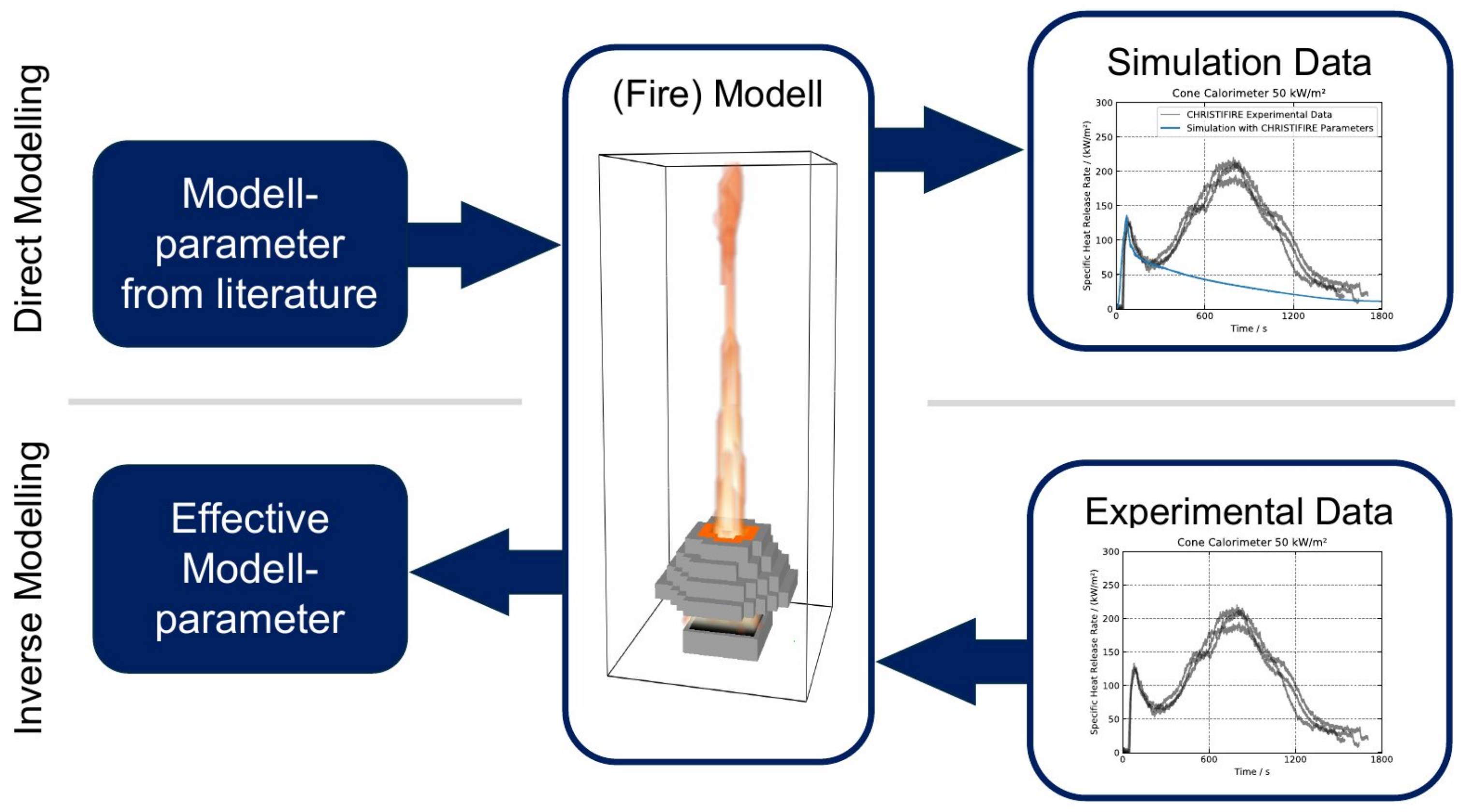
PYROLYSIS MODELLING

Lukas Arnold[1], Fabian Brännström[2], Tristan Hehnen[1], Patrick Lauer[2] and Corinna Trettin[2]
[1]Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich (Germany)
[2]School of Mechanical Engineering and Safety Engineering, University of Wuppertal, Wuppertal (Germany)

Methods of and Applications for Inverse Pyrolysis Modelling


Direct Modelling

Modell-parameter from literature

(Fire) Modell

Simulation Data

Inverse Modelling

Effective Modell-parameter

Experimental Data

Fig. 1: Direct modelling vs. inverse modelling

Modelling fire including burning behaviour of solid materials needs to consider pyrolysis – the decomposition of a solid material and its transition into the gas phase. Appropriate reaction kinetic and thermophysical parameters for pyrolysis modelling cannot be measured directly but have to be inferred from experimental data. A widely used approach is inverse modelling as shown in figure 1. Experimental data, e.g. from thermogravimetrical analysis (TGA) or cone calorimeter (CC) tests, is fed into the inverse model and the model parameters are determined. Several methods for the actual determination exist.

PROPTI – Cost Function

One common method is utilizing optimisation algorithms. The set of model parameters is altered through an algorithm until the model output fits to the experimental data to a chosen fit. This fit is determined by a cost function. We developed a framework (PROPTI) to automatize this procedure [1]. To enhance PROPTI, we investigated this cost function and introduced methods to combine point, threshold and range comparison of different data series. Additionally, we also introduced functionalities to take noise and uncertainties into account. This is making PROPTI a more versatile application and allows optimisation in a less stiff environment. An example for these different cost functions is given in figure 2. [2]

Ensemble Learning

Another method are pre-trained inverse surrogate models to predict reaction kinetic parameters instantly. We investigated a surrogate model based on a ensemble learning technique called extremely randomized trees (ERT). This machine learning method randomly generates several decision trees from training data in a supervised learning scenario for classification and regression tasks. The final result is gained through averaging from the individual decision trees. The model consists of an ERT classifier to predict the number of pyrolysis reactions taken place in a material, a non-linear least squares optimizer to predict the fractions of these reactions and an ERT regressor to predict the actual reaction kinetic parameters. The model is capable of predicting values for a huge range of synthetic TGA data as well as for real material TGA data. A total R² score of 0.77 was reached.

