls and floors of commercial buildings are tabulated as area ratios in the SFPE handbook, Table 4-12.1 (DiNenno et al., 2002) in which buildings are categorized into four leakage classes; tight, average, loose and very loose. These data are based on a relatively small number of tests performed by the National Research Council of Canada (Tamura & Shaw, 1976; Tamura & Wilson, 1966; Tamura & Shaw, 1978; Tamura & Shaw, 1978a). The area ratios in these tests are evaluated at typical airflows at 75 Pa for walls and 25 Pa for floors. According to the SFPE handbook it is believed that actual leakage areas are primarily dependent on workmanship rather than construction materials, and in some cases, the flow areas in particular buildings may vary from the values listed. Considerable data concerning leakage through building components are also provided in the ASHRAE Handbook (ASHRAE, 2009).

6 Computer modeling



All models that were used, either existing or developed, are presented in this chapter.

6.1 Fire Dynamics Simulator (FDS)

Fire Dynamics Simulator (FDS) was used for all the work performed for this thesis as it was easily available, well documented, largely accepted within the fire community and is open source, enabling modifications to the code base when needed. Fire Dynamics Simulator (FDS) is a computational fluid dynamics (CFD) model of fire-driven fluid flow. It *solves numerically a large eddy simulation (LES) form of the Navier–Stokes equations appropriate for low-speed, thermally-driven flow, with an emphasis on smoke and heat transport from fires.* (McGrattan et al., 2014b) For further information regarding the functionality and capabilities of FDS the reference manual (McGrattan et al., 2014b) is highly recommended.

6.2 FDS HVAC

To be able to model ventilation behavior the built-in HVAC model in FDS was used. Previous versions of FDS only had the ability to specify either fixed flow boundary conditions (velocity or mass flux) or a simple pressure boundary condition. While these inputs could adequately represent very simple HVAC features, they could not model an entire multi-room system. There was no coupling of the mass, momentum, and energy solutions amongst the multiple inlets and outlets comprising the HVAC network (McGrattan et al., 2014b). To address this limitation, an HVAC network solver was added to FDS (Floyd, 2011). The solver computes the flows through a duct network described as a mapping of duct segments and nodes where a node is either the joining of two or more ducts (a tee for example) or where a duct segment connects to the FDS computational domain. The current HVAC solver does not allow for mass storage in the duct network (i.e. what goes in during a time step, goes out during a time step) (Floyd, 2011). HVAC components such as fans and binary dampers (fully open or fully closed) can be included in the HVAC network and are coupled to the FDS control function capability. There is also an option to select from three fan models (McGrattan et al., 2014b). A series of verification exercises have demonstrated that the network model correctly models HVAC flows and that it's coupling with FDS maintains mass conservation (Floyd, 2011). A simple and a complex validation exercise showed that the combined solvers can accurately predict HVAC flows for a duct network in a complex geometry with fire effects (Floyd, 2011), but there is still need for validating the model with more complex and detailed experimental scenarios. The tests performed in the DIVA facility were a perfect candidate for this task, since it is a multi-room setup with an elaborate mechanical HVAC system and a very tightly sealed compartment (Audouin, et al., 2011b, 2013).

6.2.1 Duct network simplification

Since a ventilation system can be very complex with hundreds of different dimensions, bends, valves and dampers, a simplified approach had to be taken when modeling a full HVAC system. Instead of trying to model every pipe, bend, valve and other components, the flow resistance coefficient between nodes were calculated using initial pressure data from experiments when available. The flow resistance, or loss coefficients, between each node were calculated using Equation 4 (ASHRAE, 2009):

$$K = \frac{2 \cdot \Delta p_{nodes}}{\rho_{air} \cdot u_{duct}^2} \quad \text{Equation 4}$$

Where K is the loss coefficient, Δp_{nodes} is the pressure difference between [Pa] two nodes, ρ_{air} is the density [kg/m^3] of air before ignition and u_{duct} is the velocity [m/s] in each specific duct section (calculated by dividing volume flow by duct section area). Figure 4 shows an example of the reported experimental data and the simplified HVAC network that was used in an actual scenario. If the initial pressure data was not available a more time consuming process of adding all components manually to the network had to be used. This was done in Paper V since that actual setup did not exist.

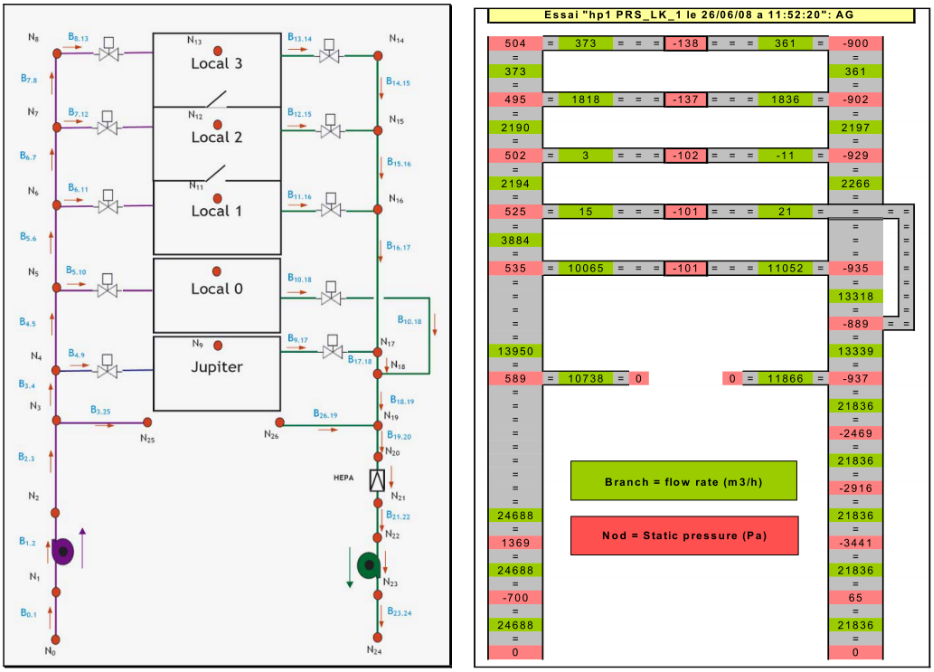


Figure 4 Example of experimental pressure and flow measurements in a simplified duct network present in the DIVA facility that was used for the PRISME experiments. Picture courtesy of IRSN.

6.2.2 Inlet- and exhaust fans

Fans can be represented in three different ways in FDS; constant volume flow, quadratic pressure/volume flow relation and user created fan curve. The simplest option is the constant volume flow which will continue to deliver the specified volume flow no matter what the upstream pressure is. The quadratic pressure/volume flow model (McGrattan et al., 2014a) is appropriate in many cases as it can fit a real fan curve within its normal operating conditions, and it is a function of the upstream pressure as seen in Equation 5:

$$\dot{V}_{fan} = \dot{V}_{max} \cdot sign(\Delta p_{max} - \Delta p) \cdot \sqrt{\frac{|\Delta p - \Delta p_{max}|}{\Delta p_{max}}} \quad \text{Equation 5}$$

where $\dot{V}_{fan}$ is the resulting volume flow of the fan [m^3/s], $\dot{V}_{max}$ is the free flow value of the fan [m^3/s], Δp_{max} is the stall pressure of the fan [Pa] and Δp is the current downstream pressure difference [Pa]. The third option, creating a custom fan curve, gives the user total freedom to create a fan curve that fits specific needs. This is done by supplying several data points of volume flow under a specific pressure which coupled with linear interpolation between points form a fan curve.

To use the same fan with different revolutions per minute (RPM), which can be useful when the same fan is used in several different scenarios, the fan affinity laws shown in Equation 6 and Equation 7 (ASHRAE, 2012) can be used to change the volume flow/pressure relation:

$$\dot{V}_{max,2} = \dot{V}_{max,1} \cdot \frac{RPM_2}{RPM_1} \quad \text{Equation 6}$$

$$\Delta p_{max,2} = \Delta p_{max,1} \cdot \sqrt{\frac{RPM_2}{RPM_1}} \quad \text{Equation 7}$$

6.2.3 Leakage

As stated in section 5.2.3 it is very important to include leakage in any scenario where a sealed compartment is present. There is a simplified leakage model included in the FDS HVAC mode which is quite similar to the quadratic fan model, as shown in Equation 8 (McGrattan et al., 2014b);

$$\dot{V}_{leak} = A_L \cdot sign(\Delta p) \cdot \sqrt{2\frac{|\Delta p|}{\rho_\infty}} \quad \text{Equation 8}$$

Where $\dot{V}_{leak}$ is the volume flow through the leak [m^3/s], A_L is the size of the leakage area [m^2], Δp is the pressure difference between the adjacent compartments [Pa] and ρ_∞ is the ambient density [kg/m^3]. The discharge coefficient is set to 1 which is in line with the findings in (McGrattan et al., 2014b). The area of the leakage can be approximated with the leakage classes reported in the Table 4-12.1 of the SFPE handbook (DiNenno, 2002), but if experimental leakage measurement data is available the required leakage area can be acquired by rearranging Equation 8;

$$A_L = \frac{\dot{V}_{leak}}{sign(\Delta p) \cdot \sqrt{2 \frac{|\Delta p|}{\rho_\infty}}} \quad \text{Equation 9}$$

6.3 Simplified environmental feedback model

The simplified environmental feedback model is divided into two parts as described in chapter 4.3, and where hence individually implemented in FDS. Each implementation is described more in detail in the following sections.

6.3.1 Oxygen depletion

Based on the model presented in section 4.3.1, Equation 1 was directly implemented in FDS with some slight modification to compensate for the actual normal dry oxygen volume fraction in FDS. The oxygen volume fraction is sampled in a volume specified by the user using a normal FDS device with a specific identity. The sampling volume is usually recommended to include all cells touching the rim of the fuel pan, essentially forming a “ring” around the fuel pan. The height of the “ring” is normally set to 1 cell originating from the fuel surface and downwards. Since the size and location of the sampling volume might have a large influence on the resulting mass loss rate, a sensitivity study was done and is presented in section 8.3.3.3.

6.3.2 External radiation heat flux

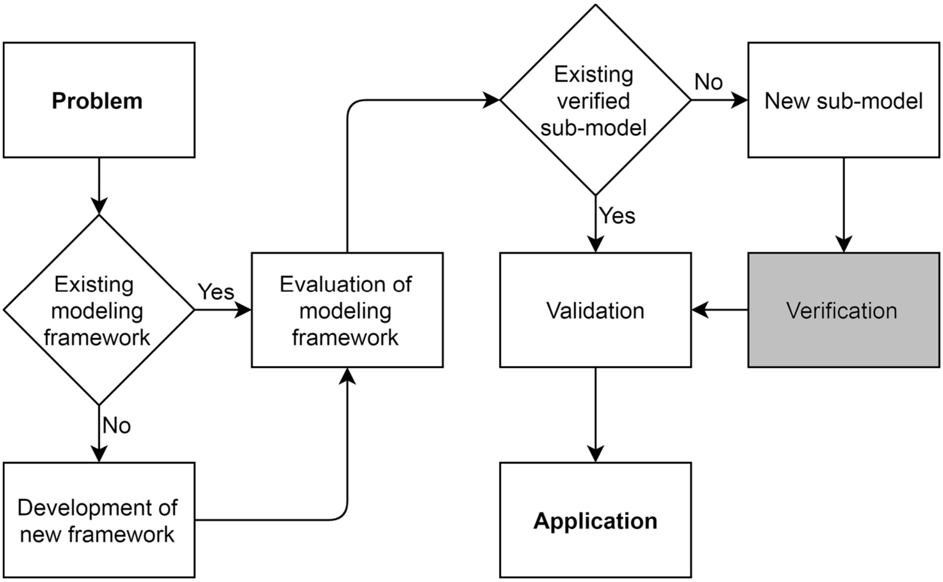
Based on the model presented in section 4.3.2, Equation 2 was implemented in FDS. This was done by adding an additional routine to the radiation calculations in FDS where all radiation from combustion was ignored. This was necessary since the initial radiation feedback from the flame was already included in the prescribed mass loss rate and the lowered radiation feedback from the flame in stages with lowered oxygen levels was compensated by the oxygen volume fraction at the fuel base. To be able to save computational power this radiation routine was not as frequently updated as the rest of the radiation routine, but more optimizations should be done in order to save computational resources, e.g. ignore all surfaces that do not require the actual quantity which is everything but the fuel surface.

To use the model, the user has to specify a similar device as described in the previous section. The external radiation is sampled on a surface specified by the user, typically the entire fuel surface, using a normal device with a specific identity.

6.3.3 Limitations

As previously discussed the model is dependent on a global prediction of oxygen consumption, which makes it dependent on the combustion model in FDS. The model is also dependent on the fact that radiation from external sources is well predicted, which makes it dependent on the radiation model in FDS. Both of these models have been subject to verification and validation (McGrattan et al.; 2013, 2014a), and both are further discussed in chapter 7 and 8.

7 Verification



Verification is defined as:

> *The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model. (AIAA, 1998)*

Verification is done to reassure that computational models are a correct implementation of the theoretical models, and this is done by trying to identify and quantify errors in the model implementation and the solution. Verification is almost always done by the developer of the model, as that person or those persons have generally better insight in all steps required. The first step is to look for bugs, incorrect implementations of conceptual models, errors in inputs, and other errors in the code and usage. The second step is to simulate one or more verification cases. These cases should be analytic or numeric solutions made for the specific cases, and in general not based on experimental data. A grid refinement study should be conducted to bring out potential errors and to check consistency with different grid sizes.

As described in section 6.3, two parts of the simplified feedback model were implemented and needed verification; the oxygen depletion feedback model and the external radiative heat flux feedback model. In Paper III which first presented the proposed model, a verification study was made to make sure the model was correctly implemented. The verification process originally presented in Paper III has been re-presented in the following sections to allow an easy overview of the results. The original study can be found in Paper III.

7.1 Oxygen depletion feedback model

To be able to verify if the proposed model was correctly implemented, a simple test case was created. It consisted of a methane burner with a surface of 1 m^2 placed in a fully open environment (no walls or ceiling, only floor) that in "normal" conditions injected 0.01 kg/s of fuel. The oxygen concentration in the atmosphere was then varied in different cases to influence the burning rate of the fuel. As can be seen in Figure 5 the model behaves as expected; a decrease in oxygen volume fraction decreases the mass loss rate linearly until extinction at approximately 11% oxygen volume fraction. The results are identical for both mesh sizes (10 and 5 cm respectively).

There are however some caveats; since the user specifies the actual oxygen volume fraction sampling volume, choosing an ill-placed volume might render unexpected results. This is however not an issue due to the implementation of the model in the code, but rather an end-user issue, and this was hence further examined in the validation process.

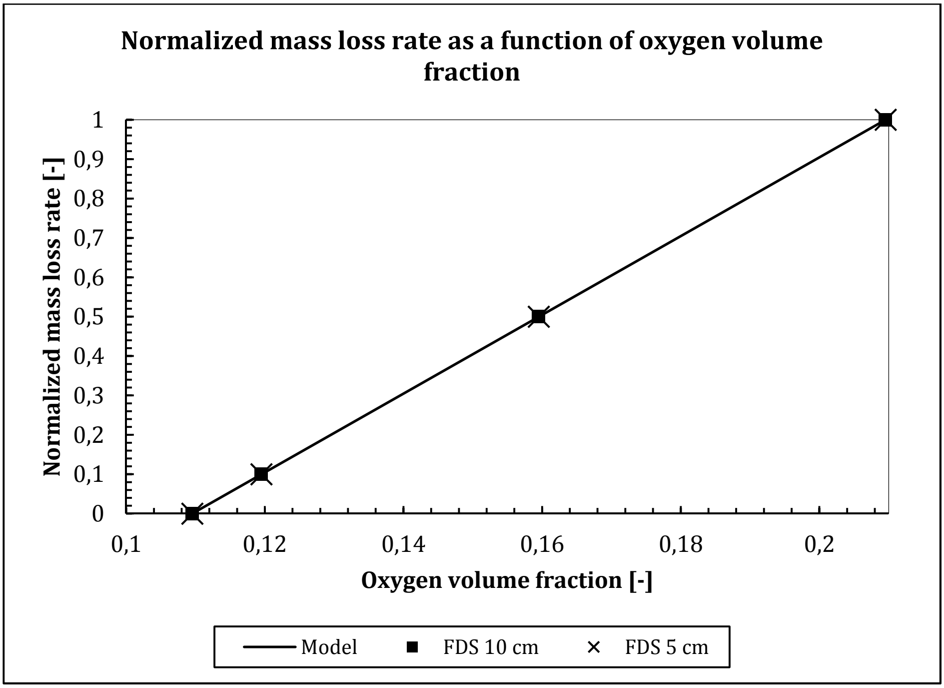


Figure 5 Comparison between predicted and expected mass loss rate.

7.2 External radiative heat flux feedback model

The external radiation model was programmed to behave identical to the standard FDS radiation model when a flame was not present, and as such it was expected to perform similar to the verification work done by McGrattan et al. (2013) in the FDS verification guide in such cases. However, to fully verify that the model was correctly implemented a simple test case was constructed to test the model both with and without combustion present. A total of four different variations were made, all using the same basic setup. This general setup consisted of a burner with the dimensions of 1 m x 1 m placed 20 cm above the ground, which had a constant surface temperature of 20 °C. 2 meters above the burner surface, a 1 m x 1 m plate with a surface temperature of 800 °C was placed. The emissivity was set to 1.0 on both surfaces. The atmosphere surrounding the setup was set to have zero relative humidity and zero carbon dioxide to prevent unwanted radiation absorption in all cases but verification test 4.

The four different verification tests and the results are explained in detail in Paper III, but a summary of the test results and test specification is listed below:

- **Verification test 1**: designed to ensure that the model had been implemented correctly when no combustion was present, as well as investigating the influence of the cell size and the number of solid angles used by the radiation model. The external radiative heat flux was compared to both the "standard" radiative heat flux and the analytical solution of the problem.
- **Verification test 2**: similar to test 1 but now fuel was allowed to enter the domain, hence introducing combustion. The purpose of this test was to make sure that the external radiative heat flux was not increased by the presence of a flame, but rather likely decreased due to absorption of radiation caused by the flame and fuel. The test was also used to verify that the resulting mass loss rate in FDS was directly proportional to the measured external radiative heat flux.
- **Verification test 3**: similar to test 2 with the exception that the mass loss rate was prescribed and constant rather than influenced by the external radiative heat flux. This was to investigate the absorption of radiation caused by the flame and fuel. By changing the mass loss rate the flame height and size was changed, and it was expected that a larger flame would absorb a larger portion of the external radiative heat flux.
- **Verification test 4**: similar to test 1 (no combustion) but in this case the absorption coefficient of the atmosphere was set to 0.15 m^{-1} (by adding carbon dioxide) instead of zero. This was done to verify that the external radiation model behaved identical to the "standard" radiation model in FDS regarding absorption.

In verification test 1 the external radiative heat flux parameter directly mirrors the results obtained by the "FDS standard" radiative heat flux, which was the intended behavior when no combustion takes place. It can also be concluded that the "standard" radiation solver in FDS is dependent on both cell size and the amount of solid angles, and this behavior is inherited by the external radiation model. As the cell size decreases and the amount of solid angles increases, the solution converges towards the analytical solution. This result agrees well with the FDS verification guide (McGrattan et al., 2013).

In verification test 2 the external radiative heat flux was slightly decreased and the "standard" radiative heat flux was significantly increased. This means that the external radiative heat flux output is ignoring the radiation from the flame while the radiative heat flux output does not, both of which are intended behavior. The radiative heat flux is decreased due to the absorption of radiation in the flame and fuel, and the absorbed amount changes with cell size. It seems as if a coarser mesh generally absorbs less radiation relatively, even though the resulting mass loss rate was larger. When the mass loss rate was identical between cell sizes this was still the case, as seen later in verification test 3. This is most likely due to differences in the predicted temperatures, species concentration and flame shape. Figure 6 shows a 2D slice of the absorption coefficient for all three cell sizes, and it can clearly be seen that there are quite significant differences of the overall flame structure; this was also true for the overall temperatures. Finally, the expected mass loss rate (measured external radiative heat flux divided by the heat of combustion of the fuel) perfectly matched the actual mass loss rate output in FDS which meant that the routine for doing so worked as intended.

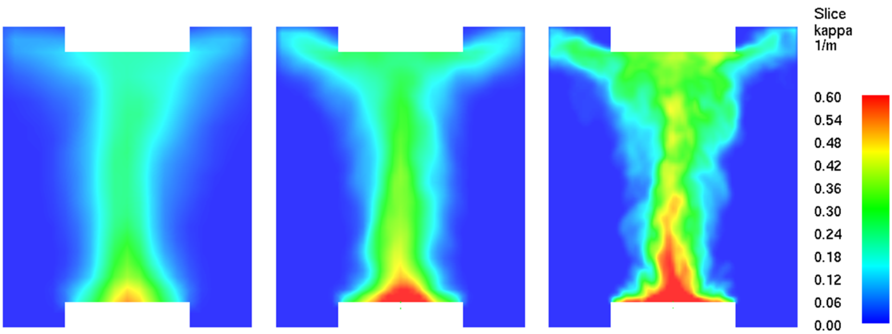


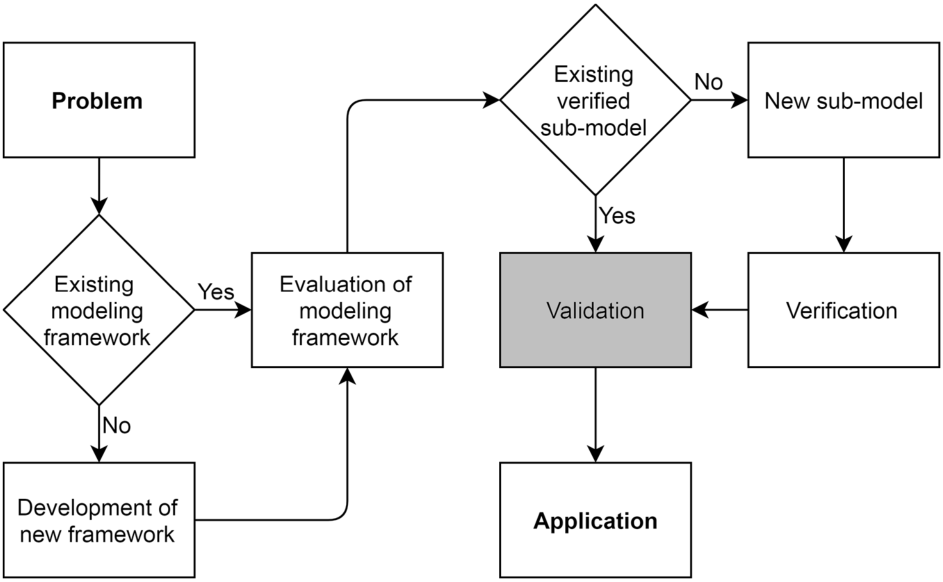
Figure 6 2D-slices of the absorption coefficient in verification test 2 (from left to right; 10, 5, 2.5 cm cell size).

In verification test 3 the external radiative heat flux consistently decreases with an increase in mass loss rate. Since it is very hard to predict the expected absorption, this is unfortunately mostly a qualitative test. As was the case in verification test 2, a coarser mesh generally absorbs less radiation relatively, and this is most likely due to differences in the predicted temperatures, species concentration and flame shape.

In verification test 4, the result showed that both the "standard" FDS output and the external radiative heat flux outputs are identical which meant that the external radiation model behaves identical to the "standard" radiation model and is implemented correctly. The results also show that the relative amount of absorbed radiation is almost identical between different cell sizes. This makes it rather likely that the differences in absorption for different cell sizes seen in verification test 3 was due to other parameters, such as the predicted temperatures, species concentration and flame shape, rather than the cell size.

The implemented model is verified to work as intended, but is coupled to the limitations of the "standard" FDS radiation model which a user must be aware of.

8 Validation



Validation is defined as:

> *The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. (AIAA, 1998)*

Validating a CFD code in its entirety is close to impossible, instead specific parts or applications are validated against experimental data. Validation examines if the models implemented into the CFD code simulation agree with real world observations, and the general approach is to identify and quantify error and uncertainty through comparison of simulation results with experimental data. However, experimental error such as bias or random errors must be considered when performing a validation study as failing to do so might lead to invalid conclusions. The accuracy required in a validation study is dependent on the application which is why the validation should be flexible to allow various levels of accuracy.

Three major validation studies were required to fulfil the objectives of this thesis; the general framework FDS and its ability to predict enclosure gas temperatures, the ventilation model built in to FDS and its ability to predict ventilation system behavior, and the newly implemented sub-model that enabled fires responding to environmental feedback. Each of these three validation studies was the focus in three different papers; Paper I, Paper II and Paper III respectively.

8.1 Enclosure gas temperature measured using ps-LIDAR measurements

Computational fluid dynamics models allow detailed calculations of, for example, multidimensional temperature distributions in a room, as the variables can be extracted for each grid cell. In turn, this puts requirements on the validation by means of experiments. Most methods that have been used so far are limited to multiple single point measurement (e.g., by thermocouples or bidirectional probes). Because of their physical size, there can be disturbances in the flow field caused by the measuring equipment (Bryant, 2005). Some detailed data using these traditional measuring techniques are available from Brown et al. (2008); however, to obtain one- (1D), two- (2D), or even three-dimensional (3D) distributions of temperature and flow (for instance, turbulence), introduction and development of novel, nonintrusive measuring techniques are necessary.

Nonintrusive techniques such as stereoscopic particle image velocimetry (SPIV) have been used to measure velocities in door openings (Bryant, 2009a, 2009b) for a similar experimental scenario, and laser tomography visualization has been used to visualize door-opening flows in a reduced-scale environment (Lucchessi et al. 2011), but in neither work were temperatures measured using nonintrusive techniques. Planar thermal imaging of a buoyancy-driven unsteady laminar hydrogen/air flame has been performed by Blunck et al. (2009) using infrared (IR) emission–absorption spectroscopy, but the method presented needs to be modified for large-scale use and is also focused on measuring the temperatures within the flame.

Kaldvee et al. (2009, 2011) have developed and demonstrated picosecond light detection and ranging (ps-LIDAR), a laser-based technique suitable for diagnostics inside large-scale combustion devices and in the field of fire safety research. Thermometry has been demonstrated for temperatures up to 1700 K, and it has been shown that Rayleigh scattering thermometry can be conducted in ethylene flames having an equivalence ratio of up to 1.3 before particulate matters in the flame disturbs the measurement. The technique is a variant of the ps-LIDAR technique frequently used for atmospheric remote sensing (Fujii and Fukuchi, 2005; Weitkamp, 2005), where backscattered light is detected time resolved to obtain range-resolved information. The major advantages of ps-LIDAR are remote sensing via only one optical access and the capability to measure over several meters while still providing spatial resolution on the order of centimeters without altering the experimental setup. However, since temperatures are extracted from the Rayleigh back-scattered light, this implies that temperatures can only be evaluated accurately in regions containing insignificant amounts of interfering particles. The measurement challenges using Rayleigh scattering techniques are thoroughly presented in a review article by Zhao and Hiroyasu (1993).

