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Prediction and validation of pool fire development in enclosures by means of CFD (Poolfire) Report – Year 1

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Abstract

Fires in nuclear power plants can be an important hazard for the overall safety of the facility. One of the typical fire sources is a pool fire. It is therefore important to have good knowledge on the fire behaviour of pool fire and be able to predict the heat release rate by prediction of the mass loss rate. This project envisages developing a pyrolysis model to be used in CFD models. In the this first year report the literature review conducted within the project is reported as well as the first tasks in the evaluation and modelling of the new model.

Key words

Fire, nuclear power plants, pool fires, modelling

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Report Year 1

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Fires in nuclear power plants can be an important hazard for the overall safety of the facility. One of the typical fire sources is a pool fire. It is therefore important to have good knowledge on the fire behaviour of pool fire and be able to predict the heat release rate by prediction of the mass loss rate. This project envisages developing a pyrolysis model to be used in CFD models. In the this first year report the literature review conducted within the project is reported as well as the first tasks in the evaluation and modelling of the new model.

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Preface

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Contents

1. INTRODUCTION.....	1
1.1. BACKGROUND	1
1.2. SCOPE	2
1.3. LIMITATIONS OF THIS REPORT.....	2
2. OVERVIEW OF THE POOLFIRE PROJECT.....	3
2.1. WORK PACKAGE 1 CURRENT STATE OF THE ART.	3
2.2. WORK PACKAGE 2 DEVELOPMENT OF ADVANCED MODEL	3
2.3. WORK PACKAGE 3 VALIDATION OF THE MODEL	3
2.4. WORK PACKAGE 4 IMPLEMENTATION OF THE MODEL IN A REAL CASE SCENARIO FOR RISK IDENTIFICATION.	3
2.5. WORK PACKAGE 5 DISSEMINATION OF RESULTS.....	4
2.6. WORK PACKAGE 6 MANAGEMENT	4
3. CURRENT STATE OF THE ART.....	5
3.1. LITERATURE REVIEW.....	5
3.2. MODEL.....	6
3.3. VALIDATION OF THE CURRENT MODEL.....	7
3.3.1. MODELS FOR PRESCRIBED BURNING AND PRESCRIBED VENTILATION	7
3.3.2. RESULTS WITH PRESCRIBED BURNING/PRESCRIBED VENTILATION.....	9
3.3.3. RESULTS WITH PRESCRIBED BURNING/VENTILATION MODULE FDS AND CFX....	11
4. DEVELOPMENT OF A NEW MODEL	17
4.1. THEORETICAL BACKGROUND AND INNOVATIONS.....	17
4.2. MODEL DESCRIPTION.....	17
4.3. PRELIMINARY COMPARISONS OF OLD AND NEW LIQUID EVAPORATION MODELS 17	
4.3.1. MODELS FOR OPEN ATMOSPHERE PRISME TESTS (PRISME SOURCE).....	17
4.3.2. RESULTS FOR OPEN ATMOSPHERE PRISME TESTS (PRISME SOURCE).....	19
4.4. NEXT STEPS	20
4.5. FIRST EXPERIMENTAL SET-UP FOR VALIDATION	20
5. DISSEMINATION	23
6. CONCLUSIONS.....	25

REFERENCES

ANNEXES

1. Introduction

1.1. Background

Safe shutdown of a reactor after an incident is a key factor in the overall safety design of a nuclear power plant. When the incident is a fire, the fire can not only be the cause for the shutdown but can also jeopardize the safe shut down by destroying critical components needed for the shutdown process. In order to prevent this redundant systems are built up which can guarantee safety shut down if the major system fails. In fire terms one is primarily interested in the functional performance of the components such as cables, electronic circuits, etc. With respect to fire, events can be classified in 3 major groups depending on the position of the subsystems. The three cases are given illustrative in Figure 1. In the first event (left), the redundant systems A and B are in the same enclosure within a fire compartment and a fire can have a much greater impact on one or both subsystem if it happens and the risk is consequently high for failure of the redundancy. Probability for failure might e.g. be 1 on 100 years. In the second event the systems A and B are in the same fire compartment but not in the same enclosure and the risk of failure will depend on the fire spread between enclosures. Probability will be 1 on 1000 years. Finally the subcomponents A and B can be in 2 different fire compartments and risk for failure will be due to failure of fire compartments, something very seldom to happen.

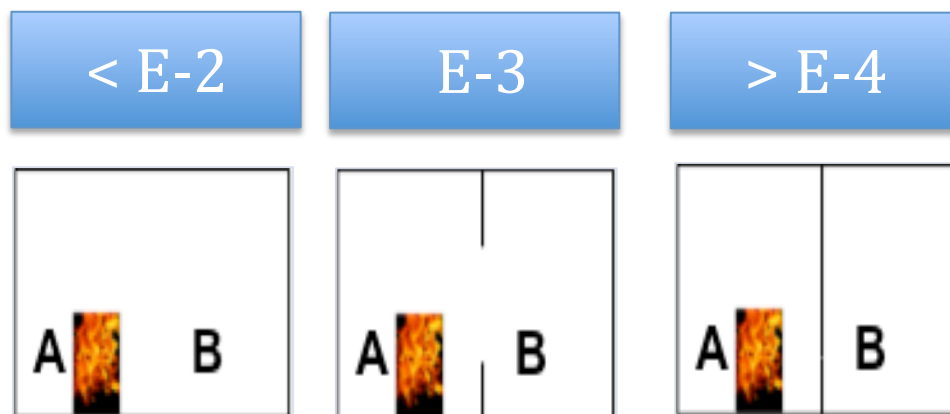


Figure 1 Example of event classification for fire incidents with probability for failure

One way to determine the overall risk in a PSA analysis is by using probabilistic methods using statistics. Another possibility is to investigate the likelihood for critical conditions by using calculation methods, which predicts fire growth, fire and smoke spread and critical temperature of the components. This is a so-called deterministic approach, which can be a complement to the probabilistic methods in PSA analysis. Today more and more CFD (Computational Fluid Dynamics) methods are used instead of empirical and zone models. The use of the method puts however high requirements on the correctness of the prediction methods and therefore validation experiments are necessary. Another key issue here is the correct prediction of the fire growth within an enclosure. This fire growth depends on the properties and geometry of the enclosure, ventilation conditions and the type and load of the fire fuel.

In an actual international OECD project called PRISME a large amount of experimental data is gathered with respect to enclosure fires where mechanical ventilation is involved. The project has been using a number of fuel loads defined by the different international partners (regulators and industry). One of the actual fuel loads is a defined pool fire using the same liquid. A liquid waste fire is namely one of the major fire incidents reported. Experiments in one or more enclosures under different ventilation conditions and by using different connections between enclosures (doors, wall openings, ducts, etc.) have been conducted. The project will be extended by another 3 years and will include also experiments with other set-ups (e.g. two enclosure above each other with a horizontal opening), another liquid fuel, cables as fire load, and extinguishment systems (sprinklers). This international project constitutes of an important and unique database set of experiments. The international project focuses mainly on the fire tests while use of the fire test results and validation of CFD models is a national or regional responsibility and subject to local funding.

Up to now Sweden and Finland have participated on national basis but it has been seen clearly that synergy is possible between the research groups involved in the project (Lund university and VTI). Activities have been related to validation of experiments with the most commonly used CFD tool called FDS and by conducting sensitivity analyses for this tool. In the future the important aspect of coupling fire growth with the enclosure conditions as mentioned above is an important aspect if a deterministic model approach would be successful for risk assessment of nuclear power plants.

1.2. Scope

The scope of the project is to provide improved tools for deterministic evaluation of the risk for loss of functional performance in redundant systems critical for shut down of the reactor within PSA analyses. The improved tool will contain an advanced pool fire model, which takes into account all aspects of the enclosure (geometry, properties, ventilation) and fuel (amount, type, surface area, thermal boundaries).

1.3. Limitations of this report

This report only deals with the results obtained during the first year of the report.

This report includes the results of work package 1 and the status of work package 2 with respect to the new model. Some results of the validation work (work package 3) within the PRISME project are also reported. A specific chapter on dissemination is also included although there are limited activities since the project is in its first year. Work package 4 (real scale application) and 6 (management) are not reported.

2. Overview of the Poolfire project

This chapter gives a short overview of the overall 3-year project. The project major core of activity is the development and validation of a pyrolysis model for pool fires in enclosures and will contain the following work packages.

