Parameter Optimization and Sensitivity Analysis
for Fire Spread Modelling with FDS

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INTRODUCTION

Recently, Baker et al. [1] conducted a programme of furniture calorimeter experiments of a mock-up armchair made of polyurethane (PU) foam. In three repeated experimental runs the ignition time and the heat release rate of the armchair were recorded. A gas burner with 100 kW output at a distance of 300 mm was used as ignition source. The objective of this research is to model the ignition and burning behaviour of the armchair using the pyrolysis model of FDS 6.0.1 [2]. In order to obtain the kinetic and thermophysical parameters which are inputs of the pyrolysis model, the kinetic parameters were derived from thermogravimetric analysis (TGA) experiments, and the thermophysical parameters were optimized based on heat release rate from cone calorimeter experiments. This research utilized the experimental results of TGA and cone experiments from Pau's research which describes the burning and pyrolysis behaviour of various types of PU foam on material scale, small scale and medium scale [3].

For the parameter optimization we make use of the increasing number of physical processes involved in the different experiments. Small-scale experiments with limited complexity allow some physical phenomena and model parameters, respectively, to be neglected. From iterative comparison of experimental and model TGA results, the best-fit kinetic parameters - activation energy, E, and pre-exponential factor, A, of the Arrhenius equation - were determined. Kinetic parameters which were not iteratively varied include reaction order, n, and the heat of reaction, Δh_r. The values of these parameters are based on assumptions made and other literature sources [4]. The heat transfer to and within the sample, which is affected by thermophysical parameters, is negligible in modelling because of the lumped capacitance nature of the sample in TGA.

Second, the modelling was carried out for the cone experiments where thermophysical parameters such as emissivity, ε, thermal conductivity, k, and specific heat, c_p were optimized based on the 1-dimensional heat transfer mode of the experiment. The kinetic parameters iteratively determined from TGA experiments remained unchanged during the optimization process. In the third and last stage of the investigation, the estimated kinetic and thermophysical properties from TGA and cone experiments were used to model the 3-dimensional flame spread of the free-burn armchair experiment. Table 1 gives an overview of the relevant physical phenomena and model parameters for the different scales of experiment. More detailed explanation of the parameters are provided in other sections of this paper.

Table 1: Overview of phenomena and parameters with effect on the decomposition and burning behaviour of the material. C 1 and C 2 denote the different material components.

	Thermogravimetric analysis	Cone calorimeter	Furniture calorimeter
Mass fraction (C 1)	×	×	×
Mass fraction (C 2)	×	×	×
Activation energy, E (C 1)	×	×	×
Activation energy, E (C 2)	×	×	×
Pre-exponential factor, A (C 1)	×	×	×
Pre-exponential factor, A (C 2)	×	×	×
Emissivity, ε (C 1)		×	×
Emissivity, ε (C 2)		×	×
Specific heat, c_p (C 1)		×	×
Specific heat, c_p (C 2)		×	×
Thermal conductivity, k (C 1)		×	×
Thermal conductivity, k (C 2)		×	×
Flame radiation			×
Convective heat transfer			×
Radiative feedback			×
3-D thermal conduction			×

The ability to use small-scale experimental data in simulations of larger-scale experiments could reduce the costs and effort for experimental testing significantly. For instance the determination of the heat release rate of a train carriage would no longer require costly and impractical large-scale experiments. Instead it would be sufficient to conduct several smaller experiments involving the most significant fuel load of the carriage. Once the refined model parameters are obtained, the burning behaviour of the whole train could be simulated. However, due to the inherent complexity of the phenomena involved, the nonlinear dependencies of the fire spread on temperature (especially with regard to radiation), the variety of fuel load in a real fire, and the limitations of current fire models this approach is far from being easy applicable, if at all possible. Therefore it should be noted that even for a simplified furniture item, like that examined in this study, a good agreement between experiment and model results cannot necessarily be expected.