This validation case was focused on two parts; firstly, a ps-LIDAR was used for the first time to measure temperature in a large-scale fire application, revealing strengths and challenges of the technique. Secondly, the collected by the ps-LIDAR method was compared to CFD simulations done with Fire Dynamics Simulator (FDS), as well as being compared to measurements done with more traditional thermocouples.

8.1.1 Experimental setup

The fire experiments were carried out in an ISO 9705 room at close to ½-scale, with dimensions 117 cm x 188 cm x 120 cm (width x length height), respectively, and a 50 cm x 107 cm door opening centered on the front 117 cm wall. The walls, floor, and ceiling were made of calcium silicate boards (Promatect-H). Two different fuel sources, placed on the floor inside the back of the room, were used for different scenarios; a 20-cm diameter cylindrical container containing methanol, as well as a square methane gas burner filled with granule and sand (sand burner) to diffuse the gas flow. However, due to the strong emission of particulate matter using a methane flame as fire source, Rayleigh scattering thermometry was only possible while using methanol as a fire source. In the case of the methane gas burner, detection of particle Mie scattering instead provided qualitative particle distribution mapping in a horizontal plane inside the room.

The temperatures in the door opening were measured with type K thermocouples along a vertical line centered in the door opening at nine different heights: 50, 60, 65, 70, 75, 80, 85, 95, and 105 cm. The second-harmonic radiation, at 532 nm, of a mode-locked Nd:YAG laser (Ekspla, PL 2143C) was used as ps-LIDAR laser pulses. The laser pulse duration was 30 ps, the pulse repetition rate was 10 Hz, the laser beam diameter was 12 mm, and the beam divergence angle was <0.5 mrad. The laser light was directed along the optical axis of the collecting telescope by a planar mirror, M1, coated for high reflectivity at 532 nm. A schematic of the experimental setup can be seen in Figure 7.

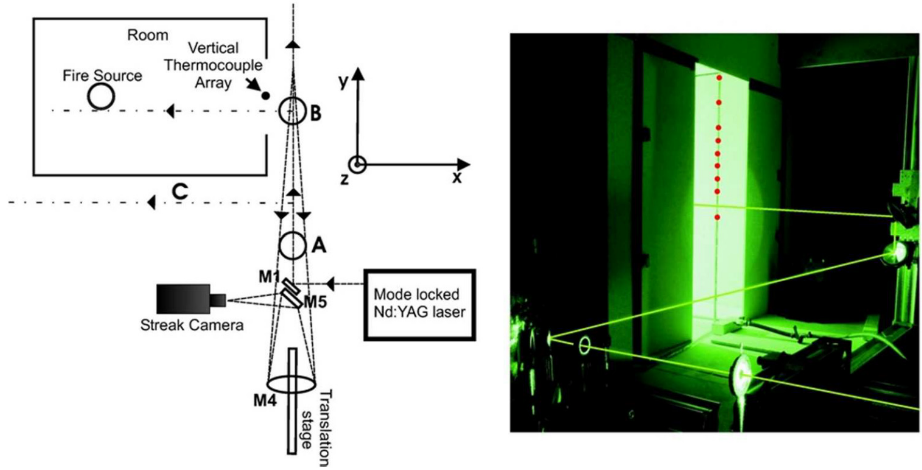


Figure 7 Schematic of the ps-LIDAR setup used in the experiments.

8.1.2 Simulation setup

The CFD simulations were carried out using FDS 5.3.3 (SVN 7060). The simulations were made as "blind" or a priori calculations where only the room configuration, material specification, ambient temperature, and volume flow in the extraction hood were known before the simulations. The hood of the calorimeter was also modeled in FDS, because the large volume flow would likely affect temperatures and flow velocities in the experiment. The experimental facility lacked capabilities to perform heat release rate (HRR) or mass loss rate (MLR) measurements, therefore the MLR was calculated using the formulation by Babrauskas (1995) and was used as a constant value for the MLR during the whole simulation time.

A uniform grid of 2 cm was used throughout the entire computational domain, and the room geometry was reproduced as accurately as the chosen grid size allowed. The 10 mm Promatect-H boards were represented as 20 mm boards in the flow-obstructing regime and 10 mm in the heat-transfer regime.

8.1.3 Results

As described in the experimental setup, the ps-LIDAR was only able to generate temperature readings when methanol was used, but in that experiment two measurement series were conducted: a doorway measurement in a y–z plane 6 cm outside the door, and a room measurement in an x–y plane at a height of 75 cm inside the room. Initial comparison between FDS and experimental data focused in the more traditional thermocouple readings as this would quickly give a general idea of how the FDS predictions performed. Figure 8 shows the average thermocouple readings between 33–35 min after ignition and the thermocouple model readings from FDS after similar amount of time in the door opening. The use of the thermocouple model allowed the effects of radiation and convection onto the surface of the thermocouple, and conduction within the thermocouple to taken into account. The results show excellent agreement, which indicates that a satisfactory grid size was used. Because the results agreed very well at this position, the general confidence in the FDS prediction was high. This was an important step in comparing the FDS results with the ps-LIDAR measurements since thermocouple measurements were not available at other positions.

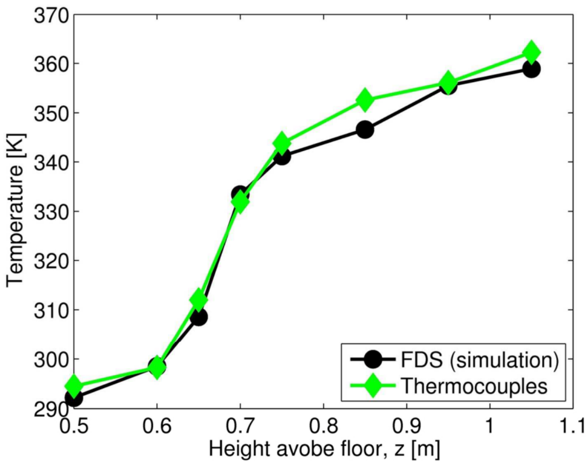


Figure 8 Comparison between experimental thermocouple readings averaged between 32-35 minutes after ignition and the CFD-simulated steady state thermocouple readings calculated with FDS.

When comparing the ps-LIDAR results across the doorway with both the thermocouple readings and the FDS simulations, they are all in relatively good agreement, which can be seen in Figure 9(b). However, it can also be seen that the ps-LIDAR temperature is underestimated at the highest thermocouple position (i.e., at 105 cm), near the top of the door opening. The underestimation is most likely because that most of the soot and particles (i.e., smoke), from the fire inside the room passes through the top of the doorway on its way out of the room. Because light scattering from homogenously distributed small particles cannot be discriminated by the filter function, the measured signal will increase and the volume will be interpreted as colder. In addition, homogenously distributed non-discernible particles will increase signal extinction, which, if it reaches a substantially high level, will give the false effect of temperature increasing with distance. The same results can also be seen in Figure 9(a) where the ps-LIDAR measurements and corresponding FDS simulations are presented as 1D temperature curves for different three heights.

The downward-pointing triangles in Figure 9b, representing simulated gas temperatures in the plane of the thermocouples (6 cm from the plane shown Figure 9d), give an indication of how sensitive both measuring and modelling of the temperature is for small translations of the y–z plane in this region. This is expected due to the turbulent flow that is present through the door opening.

The ps-LIDAR results at the x–y plane inside the room at 75 cm agree partly with the CFD results (Figure 10). Both results reveal the fast decrease in temperature outside the door and a hot structure above the region containing the flame. The position of the hot structure is translated between the two images and is more vertically extended in the ps-LIDAR results as well. However, the CFD simulations show that the position of the high-temperature region varies with time and this might explain the extended region observed in the ps-LIDAR image even though the presented CFD results have been averaged over a time interval corresponding to that of the measurements.

The overall temperatures in the plane agree well in some parts (roughly half) of the images and differ up to 20 K in other parts. The ps-LIDAR image also contains a structure, manifested as a low-temperature region in the vicinity of the door which is not observed in the simulated result. This coarse structure is mainly oriented in the vertical image direction, along the direction of the different measurement positions, which makes it reasonable to believe that at least part of the structure is due to laser pulse energy fluctuations between the measurements. However, vertical structures might also be due to real dynamics in the temperature field, causing the temperature to change in time between the ps-LIDAR measurements at the different y-axis positions. Yet another possible explanation is that the thermocouple mounting arrangement may cause gas flows, yielding a temperature structure that is not captured well in the FDS simulation. Even though the thermocouple mounting arrangement was accounted for in the simulation, it was modeled as an infinitely thin object because of grid cell size limitations.

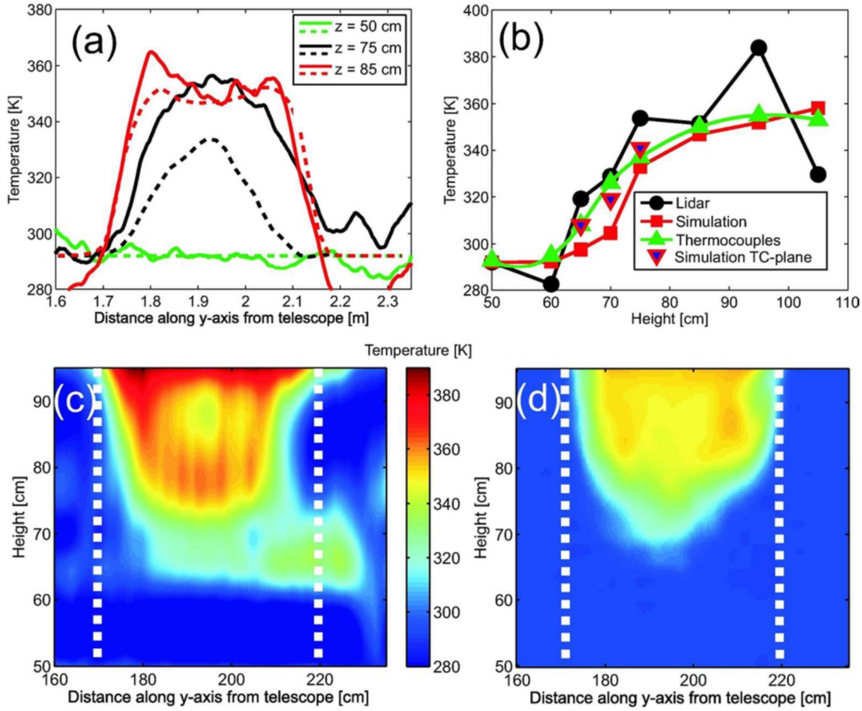


Figure 9 Temperature data in the vicinity of the door. In (a) 1D temperature curves from a vertical plane 6 cm outside the door opening corresponding to three different heights are shown (solid lines=ps-LIDAR, dashed lines = FDS). Panel (b) shows the thermocouple readings, ps-LIDAR measurements, and FDS simulations at the heights and y-position of the thermocouples in a plane 6 cm outside the door opening. A 2D temperature image of the y-z plane 6 cm outside the door measured with ps-LIDAR is shown in (c), while (d) shows the corresponding simulated result.

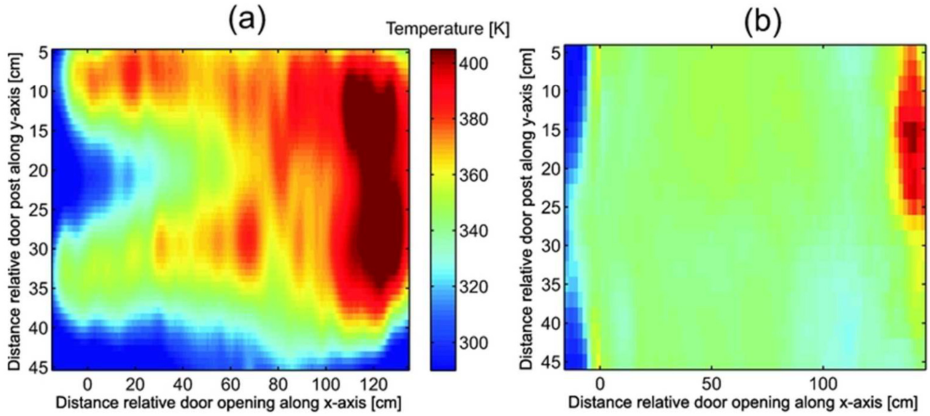


Figure 10 Two-dimensional temperature images of the x-y plane at height z=75 cm with a methanol pool fire in the room. The same color scale is used for the two images. The left picture (a) shows temperatures captured with the ps-LIDAR measurement, the right picture (b) is temperatures from the FDS simulation.

Overall deviations between simulation and measurement results could also partly be explained by the ventilation in the experiment hall, which could influence the flow in and out of the ISO 9705 room. This effect could unfortunately not be simulated because it would require a computational domain that covers the entire experimental hall and would be too computationally expensive. However, since the extraction hood had a fairly large volume flow during the experiments, this flow together with the fire-induced flow were probably the factors dominating the flow. Another reason for deviation between the experimental results and the results of the CFD simulations was the lack of transient measurements of the fuel MLR. Because no MLR data were available, steady-state simulations were compared to measurements performed while the gas temperatures inside the room were still somewhat increasing.

Although no velocities through the door opening were measured, the flow pattern through the door opening (based on the temperature profile) seems to agree well with previous work using stereoscopic PIV in a similar experimental scenario (Bryant, 2009b).

8.1.4 Conclusions

Ps-LIDAR has been demonstrated for nonintrusive diagnostics in a large-scale combustion environment, namely a room fire. The study clearly shows that the technique allows for single-ended remote laser diagnostic in hard-to-reach regions inside large combustion facilities. Elastic scattering, depending on the scattering properties of the measurement volume, has been successfully applied both for quantitative Rayleigh thermometry and qualitative monitoring of particle distributions. To reduce noise and improve the accuracy of the Rayleigh thermometry, an image filtering routine was developed and used to suppress interfering signal from discernible particle scattered light. The CFD tool FDS was validated by means of these experiments and showed satisfactory results despite some uncertainties in the HRR from the experiment.

Regarding the FDS simulations, a methane fire using a gas burner would likely provide more accurate results than a methanol pool fire since the mass flow rate is easily controlled and constant over. But because the resulting particles of such a fire inhibit the use of Rayleigh scattering thermometry, a methanol pool fire had to be used when comparing temperatures obtained using ps-LIDAR with simulated temperatures.

The agreement between the traditional thermocouple measurements and FDS simulations were well within 20%, and typically FDS has been shown to predict similar scenarios with similar accuracy (McGrattan et al., 2014a). Hence the validation exercise was considered a success.

8.2 Ventilation system behavior

To be able to validate ventilation system behavior under fire conditions requires rather specific experimental scenarios; a large scale fully enclosed space connected to a well characterized ventilation system. Fortunately, a range of tests with these characteristics were performed within the PRISME project. This work was a part of a larger effort (Audouin et al., 2011a; Audouin et al., 2011b, 2013; Klein-Heißling et al., 2010; Melis & Audouin, 2008; Nasr et al., 2011; Pretrel & Audouin, 2010; Pretrel & Audouin, 2011; Rigollet & Röwekamp, 2009; van Hees et al., 2011) to quantify comparisons between several computational results and measurements performed during a pool fire scenario in a well-confined compartment with forced ventilation.

Paper II details the experimental scenarios used, but in general all scenarios were large-scale, mechanically ventilated, tightly sealed enclosures. Since the ventilation system behavior was of primary interest the fire source was prescribed using the experimental data. Using a non-prescribed fire source would introduce two unknown variables at the same time making it extremely difficult to draw any conclusions regarding the validity of the HVAC model in FDS. This so called building-block approach is also strongly recommended by AIAA (1998).

8.2.1 Experimental setup

The experimental scenarios were conducted at the French "Institut de Radioprotection et de Sûreté Nucléaire" (IRSN) between 2007 and 2011. The DIVA facility (see Figure 11) is located in the IRSN laboratories within a facility known as JUPITER (Audouin et al., 2011b, 2013). This facility offers a large-scale multi-room set-up comprising four rooms (labeled from 1 to 4) and a corridor in 0.3 m thick concrete walls equipped with a mechanical ventilation system. The facility can be used both with a single room-setup as well as combinations of connected rooms and a connecting corridor. Inlet and exhaust ducts are normally situated in the upper part of each room, near the ceiling, unless changed for specific tests. The complete ventilation system is a very complex installation with extensive use of valves and bends as well as changes in duct dimensions to be able to control the flow and air resistance to each branch and room. All scenarios used in this validation study were performed in the DIVA facility.

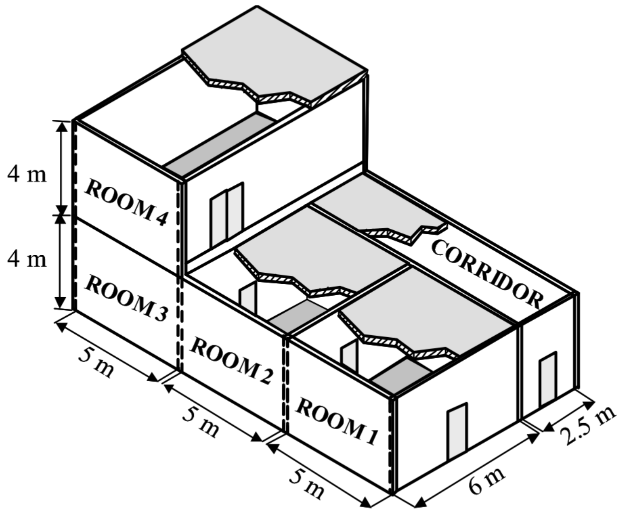


Figure 11 Schematic of the DIVA facility. Figure courtesy of IRSN.

In total 4 different test series focusing on large-scale, well-confined, mechanically ventilated fire scenarios were performed within the PRISME project, but only three of these were used to validate the ventilation system behavior since that last test series, called Integral, added unwanted complexity. An overview of the project was published for public access (Audouin et al., 2011b, 2013), but a short summary of the test series used for this validation study are presented here.

PRISME Source (SI); tests with a pool fire in one ventilated enclosure. The purpose of the PRISME Source program was to study fire behavior in an enclosure, at several different air renewal rates. Since some tests were similar with only minor changes (height placement of inlet branch) only 4 tests in total were compared to simulations performed with FDS. The pool fires were run within one (room 2) of the DIVA facility for the chosen tests. The different experimental setups have been described more in detail by Audouin et.al (2011a, 2011b, 2013). Paper II (Wahlqvist, Van Hees; 2013) gives an overview of the 4 tests conducted in this series that was chosen for further study.

PRISME Door (D); tests with a pool fire in one mechanically ventilated room connected to one or two mechanically ventilated room or rooms. The purpose of the PRISME Door test series consisted of studying the heat transfers of hot gases and smoke from the source room containing the fire towards the target rooms by "natural convection" mode, i.e. leaving a door completely open between the rooms. Thermal targets were placed in the rooms in order to simulate cable trays and the functional response of the cables, although this was not the focus of this work. The experimental setups were described by Audouin et.al (2011b, 2013) as well as Le Saux et al. (2008). Paper II (Wahlqvist, Van Hees; 2013) also gives an overview of the tests conducted in this series that was chosen for further study.

PRISME Leak (LK); tests with a pool fire in one room connected to other rooms by means of several types of leakages. The Leak test series focused on leakages between fire room and adjacent room. Two tests from this series were chosen since they were the most suitable for this study. The excluded tests included more complex leak flow mechanisms that would only aggravate the intended application of predicting the ventilation system behavior. More detailed work done on the experimental and theoretical aspect of parts of this tests series has been published for public access (Audouin et al., 2011b, 2013; Pretrel & Audouin, 2010). The two chosen scenarios were:

- Two circular ducts, one located in the upper part of the fire room close to the ceiling and the other located in the lower part of this last near the floor.
- A real fire resistance door with leakage around the borders.

The main characteristics of all the selected tests are available in Table 2. The pool fire fuel used was TPH (Hydrogenated Tetra-Propylene, $C_{12}H_{26}$) for all cases. Figure

12 demonstrates the two different intake positions (high/low) that were varied between tests.

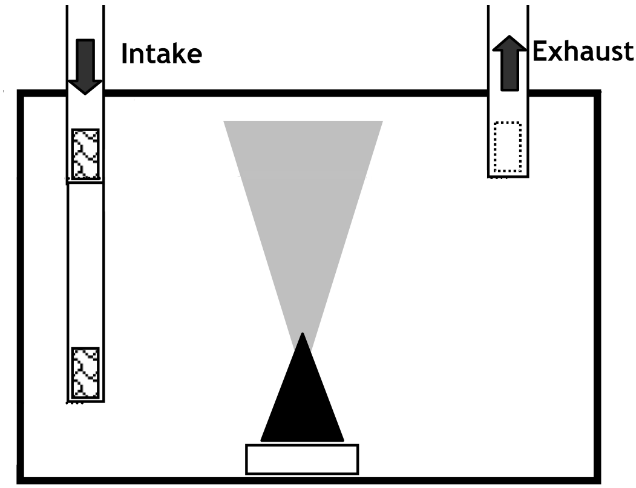


Figure 12 Schematic of a one room test set-up with position of fire and ventilation (both "high" and "low" position of intake is shown). Figure courtesy of IRSN.

Test	Pool area [m²]	Flow in and out [m³/h]			Position air inlet	Number of rooms
		R1	R2	R3		
SI-D1	0.4	-	560	-	High	1
SI-D2	0.4	-	1020	-	High	1
SI-D3	0.4	-	180	-	High	1
SI-D6a	0.4	-	200	-	Low	1
D2	0.4	180	170	-	High	2
D3	0.4	565	565	-	High	2
D4	0.4	1000	1000	-	High	2
D5	1	570	570	-	High	2
D6	1	550	550	550	High	3
LK1	0.4	1820	375	-	High	2
LK3	0.4	1915	365	-	High	2

Table 2 Overview of the test series in the PRISME project used for validation purposes.

8.2.2 Simulation setup

All simulations were done using self-compiled version of FDS 6.0.0 (SVN 11220) since the latest officially released version at the time (FDS5.5.3, SVN 7031) did not have the full functionality for simulating the HVAC network. The ventilation system was modeled by using the techniques discussed in 6.2, which meant that the ventilation system was simplified by using nodes and flow resistance between nodes. Fans were modeled by using the quadratic fan model (6.2.2) as they could be fitted to the actual fan curve.

The calculated total leakage area of the DIVA facility was in the order of 2-8 cm^2 depending on the configuration (amount of rooms). This was considered to be a very tightly sealed structure compared to “normal” leakage classes specified in the in the SFPE handbook (DiNenno, 2002) which would give a total leak area of about 135 cm^2.

The mass loss rate calculated from the experimental data (Le Saux et al., 2008; Pretrel et al., 2005) was used as input for all simulations without smoothing. No smoothing was used since filtering the fluctuations too much could end up removing certain phenomena that are dependent on short pressure peaks, such as back flow in the inlet/inlets.

8.2.3 Results

The results have been divided into two sub-sections since they served two different purposes. Firstly, simulations of the initial conditions without any fire present was first made to make sure that the ventilation system behaved as intended under normal operating conditions. Once that was confirmed, the fire scenario was simulated using the same ventilation system configuration without any changes.

8.2.3.1 Initial conditions

Initial conditions in this context are defined as the state of the ventilation system prior to any event taking place, such as a fire breaking out, and it is characterized by the pressure and volume flow in each node in the system. To predict the initial conditions accurately was an important step for giving confidence in the HVAC model, which was needed to continue with the fire scenarios and try to model more advanced HVAC system behavior. In general all predicted pressure and volume flow data are within 10% of the experimental data, and in most cases less as seen in seen in Table 3-Table 6.

	Difference between experiment and simulation [%]			
Node	SI-D1	SI-D2	SI-D3	SI-D6a
N7 (R2 in)	15.5	3.8	9.2	1.4
N15 (R2 out)	0.7	0.3	1.5	1.9

Table 3 Comparison of the volume flow at inlet and outlets in the HVAC system prior to ignition for the PRISME Source tests.

	Difference between experiment and simulation [%]						
Node	D2	D3	D4	D5	D6	LK1	LK3
N6 (R1 in)	-0.3	0.4	1.8	-0.3	-0.3	-	-
N7 (R2 in)	-0.3	0.4	1.8	-0.3	-0.2	0.6	1.8
N8 (R3 in)	-	-	-	-	-0.2	-0.9	1.5
N14 (R3 out)	-	-	-	-	0.7	2.7	-6.4
N15 (R2 out)	9.5	3.6	0.7	2.9	0.7	2.5	2.7
N16 (R1 out)	9.5	3.6	0.8	2.9	0.1	-	-

Table 4 Comparison of the volume flow at inlet and outlet nodes in the HVAC system prior to ignition for the PRISME Door and Leak tests.

	Difference between experiment and simulation [%]			
Node	SI-D1	SI-D2	SI-D3	SI-D6a
N7 (R2 in)	-4.9	0.5	0.1	-0.4
N15 (R2 out)	0.2	-2.6	-0.03	-0.3

Table 5 Comparison of the pressure at inlet and outlet nodes in the HVAC system prior to ignition for the PRISME Source tests.

	Difference between experiment and simulation [%]						
Node	D2	D3	D4	D5	D6	LK1	LK3
N6 (R1 in)	-0.8	0.3	-2.4	-1.2	-1.1	-	-
N7 (R2 in)	-0.8	0.3	-2.5	-1.2	-0.9	0.2	0.05
N8 (R3 in)	-	-	-	-	-0.9	-3.5	0.05
N14 (R3 out)	-	-	-	-	-3.4	0.2	-0.04
N15 (R2 out)	0.2	0.3	-1.4	-0.9	-3.4	0.2	-0.05
N16 (R1 out)	0.2	0.3	-1.4	-0.9	-4.5	-	-

Table 6 Comparison of the pressure at inlet and outlet nodes in the HVAC system prior to ignition for the PRISME Door and Leak tests.

8.2.3.2 Fire conditions

Overall FDS manages to predict the pressure and volume flows qualitatively well as seen in Table 7 and Table 8, with both behaving similar to the experimental data. However, there were two cases that showed larger discrepancies which are discussed in this section. Due to the large amount of graphs produced in this validation study only a few typical examples are shown here, as well as cases that showed anomalies and were later discussed. Paper II presents a more comprehensive set of data.

Scenario	Initial peak pressure [Pa] (exp./ FDS)	Quasi steady-state pressure [Pa] (exp./ FDS)	Initial peak inlet flow [m³/s] (exp./ FDS)	Quasi steady-state inlet flow [m³/s] (exp./ FDS)	Initial peak outlet flow [m³/s] (exp./ FDS)	Quasi steady-state outlet flow [m³/s] (exp./ FDS)
SI-D1	469.4/ 488.6	61.1/ 68.0	-0.12/ -0.23	0.13/ 0.14	0.21/ 0.23	0.19/ 0.20
SI-D2	329.9/ 316.6	22.3/ 9.3	-0.07/ -0.24	0.23/ 0.24	0.40/ 0.41	0.38/ 0.39
SI-D3	2852.0/ 1779.2	-*	-0.21/ -0.28	-*	0.12/ 0.11	-*
SI-D6a	3075.2/ 2552.8	-*	-0.217/ -0.25	-*	0.14/ 0.12	-*
D2	673.9/ 997.9	-130.6/ -116.6	-0.035/ -0.052	0.046/ 0.047	0.13/ 0.15	0.050/ 0.062
D3	388.9/ 529.4	-6.6/ -4.2	0.028/ -0.089	0.14/ 0.14	0.22/ 0.24	0.18/ 0.20
D4	87.7/ 123.0	-47.9/ -41.1	0.15/ 0.077	0.23/ 0.24	0.23/ 0.24	0.36/ 0.36
D5	1373.8/ 1338.2	-45.4/ -21.6	-0.25/ -0.25	0.14/ 0.14	0.32/ 0.32	0.19/ 0.21
D6	790.0/ 769.2	95.0/ 80.2	-0.14/ -0.16	0.11/ 0.11	0.24/ 0.26	0.202/ 0.23
L1	781.3/ 759.1	191.1/ 172.5	-0.082/ -0.24	0.38/ 0.38	0.86/ 0.94	0.87/ 0.92
L3	789.1/ 833.7	315.6/ 307.9	0.16/ 0.035	0.40/ 0.40	0.86/ 0.93	0.94/ 1.01

Table 7 Experimental and predicted (10 cm grid) ventilation system results in the fire room for the PRISME tests. *No quasi steady-state phase was present.