2.1. Work package 1 Current state of the art.

Evaluation of the actual state of the art of pool fire models within CFD codes especially FDS, and the validation data available within the OECD project PRISME. The result of this work package will be an overview of the need for further development and the requirements for additional data both as input data for the models and for validation purposes.

Responsible organisations: VTT and Lund University

2.2. Work package 2 Development of advanced model

This work will contain the development of an advanced model for pool fires, which takes into account important aspects from the enclosure and pool fire. The enclosure geometry (volume, openings, height, etc.) will define e.g. the hot smoke layer temperature, which on its turn defines the thermal radiation levels towards the burning liquid. Ventilation inside the enclosure is also an important factor since the ventilation affects the burning rate (ventilation controlled or not) and the burning rate affect on its turn the ventilation (overpressures, back flow, etc). Finally the type of fuel and how it is located in the enclosure is of importance. Fuel leakages mainly run on surface and hence the thermal boundaries are important, as they will affect the heat losses of the burning liquid and needed to be incorporated in the model. Advanced pyrolysis models for liquid pools need special input data. It will be investigated how these can be obtained from literature or small-scale test data.

Responsible organisations: VTT and Lund University

2.3. Work package 3 Validation of the model

Test from the international OECD project PRISME will be used for validation of the model. Both previously run experiment in the first project will be used but also data from the second project to be started in 2011. Both experiments in single and multi rooms will be used and validation will not only be limited to the pool fire growth but also to parameters such as temperature of the gas layer, gas concentrations, door flows, surface temperatures and temperatures of components. As part of the validation also a parameter investigation will be performed.

Responsible organisations: Lund University, VTT and Hugesund University College.

2.4. Work package 4 Implementation of the model in a real case scenario for risk identification.

In this work package the obtained knowledge will be applied on a real case study in a nuclear power plant within a deterministic evaluation of the risk for loss of functional performance of critical components.

Responsible organisations: Lund University and Vattenfall Ringhals.

2.5. Work package 5 Dissemination of results

Results from the project will be reported in scientific journals and at conferences. A small workshop for interested parties will be organised at the end of project.

Responsible organisations: All partners

2.6. Work package 6 Management

Management of the project includes aspects such as communication with partners, meeting organisation, economical follow up and progress follow up.

Responsible organisation: Lund University

3. Current State of the art

3.1. Literature review

The pool fire scenario has been widely used by researchers to study the vaporization process at the fuel surface since the pyrolysis process of fuel is one of the most important stages of combustion, along with the ignition and the flaming processes. Prescribed constant conditions for burning rate or fuel mass loss rate, so called open simulations or *a posteriori*, have been used in various numerical fire studies using CFD codes showing good agreement with experimental results. But the burning rate or fuel mass loss rate is often not easy to obtain without experiments. Therefore it is desired to be able to predict these parameters beforehand, *a priori*.

A practical way to determine the burning rate of large pool fires was described by Babrauskas (1). He showed that the fuel mass loss rate or the burning rate in an open-atmosphere system could be estimated with a simple correlation that only requires the knowledge of certain fuel properties. It is generally based on a simple heat balance of the poolfire taking into account mainly the effect of radiation. Other investigations of hazardous conditions associated with compartment fires have included empirical methods such as that given by the work of Peatross and Beyler (2) as well as theoretical approach proposed by Quintiere and Rangwala (3) and Utiskul (4). The empirical correlation, obtained from a steady-state combustion regime by Peatross and Beyler (2), provides fuel mass loss rate against oxygen concentration measured at the flame base for large-scale fire compartments. One of the main drawbacks of this empirical relationship lies in that it was obtained in conditions for which external heat fluxes were negligible. This limits its relevance to situations where high gas and wall temperatures, affecting incoming heat fluxes, are present. In more recent theoretical work by Melis et al (5), which made use of a well-stirred reactor approach, a good agreement between the measured fuel mass loss rate with the linear correlation of Peatross and Beyler was obtained.

Utiskul (4) presented a theoretical model that is based on the burning rate approach in an open-atmosphere and includes fuel response to vitiated air along with burning enhancement due to hot gases and confinement. In this study, the predicted mass loss rate was properly validated with small-scale heptane pool fire experiments. However, because flame radiant heat feedback to the pool fire was ignored, this theory was found to be insufficient for large-scale fires, which later was shown by Nasr et al. (7). Only a few studies have addressed the problem of the determination of the heat fluxes back to the fuel surface in order to determine the fuel mass loss rate. One of these studies was performed by Tewarson et al. (8), which focused on the determination of convective and radiant 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 (9), 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. Later Klassen et al. (10) developed an equation of radiative transfer to account for the effects of fluctuations on the heat feedback. An experimental study was also performed to obtain measurements of radiative heat feedback in a 30 cm diameter, heavily sooted, toluene pool fire (10). This work was

further developed by Hamins et al. (11, 12) 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 (13), and the convective heat transfer was determined using the stagnant film layer model.

Beaulieu and Dembsey (14) later carried out an analytical study to quantify the effect of enhanced ambient oxygen concentration on flame heat flux. An advanced flammability measurements apparatus was used to measure the flame heat flux back to the burning surface for 20.9% and 40% ambient oxygen concentrations. In this work, the flame was considered as a surface emitter, so that a view factor was used to express the flame radiant heat flux. They also measured the flame emissivity, temperature, and height to calculate the convective and radiant heat fluxes. Although the calculated values were in good agreement with the experimental measurements, there was no relationship reported between the heat fluxes from the flame or the effect of the oxygen concentration.

Concerning the complete coupling between the liquid/solid and gas phases, few computational fluid dynamics (CFD) works (15, 16) have been carried out, in which the burning rates are satisfactory reproduced in the wide range from small to large pool sizes. 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. For this reason, any predictive fire simulations in a large compartment have yet to be reported. A simpler modeling approach, based on an energy balance at the fuel surface and on the stagnant film layer theory, was derived by Nasr et al. (7) and first applied in a CFD code to predict the fuel mass loss rate of a hydrogenated tetrapropylene (TPH) pool fire in a confined and mechanically ventilated compartment as a part of the PRISME program (6). This model was validated against experimental measurements and showed good agreement for the prediction of the transient heat release rate of a fire compartment (17, 18). However, air vitiation effect on the fuel mass loss rate was not investigated in this study.

This literature review displays the need of further work in the area of predicting burning rate or fuel mass loss rate instead of simply prescribing it, especially in the case of significant external heat fluxes, where the current published work is incomplete.

3.2. Model

In FDS, fires can be modelled in two ways: as a prescribed fuel inlet boundary condition or utilizing the built in pyrolysis model. In this section, a description of the FDS liquid pyrolysis model is given and the two investigated evaporation models are presented.

When the liquid pyrolysis model is invoked FDS solves a one dimensional heat conduction equation for the liquid fuel

$$\rho_f c_f \frac{\partial T_f}{\partial t} = \frac{\partial}{\partial x} \lambda_f \frac{\partial T_f}{\partial x} + \dot{q}''' \quad (1)$$

Here ρ_f , c_f , λ_f and T_f are respectively the fuel density, specific heat, thermal conductivity and temperature. The radiative transport can be described as volumetric heat-source term \dot{q}''' in Equation 1.

The FDS condensed phase model uses a “two-flux” model, where the radiative intensity is assumed to be constant in “forward” and “backward” hemispheres. The forward radiative heat flux into the fuel is

$$\frac{d\dot{q}_r^+}{dx} = \kappa_s (\sigma T_f^4 - \dot{q}_r^+). \quad (2)$$

A corresponding formula can be written for the backward flux \dot{q}_r^- . The heat source term in Equation 1 is the difference between the forward and backward fluxes

$$\dot{q}''' = \frac{d\dot{q}^+}{dx} - \frac{d\dot{q}^-}{dx}. \quad (3)$$

Boundary condition at the fuel surface is given by

$$\dot{q}_r^+ \Big|_{x=0} = \dot{q}_{r,in}'' + (1 - \varepsilon) \dot{q}_r^- \Big|_{x=0}, \quad (4)$$

where ε is the fuel emissivity.