However, due to the general applicability of the proposed method, its advantages go beyond the parameter optimization for pyrolysis modelling. Apart from the proposed application in this study, such optimization techniques can be useful in different areas of fire safety engineering, such as forensic analyses, or the determination of critical states when designing fire safety systems. For the automated parameter optimization of the cone calorimeter experiments we use a coupling of FDS with Dakota (Design Analysis Kit for Optimization and Terascale Applications) [5], an open source software toolkit that amongst other things includes algorithms for design optimization, parameter estimation, and sensitivity analysis. This approach seems advantageous, because – once FDS is coupled with Dakota – the whole range of optimization schemes can easily be applied to the problem being investigated.
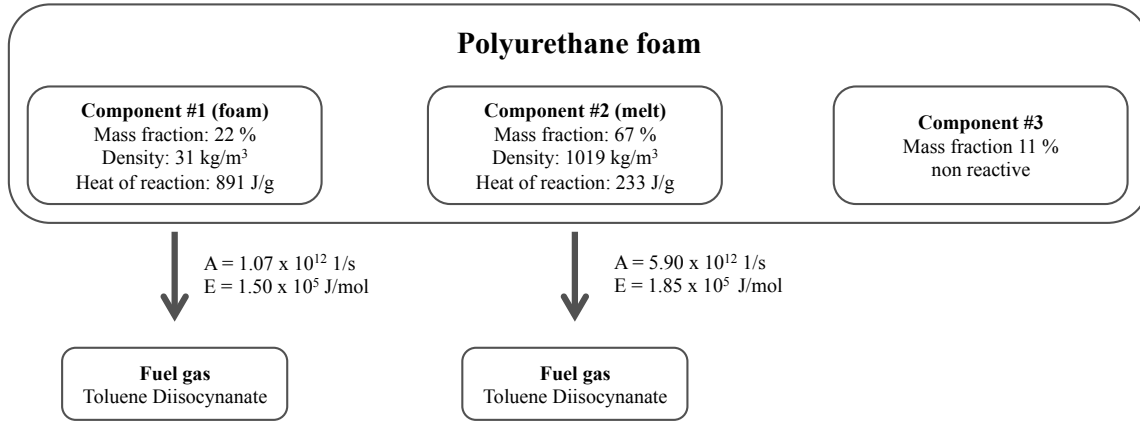
Figure 1: Reaction scheme for the pyrolysis modelling of polyurethane with FDS

MODELLING OF THERMOGRAVIMETRIC ANALYSIS – DERIVATION OF KINETIC PARAMETERS

Due to the controlled conditions of TGA the modelling in FDS is straightforward. For a small sample of the material a time-dependent increase in temperature is prescribed. Processes in the gas phase as well as heat transfer to the sample are negligible because the prescribed increase in temperature is small and the sample is a lumped capacitance model. As such, only the mass loss rate is relevant, which is controlled by the applied pyrolysis model depending on the sample temperature. In this study the reaction rate, r, at a temperature, T_s, of a material undergoing a single reaction without oxidation is defined by Equation 1 [2]:

$$ r = A \, Y_s^{n_s} \, exp \left(-\frac{E}{R \, T_s} \right) \quad \text{with} \quad Y_s = \frac{\rho_s}{\rho_s(0)} \quad ; \quad R = 8.314 \, \frac{J}{mol \, K} \tag{1} $$

Where Y_s is the ratio of the density of the material component to the initial density of the sample. The reaction order, n_s, is set to 1, which is the recommended assumption, if the exact value is unknown [2].

The reaction rate of the decomposition of PU foam in TGA experiments at heating rate of 5 K/min has two clearly distinguishable reaction regions. The first region ranges from around 200 °C to 300 °C and leads to a mass loss of one quarter of the total sample mass. In the second region from around 310 °C to 400 °C most of the remaining material decomposes. Such decomposition behaviour can mean that either the material undergoes two reactions at different temperatures, it consists of at least two components reacting at different temperatures, or the first reaction leaves behind a residue, which again reacts at a higher temperature. In accordance with the different decomposition schemes studied by Pau [3], this research further investigated the application of the *multi reactions scheme*, the *mass fraction scheme* and the *residue formation scheme*.