Scenario	Initial peak pressure [%]	Quasi steady-state pressure [%]	Initial peak inlet flow [%]	Quasi steady-state inlet flow [%]	Initial peak outlet flow [%]	Quasi steady-state outlet flow [%]
SI-D1	4.1	11.2	-98.3	5.6	11.2	7.3
SI-D2	-4.0	-58.5	-220.6	2.0	2.8	1.8
SI-D3	-37.6	-*	-37.4	-*	-9.3	-*
SI-D6a	-17.0	-*	-19.0	-*	-15.1	-*
D2	48.1	-10.7	-49.4	2.4	21.6	24.2
D3	36.2	-36.4	-416.0	3.0	13.5	6.6
D4	40.6	-14.3	-49.8	1.2	7.2	0.6
D5	-2.6	-52.5	-0.8	-1.3	0.6	8.3
D6	-2.6	-15.6	-18.0	1.4	6.5	10.8
L1	-2.8	-9.7	-192.8	-1.4	9.4	5.1
L3	5.7	-2.4	-77.8	-1.6	8.8	7.8

Table 8 Relative difference between the experimental and predicted ventilation system values in the fire room for the PRISME tests. *No quasi steady-state phase was present.

Source D1 and Source D2 were predicted qualitatively well, with both pressure and volume flows behaving similar to the experiments. A typical result, taken from the test Source D2, is shown in Figure 13 and Figure 14. Figure 13 shows that the pressure peaks caused by the fire is predicted, and Figure 14 shows that the ventilation system responds appropriately with reduced inlet flow and increased outlet flow due to the increased pressure. The fact that the flow of the inlet was reversed was also predicted, which is a key factor in predicting secondary damage due to smoke spread in the ventilation system. However, even though the initial pressure peak was predicted within 5% for both these cases, the reduction of the inlet flow is over-predicted by about 100-200% while the outlet flow is more accurate in magnitude (3-11%). This behavior seems to be general for all cases, which means that FDS likely will over-predict the amount of combustion gases being spread through the inlet system.

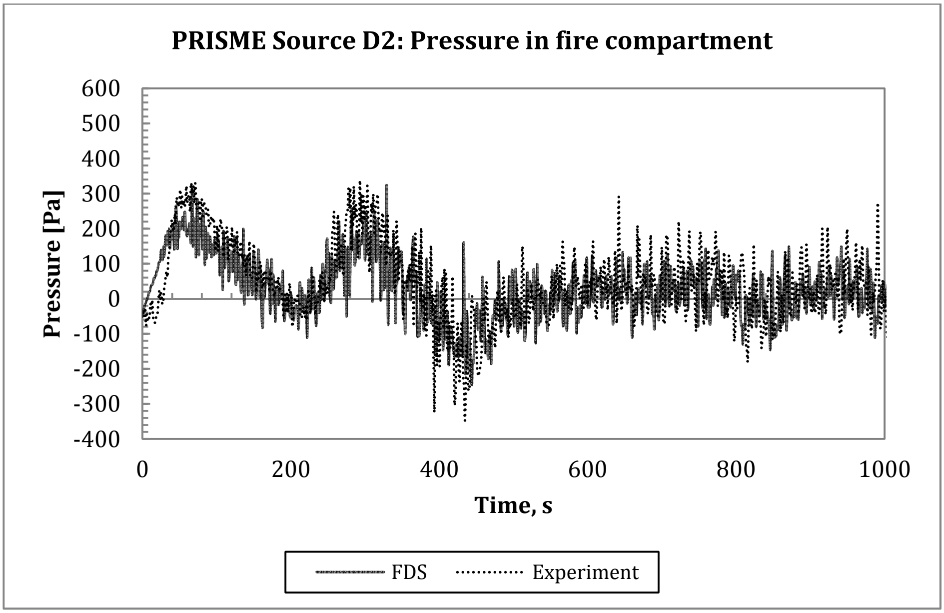


Figure 13 The predicted pressure inside the fire compartment compared to the experimental data from test Source D2 (SI-D2).

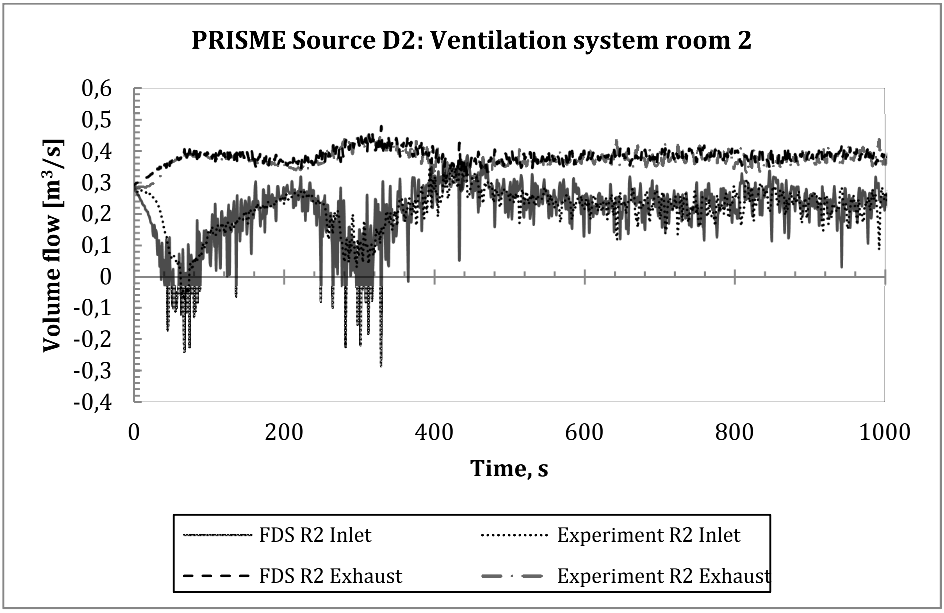


Figure 14 The predicted flow rates at inlet and exhaust in the fire compartment compared to the experimental data from test Source D2 (SI-D2).

As mentioned earlier there were two cases that were not qualitatively, or quantitatively, well predicted; Source D3 as well as Source D6a. In the case Source D3 the magnitude of the pressure peaks are not well captured, underestimating the first pressure peak by almost 1000 Pa as seen in Figure 15. Looking at the ventilation results for the same case (Figure 16) it is evident that the inlet starts to reverse under less pressure than in the experiment. The inlet acts as a pressure relief, making the predicted pressure peak much lower. The most probable cause is some discrepancy in the experimental data used for calculating the loss coefficients in the inlet branch. The fact that the temperatures inside the fire compartment were in good agreement with the experimental data supports this hypothesis and the same can be said for the case Source D6a. The noted discrepancies were inconsistent volume flow measurements in branches (not the same inflow as outflow) and pressure measurements that did not logically decrease or increase, both of which will influence calculated loss coefficients. Changing values for certain loss coefficients would probably result in a better match with experiments, but these two cases serve as good examples of how sensitive the input data can be and how hard it can be to perform measurements.

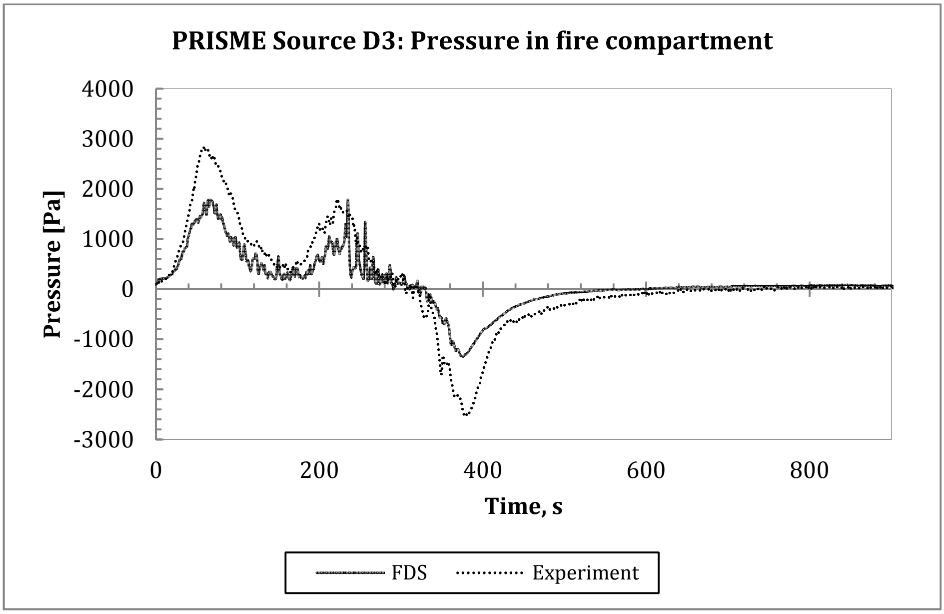


Figure 15 The predicted pressure inside the fire compartment compared to the experimental data from test Source D3 (SI-D3).

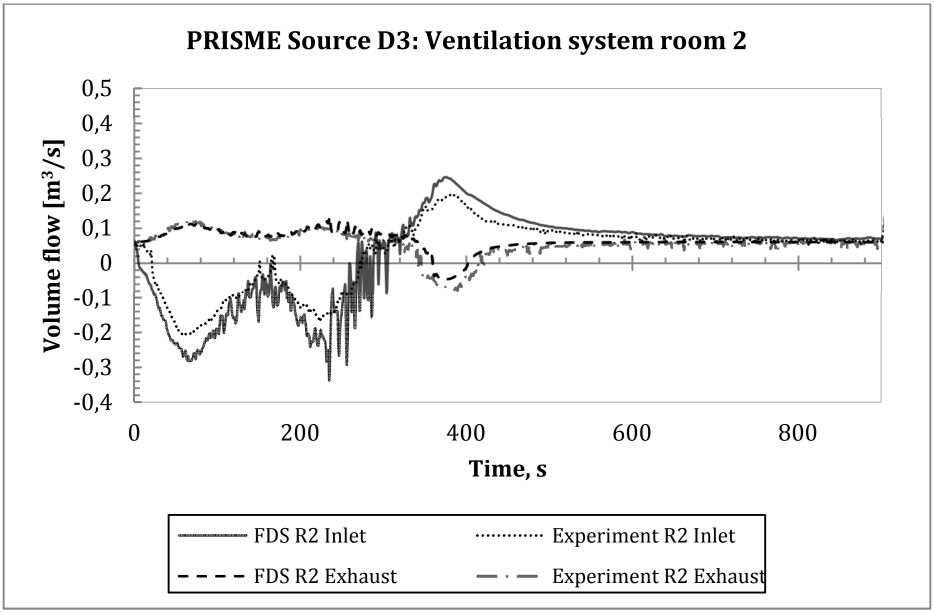


Figure 16 The predicted flow rates at inlet and exhaust in the fire compartment compared to the experimental data from test Source D3 (SI-D3).

The Door tests added additional complexity by adding one or two more rooms connected to the fire room, each room having individual inlet and outlet dampers which further upstream were connected to the same duct network branch. The general result is demonstrated in Figure 17, Figure 18 and Figure 19, which is the result for test Door D5. Here it can be seen that the pressure peak in the fire room (Figure 17) is correctly predicted, and the ventilation system response is also predicted in both rooms. This is a requirement for engineering applications since ventilation systems often serve many rooms/fire cells which are being connected to the same duct network.

The prediction of the initial pressure peak in the Door tests is over-predicted with about 36-48% in D2, D3 and D4 and under-predicted by about 3% in D5 and D6. The discrepancy for tests D2 and D3 is due to rapidly fluctuating pressure peaks in the predicted data which is not present in the experimental data. This could be due to the combustion model in FDS which can cause irregular combustion due to lack of oxygen, but could also be due to dampening of the pressure sensor used in the experiments which is not present in FDS. The inlets and outlets behave similar to the Source tests, as in the inlet flow is over-predicted while the outlet flow is generally well predicted.

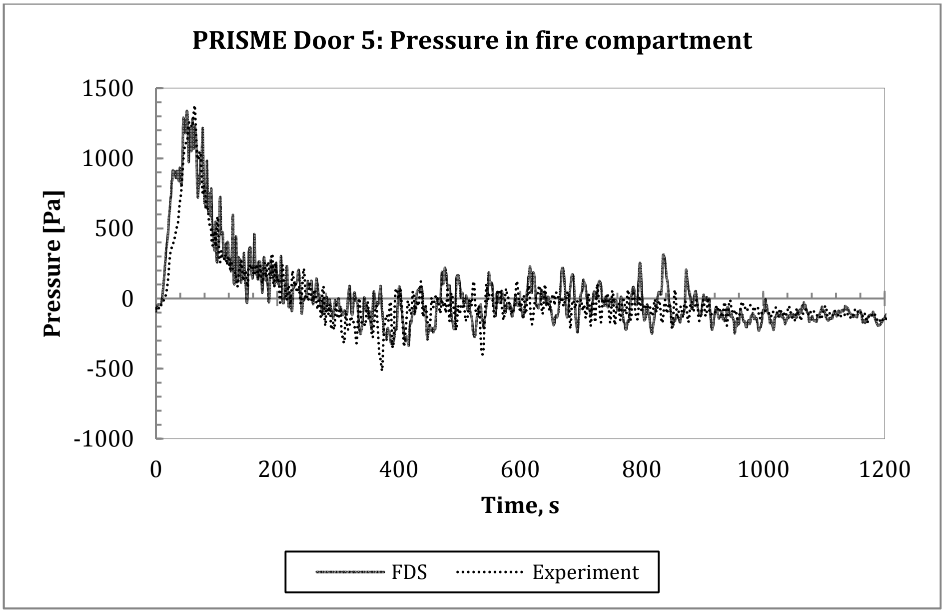


Figure 17 The predicted pressure inside the fire compartment compared to the experimental data from test Door 5 (D5).

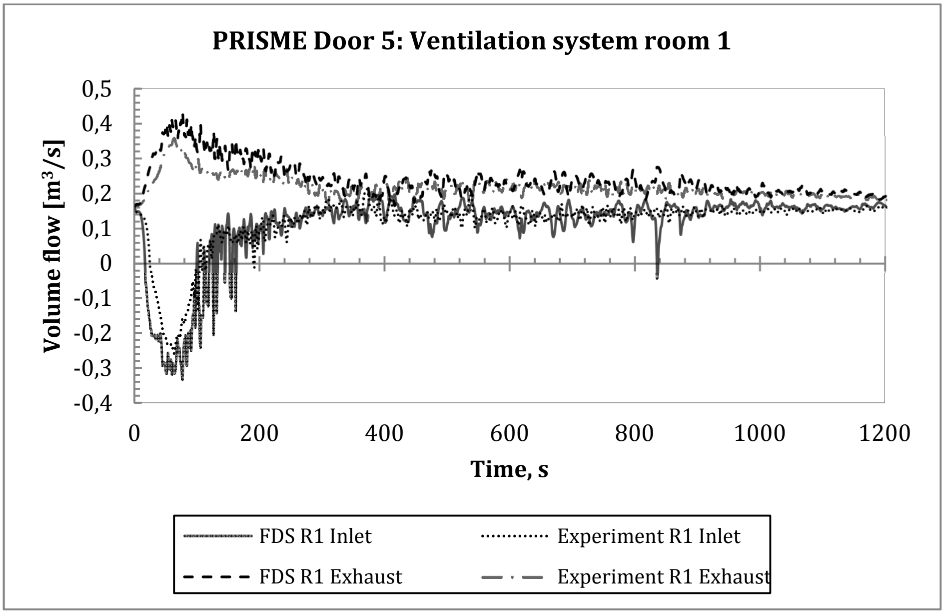


Figure 18 Predicted flow rates at inlet and exhaust in the fire compartment compared to the experimental data from test Door 5 (D5).

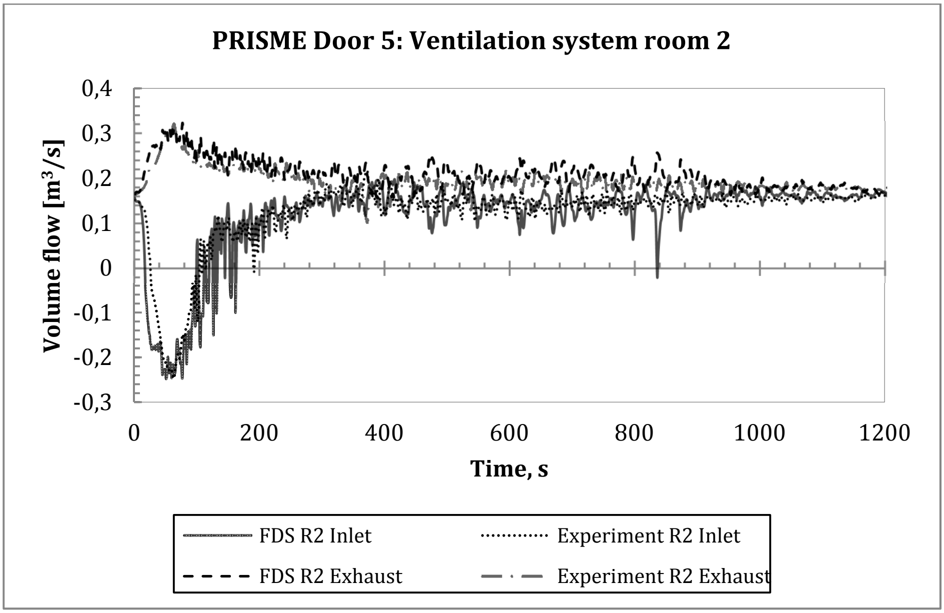


Figure 19 The predicted flow rates at inlet and exhaust in the fire compartment compared to the experimental data from test Door 5 (D5).

The Leak test series added even greater complexity due to a secondary pathway for smoke spread and pressure relief, other than the ventilation system, through different kinds of leakages typically present in a nuclear power plant or similar settings. The results for the Leak test series were similar to the other two test series; the predicted pressure inside the fire room and connected room was predicted within 6%, the reduction in inlet volume flow was over-predicted (78-193%) and the increase in outlet flow was predicted within 8%. An example of the results, taken from Leak 1, can be seen in Figure 20, Figure 21 and Figure 22. The overall results indicate that the ventilation system model does perform equally well with added complexity.

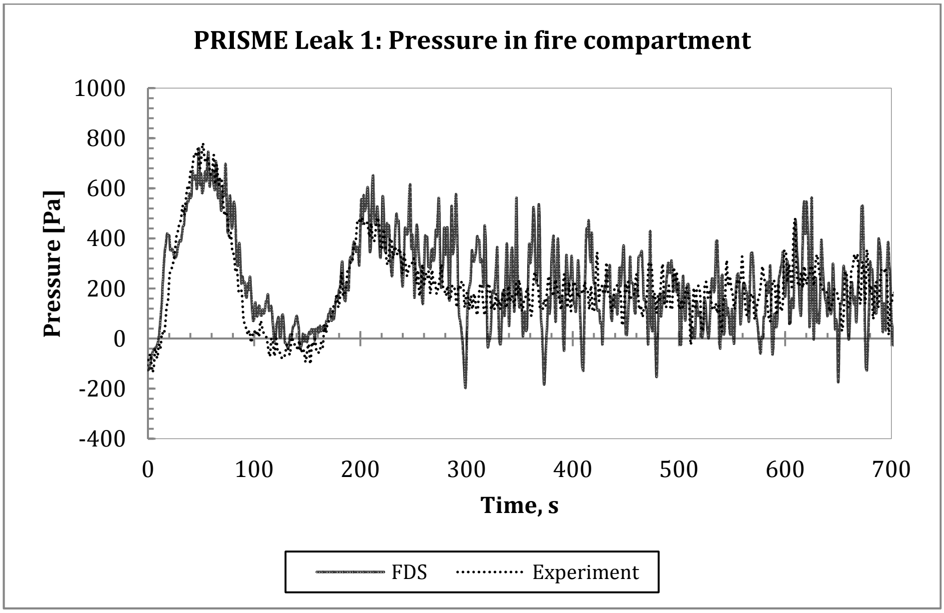


Figure 20 Predicted pressure inside the fire compartment compared to the experimental data from test Leak 1 (LK1).

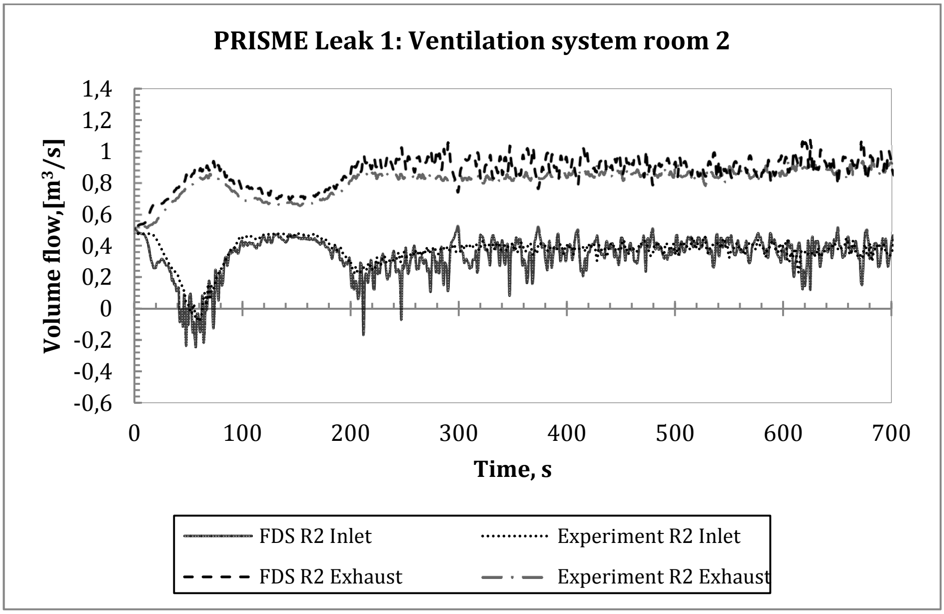


Figure 21 The predicted flow rates at inlet and exhaust in the fire compartment compared to the experimental data from test Leak 1 (LK1).

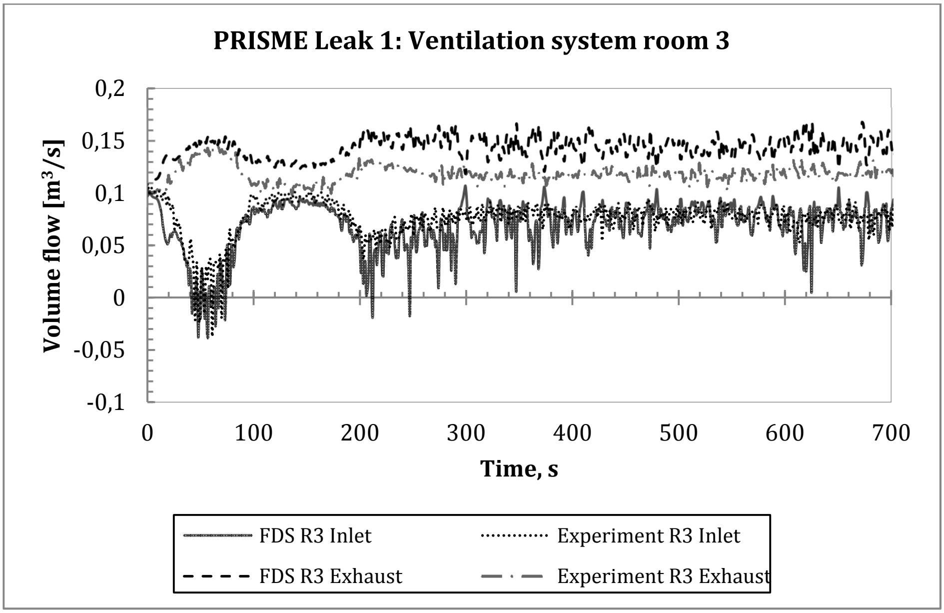


Figure 22 The predicted flow rates at inlet and exhaust in the fire compartment compared to the experimental data from test Leak 1 (LK1).

8.2.4 Conclusions

Predicting the outcome of a fire scenario consisting of a tightly sealed room or rooms connected to a mechanical ventilation network using FDS has been presented. Using data such as ventilation system specifications and material properties collected before the fire was ignited (with the exception of mass loss rate from the pool fire), FDS can be used to predict the pressure inside the fire room and consequently the effects on the ventilation system, for example backflow in the inlet branch in the early stages of the fire. However, it must be noted that the input parameters are quite sensitive, which could especially be seen in two tests where the loss coefficients of the inlet and exhaust branches were not correctly characterized. This caused FDS to inaccurately predict the magnitude of the pressure peak and subsequently the magnitude of the response of the ventilation system. Since it largely only affected two out of eleven scenarios it is very likely that this error was not due simplified representation of the ventilation system, but rather due to the measurement equipment.

It must be also noted that FDS consistently predicted a larger decrease of the inlet volume flow compared to the experimental data. This could be due to the fact that there is no time delay in the ventilation system response in FDS as no mass is being contained within the duct system, everything that comes in goes out somewhere else within the same time step. It can however not be ruled out that the difference is due to loss coefficients not being correctly calculated due to experimental measurement uncertainties. In an engineering application however, it can be argued that FDS will predict conservative values which can be considered beneficial in many applications.

8.3 Environmental feedback

To be able to fully validate the simplified environmental feedback model a range of different experiment scenarios would be required. It was desirable to first validate the model without any external radiation feedback present to focus on the oxygen depletion feedback model. It was then also desirable to have two different modes of ventilation for those cases, natural and mechanical, since they both can be present in an engineering application. Lastly it was required to have an experimental scenario where the surrounding temperatures reached high enough temperatures to warrant external radiative heat flux back to the fuel surface. Having an experimental scenario where only external radiative feedback was present was not seen as required since very high temperatures without lowered oxygen levels was deemed improbable.

To fulfil all of these requirements two different test series were used. Firstly, a steel ship compartment scenario performed by Peatross et al. (1993) in a closed off section of a ship. This scenario had several configurations containing either natural or forced ventilation, varying levels of oxygen concentration and no external radiative heat flux was to be expected due to relatively low temperatures inside the compartment. The second test series that was found to be suitable was the PRISME project tests that was also used in chapter 8.2 to validate the ventilation system behavior. These tests all had mechanical ventilation, varying levels of oxygen concentration as well as some, although relatively low, expected external radiative heat flux feedback. However, to include a scenario where significant levels of external radiative heat flux was present a test from the PRISME Integral test series was added.