In the present (FDS version 5) model, the rate of liquid fuel evaporation is a function of the liquid temperature T_s and the concentration of the fuel vapour above the pool surface. The volume fraction of fuel vapour above the pool surface is found from the Clausius - Claupeyron relation

$$X_f = \exp \left(- \frac{h_v W_f}{R} \left(\frac{1}{T_s} - \frac{1}{T_b} \right) \right). \quad (5)$$

Here h_v is the heat of vaporization, W_f is the molecular weight, T_s is the surface temperature of the pool and T_b is the boiling temperature of the fuel. In the old evaporation model the mas flux on the fuel surface is adjusted so that the fuel vapour equilibrium above the pool is maintained.

3.3. Validation of the current model

3.3.1. Models for prescribed burning and prescribed ventilation

The PRISME DOOR and PRISME SOURCE tests consider pool fires in ventilated compartments. The ventilation rates and pool sizes are varies between the tests. Different air supply locations are also considered. The PRISME SOURCE series considers a single room and the PRISME DOOR series considers two rooms with a door connecting them.

Room dimensions and material properties used are taken from the PRISME documentation (19-23). 10 cm discretization interval is used in all cases. In addition to the ventilation system, a leak with an area 0.009 m² is described for the whole compartment. Without the small leak, the simulations often stopped with numerical instabilities.

The PRISME SOURCE test series considers a single room connected to other rooms through ventilation. The computational model used in the simulations consists of only the fire room, with ventilation modelled as inflow and outflow boundaries with prescribed flow rates. The flow rates on the inflow and outflow

boundaries follow the measured inflow and outflow rates closely. The pool fire is likewise modelled as a fuel inlet boundary with a prescribed mass flux of fuel (burning rate). The mass flux is again obtained from mass loss rate measurements. Figure 2 shows the computational model used for the SOURCE series of tests. The room dimensions are $5 \times 6 \times 4$ meters. The pan is 0.4 meters high. Walls are 30 cm thick and made of concrete. In the ceiling there is a 5 cm layer of rock wool on top of the concrete. The concrete is backed by void.

Notice that the air supply had two possible positions: 'high' or 'low'. In Figure 2 the air supply is in the 'low' position. The parameters varied were the ventilation and burning rates (pool size) and the air supply position. Table 1 gives a summary of the simulation cases.

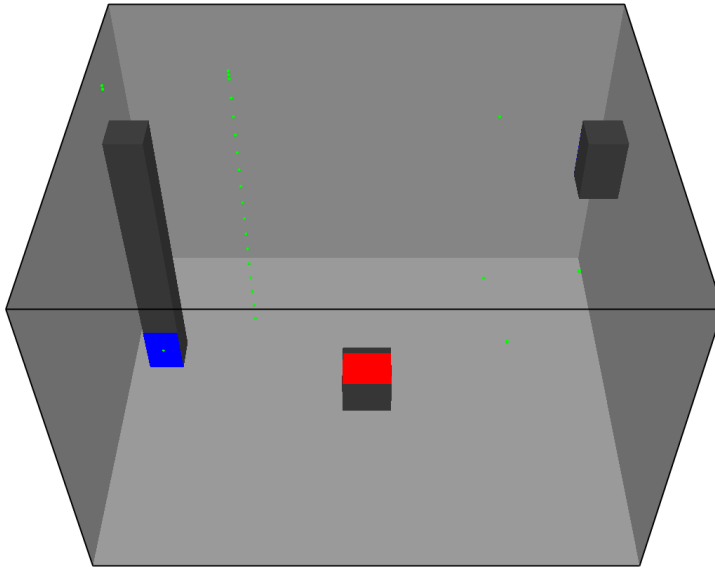


Figure 2 Model of the PRISME SOURCE series test PRS-SI-D6a. Air supply vent is in the 'low' position.

Table 1 Description of PRISME SOURCE test series

<i>Test name</i>	S m^2	D m	Tr $1/b$	dv_{air}/dt m^3/b	<i>Air supply</i> <i>position</i>
PRS-SI-D1	0.4	0.71	4.666667	560	High
PRS-SI-D2	0.4	0.71	8.416667	1010	High
PRS-SI-D3	0.4	0.71	1.5	180	High
PRS-SI-D4	0.4	0.71	4.708333	565	High
PRS-SI-D5	0.2	0.50	4.625	555	High
PRS-SI-D5a	0.2	0.50	1.583333	190	High
PRS-SI-D6	0.4	0.71	4.666667	560	Low
PRS-SI-D6a	0.4	0.71	1.666667	200	Low

The PRISME DOOR series considers two rooms, the fire room and the target room, connected by a door as shown in Figure 3. The purpose of this test series is to study the propagation of smoke and hot gases from the fire room to the target room. The room dimensions are the same as in the SOURCE test series. The dimensions of the computational domain are $10.2 \times 6 \times 4$. There is a 20 cm thick wall separating the two 5 meter wide rooms. The door is 70 cm wide and 215 cm high.

Table 2 gives a summary of the simulated PRISME DOOR tests. The varied parameters are burning rate and ventilation rate. This time there are two air supply vents and two air exhaust vents: one of each in each room. All the vents are in the 'high' position for all the simulations. In addition two gas phase measurements, additional cable targets have been added to both rooms. Temperatures on the surface and inside these cables and the flow rates and temperatures in the doorway are the focus of this test series. The cable targets are located on the walls opposite the door in both rooms and on top of the door in the target room.

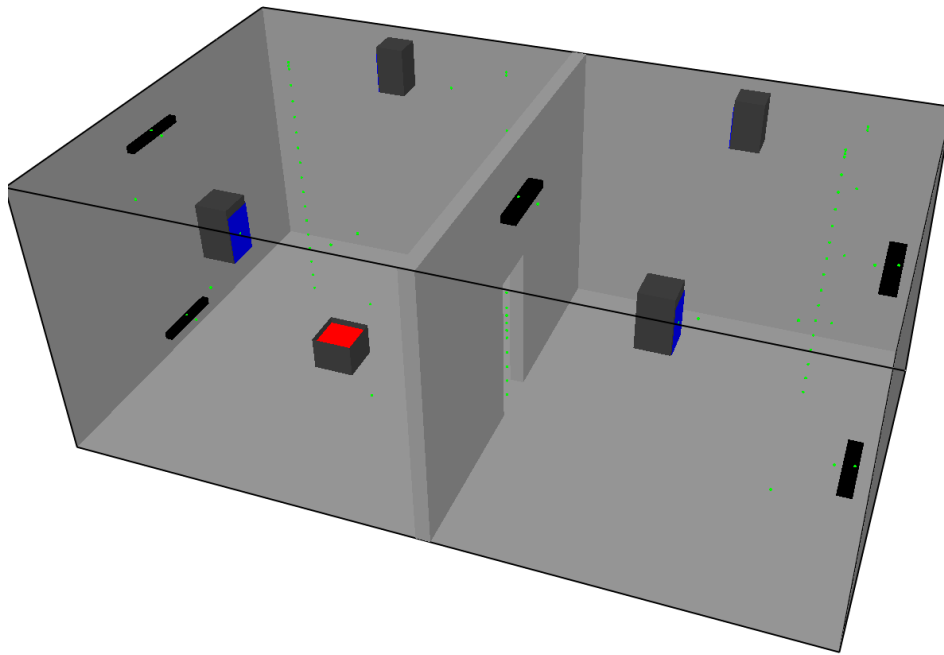


Figure 3 Model of the PRISME DOOR test PRS-D1. Both air supply vents in the 'high' position.

Table 2 Description of PRISME DOOR test series

<i>Test name</i>	<i>S</i> <i>m</i> ²	<i>D</i> <i>m</i>	<i>Tr</i> <i>1/h</i>	<i>dv_{air}/dt</i> <i>m</i> ³ / <i>h</i>	<i>Air supply</i> <i>position</i>
PRS-D1	0.4	0.71	0	0	High
PRS-D2	0.4	0.71	1.5	180	High
PRS-D3	0.4	0.71	4.666667	560	High
PRS-D4	0.4	0.71	8.333333	1000	High
PRS-D5	1	0.5	8.333333	1000	High
PRS-D6	1	0.5	8.333333	1000	High

3.3.2. Results with prescribed burning/prescribed ventilation

The uncertainty of the simulation predictions is determined using the methodology described in FDS Validation guide (24). Figure 4 shows scatter plots of predicted vs. simulated quantities in the compartment fire tests. The values in the plot correspond to maximum values of given quantity over the entire fire test or simulation. The red dashed lines indicate the confidence limits of the simulated quantities and solid line indicates the bias. The uncertainty in the experimental results was not known at the

moment of this writing, and therefore the relative standard deviations are probably too large.