In this study the *mass fraction scheme* was chosen for the modelling, as depicted in Figure 1. For this scheme 22 percent of the material is considered to be component 1 with a density of virgin foam, 67 percent is considered to be component 2 with a density of melted foam and the remaining 11 percent of the material is non reactive or inert. Toluene diisocynanate (TDI) was chosen as the pyrolysate as it is one of the main raw materials for the production of polyurethane [6]. The heat of reaction is set to 891 J/g for component 1 and 233 J/g for component 2 and
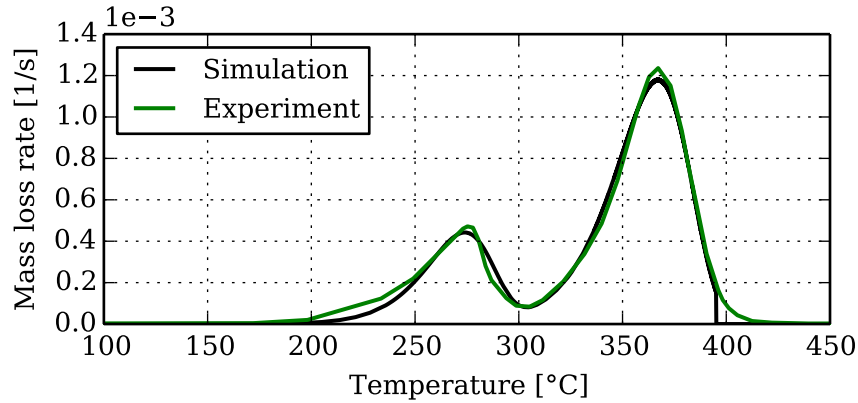
Figure 2: Comparison between experimentally determined and modelled mass loss rate of PU in TGA analysis. The sample was heated constantly at a rate of 5 K/min.

the effective heat of combustion for the gas phase combustion is set to 24.9 MJ/kg. The heat of reaction and effective heat of combustion were determined by Pau [3], who also investigated five different modelling approaches for the decomposition of PU foam. As part of this research the *multi reactions scheme* and the *residue formation scheme* were also investigated, both of which performed worse for either the modelling of the TGA or cone calorimeter experiments.

By using manual adjustments to the activation energy, E, Arrhenius pre-exponential factor, A, and the mass fractions of the two components a good agreement with experimental measurements was achieved, as shown in Figure 2. Due to the rather straightforward effect of the relevant parameters, a sophisticated optimization strategy was not necessary at this stage.

## MODELLING OF CONE CALORIMETER EXPERIMENTS – OPTIMIZATION OF THERMOPHYSICAL PARAMETERS

The parameter set that was derived based on TGA experiments is now used for the modelling of cone calorimeter experiments. The objective at this stage is the optimization of thermophysical parameters, which have been negligible before.

Simulation set-up

In a cone calorimeter, the PU foam sample is exposed to heat flux from a conical heater situated above the sample. For the simulations in this study the incident heat flux is prescribed as a boundary condition on the top surface of the sample. In this manner the radiative heat transfer can be controlled more precisely than by modelling the conical heater itself, especially for coarse meshes. The simulated computational domain is 200 mm × 200 mm × 600 mm with all sides and the top boundary defined as open, as seen in Figure 3. The backing of the sample is prescribed as void and the stretch factor for the mesh cells within the solid is set to 1, which results in a uniform solid phase mesh within the sample for solving heat transfer into the solid. According to Pau [3] a uniform solid phase mesh reduces the simulation noise in the heat release rate, which is the crucial result for the comparison of simulation and experiment.
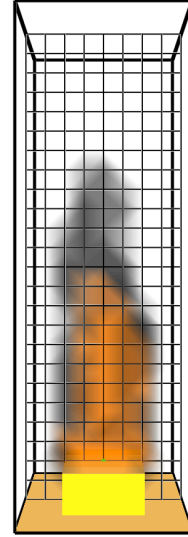
(a) In experiment   (b) In simulation

Figure 3: Cone calorimeter in experiment and simulation. In the model a mesh resolution of 25 mm is used and the sample is exposed to a prescribed heat flux on the top surface.