8.3.1 Experimental setup

As mentioned, two different sets of experiments were used, each with different range of complexity and challenges and mechanisms of interest. Each test will be explained further in detail in the following sections, but the main characteristics of the tests are presented in Table 9.

Test name	Characteristics	Fire source	Mechanisms of interest
Steel ship compartment (Peatross et al., 1993)	Single room with natural opening; single room with mechanical ventilation and a natural opening.	Pool fire (diesel), 0.302 m^2 and 0.554 m^2.	Interaction between the fire source and natural ventilation; interaction between the fire source and mechanical ventilation; oxygen depletion; possible external radiation from enclosure boundaries and smoke layer due to high temperatures.
PRISME Source D1, D2, D3 (Audouin et al., 2011b, 2013)	Closed single room with mechanical ventilation, different ventilation volume flow for each case.	Pool fire (hydrogenated tetra-propylene), 0.4 m^2.	Interaction between the fire source and mechanical ventilation; oxygen depletion; possible external radiation from enclosure boundaries and smoke layer due to high temperatures.
PRISME Door D5 (Audouin et al., 2011b, 2013, Le Saux et al., 2008)	Two closed compartments with mechanical ventilation connected through a door opening.	Pool fire (hydrogenated tetra-propylene), 1.0 m^2.	Interaction between the fire source and mechanical ventilation; oxygen depletion; probable external radiation from enclosure boundaries and smoke layer due to high temperatures.
PRISME Integral INT1 (Audouin et al., 2011b, 2013, Pretrel & Audouin, 2011)	Three closed compartments with mechanical ventilation connected through door openings.	Pool fire (hydrogenated tetra-propylene), 1.0 m^2.	Interaction between the fire source and mechanical ventilation; oxygen depletion; probable external radiation from enclosure boundaries and smoke layer due to high temperatures.

Table 9 Overview of the experiments used in the validation study of the environmental feedback model.

8.3.1.1 Steel ship compartment experiments

A number of experiments with various fuels and ventilation conditions were carried out by Peatross, Beyler and Back in a closed off section of a ship (Peatross et al., 1993). The test compartment was approximately 3.4 m x 3.3 m x 3.05 m (W x D x H) and had solid steel walls, ceiling and floor which varied between 12.7 and 15.9 mm in thickness. Four different fire sources were used; 62 cm diameter diesel pool, 84 cm diameter diesel pool, polyurethane slabs and wood cribs but this study was based only on the pool fire tests. The ventilation conditions were varied in 6 different ways; naturally vented door opening, naturally vented ¼ door opening, naturally vented window opening and three different mechanically (forced) vented scenarios with different flow rates (but with the same passive outlet opening size). Gas temperatures, surface temperatures (back and front sides), incident heat fluxes, oxygen concentrations, carbon dioxide concentrations, carbon monoxide concentrations, unburned hydrocarbons concentrations and fuel mass loss were measured in all tests. For more details on the experimental setup please refer to (Peatross et al., 1993; Peatross & Beyler, 1997). Table 10 outlines the details of the scenarios that were used for validation purposes.

Scenario	Fire source	Ventilation conditions
S101	62 cm diesel pool	Natural, 0.9 x 2.0 m door opening
S102	84 cm diesel pool	Natural, 0.9 x 2.0 m door opening
S105	62 cm diesel pool	Natural, 0.8 x 0.8 m window opening
S107	84 cm diesel pool	Natural, 0.8 x 0.8 m window opening
S111	62 cm diesel pool	Natural, 0.225 x 2.0 m ¼ door opening
S112	84 cm diesel pool	Natural, 0.225 x 2.0 m ¼ door opening
S201	62 cm diesel pool	Forced, 0.38 m^3/s (0.3 x 0.3 m outlet)
S203	84 cm diesel pool	Forced, 0.38 m^3/s (0.3 x 0.3 m outlet)
S207	62 cm diesel pool	Forced, 0.61 m^3/s (0.3 x 0.3 m outlet)
S208	84 cm diesel pool	Forced, 0.61 m^3/s (0.3 x 0.3 m outlet)
S210	62 cm diesel pool	Forced, 0.25 m^3/s (0.3 x 0.3 m outlet)
S211	84 cm diesel pool	Forced, 0.25 m^3/s (0.3 x 0.3 m outlet)

Table 10 Specifications of the scenarios selected for validation purposes from the steel ship compartment experiments.

As mentioned diesel was used as fuel, but since diesel is not a well-defined substance the exact composition of the fuel was not known. In the report by Peatross et al. (1993), they approximate the chemical composition to $C_{10}H_{19}$ and the heat of combustion to 45 000 kJ/kg; both these values were used in the FDS simulations. The boiling temperature was assumed to be 288 degrees Celsius and the heat of vaporization was set to 235 kJ/kg. No total fuel mass was specified for the tests so all simulations used 1000 kg fuel to avoid pre-mature burnout.

No actual free burning mass loss data was provided for these fuel sources, so they were approximated from the two tests that were most similar to free burning conditions (S101 and S102). This procedure was motivated by the fact that the oxygen levels at the lower positions did not change significantly within the time frame of the growth phase (Peatross et al., appendix A, 1993). This resulted in mass loss rate inputs that were approximated to be 10 g/s and 20 g/s respectively, both linearly increasing from 0 g/s over 200 seconds according to the experiments.

8.3.1.2 PRISME experiments

All experiments, but one, used for the validation study have been already been specified in chapter 8.2. The additional test added was PRISME Integral (INT) 1 (Pretrel & Audouin, 2011), which was added due to the recorded temperatures being significantly higher and was therefore of interest when validating the external radiative heat flux feedback model. The purpose of the PRISME Integral test series was similar to the PRISME Door series, but with mechanical ventilation flows between rooms. Figure 23 illustrates the ventilation setup that was used, with the intake located in room 1 and the exhaust located in room 3. Other than the ceiling, some parts of the walls were insulated to protect the structure from thermal-induced damage, but also to increase the hot gas temperature. Both door openings had the dimensions of 0.7x2.1 m (width x height). The liquid pool was located in the center of the middle room (room 2), being slightly elevated due to being placed on a scale with insulation in between. For more information on the experimental setup refer to (Pretrel & Audouin, 2011).

The fuel used in all cases was HTP (Hydrogenated Tetra-Propylene, $C_{12}H_{26}$) and the heat of combustion was reported to be 42 000 kJ/kg. The boiling temperature was assumed to be 188 degrees Celsius and the heat of vaporization was set to 365 kJ/kg, both which were used in the external feedback model. The total fuel mass was between 14.6-15.9 kg in the PRISME Source cases and 15.9 kg in PRISME Door D5.

Free burning data was fully provided for PRISME Source D1 and in part for PRISME Leak 1 as a part of the PRISME program. For PRISME Source D1 two identical tests using HTP (same as in actual experiment) and a pool size of 0.4 m^2 (same as in actual experiment) were performed.

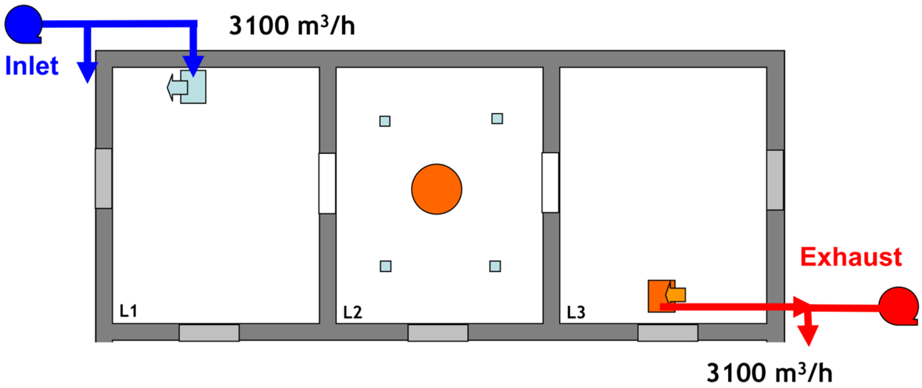


Figure 23 Schematic of the test PRISME Integral INT1 (seen from above). Figure courtesy of IRSN.

For PRISME Door D5 and PRISME Integral 1 there were two tests performed using the same pool size as the actual experiment (1.0 m^2) but with a slightly different fuel (dodecane instead of HTP; dodecane is an isomer of HTP). The burning behavior however was assumed to be similar since this had been shown in earlier tests. For this reason, this data was used to determine the free burning input. However, only one of the two free burning cases had a similar amount of total fuel (the two free burning cases had 8 kg and 18 kg fuel respectively) which drastically impacted the burning behavior as shown in Paper III. Hence only the data for the free burning case with the most fuel was used as basis for the FDS input data. The experimental measurements used for input was simplified by selecting critical points from the data set, and then using linear interpolation between the selected points. The actual input data used can be seen in the results section for each case.

8.3.2 Simulation setup

All simulations were done using a custom built version of FDS 6 (6.1.1, SVN 19953) with the simplified environmental feedback model implemented (described in chapter 4.3). For all cases, two different cell sizes were used in order to investigate the sensitivity of the results due to this parameter. The D*/dx value was calculated to get an idea of the resolution of the fire source as described in (McGrattan et al., 2014b). A uniform cell size was used in all cases. Table 11 outlines the cell size and resolution for the steel ship compartment scenarios, while Table 12 does the same for the PRISME scenarios.

Cell size	D*/dx, 62 cm diesel pool	D*/dx, 84 cm diesel pool
10 cm	7.0	9.2
5 cm	13.9	18.4

Table 11 Grid cell sizes used in FDS when simulating the steel ship compartment experiments.

As can be seen in Table 12 the general resolution is considered to be somewhat coarse for the PRISME test scenarios. However, using a 10 cm grid size has previously deemed giving acceptable prediction compared to the experimental data (Paper II, Wahlqvist & van Hees, 2013). The coarser mesh was used to investigate the sensitivity of the results.

Cell size	D*/dx, 0.4 m2 TPH pool	D*/dx, 1.0 m2 TPH pool
20 cm	3.88	5.84
10 cm	7.75	11.68

Table 12 Grid cell sizes used in FDS when simulating the PRISME experiments.

The ventilation system was modeled by using the techniques discussed in 6.2, as in every component of the ventilation system was not present, but rather simplified by using nodes and flow resistance between nodes. Fans were modeled by using the quadratic fan model (chapter 6.2.2) as described in chapter 8.2.2.

The needed fuel data for each case was based on the data given in the experimental specifications, and the needed "base" mass loss rate for each fuel source was taken from free burning mass loss rate experiments or experiments with very similar conditions (i.e. little to no change in oxygen volume fraction, no external radiative feedback).

8.3.3 Results

Since the objective of the paper was to predict the mass loss rate and the fire source interaction with the enclosure environment, most results presented concern the mass loss rate and the critical parameters which influence the mass loss; the oxygen volume fraction and external radiation onto the fuel surface. Due to the large number of graphs and data produced by the simulations only representative scenarios, as well as graphs needed as basis for discussion are shown here. However, Paper III adds further detail in this regard.

Due to some complications with the computer cluster used to do the simulations, some of the cases with refined meshes were not able to complete the full simulation time before being terminated. However, they were all considered to have been simulated long enough to compare with both the experimental data and the coarse mesh results of the same case.

8.3.3.1 Steel ship compartment

An overview of the results from the steel ship compartment experiments can be seen in Table 13. The overall agreement between the experimental data and the predicted values is acceptable with a few exceptions which will be discussed.

The mass loss rates were predicted within 3-25% in most cases for both the naturally ventilated cases and the mechanically ventilated cases. However, there were two cases that stood out with less accurate (36-40%) predictions; S111 and S112. Both of these cases were using the quarter door opening which could be part of the explanation; the grid is simply not fine enough to predict the flow through the quarter door opening correctly. These two cases were also the only cases too display large differences between the two different grid sizes which only reinforce the argument that the flow is not well resolved. In the coarse grid configuration there were only 2 grid cells spanning the total width of the opening which is most probably insufficient to accurately predict the inflow through the opening. With the refined grid there were 4 grid cells spanning the slot which was also assumed to be insufficient to render an accurate prediction. Two modifications were done on both these cases to investigate the influence on how the door slot was represented. These changes were based of the findings made in *CFD-beräkningar med FDS (Eng. CFD calculations using FDS)* (BIV, 2013) where it was observed that both wall/ceiling thickness and grid size affected flows through orifices when using FDS. First off, the thickness of the front wall was increased from 0 cm to 5 cm. The reason it initially was set to 0 cm was due to the fact that both the coarse and refined grid were still too coarse to accurately represent the real thickness of the wall (between 13-16 mm). What will probably happen in such a case (the wall is too thin) is that the flow contraction (vena contracta) is under-estimated since it behaves like flow through an orifice with a sharp edge, which means that the inflow probably is over-estimated, which in turn increases the mass loss rate due to more oxygen being available.

In the two cases S111b and S112b the thicker wall was added, which brought the predicted values closer to the experimental values. The prediction is however not as good as the rest of the cases, which is why a second modification was tested. Even if the flow contraction might be predicted a bit better with a thicker wall, it might still not be predicted well enough considering the sparse amount of cells in the opening slot. In many other applications a flow coefficient (a number between 0 and 1) is used to account for this effect, and a factor of 0.6-0.7 is commonly used in similar applications. Computational fluid dynamics software such as FDS does not generally rely on such empirical flow coefficients, but in *CFD-beräkningar med FDS (Eng. CFD calculations using FDS)* (BIV, 2013) it was observed that it might be necessary in cases where the grid is relatively coarse to not over-predict the flow through an opening. Applying this in both cases (S111 and S112) the door slot opening was instead modeled as 0.15 cm while keeping the wall thickness changed to 5 cm. The results with both these changes can be seen in Table 13 represented by case 111c and 112c. The predicted results are in better agreement (9-10%) with the experimental data, and in line with the other cases. Due to a current limitation in the external radiation model (not working over multiple meshes) it was unfortunately not possible to perform further refinements of the mesh in these cases. Combined with the fact that there were no detailed experimental measurements available that monitored the flow through the door slot, a more detailed study, both experimental and numerical, would be needed to determine the cause of the difference between the predicted and experimental values. However, it seems likely that the flow through the narrow slot is being over-predicted without the modifications. It is not believed that the discrepancy is due to the combustion process not being predicted well by FDS since the oxygen volume fraction in the lower part of the room is still 19% in the experiment.

The oxygen fraction at the lower part of the room was also largely in good agreement (2-8%) with the experimental data with two exceptions; again case S112 but also case S107. As stated above, the mass loss rate was over predicted in the cases S111 and S112, which would lead one to believe that the oxygen volume fraction would be over predicted on both these cases as well; but in case S111 the oxygen volume fraction is well predicted and case S112 is under predicted. The only reasonable explanation for this is two-fold; the oxygen volume concentration is overall not very well predicted due to the under resolved quarter door opening. Second, the experimental measurement was done in the corner of the room and the measured value is not representative of the actual oxygen volume fraction at the fuel base. The latter explanation can also be applied to case S107 which actually predicts the mass loss rate with satisfactory accuracy while the oxygen volume fraction in the bottom corner of the room is not well predicted. This could be due to the nature of the case; a relatively large fire with a relatively small opening placed in the center of the wall, both of which induces rather complex flows.

Scenario	**Mass loss rate [g/s]**		**Oxygen volume fraction [-] in lower part of the room**		**Oxygen volume fraction [-] in sampling volume**	**External radiative heat flux to fuel surface [kW/m²]**
	Experimental	FDS (10 cm/ 5 cm)	Experimental	FDS (10 cm/ 5 cm)	FDS (10 cm/ 5 cm)	FDS (10 cm/5 cm)
S101	8	9/9	0.205	0.21/0.21	0.2/0.2	0.0/0.0
S102	19	18/18.5	0.2	0.205/ 0.205	0.195/0.2	0.0/0.0
S105	8	7/7	0.185	0.19/0.185	0.18/0.18	0.0/0.0
S107	9	11/10	0.185	0.17/0.15	0.165/0.16	0.0/0.0
S111	5.5	7.5/8.5	0.19	0.19/0.185	0.18/0.195	0.0/0.0
S111b	5.5	-*/7.5	0.19	-*/0.17	-*/0.185	0.0/0.0
S111c	5.5	-*/6	0.19	-*/0.145	-*/0.17	0.0/0.0
S112	10	10/14	0.185	0.16/0.17	0.16/0.18	0.0/0.0
S112b	10	-*/12	0.185	-*/0.16	-*/0.165	0.0/0.0
S112c	10	-*/9	0.185	-*/0.14	-*/0.15	0.0/0.0
S201	5	5/5	0.175	0.175/ 0.175	0.16/0.16	0.0/0.0
S203	8	7.5/7.5	0.16	0.165/ 0.165	0.145/0.145	0.0/0.0
S207	6	6/6	0.185	0.19/0.19	0.165/0.165	0.0/0.0
S208	9.5	8.5/9.5	0.165	0.18/0.175	0.15/0.155	0.0/0.0
S210	4	5/5	0.17	0.165/ 0.165	0.16/0.16	0.0/0.0
S211	6	6/6	0.14	0.15/0.15	0.14/0.14	0.0/0.0

Table 13 Summary of the results from the steel ship compartment experiments. *Since the geometry changes made in these cases were not possible to make with a coarse grid no results were obtained.

Scenario	Mass loss rate [%]		Oxygen volume fraction on lower part of the room [%]	
	10 cm	5 cm	10 cm	5 cm
S101	12.5	12.5	2.4	2.4
S102	-5.3	-2.6	2.5	2.5
S105	-12.5	-12.5	2.7	0.0
S107	22.2	11.1	-8.1	-18.9
S111	36.4	54.5	0.0	-2.6
S111b	-*	36.4	-*	-10.5
S111c	-*	9.1	-*	-23.7
S112	0.0	40.0	-13.5	-8.1
S112b	-*	20.0	-*	-13.5
S112c	-*	-10.0	-*	-24.3
S201	0.0	0.0	0.0	0.0
S203	-6.3	-6.3	3.1	3.1
S207	0.0	0.0	2.7	2.7
S208	-10.5	0.0	9.1	6.1
S210	25.0	25.0	-2.9	-2.9
S211	0.0	0.0	7.1	7.1

Table 14 Relative difference between predicted and experimental values for the steel ship compartment scenarios. *Since the geometry changes made in these cases were not possible to make with a coarse grid no results were obtained.

The grid cell size dependency of the oxygen volume fraction and the resulting mass loss rate was in most cases relatively small, although there were yet again two instances where the differences were more noticeable; case S111, and even more case S112. This is yet again most likely due to the relatively poor resolution over the quarter door slot. This argument is enhanced by the fact that the larger fire (S112) induces larger differences between the two cell sizes due to its more turbulent behavior.

Temperatures inside the compartment were not high enough to generate external radiative heat flux enough to increase the mass loss rate in any case. Coupled with the estimated relatively high boiling point of the diesel fuel none of the simulated mass loss rates were affected by the external radiation which was to be expected.

8.3.3.2 PRISME

An overview of the results from the PRISME experiments can be seen in Table 15. The quasi steady-state mass loss rates were predicted within 2.5-25% in all cases except PRISME Source D3; the extinction was not predicted (Figure 24 and Figure 25). The only criterion for extinction included in the model is oxygen volume fractions below approximately 11 % and this criterion was not met. Looking at the oxygen volume fraction close to the fire source for this case, the predicted values are actually well predicted, and even a bit lower, though the reduction is not as rapid as in the experiment. There were some problems with the ventilation system response (which is discussed further down) which might explain some of the problems displayed. However, a more advanced model might capture extinction more accurately which would be of interest in future work. PRISME Door D5 also displayed some tendencies towards not being able to predict the extinguishing correctly but overall the results were better.

The initial phase of the fire was predicted within 0-30% regarding the magnitude. But temporally in the PRISME Source D2 the peak mass loss rate was predicted earlier than in the experiment and in the rest of the cases the peak mass loss rate time frame was longer than in the experiments (Figure 26). This could be due to an error in the prediction of the external radiative heat flux feedback which in turn is reliant on the prediction of the temperatures on the walls and smoke layer. Since the radiative heat flux is dependent on the temperature to the power of 4, a relatively small error can yield a rather big response in the resulting mass loss rate which should be taken into account. Surprisingly the case PRISME Door D5 did not render more radiative heat flux feedback despite having the larger fire source. This was probably due to three rooms being available for smoke spread which distributed the heat over a larger surface and mass.

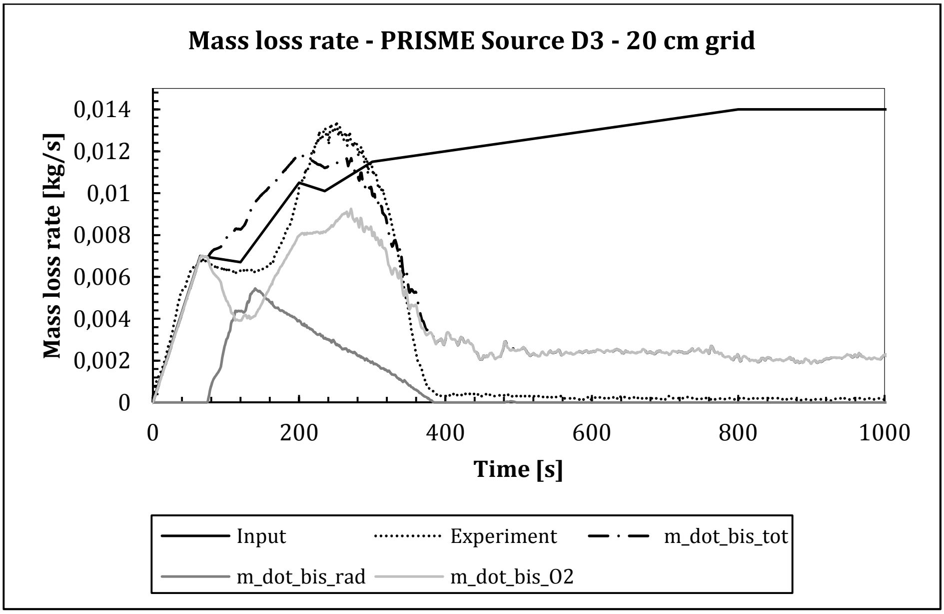


Figure 24 Comparison between the measured and predicted mass loss rates for PRISME Source D3 using 20 cm grid cells.

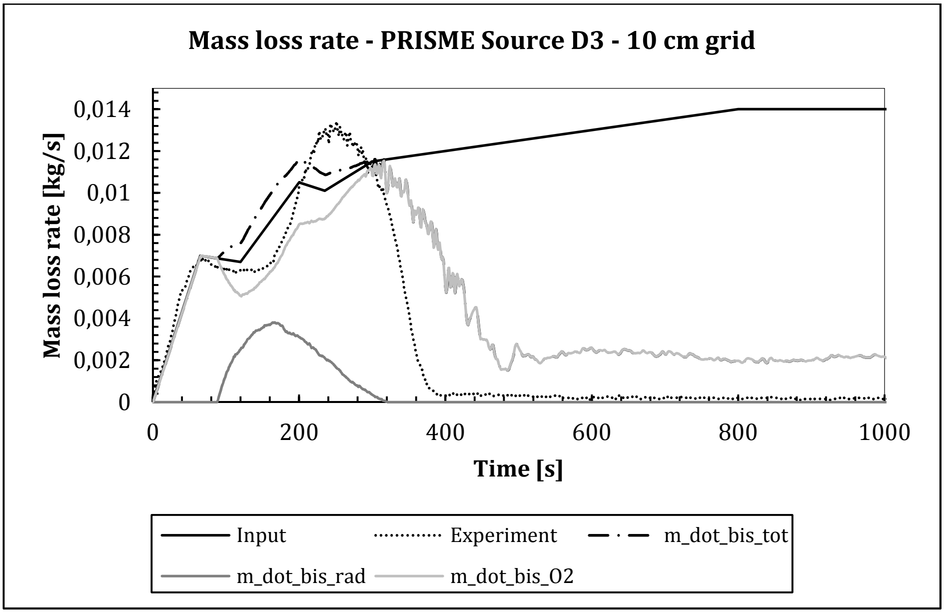


Figure 25 Comparison between the measured and predicted mass loss rates for PRISME Source D3 using 10 cm grid cells.

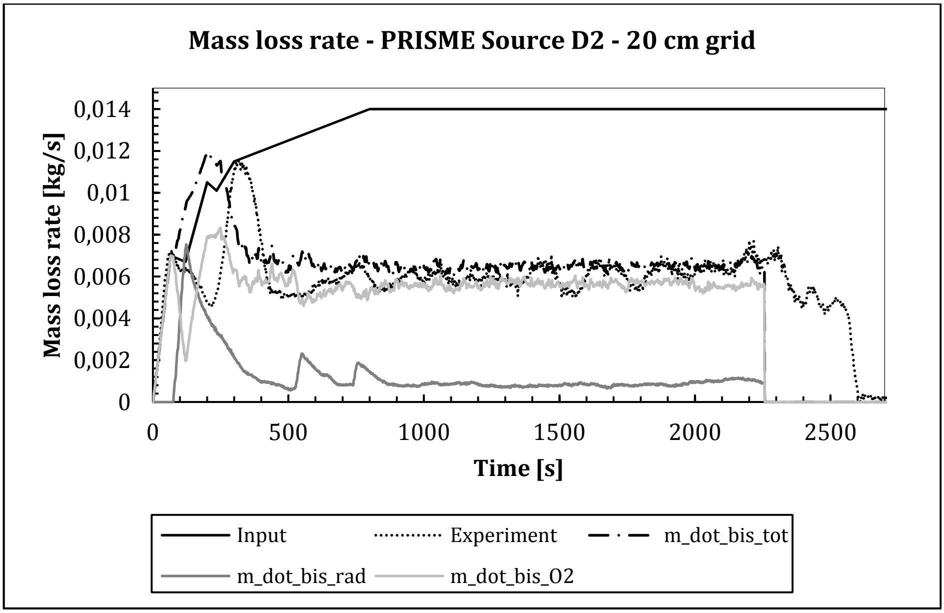


Figure 26 Comparison between the measured and predicted mass loss rates for PRISME Source D2 using 20 cm grid cells.

In PRISME Integral INT1, the initial peak mass loss rate was not as high as in the experiment but was well captured temporally, and the general behavior was relatively well predicted. The average mass loss rate in this case was also predicted well, but the sometimes fluctuating nature was not always well predicted, e.g. the sudden peaks seen in Figure 27 and Figure 28 at around 1200-1400 seconds. These strong and sudden peaks in the experimental data are believed to be caused by a decrease of the mass loss rate, which is then followed by an increase in inflow of fresh oxygen through the ventilation system due to lowered pressure inside the fire room. This in turn then rapidly increases the mass loss rate, but is yet again quickly dampened by the fact that the pressure in the fire room once limits the inlet flow. Looking at the transient ventilation and pressure data confirms this behavior; it is however not exactly known why the mass loss rate suddenly decreases after about 1200 seconds. PRISME Integral INT1 displayed by far the highest overall external radiative heat flux feedback to the fuel, and it was the only case where the radiative feedback was a main contributor to the mass loss rate. At 15 volume-% oxygen the mass loss rate would be approximately 15 g/s without external radiation. The case INT1 had an average mass loss rate of almost 40 g/s which indicates that about 60% of the mass loss rate was due to external radiation. This can be seen in Figure 27 and Figure 28, where about 60% of the mass loss rate is caused by radiation when

20 cm cells are used, and about 50% when 10 cm cells are used. Though the overall mass loss rate was well predicted in this case, the oxygen volume fraction close to the fire source was not, as seen in Table 15 (0.09 in the experiments, 0.14-0.15 predicted). This could be due to local sensitivity of this parameter in this specific case; the combination of a relatively high mass loss rate and low oxygen volume fraction could indicate that detachment of the flame from the fire source occurs, resulting in irregular flames or even ghosting flames which would affect the oxygen volume fraction very locally. Another possible explanation could be that the flame extinction model in FDS cannot predict the combustion under these specific conditions, which would affect the predicted oxygen volume fraction.