The gas species quantities considered are the CO_2 concentration and the reduction of O_2 concentration. The bias factor is very close to one and the relative standard deviation is 10 %. Uncertainties in predicted gas concentrations seem to be slightly larger at smaller concentrations.

The gas phase temperatures show a significantly larger amount of scatter. In the PRISME DOOR simulations, a significant number of peak gas temperatures is underestimated even by hundreds of degrees. The PRISME SOURCE shows much better agreement with the observations, although there are few considerable over predictions.

Many of the predicted wall heat fluxes are clearly too high, and the bias factor is 1.36. There is also considerable variation in the values which is reflected in the large relative standard deviation. The accuracy of the wall temperature predictions is much better, which is somewhat surprising, considering that the wall heat flux predictions were too large in average.

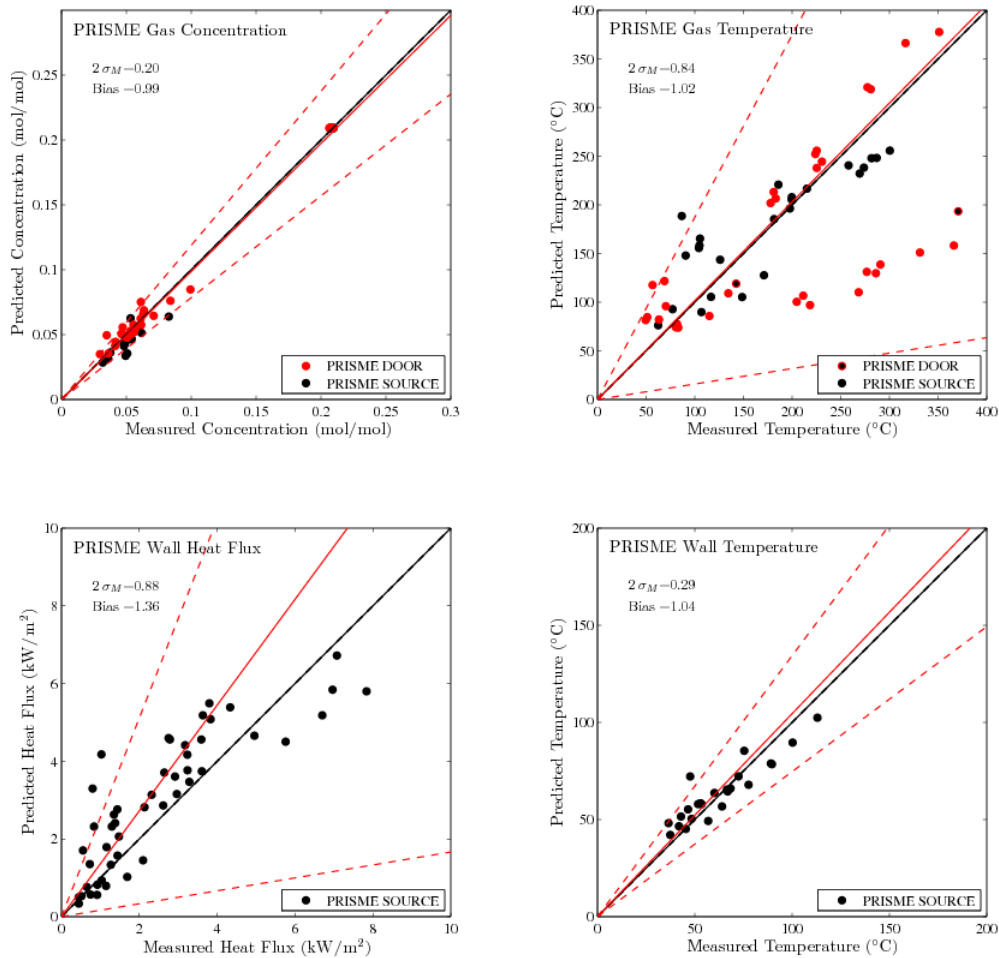


Figure 4 Measured vs. predicted quantities in the PRISME SOURCE and PRISME DOOR test series.

3.3.3. Results with prescribed burning/ventilation module FDS and CFX.

In the previous paragraphs simulation results were shown of a number of the PRISME tests where both the burning and ventilation were prescribed. In this project focus is put on developing a pyrolysis model for the pool fire but since part of the validation will be done on the PRISME project results it is also important to see if the newly developed ventilation model (25) in FDS can be used to predict the ventilation changes during a test. Therefore validation of this model was done. Simulations with data from the PRISME SOURCE test used in Benchmark 1 (26) were performed and reported below. Both FDS (24) and CFX (27) were used.

The leak area from the fire room to surroundings was calculated using data from PRISME SOURCE – Ventilation Tests. Leakage between the fire room and surroundings was assumed to be a quadratic function of pressure difference. The calculated total leakage area from the fire room was in the order of 4 cm^2 . The sensitivity of this parameter was tested by doing two more calculations with FDS, one with zero leakage, and one with 10 cm^2 leakage. As seen in Figure 5, the impact is quite large. When changing the total leakage with $4\text{--}6 \text{ cm}^2$, the first pressure peak in the experiment changes in the order of 50 Pa .

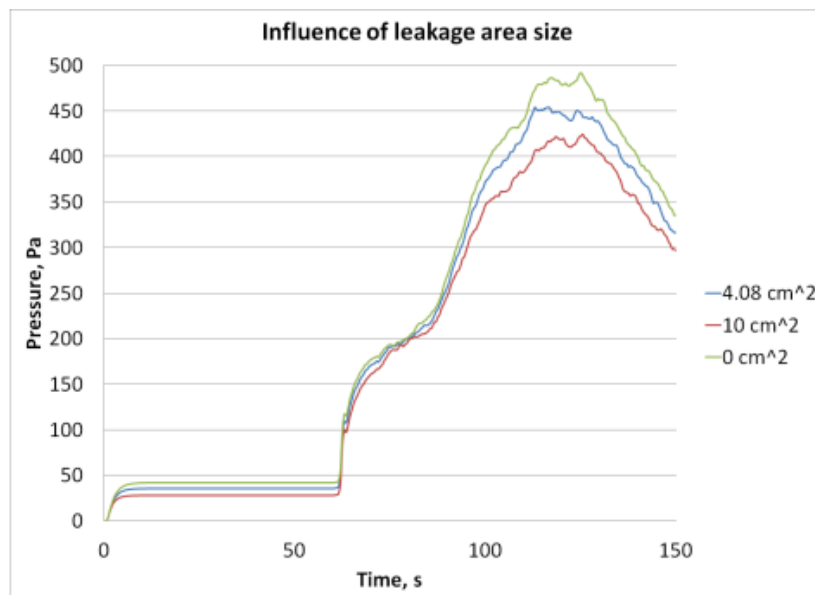


Figure 5 Influence of changing the room leak area in FDS.

Since the full ventilation system (Figure 7) was modelled with FDS, it was necessary to compare the experimental data in every node of interest with the data produced with FDS, prior to the fire being ignited. If this proved to give a good prediction, the likelihood of getting good results when compared to the full experiment would be far larger. As seen in Table 3, the results agree very well with the experimental data. Only one node shows a relative pressure difference larger than 10%, though the pressure difference is only about 40 Pa.

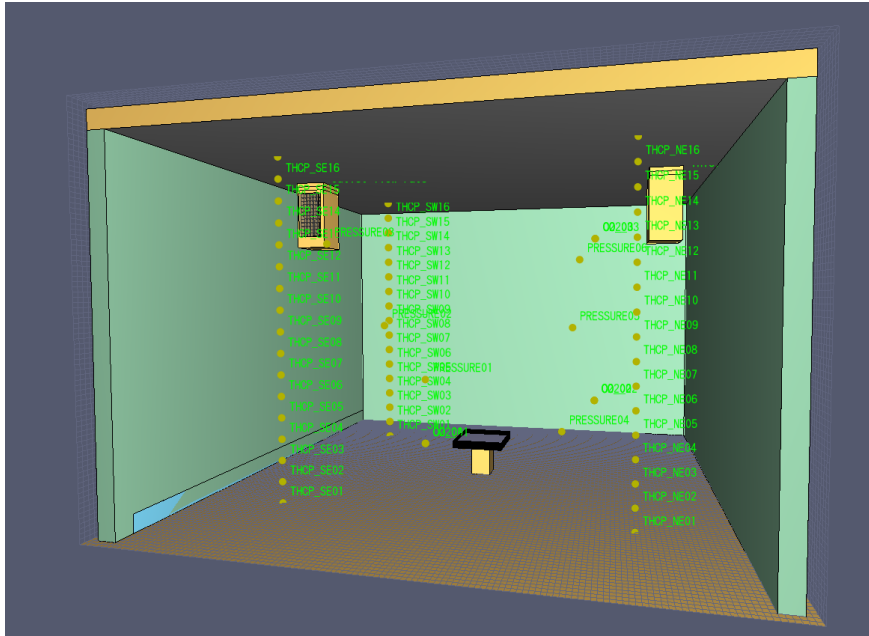


Figure 6 Geometry for the simulations with ventilation module.