For several reasons a coarse resolution of 25 mm is chosen for the gas phase mesh. First of all it guarantees the same resolution can also be used for the simulation of the furniture calorimeter. This is important to eliminate any additional source of uncertainty when transferring the optimized parameter set from the cone to the furniture calorimeter. A coarse mesh is also beneficial to minimize computation time for the optimization process, which is based on many repeated simulations of the cone calorimeter. However a grid sensitivity study is carried out using results from experiments conducted at an incident heat flux of 50 kW/m^2 to investigate the influence of different mesh resolutions on the heat release rate. Figure 4 shows that a finer mesh leads to a slightly higher maximum heat release rate (HRR) and a more rapid growth of the heat release rate. However, the differences are small. Regardless of the resolution, the simulation is not reproducing the typical two-stage burning behaviour of PU foam.

Automated parameter optimization workflow

At this stage the thermophysical parameters emissivity, specific heat, and thermal conductivity for foam and melt respectively are optimized. As mentioned before, the kinetic parameters, which have been derived using the TGA experiments, are kept constant. Here the crucial values for the comparison of simulations with experiments are the heat release rates for different heat fluxes. In our study we used two representative heat fluxes (30 kW/m^2 and 50 kW/m^2), which means, for the testing of one parameter set, two simulations had to be done.

To be able to compare model and experimental heat release rates quantitatively, we calculated the euclidean relative difference between the heat release rate from each simulation and the corresponding experimental measurement. This method of functional analysis treats a series of measurements over time as a multi-dimensional set of vectors in the same manner as Peacock et al. in 1999 [7]. The euclidean relative difference as determined by Equation 2 is a scalar value that gives an indication of the overall agreement of two time-dependent curves. The vectors **E** and **m** represent the experimental and simulated data respectively, E_i and m_i are experimental
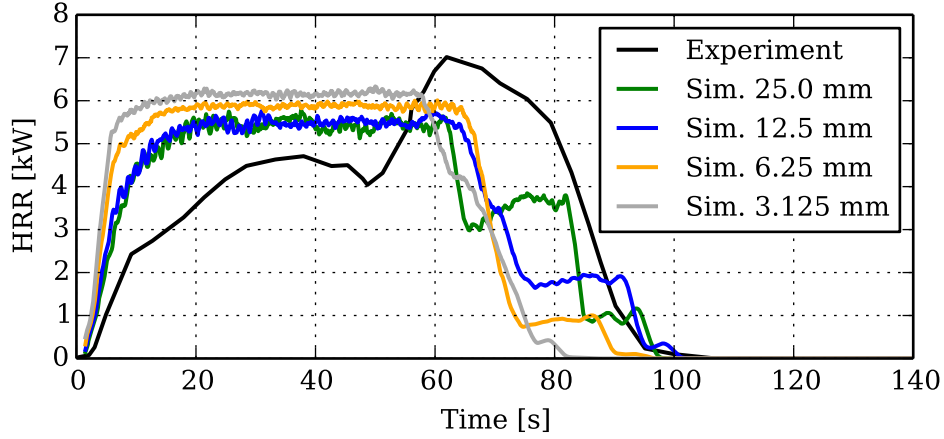
Figure 4: Grid study for cone calorimeter simulations with 50 kW/m² heat flux. The simulation results are smoothed with a moving average of 3 s.

and simulated values at the time i.

$$\frac{\|\mathbf{E} - \mathbf{m}\|}{\|\mathbf{E}\|} = \sqrt{\frac{\sum_{i=1}^{n}(E_i - m_i)^2}{\sum_{i=1}^{n}(E_i)^2}} \qquad (2)$$

For the automated parameter optimization, FDS was coupled with Dakota. The method to couple the two programs is called a loosely-coupled or "black-box" approach, meaning Dakota has no information about the internal structure of the simulation program. The communication between the programs is based on data files. Dakota writes a file containing a parameter sample and waits for the simulation program to return a loss function value that indicates the quality of this very parameter set. The same procedure is repeated for several samples (up to ~100) while Dakota applies optimization techniques in order to determine the minimum of this loss function, i.e. finding the best fitting parameter set. In our study the loss function, L, is the sum of the squared euclidean relative differences.

$$L(ERD_{30kW}, ERD_{50kW}) = ERD_{30kW}^2 + ERD_{50kW}^2 \qquad (3)$$

For the coupling of FDS and Dakota it is necessary to set up a framework that is able to

- implement the material parameters given by Dakota into a template of an input file,

- create an input file for each heat flux and start the FDS simulations,

- compute the euclidean relative difference to the experiment for each simulation,

- calculate the loss function and return the value to Dakota.