Table 15 & Table 16 legend:

*Extinction occurred before any quasi steady-state conditions were reached.

**No quasi steady-state conditions were reached so this value is an average over the latter part of the fire duration.

***The experiment recorded a very noisy mass loss rate which after the initial peak shifted between 20-50 g/s, this value is in the later part of the fire duration once the mass loss rate was somewhat stable.

****The oxygen concentration was never stable and almost constantly decreasing due to the relatively high mass loss rate, these values are an approximated average during the part with a relatively stable mass loss rate.

*****The radiation feedback to the fuel surface was increased over time without reaching a semi semi-state; these values are representative of the latter part of the fire duration.

	Source D1	Source D2	Source D3	Door D5	Integral INT1
Initial peak mass loss rate (exp./20 cm/10 cm) [g/s]	12/12/12	11.6/12/ 12	13.2/12/ 11.8	34/42/3 8	74/53/52
Quasi steady-state mass loss rate (exp./20 cm/10 cm) [g/s]	4/4.5/4	6/7/7	0*/2/2	8**/ 10/ 10	40**/ 39/ 37
Initial peak inlet flow (exp./20 cm/10 cm) [m^3/s]	-0.12/ -0.22/ -0.17	-0.07/ -0.15/ -0.1	-0.21/ -0.25/ -0.26	-0.26/- 0.33/- 0.24	-0.38/ -0.48/ -0.42
Initial peak outlet flow (exp./20 cm/10 cm) [m^3/s]	0.23/ 0.24/ 0.23	0.45/0.5/0 .45	0.12/ 0.12/ 0.10	0.36/ 0.38/ 0.32	1.48/ 1.73/ 1.68
Quasi steady-state inlet flow (exp./20 cm/10 cm) [m^3/s]	0.13/ 0.13/ 0.14	0.24/ 0.23/ 0.25	*	0.14/ 0.14/ 0.14	0.67**/ 0.75**/ 0.76**
Quasi steady-state outlet flow (exp./20 cm/10 cm) [m^3/s]	0.19/ 0.20/ 0.22	0.41/ 0.39/ 0.38	*	0.22/ 0.21/ 0.19	1.53**/ 1.72**/ 1.69**
Quasi steady-state volume fraction close to fire source (exp./20 cm/10 cm) [-]	0.14/ 0.13/ 0.135	0.16/ 0.15/ 0.15	0.124*/ 0.114/ 0.12	0.13/0.1 24/ 0.126	0.09****/0 .14****/0. 15****
Quasi steady-state volume fraction in sampling volume (20 cm/10 cm) [-]	0.135/ 0.14	0.155/ 0.155	0.12/ 0.12	0.134/ 0.138	0.14/ 0.16
Initial peak net radiative heat flux to fuel source (20 cm/10 cm) [kW/m^2]	2.8/ 1.9	2.7/ 1.4	1.9/ 1.4	3/0.8	7.0/ 5.6
Semi steady- radiative heat flux to fuel source (20 cm/10 cm) [kW/m^2]	0.7/ 0.0	0.3/ 0.5	0/ 0	0.3/ 0.0	8.4*****/6. 4*****

Table 15 Summary of the results for all PRISME scenarios.

	Source D1	Source D2	Source D3	Door D5	Integral INT1
Initial peak mass loss rate (20 cm/10 cm) [%]	0.0/0.0	3.4/3.4	-9.1/-10.6	23.5/11.8	-28.4/-29.7
Quasi steady-state mass loss rate (20 cm/10 cm) [%]	12.5/0.0	16.7/16.7	*	**25.0/25.0	**-2.5/-7.5
Initial peak inlet flow (20 cm/10 cm) [m^3/s]	83.3/41.7	114.3/42.9	19.0/23.8	26.9/-7.7	26.3/10.5
Initial peak outlet flow (exp./20 cm/10 cm) [%]	4.3/0.0	11.1/0.0	0.0/-16.7	5.6/-11.1	16.9/13.5
Quasi steady-state inlet flow (exp./20 cm/10 cm) [%]	0.0/7.7	-4.2/4.2	*	0.0/0.0	**11.9/13.4
Quasi steady-state outlet flow (exp./20 cm/10 cm) [%]	5.3/15.8	-4.9/-7.3	*	-4.5/-13.6	**12.4/10.5
Quasi steady-state volume fraction close to fire source (exp./20 cm/10 cm) [%]	-7.1/-3.6	-6.3/-6.3	*-8.1/-3.2	-4.6/-3.1	****55.6/66.7

Table 16 Relative difference between predicted and experimental values for the PRISME scenarios.

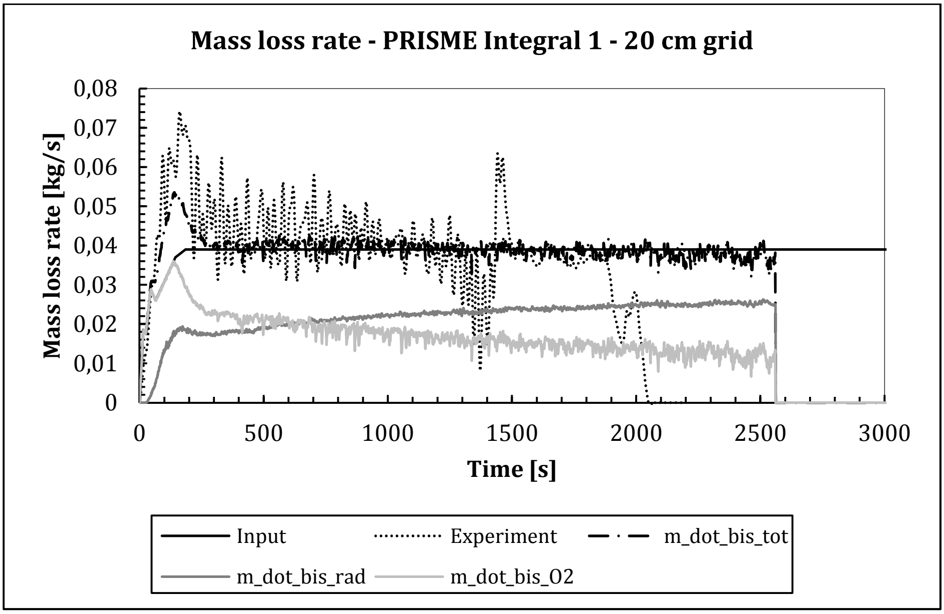


Figure 27 Comparison between the measured and predicted mass loss rates for PRISME Integral INT 1 using 20 cm grid cells.

An explanation for the initial under-estimation of the mass loss rate peak could be that the model cannot take into account a more intense flame than was originally present in the free burning case. This is due to the fact that only external radiative feedback is being included; a flame that yields higher radiative feedback to the fuel source than a free burning flame would, will not contribute any additional mass loss rate as the radiation from the flame itself is always excluded when calculating the external radiation. To be able to include the increased mass loss rate due to a more intense flame (which is not caused by elevated oxygen volume fractions, which could be included in Equation 1) an accurate prediction of the radiative feedback from the flame would have to be done. And if the radiative feedback from the flame could be accurately predicted it would probably be better to use a more advanced and complete pyrolysis model, as the one already included in FDS. But this would then elevate the requirements of the cell size used and increase the computational cost, which would be the opposite of the objectives if this work which aims to provide a practical engineering model. In certain scenarios this might be a significant limitation in the simplified model compared to a more advanced pyrolysis model. Since all other cases showed good agreement with the experimental data, it is believed that the INT1 case poses a more challenging scenario that would have to be investigated deeper, performing additional experiments with detailed measurements of the radiative feedback to the pool surface to draw any final conclusions. However, since the overall behavior was well predicted, the performance of the proposed simplified model was considered to be a good within the given limitations of the model.

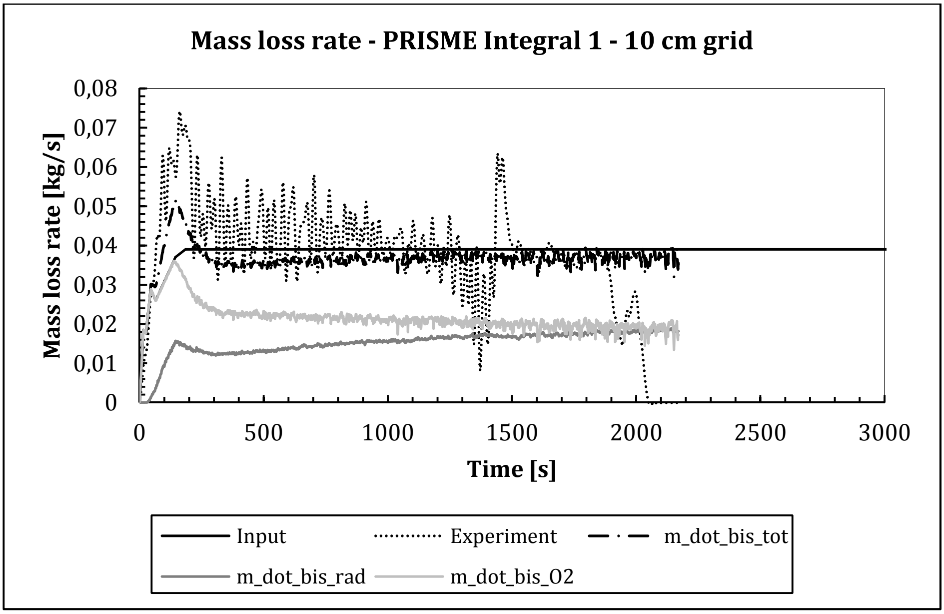


Figure 28 Comparison between the measured and predicted mass loss rates for PRISME Integral INT1 using 10 cm grid cells. Due to issues with the data cluster used, the last part of the simulation was lost but was not considered crucial to be able to compare the results.

Overall the predicted ventilation system response was in agreement with previous validation of the HVAC sub-model. Again PRISME Source D3 was not predicted well which was expected since the previous work done on the same case (Paper II; Wahlqvist, van Hees, 2013) also had problems getting a good agreement compared to the experimental data. The problem was narrowed down to the fact that some of the input data provided by the experimental data did not match the actual response of the system; hence it would not be possible to predict the behavior due to inaccurate input data. This could also explain why the general agreement with the experimental data was worse than other cases.

The difference in total mass loss rate between the two grid sizes was in most cases relatively small, at most 4 g/s which were about 10% of the total mass loss rate. One of the main objectives with the proposed model was to reduce the influence of the grid size which seems to be the case. This would imply that the proposed model could be suitable for more practical engineering purposes sine it can be relatively easy to setup and use. However, the radiative heat flux feedback to the fuel surface was in general higher when a coarser mesh was used, but this was balanced out by the oxygen depletion, rendering very similar mass loss rates independent of grid size.

Since there were no experimental data to compare the radiative heat flux feedback with, it is still unclear which prediction is the most correct one.

8.3.3.3 Sensitivity of oxygen volume fraction sampling volume

Since the oxygen volume fraction sampling volume has to be chosen by the end-user it can be a significant source of error if not done properly. To test the sensitivity of the oxygen volume fraction volume, eight different locations were sampled in the two different test cases; test S105 and S111 from the steel ship compartment experiments. These tests were chosen for different reasons; S105 was chosen due to the relatively high accuracy of the predicted oxygen volume fraction in the lower part of the room; if the prediction and the experimental results were in good agreement at that position it would probably be in good agreement close to the fuel base and would hence give a good prediction of the mass loss rate (as seen in Table 13). S111 was chosen for the opposite reason; the prediction of the oxygen volume fraction in the lower part of the room was not satisfactory hence it would be of interest to see whether this was due to the placement of the oxygen volume fraction sampling volume. Exact location size of the eight different sampling volumes can be found in Paper III, but in general the total volume size and location relative to the burner and flame was varied in various ways.

The results were almost identical for both cases (S105 and S111), and in Figure 29 the results for the case s105 is shown. And as can be seen there is only one sampling volume which would render significant changes on the resulting mass loss rate in both cases; the sampling volume that has cells inside the flame. This naturally causes a lower oxygen volume fraction to be sampled and should be avoided. Sampling a larger volume seems to have a small impact as long as it is relatively close to the fuel base, although additional space averaging might be acquired compared to a smaller overall volume. Sampling on only one side of the burner instead of all sides will on average give approximately the same results but will fluctuate more over time; this is in part due to the smaller overall sampling volume but could also be due to non-symmetrical entrainment of air into the flame.

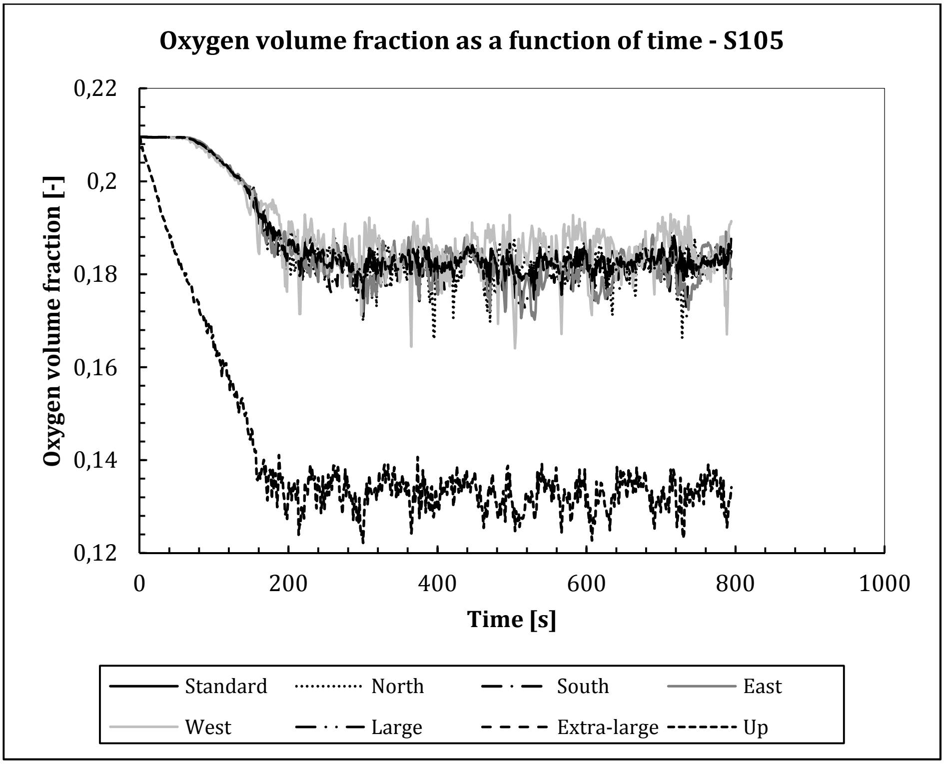


Figure 29 The oxygen volume fraction in different sampling volumes for test S105.

Some additional analysis of the simulated data indicates that it would not be suitable to use a two-layer approach to directly obtain the oxygen volume fraction. This is due to the average volume fraction in the lower layer likely being higher than the value used by a local sampling volume located by the flame base. It might however be feasible with some minor modifications to Equation 1 if needed.

In conclusion, it is important to note that the placement of the oxygen volume fraction volume will always be very dependent on the experimental/fictional setup and should always be carefully considered. The user should avoid placing it above the fuel surface or any other placement that would likely end up inside the flame.

8.3.3.4 Sensitivity of soot yield

Since soot often is the most dominant contributor to radiation from the smoke layer, it was relevant to test the sensitivity of this parameter as the soot yield is controlled by the user in FDS. To do so, two of the previously presented cases were chosen for sensitivity analysis; one with relatively low radiative feedback and one with relatively high radiative feedback. For low radiative feedback the case PRISME

Source D2 was chosen, and for high relative feedback PRISME Integral INT1 was chosen. The soot yield was increased and decreased by 30% from the experimentally measured value, 0.015, to 0.0195 and 0.0105 respectively. As can be seen in Figure 30, there was very little change in radiative heat flux feedback to the fuel surface when the “normal” radiative heat flux feedback was relatively low (PRISME Source D2). The resulting change in mass loss rate was hence also very small. However, once the “normal” radiative heat flux to the fuel surface was relatively high (PRISME Integral INT1) the soot yield have a relatively large effect on the radiative feedback to the fuel, as seen in Figure 31.

The results are rather interesting since generally it is expected that a higher soot production produces higher radiation intensities, but in this case the lower soot yield renders a higher radiative heat flux feedback to the fuel surface than the two other cases, and the highest soot yield renders the lowest radiative heat flux feedback to the fuel surface. The wall temperature with a higher soot yield is higher in the upper part of the room, but lower in the lower part of the room, meaning that a lower soot yield renders a more even temperature distribution inside the compartment. It seems as if the more optically thick smoke layer absorbs radiation from the walls and itself, reducing the radiative heat flux feedback to the fuel surface. The overall gas temperature is somewhat higher in the upper region of the compartment with a higher soot yield, but this does not seem to overpower the other absorption. However, the effect on the resulting mass loss rate is rather small since the oxygen volume fraction is consequently lowered by the increase in mass loss rate, resulting in similar total mass loss rates as the two parameters seem to balance each other out. The largest difference is during the initial transient stage, specifically during the initial mass loss rate peak, since the oxygen depletion has not yet started to affect the mass loss rate. It could be argued that a lower soot yield should have been used when the compartment temperature was relatively high, since the increased temperature might increase the effectiveness of the combustion. This phenomenon must however be studied in a more controlled environment than the one provided in current experiments.

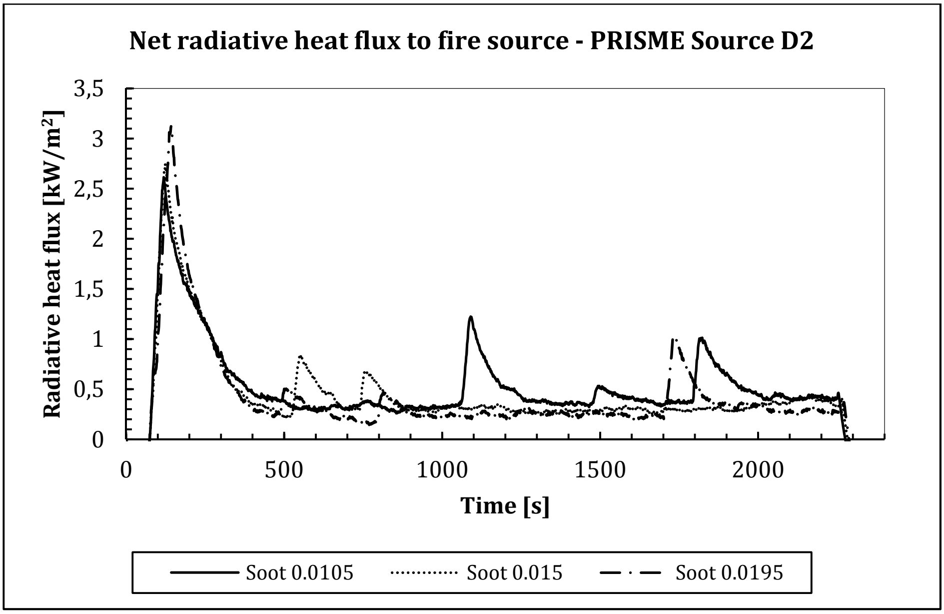


Figure 30 Radiative heat flux feedback to the fuel surface obtained using different soot yields and a coarse grid.

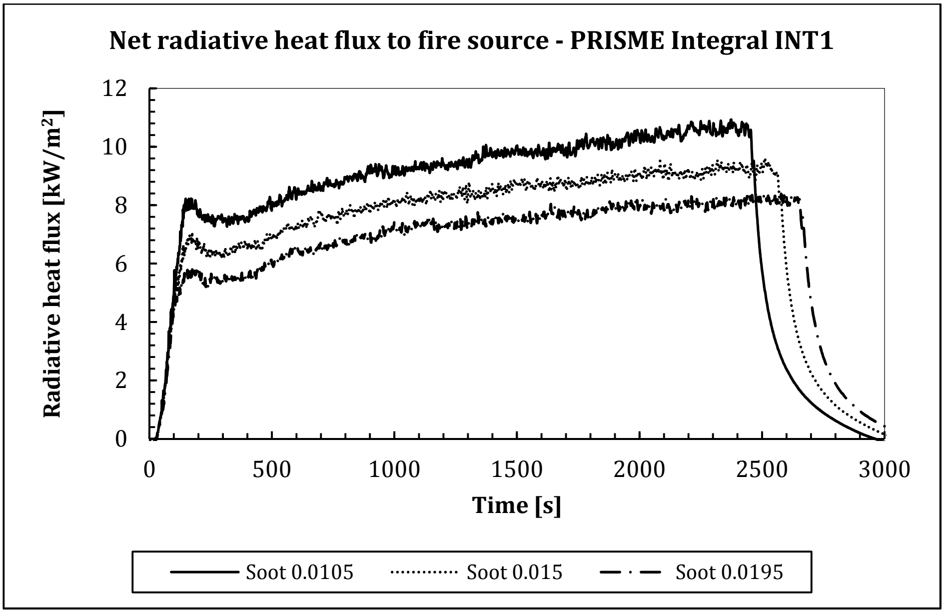


Figure 31 Radiative heat flux feedback to the fuel surface obtained using different soot yields and a coarse grid.

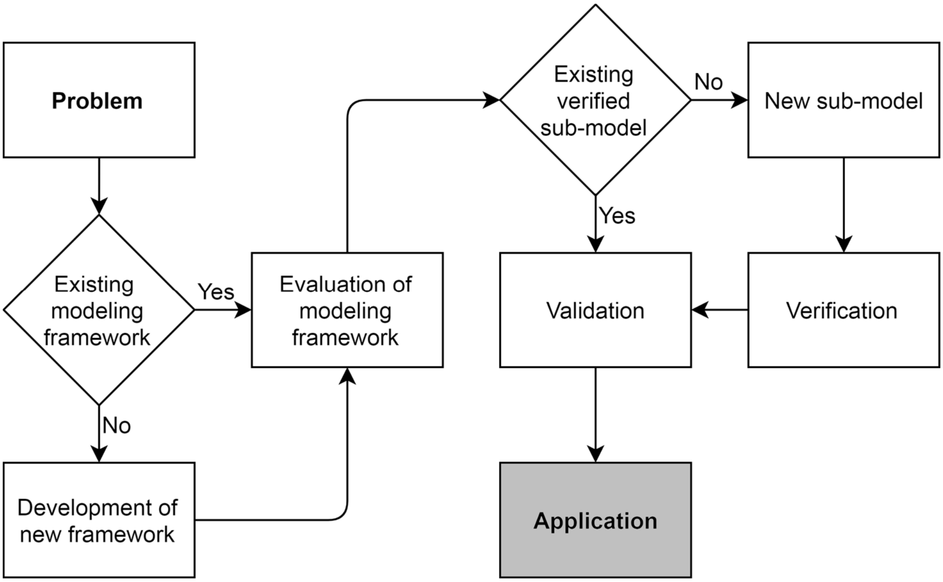
8.3.4 Conclusions

Prediction of the mass loss rates in enclosed spaces using the simplified environmental feedback model has been done qualitatively well with some exceptions. The predicted mass loss rates are within 20% of the experimental measurements with the exception of three cases which are discussed. Using relatively simple data collected from free burning pool fires the mass loss rate is predicted using the oxygen volume fraction close to the flame base, and in some cases the radiative heat flux from external sources (sources other than the flame itself) such as the walls and smoke layer. The prediction of the mass loss rate is reasonably accurate as long as the overall flow is reasonably resolved by the model, and natural as well as mechanical induced flows both give accurate predictions. The grid dependency of the sampled oxygen volume fraction has been observed to be relatively small even on coarse meshes, which can be a large benefit for engineering purposes compared to more detailed and advanced models.

The grid dependency of the external radiation model is coupled to the "standard" radiation model in FDS, hence the grid dependency of the external radiative heat flux feedback has been observed to be larger compared to the oxygen volume fraction, but the actual predicted mass loss rate was not largely affected. This was due to two reasons; in the cases where the relative difference between the two grid sizes was large, the actual external radiative feedback resulted in a very small portion of the total mass loss rate. In the case (INT1) where the external radiative feedback was the cause of a significant part of the mass loss rate, the oxygen depletion had the inverse relation compared to the external radiative feedback, resulting in similar total mass loss rate except for the very beginning of the fire duration when the oxygen fraction in the compartment was still sufficient.

The general goals with the proposed model have been met since the grid dependency seems to be relatively low and the prediction accuracy is considered to be acceptable (within 20%). It should however not be used as a substitute to more advanced pyrolysis models since accurate extinction, boiling/boil-over of the fuel, movement/leaning of the flame and other phenomenon simply are not taken into account. It can however be a valuable tool for more global phenomenon such as ventilation system behavior and determining input for design fires, which in turn can be used for evaluating the safety of a certain structure or building.

9 Application of the model



The last objective was to make useful engineering tools and methods that could be applied based on the research. Two different applications that rely on either predicting the behavior of ventilation systems or environmental feedback were identified:

- Predicting fire growth related to building characteristics.
- Predicting performance of measures against smoke spread in ventilation systems.

These applications were chosen since they are dependent on accurate prediction of several key mechanisms:

- Prediction of mass loss rate changes due to changing oxygen levels.
- Prediction of mass loss rate changes due to radiative heat flux feedback to the fuel surface.
- Prediction of mechanical ventilation system response with interconnected compartments.

All of the needed tools for doing this have been verified and validated within the framework of this thesis and have been discussed in the previous chapters.

9.1 Numerical experiments

A numerical experiment is an experimental study with a numerical model (Johansson et al., 2014) and the reasoning behind using numerical experiments is many; it can be a cost effective approach to collect large sets of data, it enables full control of the surroundings and boundary conditions and it also enables scenarios that would be very hard and costly to build in real life.

Johansson presented a flow chart (seen in Figure 32) that can be used to determine if using numerical experiments is feasible for a certain application. The two presented applications were good candidates for the process of numerical experiments due to several key points:

- Performing full-scale experiments would not be practically or economically feasible.
- Due to the nature of radiation and pressure build-up it would next to impossible to perform less resource intensive small-scale experiments, as they would behave significantly different to a full-scale experiment.
- The validation work performed within this thesis showed that the models needed to perform the numerical experiments agreed well with experimental data and could hence be used for numerical experiments in similar settings and applications.