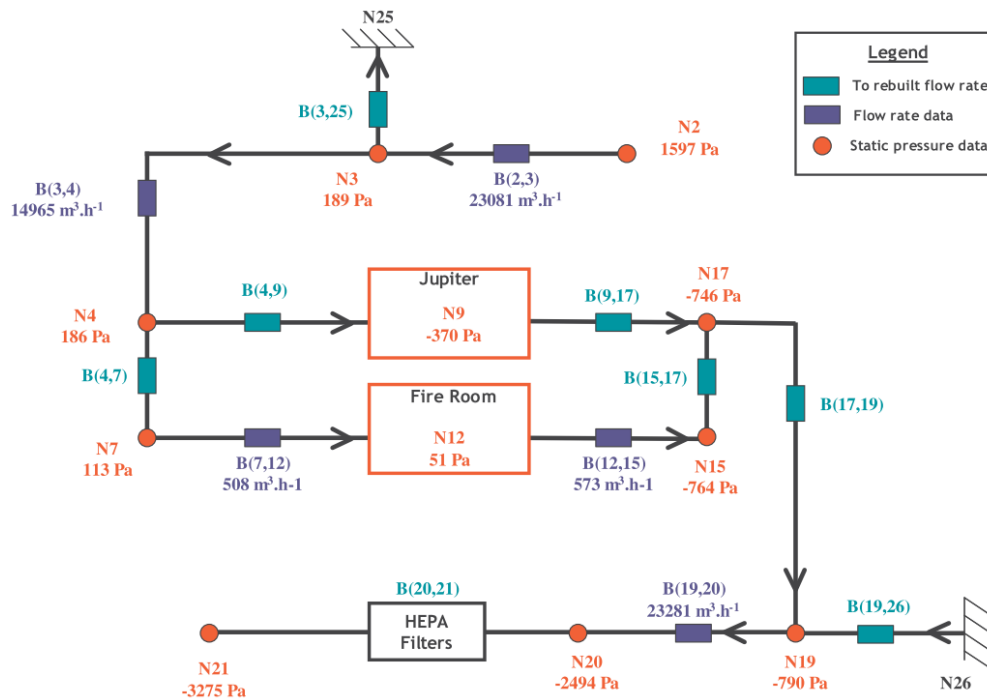


Figure 7 Layout of the ventilation network (picture IRSN, courtesy to IRSN) and a comparison between FDS data and experimental data

Table 3 Comparison of FDS5 results and measured pressure in each ventilation node.

	N2	N3	N4	N7	Fire room	N15	N17	N19	N20	N21
FDS, Pa	1575.73	191.71	188.81	162.77	35.5	-706.71	-726.09	-769.46	-2446.5	-3228.18
Experiment, Pa	1597	189	186	113	37.9	-764	-746	-790	-2494	-3275
Difference, %	1.33	1.43	1.51	44.04	6.33	7.50	2.67	2.60	1.90	1.43

An overview of the temperatures calculated with both CFX and FDS compared to the experimental data can be seen in Figure 8. FDS manages to give a good prediction of the temperatures (within 10-15 %) on a relatively coarse grid (10 cm cubes), providing a good basis for evaluating the ventilation system behaviour. Unfortunately the same cannot be said about CFX. CFX over-predicts the temperature by far (30-50 %), however, it cannot be ruled out that errors made by the software operator influences this deviation. Also, the way CFX handles combustion, for example internally calculating heat of combustion, prevented use of the experimental value obtained. This will likely impact the temperatures in the fire room. Also, heat transfer to the surrounding walls has been taken into account, but it was unclear if it was properly set up even though initial tests were performed.

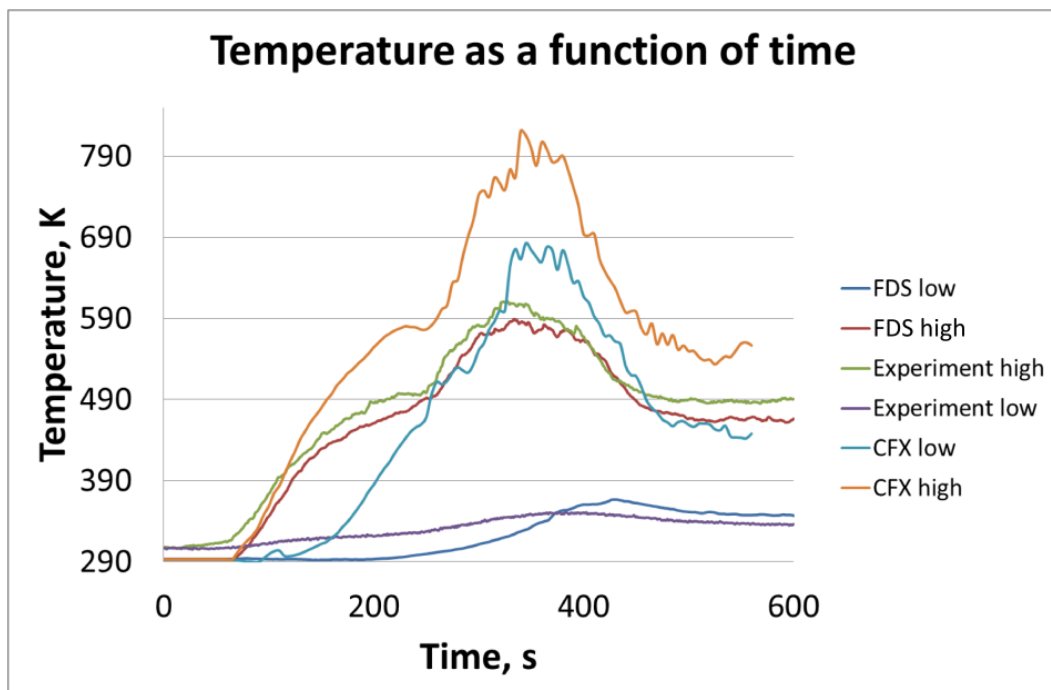


Figure 8 Temperature (highest and lowest measure point) as a function of time for the first 600 seconds.

Since full capabilities concerning ventilation system modelling is not present in CFX (simplifications were made at the in- and outlet branch, specifying appropriate boundary conditions to get realistic pressures in the fire room), only results from calculations made with FDS are presented when comparing pressure in fire room and mass flow in the ventilation branches. As seen in Figure 9, the calculated pressure in the fire room is very close to the experimental data. All pressure peaks

are fairly well predicted, and this is using only data available prior to the fire being ignited (except for HRR).

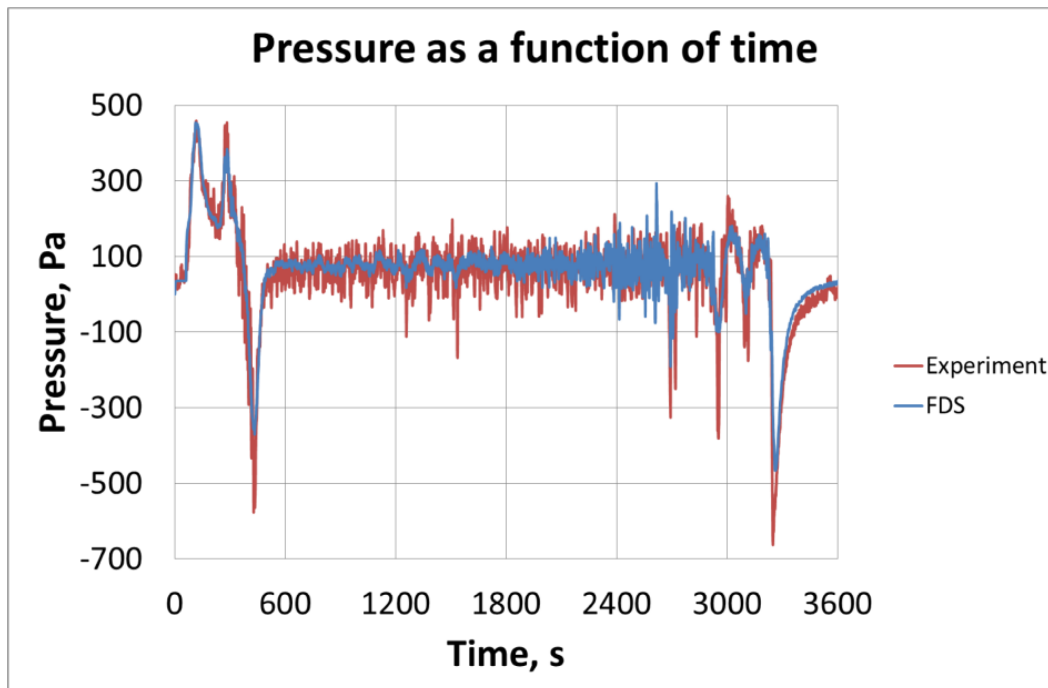


Figure 9 Pressure in the fire room as a function of time, the blue line is the pressure predicted with FDS.