The overall workflow and the execution of FDS is controlled by a shell script. The automated generation of FDS input files based on XML (Extensible Markup Language) and the evaluation of the simulation results are based on Python scripts. Figure 5 illustrates the workflow that was used for this study.
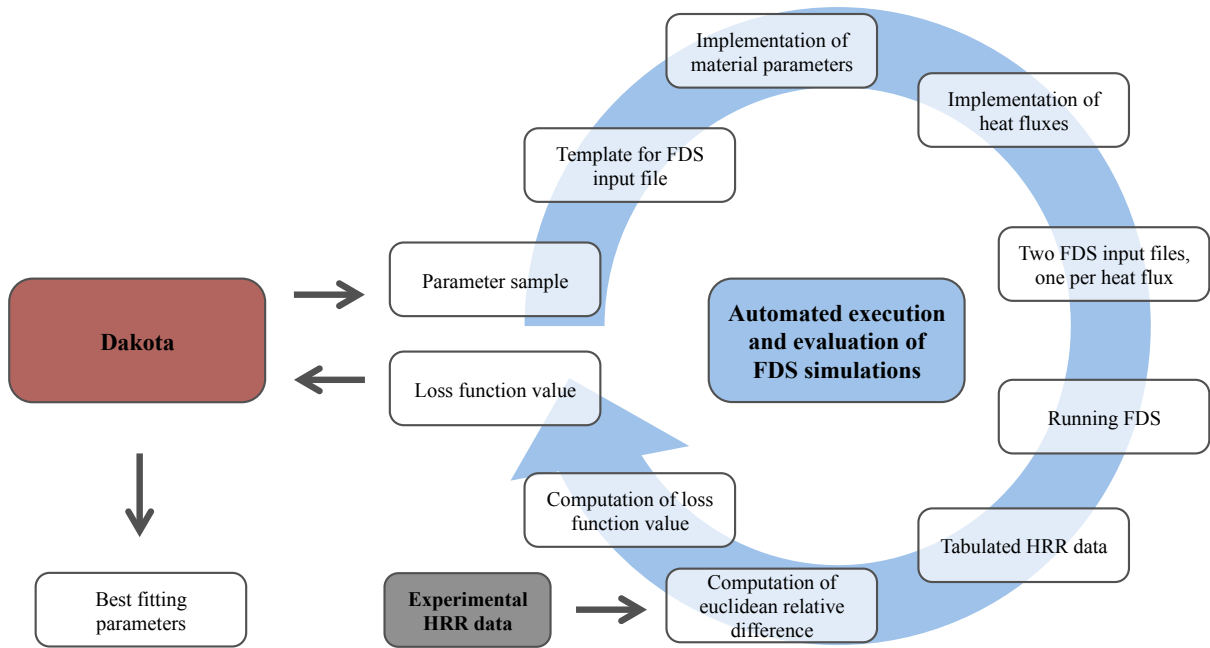
Figure 5: Automated parameter optimization workflow using a coupling of FDS and Dakota.

The optimization strategy we used is called *efficient global optimization*. It is a gradient-based global method, which is capable of handling nonsmooth response functions. Compared to other strategies such as *surrogate based global optimization* or an optimization based on *numerical gradients* it led to the best results. For more information about different strategies see the Dakota manual [5]. The parameter bounds that were prescribed for the optimization with Dakota are very wide. That is why the resulting best fit parameters should be considered to be model and scenario-specific. Unless the model being used is perfect, they are not the same as real material parameters. Despite the wide parameter bounds, some of the optimized parameters lie on the boundary. This is an indication, that there are still issues with the modelling approach. The chosen parameter bounds and the best fit parameter set are shown in Table 2.