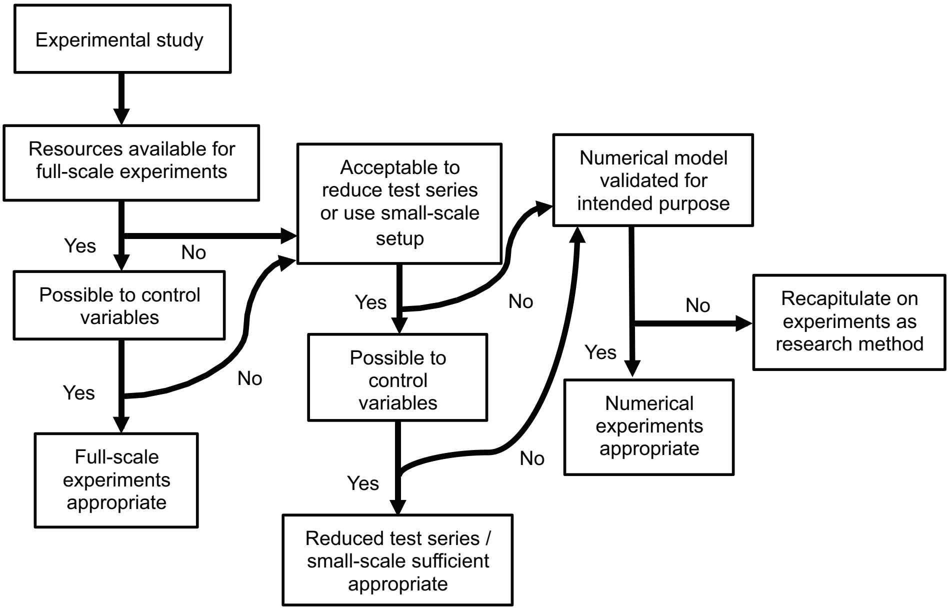


Figure 32 Flow chart for determining the applicability of numerical experiments. Courtesy of Nils Johansson.

With the use of numerical experiments, both Paper IV and V investigated real life applications that would be cost-prohibitive to perform in a real, full-scale experiment setting.

9.2 Predicting fire growth related to building characteristics

The simple design fire concept has been used extensively to evaluate performance based designs all over the world and is an invaluable tool for many fire protection engineers. However, the design fire is a rough simplification of the real world and using it in applications outside the boundaries of its original intent might result in erroneous conclusions in regard to fire safety. The Swedish National Board of Housing, Building and Planning (Boverket in Swedish) recommends e.g. different fire growth rates depending on the type of activity in a building (Table 17), but one problem that can arise from directly using proposed growth rates is that the characteristics of the fire compartment is never accounted for. Will a heavily insulated building behave e.g. the same as a steel sheet building or does the radiative feedback increase the fire growth and maximum heat release rate? Does a smaller room behave different from a big room? How much does the amount of openings (both normal openings and those caused by evacuating people, as in doors being opened) to the fire room affect the development of a fire? Some studies have been made on this topic, e.g. an experimental study done by Evegren et al. that indicates that the effects of using highly insulated compartments will influence the mass loss rate (Evegren & Wickström, 2015) to some degree, but the scope of different scenarios was rather limited in that work. This work focuses on investigating typical building materials, the amount of door openings supplying air to the fire room, fire room floor area and ceiling height and how they affect the fire growth and maximum heat release rate by doing numerical experiments (Johansson et al., 2014).

Activity	**Growth rate [kW/s^2]**	**Maximum heat release rate [MW]**	**Heat of combustion, [MJ/kg]**
Offices and schools	0.012	5	16
Dwellings, hotels, nursing homes etc.	0.047	5	20
Shopping centers, entertainment centers etc.	0.047	10	20

Table 17 Recommendations on design fire growth rates and maximum heat release rates given by the Swedish National Board of Housing, Building and Planning (Boverket, 2011).

The design fire concept is divided into three parts; the growth phase, the steady phase and the decay phase. In this work the primary phase of interest is the growth phase, but also on the steady phase, specifically the maximum heat release rate. The most common way to describe the growth phase is to use the following mathematical formulation:

$$\dot{Q} = \alpha \cdot t^2 \quad \text{Equation 10}$$

What this means is that the heat release rate $\dot{Q}$ at a certain moment determined by a number α and the time t since the fire started. A larger α value would mean that the heat release rate would increase more quickly than a smaller number, and a common classification of this number has been done by the National Fire Protection Association (NFPA), which can be seen in Table 19. This standard classification will be used throughout this paper by using references to both the name of the growth rate classification as well as the given -value.

Growth rate	α **[kW/s²]**	**Time to reach 1055 kW**
Ultra-fast	0.19	75
Fast	0.047	150
Medium	0.012	300
Slow	0.003	600

Table 18 Standard classification of different growth rates according to NFPA 204M (NFPA, 1985).

To be able to predict the changes in heat release rate and growth rate two things are essential; a model for radiative feedback to the fuel and a model for taking into account oxygen depletion. The model described in chapter 4.3 (Paper III, Wahlqvist & van Hees, 2013) was used for this purpose which enabled lowered mass loss rate due to lowered oxygen levels close to the fire source and increased mass loss rate due to radiation from external sources, such as walls and smoke layer.

To investigate the influence of the building material and opening factor on the design fires a simple room was created with the following dimensions; 10 m x 10 m x 3 m (width x length x height), see Figure 33. The compartment dimensions were selected as the “default” room to represent a reasonable “normal” case, but also adapted to be able to see a clear distinction for each material. If the ceiling would have been very high the radiation from the ceiling and hot gasses might potentially be relatively low which in turn would mean that the growth rate probably would never be changed. The same thing would probably happen if the room floor area was relatively large, since there would be very little build-up of a hot gas layer and there would probably be very little radiative heat flux feedback from the walls. To further analyze these assumptions additional simulations were done to investigate the influence of the room floor area size and the room ceiling height.

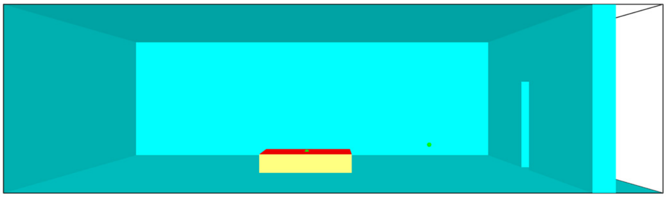


Figure 33 The 10 m x 10 m x 3 m room that was used in the simulations with one door opening and the fire source with constant burning area placed in the middle of the room.

9.2.1 Influence of building material and growth rate

Four different materials were selected, each having different properties and responses (thermal properties and thickness/heat storing capacity); a drywall construction (13 mm gypsum, 70 mm insulation 13 mm gypsum), 200 mm concrete, 2 mm sheet steel and finally 100 mm insulation (to represent a modern light sandwich construction). All materials were assumed to be incombustible and used the same emissivity. It was observed that there were minor changes in the growth rate depending on the building material (concrete 1-7%, drywall 8-35% and steel 0-20%) with the exception of the insulated walls where the difference in growth rate is at most almost 300% and the least about 115%. The actual growth rate when using the insulating walls and specifying a growth rate of 0.003 kW/s^2 is calculated to 0.012 kW/s^2; the same as the next standard classification “medium”. The relative increase is not as great (114-213%) using the higher growth rates, but it could still be considered significant when used to assess the fire safety in a building.

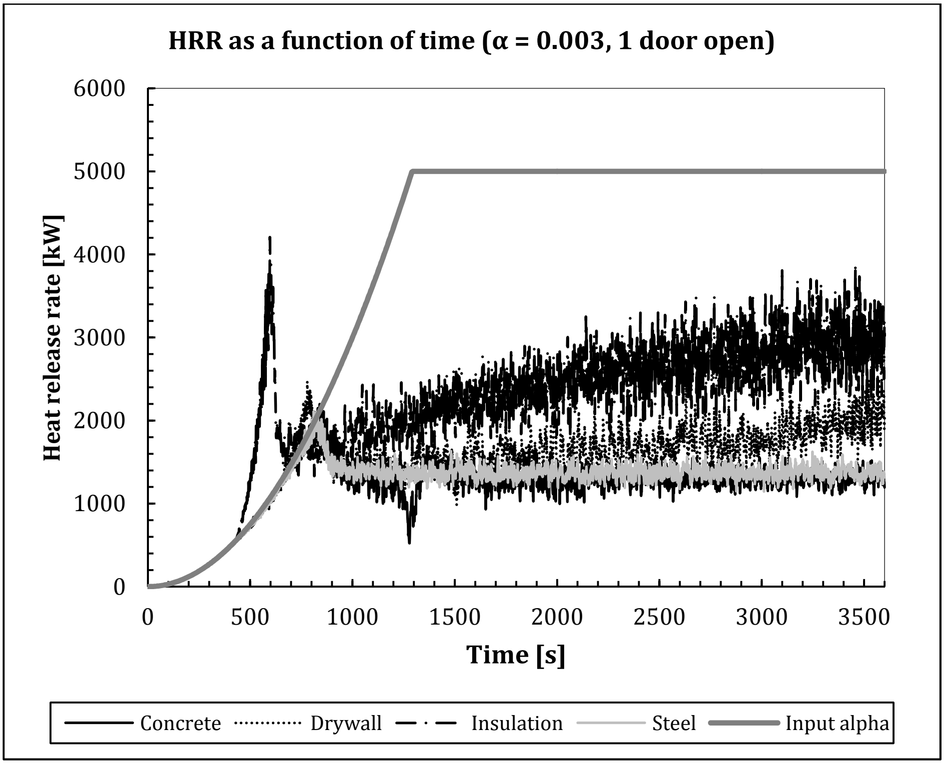


Figure 34 Heat release rate as a function of time using different building materials, one door opening and a growth rate of 0.003 kW/s^2.

It can also be noted that the maximum heat release is increased with increased growth rate for all building materials. But, as observed in the example given in Figure 34 the peak heat release rate duration is rather short (similar for all growth rates) since the oxygen depletion starts to affect the mass loss rate rather quickly. It is evident that the growth rate was hampered by the lack of oxygen being supplied to the compartment. An example of what causes the heat release rate dynamics can be explained by looking at Figure 35 and Figure 36; the heat release rate initially increases according to the specified growth rate causing the oxygen volume fraction to decrease inside the compartment. As the walls heat up and compartments is filled with hot gasses the radiation to the fuel source is increased which in turn increases the mass loss rate, which in turn further decreases the oxygen volume fraction but also further heat up the walls and hot gasses. Once the oxygen volume fraction is very low (around 11%) most combustion will happen detached from the fuel base and the local heating of the walls and hot gases decreases (and therefore also the radiative heat feedback to the fuel source) will start to decrease. This loss of radiative feedback in combination with the already oxygen depleted environment then causes a rapid decrease in the mass loss rate until the room once again starts to heat up which again increases the radiative feedback, this time in a slower more controlled pace. The fact that the maximum heat release is increased with increased growth rate is simply due to the fact that a faster growth rate reaches a higher heat release rate before the effects of oxygen depletion sets in.

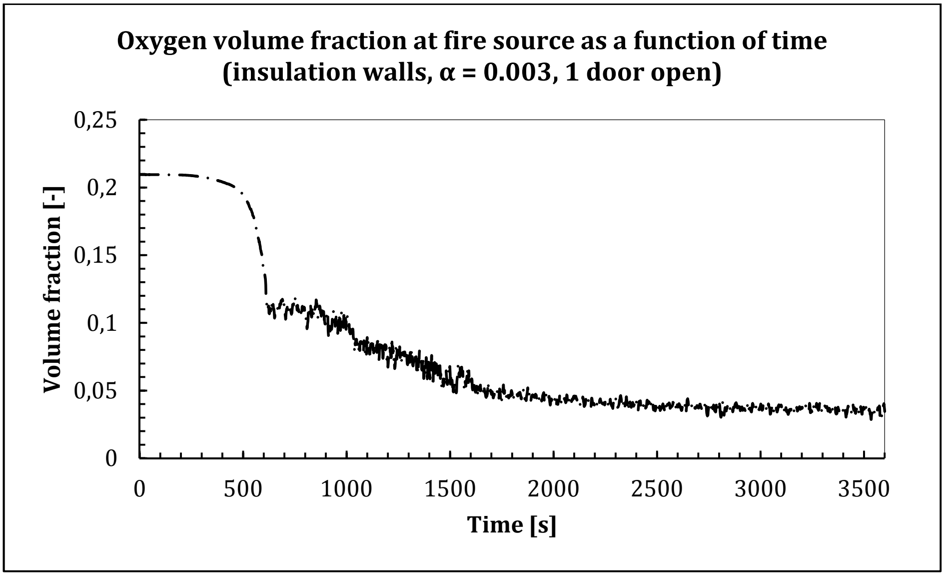


Figure 35 Oxygen volume fraction close to the fire source as a function of time using insulated walls, one door opening and a growth rate of 0.003 kW/s^2.

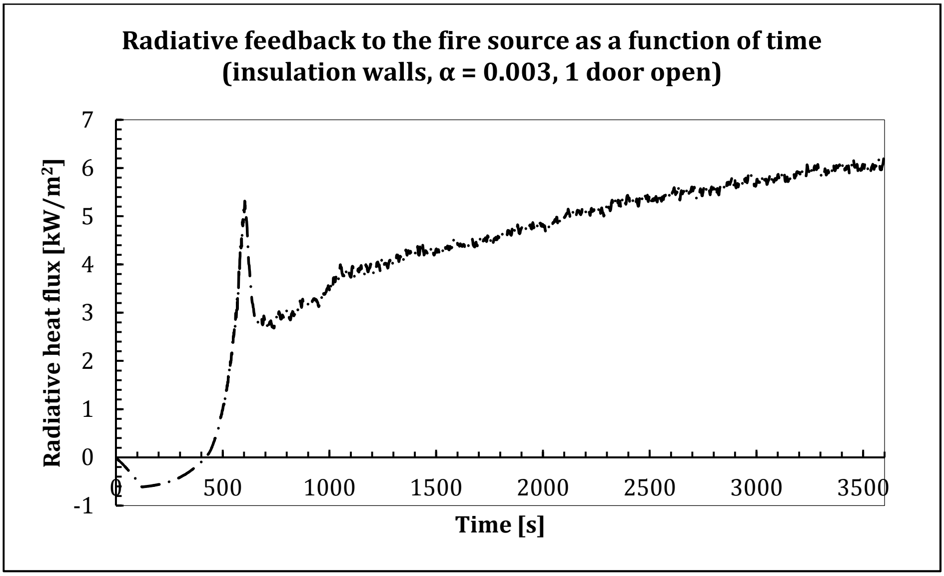


Figure 36 Radiative feedback to the fuel surface as a function of time using insulated walls, one door opening and a growth rate of 0.003 kW/s^2.

9.2.2 Influence of door openings

Two different opening configurations were used to investigate the effect of this parameter; one door opening and four door openings. The growth rate is larger in all cases when using four doors compared to when only one open door was present. For example, the growth rate when using the insulating walls and specifying a growth rate of 0.012 kW/s^2 now exceeds the next standard classification (fast, 0.047 kW/s^2) with a calculated growth rate of 0.057 kW/s^2. In fact, all specified growth rates are higher or close to the next standard classification (when available), even the specified “fast” growth rate (0.047 kW/s^2) closes in on the “ultra-fast” growth rate (0.19 kW/s^2) with a value of 0.16 kW/s^2. Looking at recommendations from the Swedish National Board of Housing, Building and Planning in Table 17, this would mean that the time available to perform safe egress from a building would probably be overestimated in such a case as larger quantities of smoke and hot gases would be produced within the same time frame.

Looking at example given in Figure 37 the heat release rate is not abruptly cut off due to oxygen depletion as in the case when only one door was present. The general maximum heat release rate is also no longer always increasing with increased growth rate, and the heat release rate increases as time progresses due to radiation from the ceiling and the hot gas layer. Since more air is supplied a larger portion of the combustion can occur inside the compartment and closer to the fire source and this increases the temperature of the walls and hot gasses, hence intensifying the radiative feedback. This can clearly be seen since the radiative heat flux to the fuel source with four doors reaches approximately 30 kW/m^2, compared to 6 kW/m^2 when only one door opening was present. It can however be noted that each building material seem to have an allowed maximum heat release rate controlled by the radiative feedback; the insulated walls having the highest heat release recorded and the steel walls having the lowest due to relatively large heat losses.

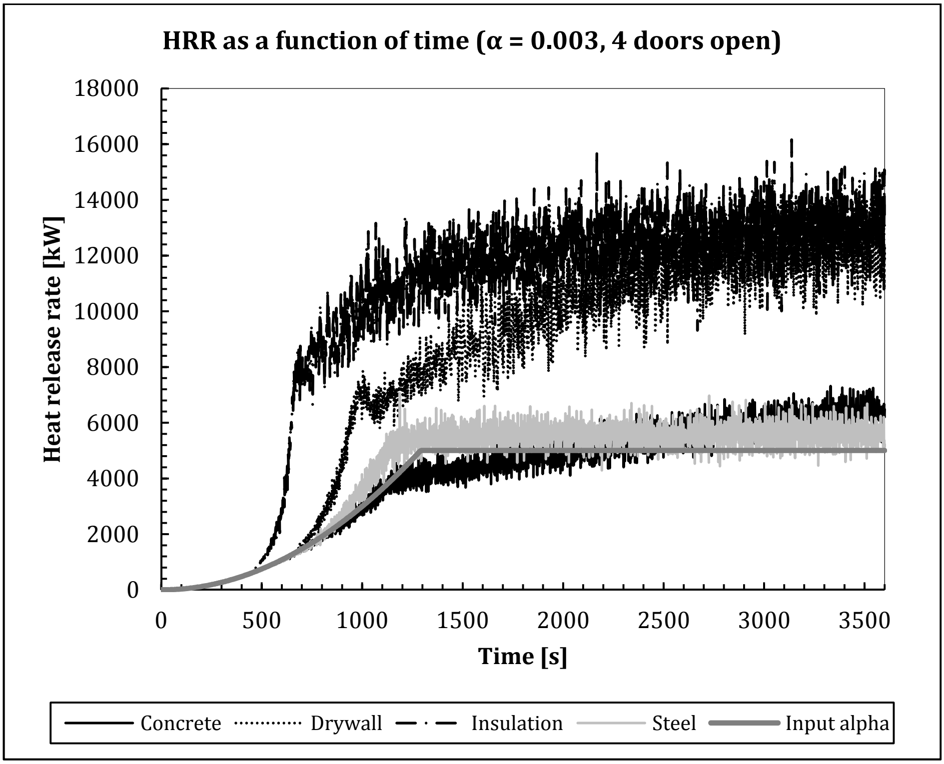


Figure 37 Heat release rate as a function of time using different building materials, four door openings and a growth rate of 0.003 kW/s^2.

9.2.3 Influence of the room floor area

Three different room sizes were used to investigate this parameter; 5 m x 5 m, 10 m x 10 m and 20 m x 20 m. It was observed that the room floor area can have a significant influence on the growth rate and maximum heat release rate. In almost all cases the main driving force is the radiative feedback since the oxygen volume fraction close to the fire source reduces to a value close to or below the limit for extinction (around 11 volume-% without external radiation).

The external radiation heat flux does get significantly larger in the cases with 4 door openings due to the same reasons given before; since more air is supplied more combustion can occur inside the compartment and closer to the fire source and this increases the temperature of the walls and hot gasses; hence the radiative feedback intensifies. It is also important to note that the radiative feedback increases as the room floor area decreases independent of how many door openings are present (although to a larger extent when four door openings are present). The reasons for this are two-fold; firstly, it takes longer time to heat up the walls and ceiling the larger the floor area is. Secondly, even if the walls and ceiling would be of the same temperature in all cases only the ceiling would consistently contribute the same amount of radiative feedback, the walls would not simply due to the fact that they are further away from the fire source. This could have implications when the fire is placed in a corner or when other nearby objects heat up and can contribute with radiative feedback.

Another interesting observation is on the maximum heat release; when only one door opening is present the highest recorded heat release rate is in the largest floor are but only for a very brief time. When four door openings are present the smallest floor area reaches the highest heat release rate and over a much longer period of time. The reason that the maximum heat release rate is found in conjunction with the largest floor area when only one door opening is present is due to the larger "oxygen reserve" stored inside the compartment. It takes longer time to reach lower oxygen levels with increased floor area, and when only one door opening is present the radiative feedback is not contributing as much to the heat release rate as when four door openings are present. This dynamics changes however once four door openings are present; the maximum heat release rate is decreased with increased floor area as seen in Figure 38.

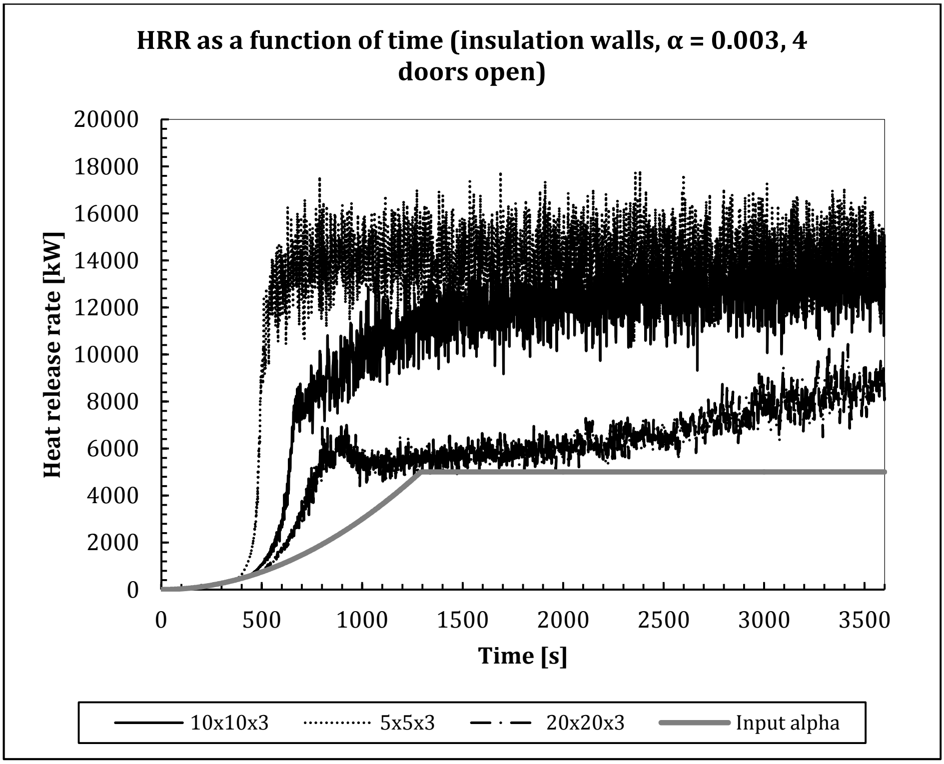


Figure 38 Heat release rate as a function of time using different room floor areas, four door openings and a growth rate of 0.003 kW/s^2.

9.2.4 Influence of the ceiling height

Three different ceiling heights were used to investigate this parameter; 3 meters, 5 meters and 7 meters. It was observed that the room height has a significant effect on the growth rate and maximum heat release. Having only one door opening, the growth rate drastically decreases as the ceiling height increases. This is due to the decrease of external radiative heat flux feedback with increasing ceiling height in combination with the fact that some degree of oxygen depletion occurs regardless of ceiling height. When four doors are present the effect is very similar although to a larger degree as seen in Figure 39. However, the effect of the room height is not as significant if the room floor area is smaller since the walls seems contribute to a larger degree. A combination of a larger floor and high ceiling height actually renders very little or almost no radiative feedback which might be "good news" for scenarios where performance based design often is applied (big open spaces). It should however be remembered that nearby objects or walls still can provide radiative feedback.

With room floor area sizes of 10 m x 10 m and 20 m x 20 m the maximum heat release rate is decreased with increased ceiling height. This can yet again be attributed to the lack of radiative heat flux feedback, though the effect is somewhat lessened when the room floor area is smaller (10 m x 10 m) since the walls can contribute more radiative feedback compared to when the walls are distant from the fire source. When the room floor size is 20 m x 20 m there is very little difference between a ceiling height of 5 or 7 meters and this difference seems to be sourced from lesser oxygen depletion since the radiative feedback is virtually non-existent for both ceiling heights. When the room floor area is 5 m x 5 m the maximum heat release rate is the same regardless of the ceiling height; it is simply not possible to increase it further in that system even though the radiative feedback increases.

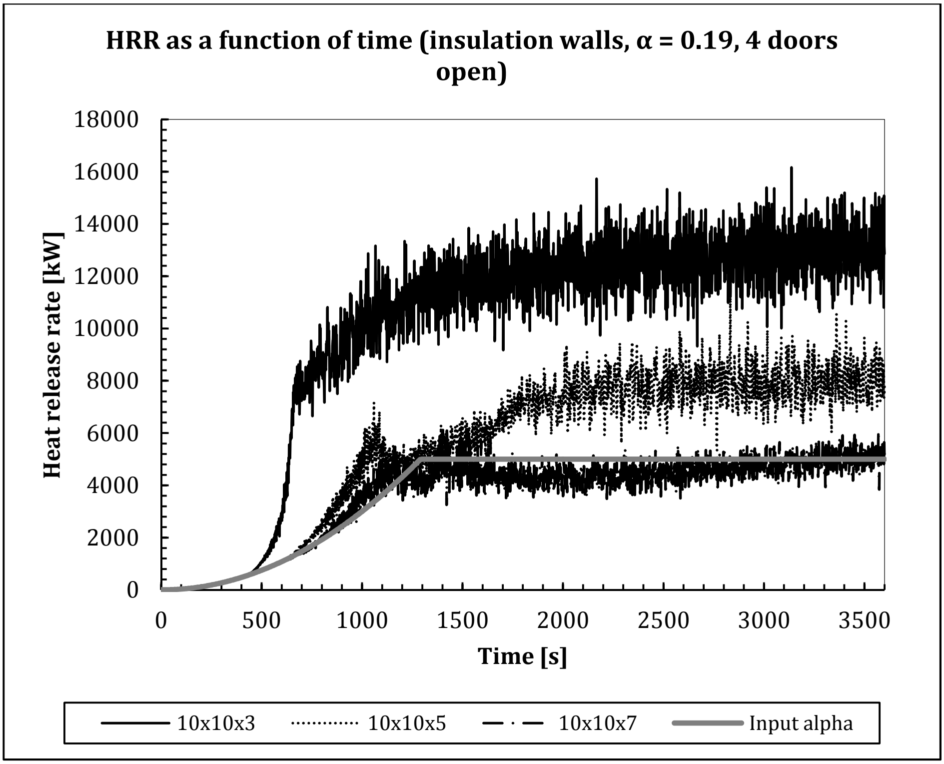


Figure 39 Heat release rate as a function of time using different ceiling heights, four door openings and a growth rate of 0.003 kW/s^2.

9.2.5 Conclusions

It has been shown that the type of incombustible building material used in a fire compartment might influence the growth rate of a design fire in a significant way; insulating wall/ceiling materials will probably increase the growth rate which in turn will mean that the time to critical conditions will be shorter compared to the expected result. This can be relevant in modern buildings where highly insulating building materials are used to be more environmentally friendly. However, if the building material used is thermally thin or has a large heat storing capacity the influence is rather negligible. The maximum heat release rate and transient behavior of the fire was shown to be very dependent on ventilation factor in combination with the building material; with only one door opening present the initial fire growth was rapid due to radiative feedback but was then hampered by the oxygen depletion which caused the heat release rate to decrease significantly during the course of the simulation duration. The heat release rate increased slowly over time but never reached above the preset maximum (5000 kW). This applied to all building materials. Using 4 door openings however allowed the initial peak heat release rate to become larger for the insulated and drywall compartments which meant an increase in calculated growth rate. Since more air was supplied more combustion could occur inside the compartment and this increased the temperature of the walls and hot gasses and hence the radiative feedback became more intense.