Looking at the inlet and outlet branches (Figure 10) it is shown that FDS manages to predict the backflow in the inlet branch correctly. However, due to differences in the reported data from the experiment (actual measured mass flow not the same as reported in figure 3), the mass flow at the in- and outlet before the fire was ignited does not correspond to the FDS values. This in turn affects the “steady-state” mass flow in the later part of the experiment (after 600 seconds) making the FDS prediction somewhat incorrect. But it can be seen that the difference is constant, indicating that with the right starting values, FDS would give a better prediction.

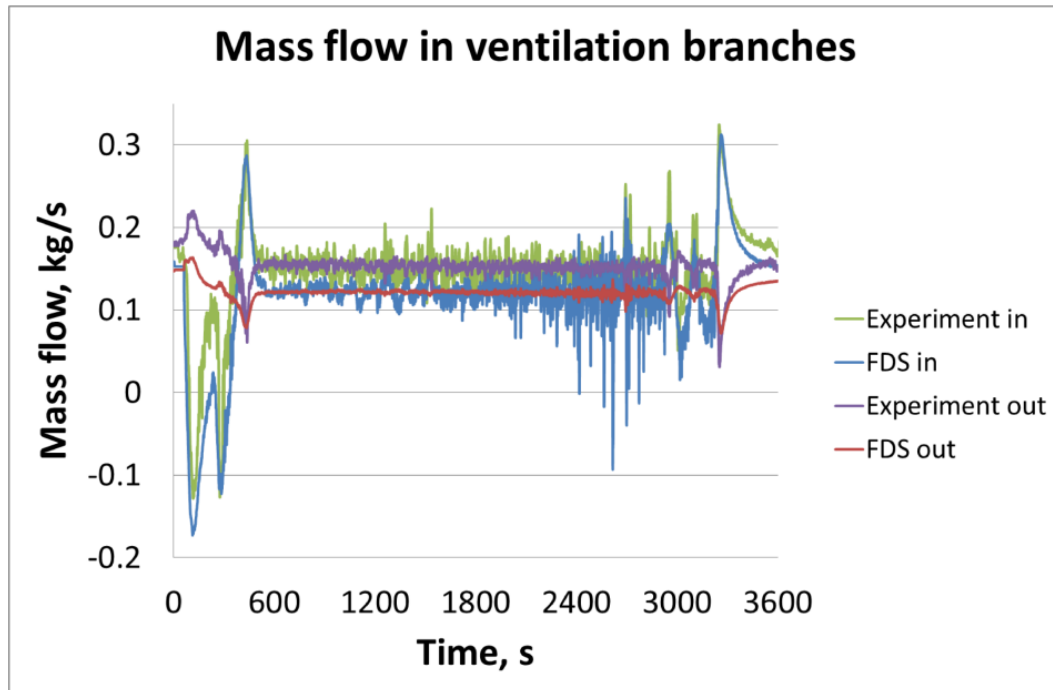


Figure 10 Mass flow in the ventilation branches as a function of time during the experiment.

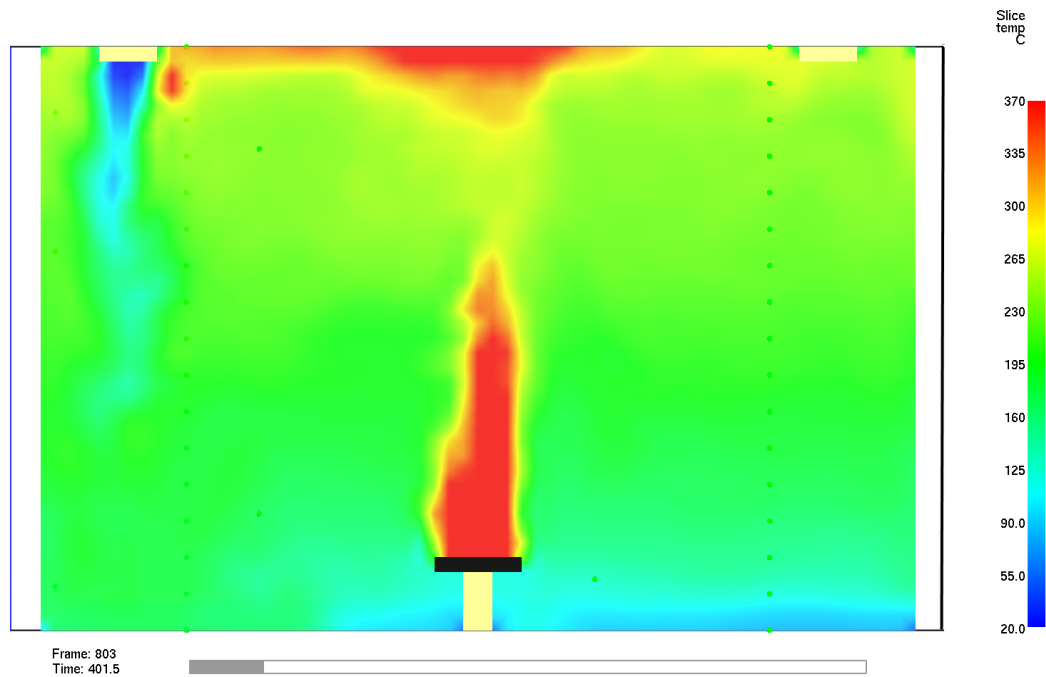


Figure 11 Snapshot of a temperature slice during the simulations done with FDS5. The incoming cold air is clearly visible at the top left corner.

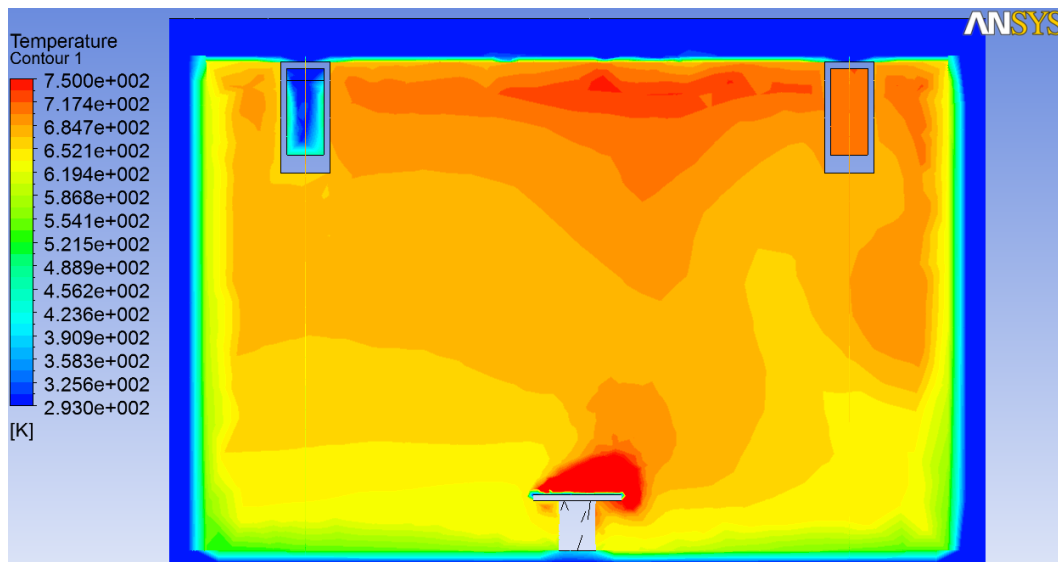


Figure 12 Snapshot of a temperature slice during the simulations done with CFX. The incoming cold air is clearly visible at the top left corner. It can also be seen that the temperature gradient from ceiling to floor is not as steep as shown with FDS5. The maximum temperature is also overestimated to a quite large degree.