Results

Figure 6 shows the agreement between simulation and experiments [3]. For low incident heat fluxes a good agreement is achieved, however with increasing heat flux the similarity between the simulation and experimental results reduces. In the experiments a characteristic two stage burning behaviour can be observed. The first stage coincides with the release of volatile pyrolysate and the collapse of the foam structure. The second stage occurs after the formation of a burning layer of melt in the sample holder, which behaves like a pool fire [8]. The difference between experimental and model results is probably due to the inability of the chosen decomposition scheme to appropriately model this physical behavior. As a result the heat release rate is overestimated during the first half and underestimated during the second half of the burning process for high heat fluxes. The overall burning time as well as the average heat release rate is a good match to the experimental results.
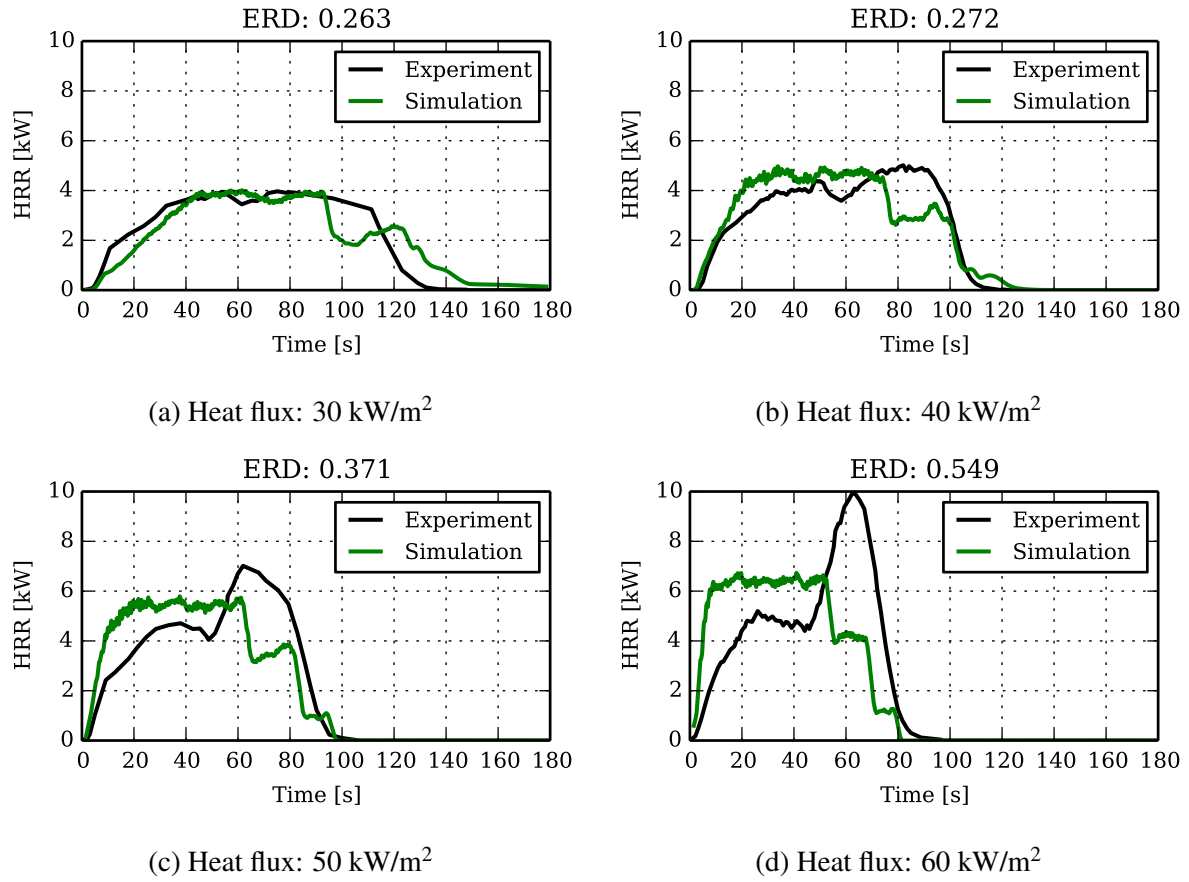
Figure 6: Results of cone calorimeter simulations with different heat fluxes using the best fitting parameter set. The simulation results are smoothed with a moving average of 3 s.