Furthermore, it was shown that the room floor area might have a significant effect on the growth rate and maximum heat release rate. With one door opening a larger room (floor area 20 m x 20 m) would have a higher initial peak heat release rate than the smaller rooms (5 m x 5 m and 10 m x 10 m), but they would all get oxygen depleted soon thereafter and behave similarly for the rest of the simulation. If there were four door openings present, the radiative feedback would overpower the oxygen depletion and the smaller the room the higher the maximum heat release rate and growth rate.

It was also shown that the ceiling height does have a significant effect on the growth rate and maximum heat release when coupled with four door openings. Having only one door opening present quickly decreases the oxygen volume fraction close to the fire source which decreases the heat release rate rapidly and this effect seem to happen with very little time delay independent of the room height. However, the effect of the room height was not as significant if the room floor area was smaller since the walls seems contribute to a larger degree in that case. Another important note was the fact that a combination of a larger floor area (20 m x 20 m) and high ceiling height (above 5 meters) actually rendered very little or almost no radiative feedback which might be beneficial for scenarios where performance based design often is applied (big open spaces).

In conclusion it is recommended to further investigate current use of design fires in compartments with highly or moderately insulating building materials as the environmental feedback might increase the growth rate significantly. If the building material also is combustible, the growth rate would also likely increase which also should be taken into account in future work.

9.3 Predicting performance of measures against smoke spread in ventilation systems

As the validation cases showed, much effort has been put into predicting ventilation system behavior of a well-defined, full-scale scenario in the presence of a fire. It was shown that the pressure peaks and ventilation system response could be well predicted given that the input data generated from experimental measurements was accurate. However, in any real application the behavior observed in those cases would be highly undesirable. In all cases the inlet was reversed, thus allowing hot gases and soot to spread to nearby compartments. The exhaust was also continuously running which meant a great deal of hot gases and soot would enter the ventilation system and potentially damage filters, fans and ducts. Paper V sought to compare different measures to prevent hot gas and soot spread to a ventilation system, as such a system would likely be in place in any real application.

As stated in the introduction, a wide variation of methods for preventing smoke spread in the ventilation system exist and are applied in performance based designs. This is especially true in Sweden where the fire code is performance based, stating that satisfactory protection against the spread of fire gases may be obtained by:

> *Allowing fire gases to enter the ventilation system but designing the system in such a way that the spread of fire gases between fire compartments is prevented or considerably impeded depending on the design and the nature of the premises. (Boverket, 2011)*

As a basic rule, the ventilation system must not impair the fire safety provided by the general building structure. Accordingly, fire dampers are usually selected to meet the fire resistance period of the fire compartment-separating element. However, this traditional approach is often very expensive since the cost of every fire damper and its electronics is relatively high. Combined with the need of several fire dampers in e.g. a multi-family building, the cost quickly becomes a determining factor. However, there are alternatives to using fire dampers. These solutions are often used as a mean to cut costs compared to using fire and smoke dampers since they include using existing or cheaper parts to achieve a similar level of safety. The different methods used in the evaluation are further detailed in Paper V.

To be able to test the different methods for preventing smoke spread through the ventilation system, a relatively simple setup consisting of compartments and an interconnecting ventilation system had to be used. Since no suitable experimental setup could be found a purely numerical environment was designed for the purpose to demonstrate the usefulness of the methodology. The simulation setup used in this paper consists of five rooms connected to each other only through the ventilation system. All compartments have both an inlet and an exhaust with the same flow rate at normal operating conditions. Each compartment is 10 meters wide, 10 meters long and 2.8 meters high, which results in a total of 280 m^3 per compartment. The simulation setup can be seen in Figure 40.

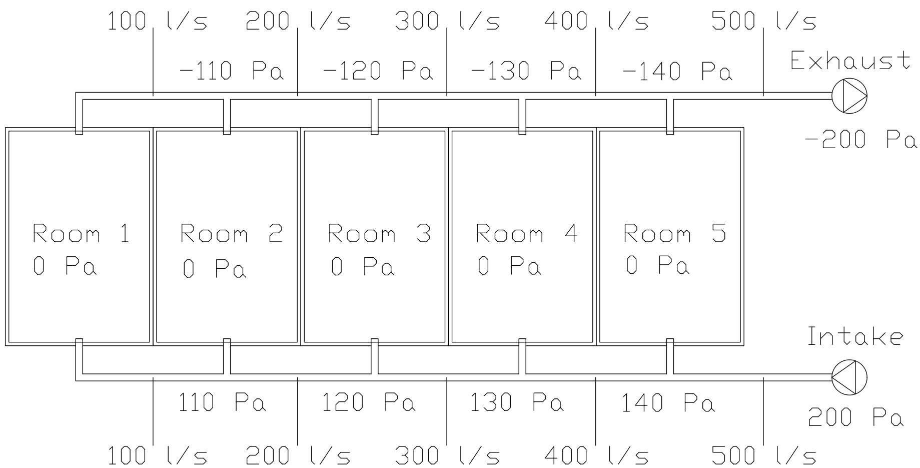


Figure 40 Node pressures, flow rates and room pressures during normal operating conditions.

The fire was placed in room 1, since smoke spread would occur the fastest from this room due to the fact it has the lowest pressure at the inlet junction and the lowest flow at the closest outlet junction (Jensen, 2002) The growth factor of the fire has a significant impact on the pressure build-up inside a compartment (Jensen, 2002), but unfortunately, determining the "real" heat release rate of an apartment fire is a very complex issue. For this reason, traditional design fires were used following the NFPA standard (NFPA, 1985) as can be seen in Table 19.

Growth rate	α [kW/s^2]	Time to reach 1055 kW
Ultra-fast	0.19	75
Fast	0.047	150
Medium	0.012	300
Slow	0.003	600

Table 19 Standard classification of different growth rates according to NFPA 204M (NFPA, 1985).

In most cases where design fires are used it is assumed that solid objects are combusted. However, since simulation of solid combustion is often considered relatively complicated and unreliable, a simpler approach was desired. Using the approach described in the next section, a liquid with well-known thermal and chemical properties can be relatively well modeled; hence this approach was taken in this paper. This approach could have limited the direct practical use of the findings since solid fuels typically have higher pyrolysis temperature and lower heat of reaction, which would influence the fire behavior. However, since no radiative feedback was found in any of the simulations the results were believed to have largely not been affected by this approach.

The burning behavior of heptane (C_7H_{16}) has been rather well studied (Casale & Marlair, 1994; Evegren & Wickström, 2015; Truchot et al., 2010; Yina et al., 2013) and the needed thermal and chemical properties are well-known which made it a perfect candidate to use in this work. The maximum specified heat release rate was set to 5000 kW in all cases with the fire source being 4 m^2, resulting in a heat release per unit area to be 1250 kW/m^2, both values in line with common design fire inputs.

“Windows” were placed in each room that was designed to be removed to normalize pressure if the over-pressure exceeded 3000 Pa. This was implemented since most buildings walls and windows would not be able to withstand larger pressure without partial collapse.

Three different criteria were chosen to evaluate the performance of the different methods for preventing smoke spread in the ventilation system; total amount of soot transported to each of the rooms, the thermal load on the fans which could potentially destroy or damage the fans and the severity of the fire (average and maximum heat release rate).

9.3.1 Influence of building leakage

As discussed in section 5.2.3, it is important to consider building leaking when modeling ventilation systems since air movement through these leaks is to be expected when relatively large pressure differences are present. The area of the leakages was calculated by using the values provided by the SFPE handbook of fire protection engineering mentioned in chapter 5.2.3, but since these vary in the order of 100 choosing an inappropriate leakage class could have significant impact on ventilation system behavior in a fire. As the quantification of smoke spread through the ventilation system was of prime interest, only the most stressing leakage class was of interest when evaluating the different methods for preventing smoke spread. Since a tighter room practically means that it is harder for the hot gases (produced by the fire) to escape through the leakage (compared to exiting through the ventilation) the leakage class “Tight” was likely to produce the worst results. This was also confirmed by doing simulations with varying leakage area as seen in Table 20. The different simulations and results are further explained and discussed in Paper V.

	Very loose	Loose	Average	Tight
Accumulated soot Room 2 in [kg]	0	0.0049	0.014	0.016
Accumulated soot Room 3 in [kg]	0	0	0.0027	0.014
Accumulated soot Room 4 in [kg]	0	0	0	0.0072
Accumulated soot Room 5 in [kg]	0	0	0	0.00024
In total [kg]	0	0.0049	0.017	0.038
Accumulated soot Room 2 out [kg]	0	0	0	0
Accumulated soot Room 3 out [kg]	0	0	0	0
Accumulated soot Room 4 out [kg]	0	0	0	0
Accumulated soot Room 5 out [kg]	0	0	0	0
Out total [kg]	0	0	0	0
Total [kg]	0	0.0049	0.017	0.038
Accumulated soot outlet fan [kg]	0.24	0.23	0.23	0.22
Accumulated soot inlet fan [kg]	0.0	0.0	0.0	0.0
Max temp. outlet fan [C°]	73	91	107	144
Max HRR [kW]	2885	2574	2589	2842
Avg. HRR [kW]	846	780	688	579
Max pressure [Pa]	94	391	826	2289

Table 20 Summary of the results using different leakage classes.

As can be seen in Table 20 the soot to the connected rooms was transported through the inlet branch. This is due to the pressure created by the fire which reverses the inlet flow as it over-powers the capacity of the fan. As the fire room has less leakage the pressure increases and the reversed flow is increased, causing soot being spread further down-streams to rooms closer to the fan. The magnitude of the reversed inlet flow for each tightness class is shown in Figure 41.

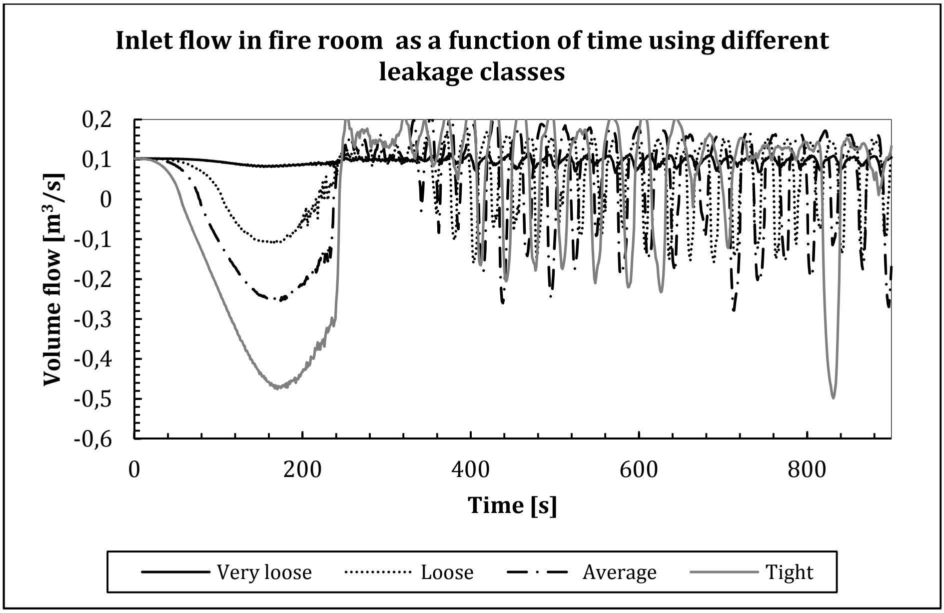


Figure 41 The inlet volume flow rate in the fire room using different leakage classes.

9.3.2 Influence of fire growth rate

Since only the worst possible scenario was of interest when evaluating the smoke spread in the ventilation system, the fire growth rate which produced the most taxing conditions had to be identified. It was likely that either the "Fast" or "Ultra-fast" fire growth rate would produce the largest smoke spread in the ventilation system, but to be able to quantify the difference all "standard" fire growth rates were tested and evaluated using a "Tight" leakage rate (as that was determined to be the worst performing leakage class previously). The results were a little surprising; the "Fast" fire growth rate amounts to the overall worst smoke spread followed by "Medium" growth rate. The "Ultra-fast" growth rate does initially produce the strongest reaction on the ventilation system, but since the windows were assumed to break at 3000 Pa over-pressure (due to most buildings not able to withstand higher pressures before collapse) the pressure quickly dropped to nearly zero. This meant that there is hardly any risk of smoke spread to the other rooms (although the outlet still takes in hot gases which can damage the fan, ducts and filters). The results for all simulations are shown in Table 21.

Similar to when testing the different tightness classes, soot spread only occurred though the inlet branches. The behavior of the inlet flow in the fire room is shown in Figure 42, where the pressure breaking point that occurred when the growth rate

“Ultra-fast” was used is also clearly visible. In the same figure it is also evident that oxygen depletion has started to affect the heat release rate which causes oscillations of the system. These kinds of oscillations might occur in an under-ventilated environment, but the frequency and amplitude has not been validated properly in this study; partly due to it being out of scope and partly due to very limited access to experimental work which could be used and is needed for validation. It might also happen that these oscillations are caused by the numerical models used, and for these reasons smoke spread recorded during these oscillations were not added to the total amount of soot being spread. The oscillations are however further discussed in Paper V.

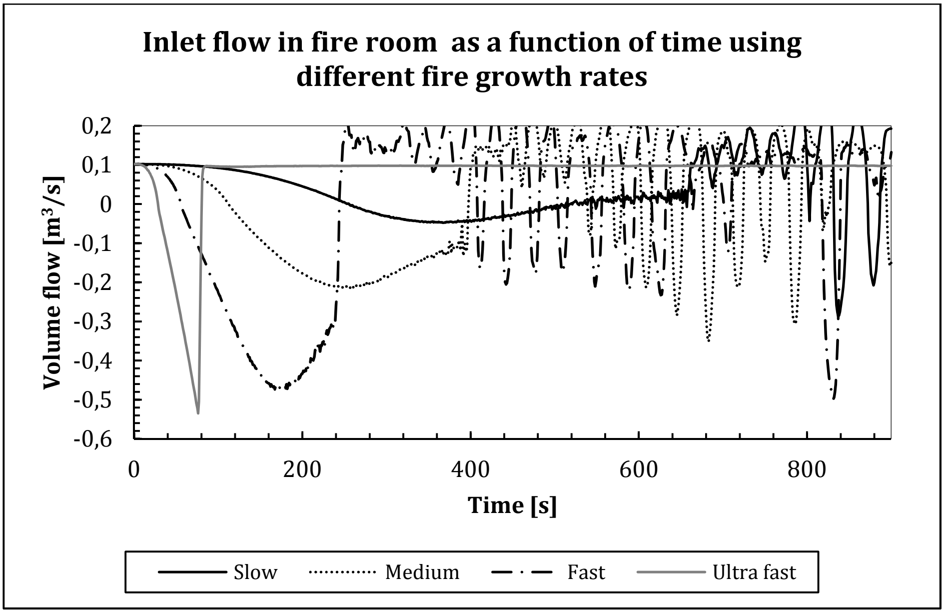


Figure 42 The inlet volume flow in the fire room using different fire growths.

	Slow	Medium	Fast	Ultra-fast
Accumulated soot Room 2 in [kg]	0.0037	0.025	0.016	0.00097
Accumulated soot Room 3 in [kg]	0	0.0030	0.014	0.00083
Accumulated soot Room 4 in [kg]	0	0	0.0072	0.00056
Accumulated soot Room 5 in [kg]	0	0	0.00024	0.00021
In total [kg]	0.0037	0.028	0.038	0.0026
Accumulated soot Room 2 out [kg]	0	0	0	0
Accumulated soot Room 3 out [kg]	0	0	0	0
Accumulated soot Room 4 out [kg]	0	0	0	0
Accumulated soot Room 5 out [kg]	0	0	0	0
Out total [kg]	0	0	0	0
Total [kg]	0.0037	0.028	0.038	0.0026
Accumulated soot outlet fan [kg]	0.12	0.17	0.22	0.27
Accumulated soot inlet fan [kg]	0.0	0.0	0.0	0.0
Max temp. outlet fan [C°]	86	94	144	81
Max HRR [kW]	1323	1953	2842	3686
Avg. HRR [kW]	467	541	579	960
Max pressure [Pa]	870	1258	2289	3000*

Table 21 Summary of the results using different fire growth rates. *Since 3000 Pa was reached the pressure boundary fail safe was opened, creating an opening to the atmosphere.

9.3.3 Results

All of the results presented in this section are using the “Tight” leakage class and the “Fast” fire growth rate since they were found to be the worst case scenario.

None of the cases got any radiative feedback that affected the mass loss rate, which was expected due to the fact that concrete was chosen as material for the walls. This was purposely done since the ventilations system and its interaction with the fire was the primary interest. This also meant that the use of heptane instead of a more complex, solid material likely did not affect the results to a very large degree since the prescribed mass loss rate was never increased due to radiative feedback.

The soot yield that was used in FDS was determined under well ventilated conditions, which is not the case in this study. Therefore, the results presented should only be considered as a qualitative difference between all of the scenarios that were simulated. This would also apply to other species such as CO which can be relevant for egress safety.

In three cases (fire dampers and both cases using reverse valves) the pre-set pressure limit of 3000 Pa was reached, which opened up a hole from the fire room to the atmosphere in order to represent a wall or window breaking. In these cases, together with the pressure relief case, the average heat release rate was higher than in other cases since more oxygen was being supplied through the pressure relief opening. This could have negative consequences on the thermal stresses of the building and other heat sensitive equipment, but would also likely have positive effect (as in lowered) on the soot production due to more well-ventilated conditions.

The maximum heat release rate was rather similar in all cases since the oxygen depletion evidently affected all cases in the same way. The only way this would have changed between cases was if the inlet to the fire room would have continued to supply fresh air without interruption, but this would require the inlet fan to withstand much higher pressures which is often not the case. Even if the outlets were also converted to inlets the maximum heat release remained the same since the pressure/flow relation for the fans remained the same. The average heat release rate also remained similar in cases where the pressure boundary was not broken. Once the pressure boundary was broken the average heat release rate was increased by about 50%, but since the flow from the fire room to the atmosphere was also increased in these cases the thermal load on the fans was not increased compared to other cases, it was actually decreased.

The quantitative results are sensitive to changes in the ventilation system setup. Changes such as the fan characteristics, placing the compartments on different z-levels or changing the loss coefficients in the ventilations system will have a great impact on the final results since the system will inherently behave different. The system is also symmetrical and all rooms have the exact same volume flow, which in many cases will not be true. This will of course also affect the quantitative results. All this information should be kept in mind if the methodology is to be applied to a real case, and the actual system will have to be well represented in FDS. The qualitative conclusions can however be of use when designing or opting a counter measure for smoke spread through a ventilation system.

9.3.4 Conclusion

It has been shown that it can be possible to simulate and evaluate different methods for preventing smoke spread through ventilation systems using FDS. Using the presented methodology, it can be possible to evaluate the performance of different systems in great detail which can make it possible to choose a better suited system for a specific application, but also to identify specific risks. This could be applied to situations where the safety of evacuating people or people in adjacent compartments is of interest, for example in a hotel or apartment building. However, there is a need for more experimental validation to ensure the quality of any of the proposed applications, as well as the application in this study. But the results of experimental validation done so far (Floyd, 2011; Wahlqvist & van Hees, 2013; van Hees et al., 2011; Wahlqvist, 2011; Wahlqvist, 2016) shows great potential for future use in performance based design and the study should be considered as an introduction to implementing a similar methodology in specific cases since different ventilations systems will present very different challenges and weaknesses.

10 Discussion

10.1 Research objectives

Based on the identified problems in the introduction and background, five distinct objectives were formulated to ensure that those problems would be addressed successfully. Each of those objectives will be evaluated, whether or not they can be considered successfully addresses, and discussed in this chapter, starting with the first objective:

- *Evaluate a CFD modeling framework to ensure that it can accurately predict thermally-driven flow, with an emphasis on smoke and heat transport from fires.*

FDS is generally well-accepted within the fire community for its ability to predict smoke movement and temperature in enclosure fires. Coupled with the fact that it is open source, which enables anyone to add or alter the inner workings of the code, made it a natural fit to use as a framework for successfully complete the set objectives.

Other frameworks were considered and evaluated, such as Ansys CFX, but the initial results when validating it against the PRISME scenarios did not look promising compared to FDS (Wahlqvist & van Hees, 2011). It was also evident that since most commercial software packages are closed source, and hence would not allow for changes or additions to the code base, that FDS was the most suitable modeling framework at the time. However, in the last years another open source alternative has been actively developed in the form of FireFOAM. FireFOAM is based on OpenFOAM (FireFOAM, 2017) which is a free and open CFD software with an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to acoustics, solid mechanics and electromagnetics (OpenFOAM, 2017). FireFOAM utilizes the finite volume method on arbitrarily unstructured meshes, and is highly scalable on massively parallel computers (FireFOAM, 2017). For future work it would be interesting to add the same capability to FireFOAM as that could likely complement FDS in some cases.

Even though FDS was already generally well validated for smoke and heat transport (McGrattan et al., 2014a), an additional validation exercise was performed comparing FDS with measurements made using the novel technique ps-LIDAR. As modeling software become more complex, the experimental setups get more complex, and more complex and non-intrusive measuring methods will be high in demand. FDS showed good agreement with collected data, both using ps-LIDAR and traditional thermocouples, but the 2D-data collection made possible by using the ps-LIDAR measurement technique provided valuable comparison to FDS and any other CFD software since the enclosure fire dynamics could be studied more in detail. As ps-LIDAR and similar techniques improve they will be an invaluable tool to provide validation data for CFD models.

In conclusion, the first objective was considered to be fulfilled by using FDS as a framework for further development and validation.

- *Validate, and if necessary improve or develop, a CFD sub-model that can predict the behavior of a ventilation system connected to one or several enclosures, both with and without any fire present.*

At the very start of the work that has been used as basis for this thesis FDS released its new HVAC sub-model. Although not fully developed or documented at the time, it provided new highly sought after capabilities which were very much needed to meet the second objective. Other ventilation calculation software such as PFS (Jensen, 2007) has traditionally been used to predict ventilation system behavior, but that approach does not provide a two-way coupling between the ventilation system and the fire. It is also only capable to generate steady-state results, lacking any time resolution and therefore any quantitative predictive capabilities of smoke spread. The obtained results only showed to which degree smoke spread was likely to occur or not. The HVAC model introduced to FDS opened up new possibilities in this application.

Prior to using the HVAC model in FDS other techniques for representing the ventilation network were evaluated, treating room inlets and outlets as a volume flow controlled by room pressure which was an available functionality in FDS. It was done with moderate success being able to predict qualitatively similar results, but as the complexity of the ventilation network in the validation cases increased it was evident that this approach was not quantitatively comparable.

The validation of the HVAC model in FDS was considered a success, which made it fulfill the second objective. There were however some interesting observations made related to FDS.

Using a prescribed mass loss rate, which was used in Paper II to focus on the validation of the ventilation system behavior, FDS generally produced more frequent and ampler pressure fluctuations for all cases. This could either be due to smoothing of the signal in the pressure measurement device used in the experiments, or it could be due to the difference between input mass loss rate and actual heat release rate in FDS. For example, as seen in Figure 43, the heat release rate fluctuates to a greater extent compared to the prescribed mass loss rate in Leak 1, specifically during the initial mass loss peak (around 60 seconds) when the fire becomes oxygen controlled (the effect here is however seen to a less extent compared to the later stages) and after the initial phase (after 200 seconds) once oxygen levels are lowered again. Up until about 260 seconds there is a good fit between the experimental values and the simulation, both regarding mass loss rate with corresponding heat release rate (Figure 43), and also pressure response (Figure 20). The oscillations of the heat release rate after 260 seconds seem to correspond to the fluctuations that can be seen in the pressure graph (Figure 20) according to the comparison of the oscillation frequencies made in Figure 44. Here it can be seen that the peaks correspond well with a very slight delay of the pressure response. The oscillation is probably caused by the lowered oxygen levels in the fire compartment(s) combined with the suppression model of FDS (McGrattan et al., 2014a). As seen in Figure 45, un-combusted gases are transported to an area with a higher oxygen fraction and are then combusted, causing a ghosting flame. This sort of transport of un-combusted gases (delays HRR over time) and local combustion (changes HRR in amplitude at specific time) causes the heat release rate to deviate from the prescribed mass loss rate and likely also causing the oscillations in the ventilation system response. The phenomena with ghosting flames are however likely also seen in the experiment, but it seems to occur to a less extent. It must also be noted that this behavior is coupled to using a prescribed mass loss rate, using an advanced pyrolysis model could dampen this effect since the mass loss rate would be coupled to the environmental feedback which is lacking with a prescribed mass loss rate.

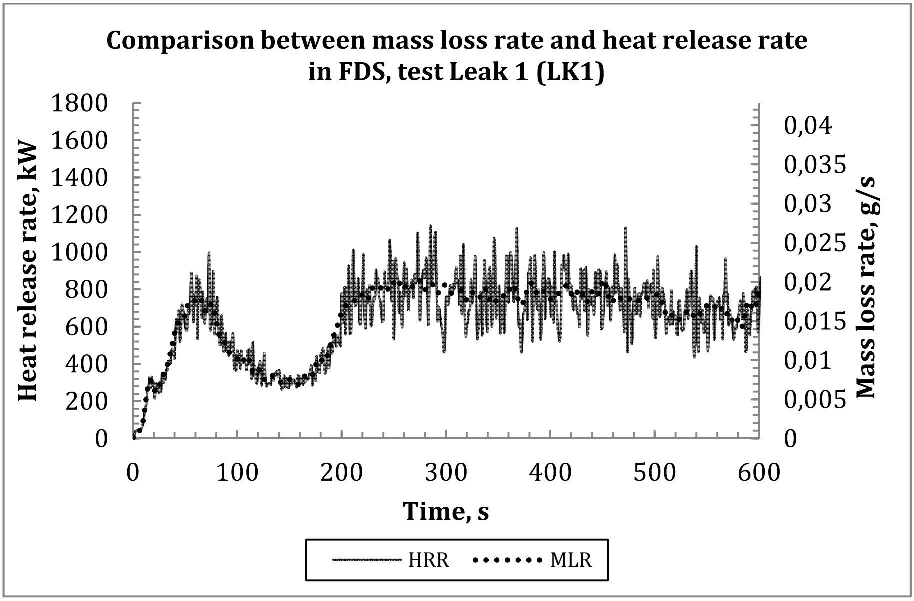


Figure 43 Comparison between prescribed mass loss rate and actual heat release rate in FDS, test Leak 1 (LK1).