From these simulation results it can be seen that the ventilation module is working well when exact data from the complete ventilation system is available. For this project FDS will only be used when it is decided to use the ventilation module.

4. Development of a new model

4.1. Theoretical background and innovations

4.2. Model description

In the new evaporation model, the effect of the unresolved concentration boundary layer near the pool surface is taken in to account. In this model the mass flux is given by

$$\dot{m}'' = h_m \rho_{f,g} \log \left(\frac{X_G - 1}{X_f - 1} \right). \quad (6)$$

Here $h_m = Sh \mu_g / Sc \Delta x$ is the mass transfer coefficient and $\rho_{l,g}$ and X_G are the density of the fuel vapour and the volume fraction of fuel vapour in the grid cell adjacent to the pool surface. The Schmidt number Sc is 1 and the Sherwood number is given by

$$Sh = 0.037 Sc^{\frac{1}{3}} Re^{\frac{4}{5}}. \quad (7)$$

The Reynolds number $Re = \rho_g v_g / \Delta x \mu_g$ is calculated based on conditions in the cell adjacent to the surface.

4.3. Preliminary comparisons of old and new liquid evaporation models

4.3.1. Models for open atmosphere PRISME tests (PRISME SOURCE)

The test data considered here is from the PRISME project. The tests were conducted in free atmosphere under the SATURNE hood (20). The fuel in all the tests considered here was hydrogenated tetrapropylene (TPH). The tests involve a single pan of TPH under the SATURNE hood. The pan is 100 mm deep and the fuel depth is 50 mm in all except one test where it was 80mm. The surface area of the pan was varied. The physical properties of the fuel are listed in Table 4. The pan is modelled as a layer of TPH followed by a steel plate, followed by insulation. The pan is defined by following FDS lines. An overview of the tests is given in Table 5.

```
&SURF ID='POOL'
      STRETCH_FACTOR=1
      CELL_SIZE_FACTOR=0.25
      COLOR='RED'
      MATL_ID(1,1)='TPH'
      MATL_ID(2,1)='STEEL'
      BACKING = 'INSULATED'
      THICKNESS= 0.05 0.005 /
```

Table 4 Properties of the fuel (TPH)(23)

Property	Value	Units
EMISSIONITY	1	-
HEAT OF REACTION	1098.94	kJ/kg
CONDUCTIVITY	0.18	W/mK
SPECIFIC HEAT	2.4	kJ/kgK
BOILING TEMPERATURE	188	°C
DENSITY	758	kg/m ³
ABSORPTION COEFFICIENT	1000	1/m

Table 5 Test scenarios under investigation

<i>Test name</i>	<i>Pool Surface Area</i>	<i>Fuel Depth</i>
Units	m²	mm
PRS-SI-S1	0.2	50
PRS-SI-S3	0.4	50
PRS-SI-S5	0.1	50
PRS-SI-S7	0.1	80

The purpose of these simulations was to predict the burning rates of the pools. The computational model of the experiments includes only the pan and not the hood. All boundaries, except the bottom boundary are defined open for flow. The bottom boundary is inert. The computational model includes the 50 mm lip of the fuel pan. Two different grid resolutions are used for both the new and the old evaporation model: 25 mm grid cells and 50 mm grid cells. The full set of experiments is run with all parameter combinations. The simulation matrix is given in Table 6.

Table 6 Simulation matrix.

#	Test name	Evaporation model	ΔX
1	PRS-SI-S1	Old	5 cm
2	PRS-SI-S3	Old	5 cm
3	PRS-SI-S5	Old	5 cm
4	PRS-SI-S7	Old	5 cm
5	PRS-SI-S1	New	5 cm
6	PRS-SI-S3	New	5 cm
7	PRS-SI-S5	New	5 cm
8	PRS-SI-S7	New	5 cm
9	PRS-SI-S1	Old	2.5 cm
10	PRS-SI-S3	Old	2.5 cm
11	PRS-SI-S5	Old	2.5 cm
12	PRS-SI-S7	Old	2.5 cm
13	PRS-SI-S1	New	2.5 cm
14	PRS-SI-S3	New	2.5 cm
15	PRS-SI-S5	New	2.5 cm
16	PRS-SI-S7	New	2.5 cm

4.3.2. Results for open atmosphere PRISME tests (PRISME SOURCE)

Figure 13 shows the comparisons of measured and predicted burning rates in the open atmosphere simulations. In all cases, the burning rate is overestimated. Both the new and the old evaporation models exhibit considerable grid dependency. The effect is slightly diminished for the smaller pools. However in these cases the problem could be that the pools are not adequately resolved by the grid.

The overall shape of the burning rate curve with slight rise in burning rate towards the end seems hard to reproduce. Some of this dynamic is visible in all the simulations but it is not as pronounced as in the experimental data.

Initially, the new evaporation model, represented by the red lines in Figure 4, suffered from large overshoots. Sharp spikes were observed in the burning rate, which often lead to numerical instabilities. These spikes were caused by the temperature in the surface cell rising very close to the boiling point of the fuel. This in turn would lead to an equilibrium vapour fraction close to unity. Occasionally this would cause the logarithm in Equation (6) to diverge leading to very large mass transfer rates. This problem was solved by limiting the fuel mass fraction at the surface to a value of 0.9999.

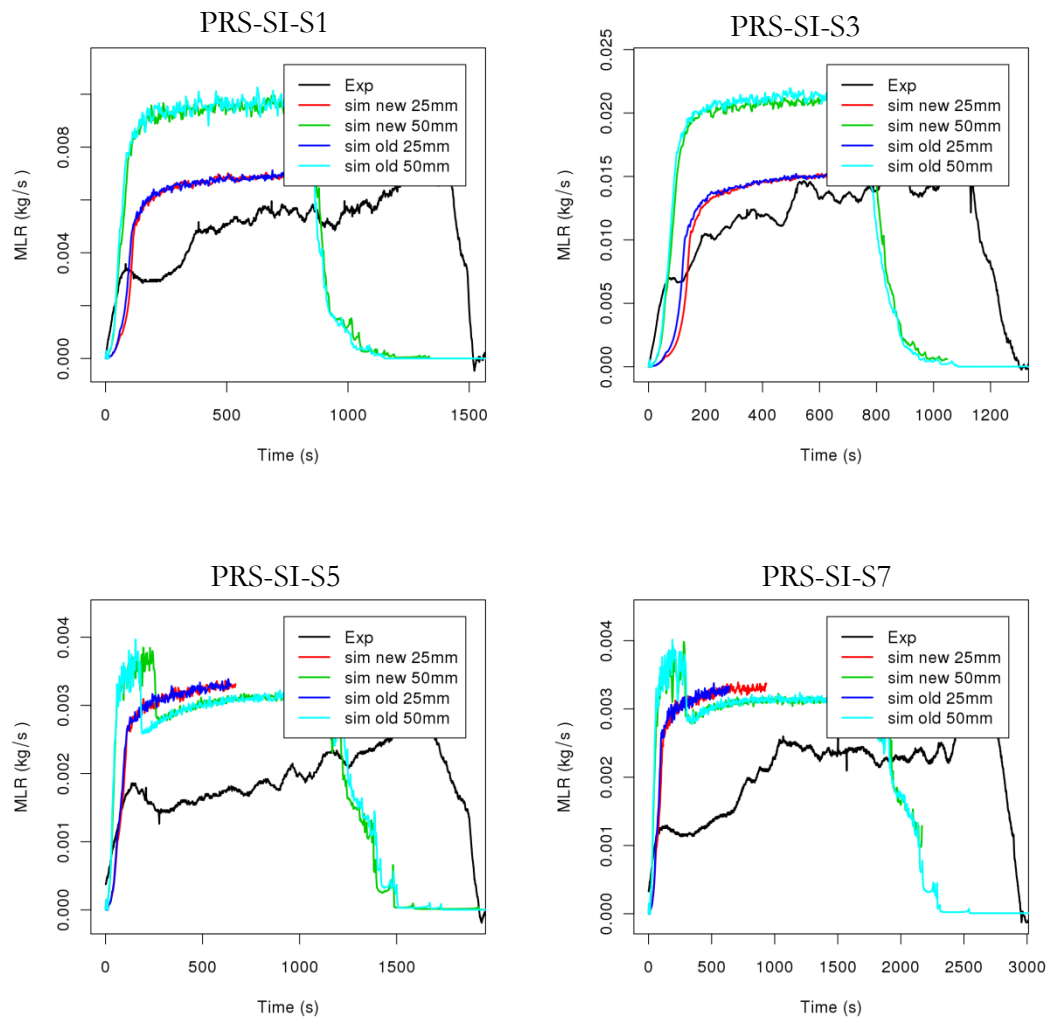


Figure 13 Comparison of pool evaporation models and different grid resolutions.