Table 2: Overview over parameter bounds and the best fit parameter set.

	Unit	Lower bound	Upper bound	Best fit
Mass fraction (C 1)	—	-	-	0.22
Mass fraction (C 2)	—	-	-	0.67
Activation energy, E (C 1)	kJ/kmol	-	-	1.50×10^5
Activation energy, E (C 2)	kJ/kmol	-	-	1.85×10^5
Pre-exponential factor, A (C 1)	1/s	-	-	1.07×10^{12}
Pre-exponential factor, A (C2)	1/s	-	-	5.90×10^{12}
Emissivity, ε (C 1)	—	0.70	1.00	0.70
Emissivity, ε (C 2)	—	0.70	1.00	0.78
Specific heat, c_p (C 1)	kJ/(kg·K)	1.50	4.00	3.17
Specific heat, c_p (C 2)	kJ/(kg·K)	1.50	3.00	3.00
Thermal conductivity, k (C 1)	W/(m·K)	0.01	0.15	0.01
Thermal conductivity, k (C 2)	W/(m·K)	0.15	0.23	0.23
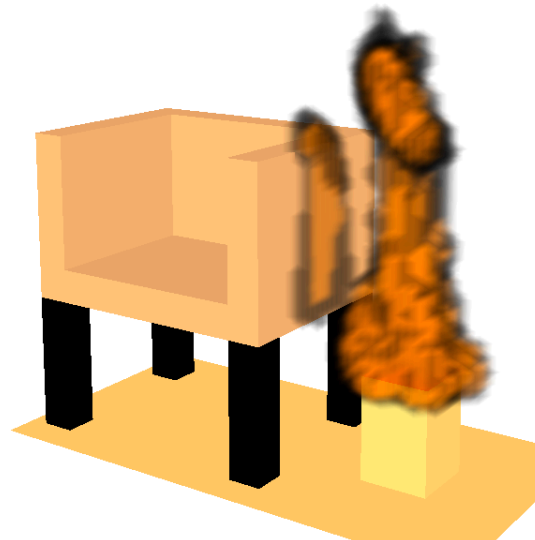
(a) In experiment   (b) In simulation

Figure 7: Representation of armchair in experiment and simulation.

COMPARISON WITH FURNITURE CALORIMETER EXPERIMENTS

Simulation set-up

When tested under the furniture calorimeter the mock-up armchair was ignited by a gas burner with a continuous heat output of 100 kW. For the experiments relevant to this study the center of the burner was located 300 mm from the side-face of the armchair, see Figure 7. Again the crucial information for the comparison between experiment and simulation is the heat release rate, which is measured by the oxygen depletion technique in the experiments. In order to assess the variability, three experiments with an identical set-up were carried out.

For the simulation of the furniture calorimeter with FDS a 25 mm grid resolution is used as for the cone calorimeter simulations. Furthermore two simulations with mesh sizes of 50 mm and 12.5 mm are examined to evaluate the sensitivity of the heat release rate to the mesh resolution. The overall domain size is 1.5 m × 0.8 m × 1.8 m with all sides and the top boundary defined as open.