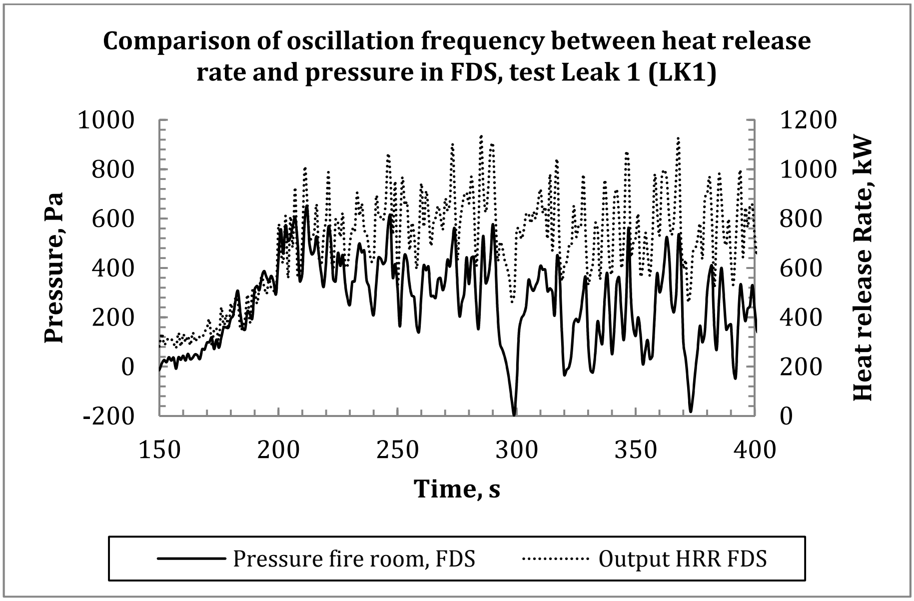


Figure 44 Comparison of oscillation frequency between the heat release rate in FDS and the pressure inside the fire room, test Leak 1 (LK1).

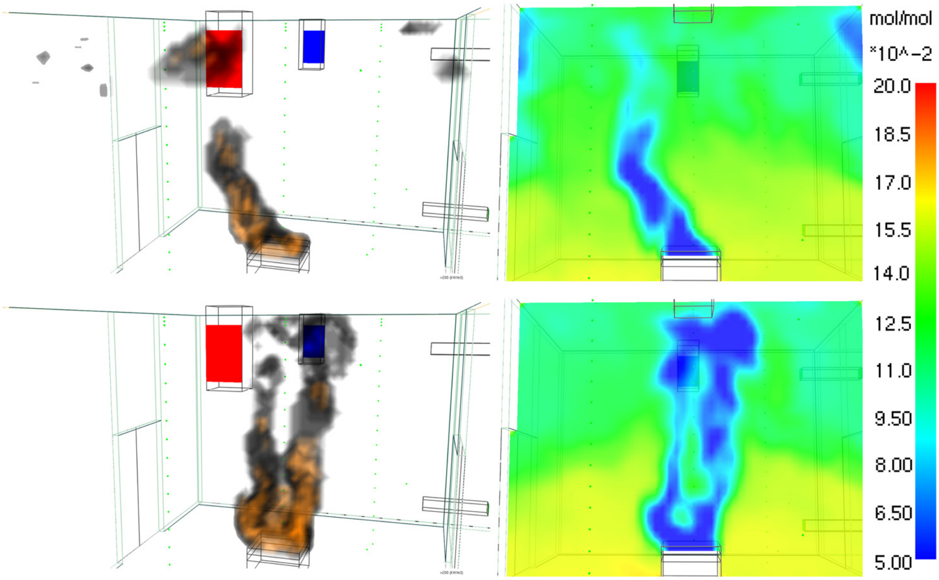


Figure 45 Example of ghosting flames and flickering flame (left part of figure) due to low oxygen levels (right part of figure) in FDS during a simulation of the Leak 1 (LK1) test. Ghosting flames can for example be seen at the exhaust on the top left half of the picture.

- *Validate, and if necessary improve or develop, a CFD pool fire pyrolysis sub-model that is capable of dynamic interaction with the surrounding environment in a feedback loop and that is robust (results largely independent to grid-size) and require relatively small amount of input data from the user.*

FDS includes both a solid pyrolysis model and a dedicated liquid pyrolysis model, but as previously stated those models are relatively complex, requiring detailed input from a user, and have been shown to be quite sensitive to the chosen grid size, as demonstrated in Paper III. Both of those characteristics are unwanted in applied engineering as user error and influence should always be kept to a minimum. But the traditional approach of using a specified design fire was limiting in many complex scenarios; therefore, it was warranted to introduce a simplified environmental feedback model to bridge the two.

Based on relatively simple pool fire physics and empirical data a model was presented, implemented, verified and validated. In general, it was concluded that the prediction of the mass loss rate is reasonably accurate as long as the overall flow is reasonably resolved by the model, and natural as well as mechanical induced flows both give acceptable predictions. The grid dependency of the sampled oxygen volume fraction has been observed to be relatively small even on coarse meshes, which can be a large benefit for engineering purposes compared to more detailed and advanced models. However, it should be noted that the oxygen volume fraction sampling volume must always be chosen with care and regards to each individual scenario since sampling inside the flame will yield significant differences. Though the model is bound to have limitations due to its simplicity, some of which are discussed in chapter 4.3.4, it has been shown to predict mass loss rates within 2.5-25% while being relatively insensitive to grid size. The model also requires a limited set of user input data which makes it suitable for applied engineering. The third objective was hence considered fulfilled. There were however some observations as described below.

One of the more challenging scenarios seems to be cases where the oxygen volume fraction inside the compartment is dependent on resolving complex flows through passive openings. For the steel ship compartment experiments all of the mechanically ventilated scenarios were well predicted, as well as the ones with "simpler" passive ventilation, such as a full door opening. However, when a quarter-door opening was present, the prediction of the oxygen volume fraction, and as a consequence the mass loss rate, was not satisfactory. The results were improved by making changes to the door slot, but a more in-depth analysis and comparison of similar cases with more detailed experimental measurements would be of prime interest.

The grid dependency of the external radiation model is coupled to the "standard" radiation model in FDS, hence the grid dependency of the external radiative heat flux feedback has been observed to be larger compared to the oxygen volume fraction, but the actual predicted mass loss rate was not largely affected. This was due to two reasons; in the cases where the relative difference between the two grid sizes was large, the actual external radiative feedback resulted in a very small portion of the total mass loss rate. In the case where the external radiative feedback was the cause of a significant part of the mass loss rate (INT1), the oxygen depletion had the inverse relation compared to the external radiative feedback, resulting in similar total mass loss rate except for the very beginning of the fire duration when the oxygen fraction in the compartment was still sufficient.

A possible limitation of the presented simplified feedback model is that it relies on the relatively simple combustion model built into FDS; the stirred reactor approach. There are more advanced extinction models built into FDS to take into account finite rate reaction rates, but for the majority of the validation cases used in this thesis the simpler combustion model performed well. There were however a few cases where the oxygen volume fractions were very low in the experiments (below

10%) which was not well predicted by the model. These discrepancies were discussed to likely be the result of incorrect inflow of air through small air-intakes, but there is a possibility that it is due to the choice of combustion model. A more detailed study should be performed to fully understand the influence of chosen combustion and suppression model.

A general limitation to the presented model is that it has only been formulated and validated with liquid pool fires in mind. To be able to extend the area of use the model should be extended to solid fuels in the future which would require additional verification and validation, most likely accompanied by new suitable experimental test cases.

- *Validate the CFD model for predicting dynamic fire behavior caused by environmental interaction, including mechanical ventilation system response.*

Once all three separate required models and sub-models were validated (general heat and smoke spread, ventilation system response and pyrolysis model with environmental interaction) the combined prediction was the final step to validate. This was done using test from the PRISME project as the experimental campaign was tailor made for this type of validation exercise. The second and third objectives were very much overlapping in Paper III, so the conclusions and findings stated under the last objective holds true also here; it was considered successful.

- *Apply the CFD model to typical engineering problems and key issues raised in the introduction and background to demonstrate practical usefulness and obtain novel knowledge.*

Applied use of the verified and validated models was purely in the form of numerical exercises and as such might be the subject of some discussion. But since each element needed to perform these applications had been verified and validated, the confidence the predicative capability of the model was quite high.

A few points regarding the prediction of fire growth related to building characteristics must however be discussed. Even though a typical case was selected as basis for the numerical study, the selected test setup will not represent every possible scenario very well; objects close to the fire source might influence the radiative feedback, mechanical ventilation may influence the rate of oxygen depletion, complex flow patterns due to the location of inlets and outlets may also influence the rate of oxygen depletion etcetera. All of these factors and more must be taken into account and evaluated before application.

The fuel used in the simulations was a liquid (heptane) due to the relatively well known properties, fire behavior and the fact that the simplified environmental feedback model used to take oxygen depletion and radiative feedback into account had previously been developed for pool fires. In a real case the fuel source would probably be solid objects which increases complexity and could very well give different results than the ones observed. More experimental data would be beneficiary to investigate the differences between solid materials and liquids but unfortunately that was out of the scope for this thesis. However, it is expected that the qualitative effects would be similar using solid fuels as on liquid fuels, though the magnitude would be very fuel dependent.

Regarding the prediction of the performance of measures against smoke spread in ventilation systems there are also a few points to discuss. A rather large performance difference was observed between the different methods for preventing smoke spread, where traditional approaches such as using fire dampers or reverse valves performed among the best regarding total amount of soot spread. Other methods such as pressure relief and converting the inlet system to an outlet system also performed very well in this regard. However, since all methods, with the exception of the fire dampers, allow soot and hot gases to enter the ventilation system to different degrees, the real life performance and actual taxing on the ventilation system might be different due the clogging of filters and deformation of the duct network due to thermal stress. And in the case of fire dampers and reverse valves the functionality will also likely change under thermal stress. The effects of these parameters would be of prime interest for future work, both experimental and numerical.

Although quite a number of methods for preventing smoke spread in the ventilation system were tested it is far from a complete overview. In more complex systems, combinations of the tested solutions could be beneficial, e.g. reverse valves on inlets combined with using a collection box on the outlets, and using FDS to evaluate specific systems might be a relatively quick and cheap examine the performance of such a system.

The system oscillations observed could be due to the models used (combination of the HVAC model, leakage model and model used for predicting the heat release rate), but they might also be a naturally occurring phenomena in an under-ventilated environment. But since the frequency and amplitude have not been validated properly in this study (partly due to it being out of scope and partly due to very limited access to the experimental work which could be used for validation) any smoke spread occurring during these oscillations was not included in the primary results. An experimental and numerical study focusing on this phenomenon would be of prime interest for future research, since system oscillations can cause complex fire behavior and smoke spread in ventilation systems.

In all simulated cases simple combustion chemistry was used. Since only a single value for the soot yield was used, this might lead to an underestimation of the soot production that will occur in an under-ventilated environment (which was present in all of the simulations). This in turn can lead to under-estimation of the actual mass of soot that is being spread through the ventilation system and into the other rooms. A potential end user should be aware of this fact and treat the definition of the soot yield accordingly.

10.2 Experimental data

Every time experimental work is performed there is always experimental error or uncertainty. In simpler experimental setups it might be possible to estimate the experimental uncertainty or correct specific experimental errors with post-processing, but in the relatively complex experimental scenarios that were used for validation this might be impossible. However, observations done in the validation study, which likely were related to experimental error are discussed in the following sections.

10.2.1 ps-LIDAR experiments

Using methanol as fuel, the overall comparison between ps-LIDAR data and traditional thermocouples were good. However, the temperature measured using ps-LIDAR was underestimated near the top of the door opening. The underestimation is most likely because that most of the soot and particles (i.e., smoke), from the fire inside the room passes through the top of the doorway on its way out of the room. Because light scattering from homogenously distributed small particles cannot be filtered out, the measured signal will increase and the volume will be interpreted as colder. In addition, homogenously distributed non-discernible particles will increase signal extinction, which, if it reaches a substantially high level, will give the false effect of temperature increasing with distance.

The measurements using the sand burner (propane) showed a result contaminated by strong scattering from particles, rendering the results very hard to interpret. This unfortunately limits the use of the ps-LIDAR in general fire engineering experiments as soot producing fuels are the norm, but the technique is ever evolving and improvements are hopefully made in this regard.

The methane fire using a gas burner was initially chosen as the mass flow rate is easily controlled and can be constant over time. The gas burner flame also has less complicated combustion chemistry in comparison with pool fires. Consequently, a methane fire using a gas burner would have been the preferred choice from a simulation point of view, but because the resulting particles of such a fire inhibit the use of Rayleigh scattering thermometry, a methanol pool fire had to be used when comparing temperatures obtained using ps-LIDAR with simulated temperatures. The use of the methanol pool with non-steady burning unfortunately added some uncertainty to the comparison between the experimental and simulated results, but the gain from using non-intrusive techniques as well as being able to measure 2-dimensional temperature slices proved to be valuable none the less.

10.2.2 Steel ship compartment experiments

The data from the steel ship compartment experiments that were used for comparisons were not available in a digital format and were therefore transferred manually from the report (Peatross et al., 1993). In addition, the overall mass loss rate data was rather noisy, which was probably due to the relatively large capacity of the used load cell (0-200 kg), but no attempts of smoothing the data was done. Both of these issues likely caused increased uncertainty but neither were considered major enough to influence the final conclusions as none of these issues could be used to explain major differences between the experimental data and the simulations as were reported in some cases.

Another minor issue that concerned the experimental data was the fact that the oxygen volume fraction was reported being measured as “dry” and then converted to represent “wet” conditions (with or without water content) using the assumption that the ratio of water to carbon dioxide production remained the same as the stoichiometric ratio. This was not taken into account in the simulations where the dry volume fraction was measured, but the report stated that no oxygen concentration was reduced by more than 10 % compared to the dry values so this difference was deemed acceptable.

10.2.3 PRISME experiments

In Source D3 and Source D6 there is a strong mismatch between the experimental results and simulation (both pressure and ventilations system response). The magnitude of the pressure peaks is not well captured at all, being underestimated by almost 1000 Pa in the worst case. By analyzing the ventilation system response for the same cases it is evident that the inlet starts to reverse under less pressure than in the experiment. This means that the inlet acts as a pressure relief, making the predicted pressure peak much lower. This is demonstrated for the test Source D3 in Figure 46 where it can be seen that the expected response of the inlet, given that the experimental initial conditions were correct, is not achieved. The pressure (initial conditions) at the inlet in Source D3 was 163 Pa and 192 Pa at the closest connecting branch. The expected response would then be that the inlet flow would start reversing at a room pressure around 192 Pa. In Figure 46 it can be seen that the FDS simulation inlet reverses at 205 Pa, but the experimental inlet reverses at 450 Pa. The most probable cause for this is some discrepancy in the experimental data used for calculating the loss coefficients in the inlet branch or that some change or damage occurred in the system during the experiments. These assumptions are further assured by the fact that the temperatures inside the fire compartment are in good agreement with the experimental data, as well as the generally good agreement between the experiments and simulations in other tests. The same conclusion can be drawn for Source D6a, but the impact on the result is not as large since the difference is smaller between the two values.

No extensive sensitivity analysis of the loss coefficients in the cases where the discrepancies were significant were made partly due to the fact that they demonstrated the sensitivity to either user of experimental errors of these kind of systems, but also due to the complexity of the ventilation system. Changing one loss coefficient would change the dynamics of the system to a rather large extent, for example changing the loss coefficients to the inlets to increase the pressure resistance before backflow would occur would mean changing most other loss coefficients to balance the flow ratio between inlet branches (including those that release air into the “atmosphere”). In turn the capacity (RPM) of the fan would have to increase since the resistance from the fan to the inlets has increased and the total flow would else be less due to the behavior of the fan curves. Changing multiple parameters would defeat the purpose of the study since it would mean changing several unknowns, meaning that the end result would not lead to better understanding and it would not be a very good validation exercise.

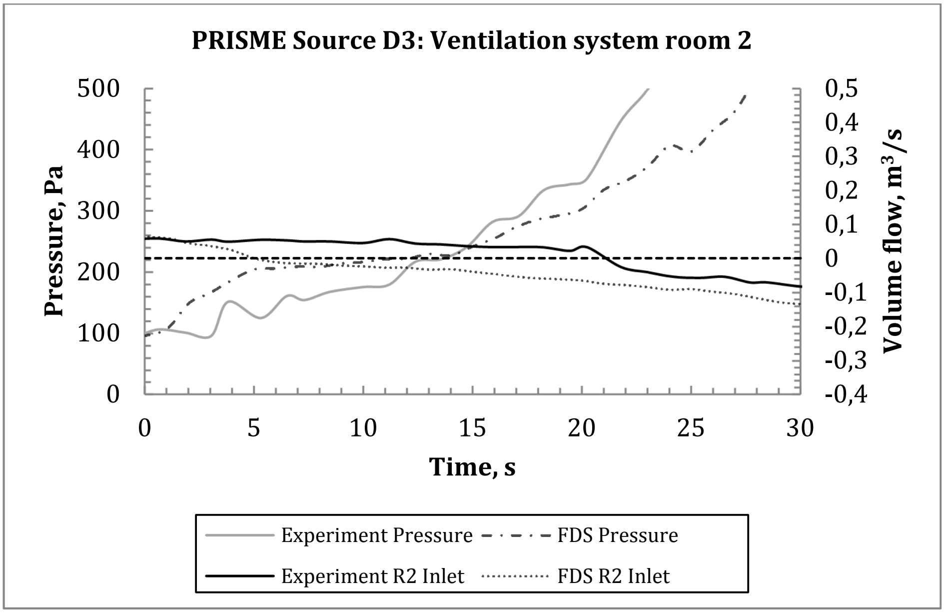


Figure 46 Detail of the initial pressure and ventilations system response in test Source D3.

There are also other minor differences observed between the experimental data and the simulations. For example, in test Door 6 (D6) the initial pressure peak was not correctly predicted. The mass loss rate (which was prescribed from experimental data) in FDS corresponds well with the small pressure peak during the initial pressure rise (Figure 47), while the pressure measured during the experiment does not. There are two probable causes for this mismatch. Firstly, a direct error in the measurement of the experimental mass loss rate, which is less likely since the phenomena is observed on several occasions. Or secondly, a difference in the measured mass loss rate and the actual heat release rate in the experiments, as in fuel evaporating in the experiment but remains un-combusted, while combustion occurs in FDS. The same initial pressure peak can also be seen in test Door 5, Leak 1 and Leak 3 although not as prominent. One possible reason for this behavior could be that the vaporization layer size of the pool is changing during the initial phase. The increase in volume of this layer would mean that a mass loss is registered on the scale, but this vaporized fuel does not contribute to any heat release. When the vaporization layer size has stabilized the actual heat release rate corresponds to the mass loss rate. Since the vaporization process in not simulated in FDS, the formation of this layer is almost instant. The argument is in part backed up by the fact that the largest effect is seen in test Door 6 and Door 5, which both have a larger pool surface area, 1 m^2, compared to the other tests with the same phenomena (Leak 1 and 3) which had pool surface areas of 0.4 m^2. A larger pool area would lead to a larger volume of the vaporization layer given the same approximate border height of the steel pool container. However, the same effect is not as clearly seen in the Source test series or the Door 2 to 4 tests, which also had pool surface areas of 0.4 m^2, so no definitive conclusion can be made without more detailed experiments on this specific topic.

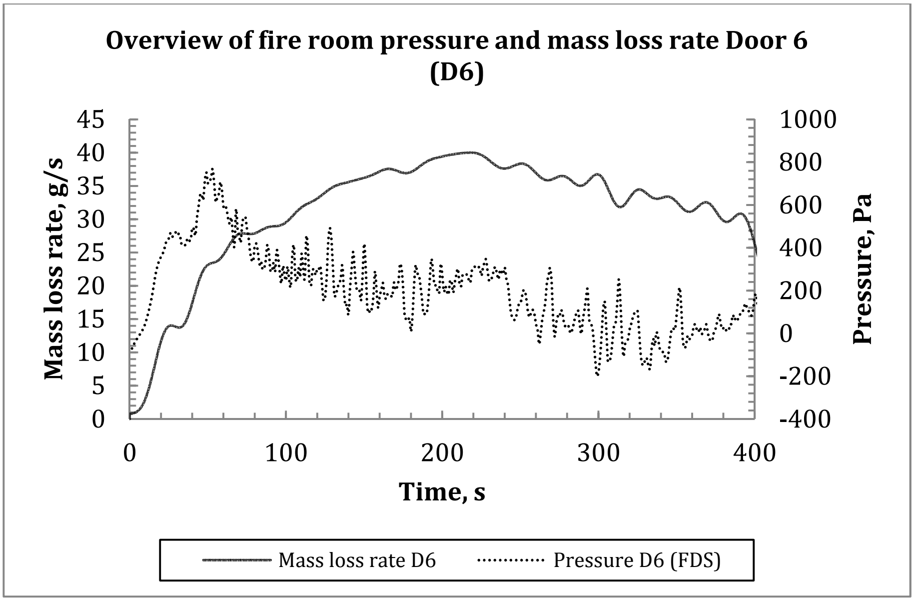


Figure 47 Overview of fire room pressure and mass loss rate during (MLR) test Door 6 (D6). It can be seen that the sudden decrease of the MLR (at 25 s) directly influences the pressure in FDS and in turn the ventilation system behavior, but the same response is not seen in the experimental data.

11 Conclusions

The general topic of this thesis was to be able predict the feedback loop that occurs between a pool fire and its environment. This was done by sub-dividing the problem into several objectives that when solved separately would come together to and be applicable to the larger problem. The major conclusions of the appended papers and this thesis are:

- The need for validation data is always in high demand, especially non-intrusive methods and methods that are capable of doing more than point-measurements. As computational models get more advanced this demand is expected to increase, and using equipment such as picosecond-LIDAR is a promising technology as it is both non-intrusive and also capable of capturing data in a 2D-plane. One downside is the need for relatively non-sooty fuels, but as the used software and hardware develops this caveat will probably decrease.
- The possibility of simulating a tightly sealed fire room connected to a mechanical ventilation network using FDS has been demonstrated with success. Using only data collected before the fire was ignited (with the exception of mass loss rate from the pool fire), FDS manages to correctly predict the pressure inside the fire room and consequently the effects on the ventilation system, for example backflow in the inlet branch in the early stages of the fire. Although it must be noted that the input parameters are quite sensitive, this could be seen especially in two tests. When the loss coefficients of the inlet and exhaust branches were not correctly characterized, FDS failed to predict the magnitude of the pressure peak and subsequently the magnitude of the response of the ventilation system.
- Predicting the mass loss rates in enclosed spaces using a simplified environmental feedback model has been done with satisfactory accuracy (within 25% or less in most cases) for fire safety engineering. Using simple data collected from free burning pool fires, FDS manages to reasonably well predict the mass loss rate using the oxygen volume fraction close to the flame base, and in some cases the radiative heat flux from external sources

(sources other than the flame itself) such as the walls and smoke layer. The prediction of the mass loss rate is reasonably accurate as long as the overall flow is reasonably resolved by the model, and natural as well as mechanical induced flows both give acceptable predictions. The grid dependency of the sampled oxygen volume fraction has been observed to be relatively small even on coarse meshes, which can be a large benefit for engineering purposes compared to more detailed and advanced models. However, it should be noted that the model does not replace a more complex pyrolysis model and any end user should be aware of its limitations.

- Two practical engineering applications with novel results have been demonstrated using numerical experiments. Numerical experimentation is a promising and useful research method in fire science and performance based design. It holds both advantages and drawbacks compared to traditional experiments, but with proper validation of the underlying models the confidence in the method can be increased. Since actual experiments have to be performed to provide validation data, numerical experiments are strongly linked to traditional experiments and both methods complement each other rather than replace another.

12 Future research

During the continuous work of this thesis there were several topics that simply could not be dealt with, either due to time or budget constraints. In many cases there was lacking or altogether missing experimental data suitable for validation work which means that extensive experimental work would had to be done in order to obtain suitable validation cases. This meant that even if a model could be developed, it would have been impossible to validate such model. Some of the topics that were explored but never concluded are discussed the following sub-sections.

12.1 Ghosting and wandering flames

One particular phenomenon was identified during search for suitable validation cases for the implemented environmental feedback model, namely ghosting and wandering flames. Ghosting flames has been observed in several experiments, but they are not very often performed in full scale. Since the contribution to the total mass loss rate between the convective and the radiative part can change significantly between small scale and full scale these experiments were not ideal for validating a model for use in full scale applications. Therefore, more experimental and numerical work is needed to fully understand this phenomenon and the consequences in an engineering setting when evaluating fire safety.

A special case of ghosting flames is the wandering flame. This has been observed in cases where the fire is enclosed in a space with an opening in only one part of the enclosure that is relatively far away from the fuel source. If the conditions are suitable the flame will then detach from the fuel source and “wander” towards the opening as oxygen depletes near the fuel source. If the temperature and resulting radiative feedback to the fuel source is not high enough the flame will wander back and re-attach or extinguish, but if the radiative feedback is high enough fuel will still be evaporated and combusted in a region with sufficient oxygen. This behavior is of prime interest in both an experimental and numerical sense, and future work would likely have to focus on both parts as existing, well-documented experiments are far and few between. Initial numerical work was carried out with some success but due to the lack of verification tests no publication could be made within the work of this thesis.

12.2 Oscillating system behavior

As noted in Paper V some oscillatory behavior was observed when combining a fire in an enclosure connected to a mechanical ventilation system. This is not always the case, but given the “right” combination of fire size, ventilation performance and building materials this phenomenon has been observed in full-scale experiments conducted within the PRISME 2 project (OECD, 2015) resulting in very particular and interesting results. Some work on the topic has been done (Beji & Merci, 2016), but it is believed that more experimental work has to be done before this can be fully understood and modelled with reasonable accuracy. This topic is also closely linked to the ghosting and wandering flames as a robust model is needed predicting the fuel mass loss rate in various conditions.

12.3 Building leakage behavior under fire induced stress

A fire is a fierce and often uncontrolled force, and in such cases the fire will likely affect the structure of the building. In several cases (paper II, III and V; Kallada Janardhan et al., 2017; Hostikka et al., 2017) the effect of building leakage has been observed, but in all of those cases it has been assumed to been constant. Since the experimental setup used in some of these cases was considered extremely robust this was not an issue, but in a “normal” residential building the fire induced pressure and thermal load would likely significantly change the building leakage over time, hence affecting the overall system behavior. Research with direct focus on this topic has not been done but it is believed to be of significant importance as building gets built tighter and tighter to be more energy efficient. A fire in a tightly sealed, well insulated building will undoubtedly put more stress on a connected ventilation system compared to a building with large leakage areas and less energy efficient materials due to higher pressure being built up. But if a fire changes the building over time, e.g. cracks walls or windows, the pressure will change and the consequences might be less severe. This topic would be valuable piece of puzzle in fully understanding the interaction between fire and environment.

12.4 Ventilation system performance under particle and thermal stress

In Paper V it was discussed that the presented results might change due to ducts deforming under large pressure differences and thermal stress as well as flow resistances in the ventilation changing due to soot deposition in filters and ducts. The general topic of soot deposition has been researched to some extent, but soot depositions inside duct networks are still not explored. Deformation of duct networks has largely not been researched at all, but if performance based designs is to be fully accepted in facilities such as nuclear power plants, this topic has to be further investigated.

12.5 Pool fire extinction criteria

One of the presented cases in the validation study (Paper III) was extinguished due to low oxygen concentrations, but since no extinction criteria other than fuel burn-out is present in the simplified environmental feedback model this was not predicted by the model. Adding an extinction criterion could prove valuable as some case might otherwise be over-conservative and force unreasonably complex and expensive engineering solutions to a potentially non-existent problem. Further experimental data would be needed to understand the mechanism of extinction in room scale-fires, but it would further increase the knowledge of the interaction between fires and their environment.

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