4.4. Next steps

In the next steps of the project the model will be further refined and also validated by a number of experiments. The experiments from literature will be investigated if they fit but also new data from tests done in the UK and gathered by Ringhals and Oscarshamn will be collected. Finally tests will be performed jointly by Lund University and Haugesund College during the second year of the project. One test series will be conducted at Lund University with participation of a master student from Haugesund. Most experimental work is planned for year 2 but in the next paragraph the set-up used in the first campaign is given.

4.5. First Experimental set-up for validation

One of the experimental set-ups was done at Haugesund College (28) and the set-up is given in Figure 14.

Several 0.5m x 0.5m heptane pool fire experiments with pipes obstructing above the fire were studied in the fire laboratory at HSH (Stord/Haugesund University College). Different obstruction areas in different heights above the obstruction were tested in order to verify what effects it had on the fire. An open calorimeter analysed the smoke from the fire. Additionally, temperature, radiative heat flux and mass loss rate were measured.

These experiments showed that when a pipe obstruction is located close to the pool fire it has a decreasing effect on the heat release rate and thermal radiation from the fire. In order to verify if this also was the case with increased fire diameter, outdoor pool fire experiments with increased area were performed. Due to wind conditions during these experiments the results were not valid for use in verification. However, the outdoor experiments showed that the pipe effect can be neglected for windy conditions.

This setup can be used to study additional liquids. Furthermore a number of total heat flux meters has been acquired, so the radiative heat flow from different part of the flames could be further investigated.

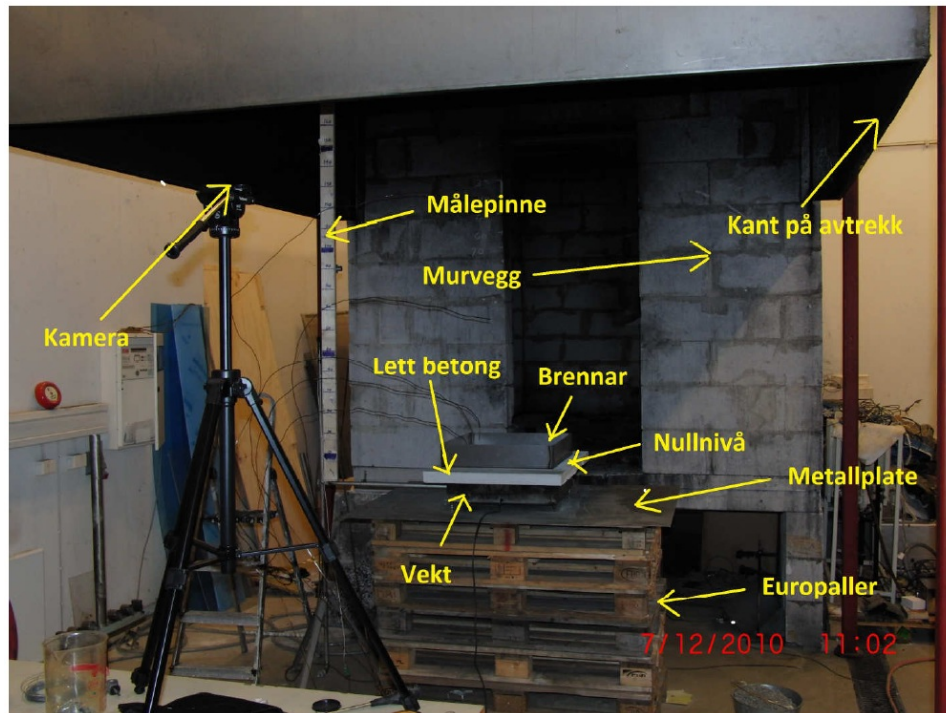


Figure 14 Set-up in Haugesund for pool fire experiments

Legend for Figure 14:

Kamera: Camera

Målepinne: Measuring reference for height measurements

Brennar: pool tray

Murvegg: wall from room

Kant på avtrekk: boundary of exhaust hood

Vekt: Load cell

Nullniva: Zero reference

Metallplatte: Metal sheet

Europaller: Europallets (wooden pallets)

5. Dissemination

This first year report is the first outcome of the project. During the first year mainly research activities were performed and different bodies were informed such as NBSG in Sweden. Most of the dissemination will be done in the second and last year but it is envisaged that the project results will be incorporated in at least master thesis's, conference papers and journal articles. At the moment the validation of the ventilation module has been presented as a poster at the IAFSS conference in Maryland, June 2011 and at the SMIRT conference in München, September 2011 (29).

6. Conclusions

Accuracy of the FDS simulation of the gas concentrations and gas phase velocities in the PRISME SOURCE and PRISME DOOR tests was determined. The simulations were carried out using prescribed burning rates and ventilation rates. Smallest uncertainties were found for the gas concentrations and highest bias for wall heat fluxes. Heat fluxes on the walls were drastically over estimated in many cases. In contrast the wall temperatures showed good agreement with the experimental values. For gas temperatures, the simulations were not biased in average, but the relative standard deviation was large.

Based on the current, rather limited set of burning rate predictions, the new evaporation model clearly outperforms the old evaporation model. When the boundary layer resistance to the mass transfer is not taken into account, the burning rates are too high and the general dynamics of the pool fire are not reproduced. In contrast the new mass transfer coefficient based model predicts burning rates that are much closer to the experimental values. In addition the general dynamics of the pool fire with HRR increasing towards the extinguishment phase is reproduced.

Although the new evaporation model is clearly step in the right direction, more work needs to be done to ensure the numerical stability of the numerical scheme. The current version is prone to overshoots that result in unphysical sharp spikes in the burning rate curve. Sometimes these spikes lead to numerical instability. An iterative procedure might be required to overcome these difficulties, instead of the current explicit method.

Good prediction is obtained by the new ventilation module in FDS, which allows us to use both models (pyrolysis and ventilation module) in order to predict some of the testdata which will be obtained and generated later in the project.

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Annex A Acronyms

Brandforsk: Swedish Board for Fire Research

CFD: Computational Fluid Dynamics

FDS: Fire Dynamics Simulator software programme

FSE: Fire Safety Engineering

IRSN: Institut de radioprotection et de sûreté nucléaire

NBSG: National Fire safety group (composed av SSM, SKB and nuclear power plants at Oscarshamn, Forsmark and Ringhals)

NEA: Nuclear energy agency

OECD: Organisation for Economic Co-operation and Development

ISO: International Standardisation Organisation

QRA: Qualitative Risk Analysis

SKB: Svensk kärnbränslehantering AB (Swedish Nuclear Fuel and Waste Management Company)

SSM: Strålsäkerhetsmyndigheten (Swedish Radiation Protection Agency)

SVN: Apache Subversion (formerly called Subversion, command name svn) is a revision control system initiated in 2000 by CollabNet Inc. Developers use Subversion to maintain current and historical versions of files such as source code, web pages, and documentation

TS: Technical Specification

Title	Prediction and validation of pool fire development in enclosures by means of CFD (Poolfire) Report – Year 1
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No. of references	29
Abstract	Fires in nuclear power plants can be an important hazard for the overall safety of the facility. One of the typical fire sources is a pool fire. It is therefore important to have good knowledge on the fire behaviour of pool fire and be able to predict the heat release rate by prediction of the mass loss rate. This project envisages developing a pyrolysis model to be used in CFD models. In the this first year report the literature review conducted within the project is reported as well as the first tasks in the evaluation and modelling of the new model.
Key words	Fire, nuclear power plants, pool fires, modelling