Results

Figure 8 shows a comparison of heat release rates from the experiments and simulations. The 100 kW heat output of the ignition source is already subtracted in both cases. For the simulations different grid resolutions of 50 mm, 25 mm and 12.5 mm are used. During the first 120 s the simulation is similar to the experimental measurements. The side-face of the armchair starts to pyrolyse and burns with a heat release rate of up to 70 kW. However, the flame does not spread to other parts of the armchair and the heat release rate eventually decreases, until after 200 s the simulated flame on the armchair has extinguished completely. This outcome is similar to Pau's findings [3], who investigated the 2-dimensional flame spread behaviour on a horizontally aligned slab of PU foam. The author used a *multi reactions scheme* with FDS 5 and a set of kinetic and thermopyhsical parameters optimized based on cone calorimeter experiments.
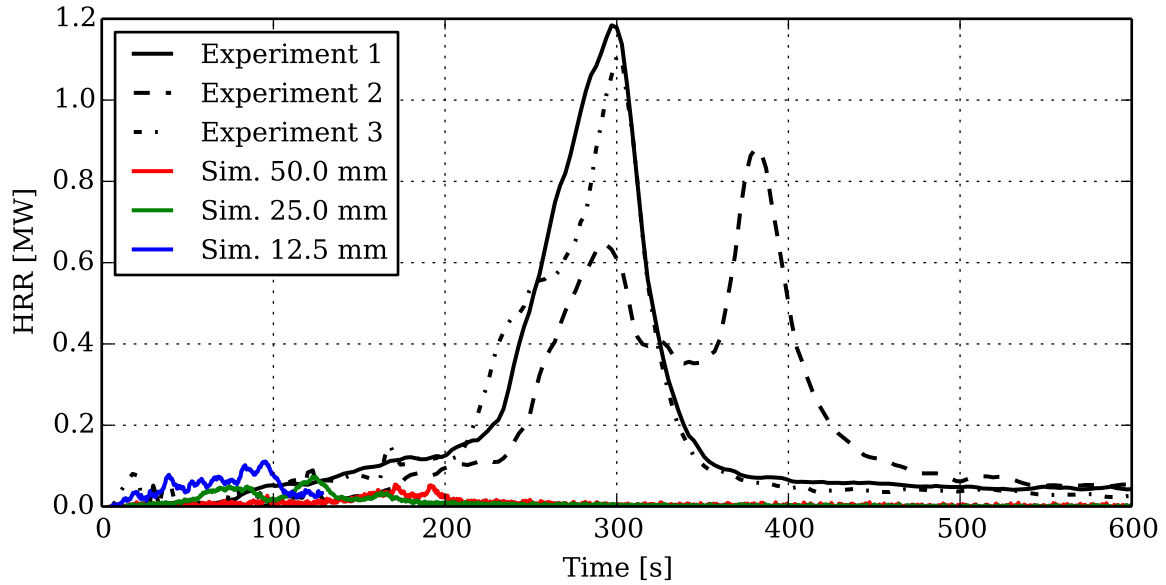
Figure 8: Comparison between heat release rates in experiment [1] and simulation with different grid resolutions. The heat output of the ignition source is removed. The data is truncated at 600 s.

CONCLUSIONS

The objective of this work was to investigate an optimization method for kinetic and thermophysical parameters based on small-scale experiments, i.e. TGA and cone calorimeter experiments. The ultimate goal was to model the ignition and burning behaviour of a mock-up armchair made of PU foam using the pyrolyis model of FDS 6. The modelling of the TGA that is used for the derivation of kinetic parameters shows promising results. By using a pyrolysis scheme with a material consisting of three different components, it was possible to accurately reproduce the decompostion of PU foam with temperature.

On the next scale, the cone calorimeter experiments, a sophisticated strategy was required for the optimization of additional thermophysical parameters. In order to couple FDS 6 with Dakota an automated workflow for the generation, execution and evaluation of FDS simulations was set up. The coupling proved to work seamlessly and could also be used for other questions regarding parameter optimization or sensitivity analysis in conjunction with FDS. However, the chosen pyrolysis scheme with FDS was not able to reproduce the typical two-stage burning behaviour of polyurethane for higher heat fluxes. For lower heat fluxes around 30 kW/m^2, a good agreement was achieved between the experimental and simulated heat release rates.

The simulation of the burning mock-up armchair under the furniture calorimeter fail to predict the flame spread seen in the experiments. Although the armchair started burning initially in the simulations and its heat release rate develops similarly to the experiments over the first 120 s it is not fully ignited and stops burning after 200 s. This finding supports similar results from a former study [3]. The cause for this burning behaviour could not be investigated completely, however the grid sensitivity study implies a higher mesh resolution might promote the propagation of flames. Further research is needed to investigate this question and improve the ability of simulation tools such as FDS.

ACKNOWLEDGEMENTS

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