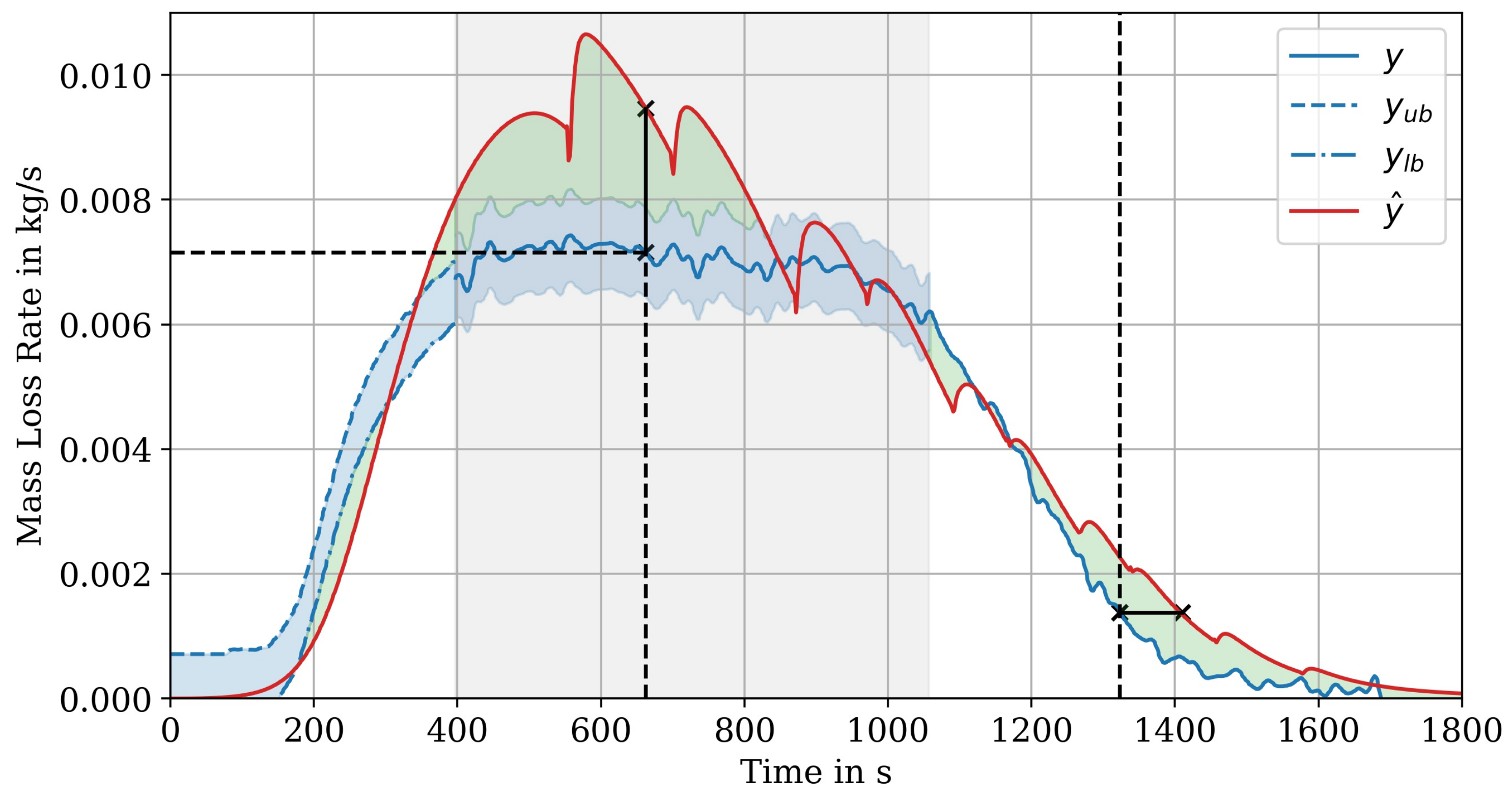


Fig. 2: Cost functions of PROPTI

Application: Cable Tray Fires

Using PROPTI, parameter sets of different cable materials are determined by an inverse modelling process (IMP) [1]. These are aimed to simulate fire spread in horizontal cable tray installations as shown in figure 3. An Arrhenius equation is used to model the decomposition reactions of the solid material. They are based on micro-scale experiment data from micro-combustion calorimetry (MCC). In a simplified cone calorimeter setup the thermo-physical parameters are determined in a second IMP step. Finally, the parameter sets are used in real-scale simulation to predict the fire spread in said setup. The simulation results are compared with experiment data, as a validation step.

Difficulties arise from the complex geometry of the cables, size and cross section. For practical simulations the fluid cells need to be relatively large (order of 5 cm), thus the cables can't be resolved well. The material parameter sets need to account for this difference and are therefore effective. The experiment data is taken from CHRISTIFIRE [3], as simulation software the Fire Dynamics Simulator (FDS) [4] is used. [5]

Outlook

Future work on the inverse surrogate model will include evaluation of different methods and validation for a broad range of real materials. Cable pyrolysis could be improved, by changes to the surrogate fuel and taking MCC and TGA data into account. Additionally, several problems and questions that arose during this project are now investigated in separate experimental and modelling studies.

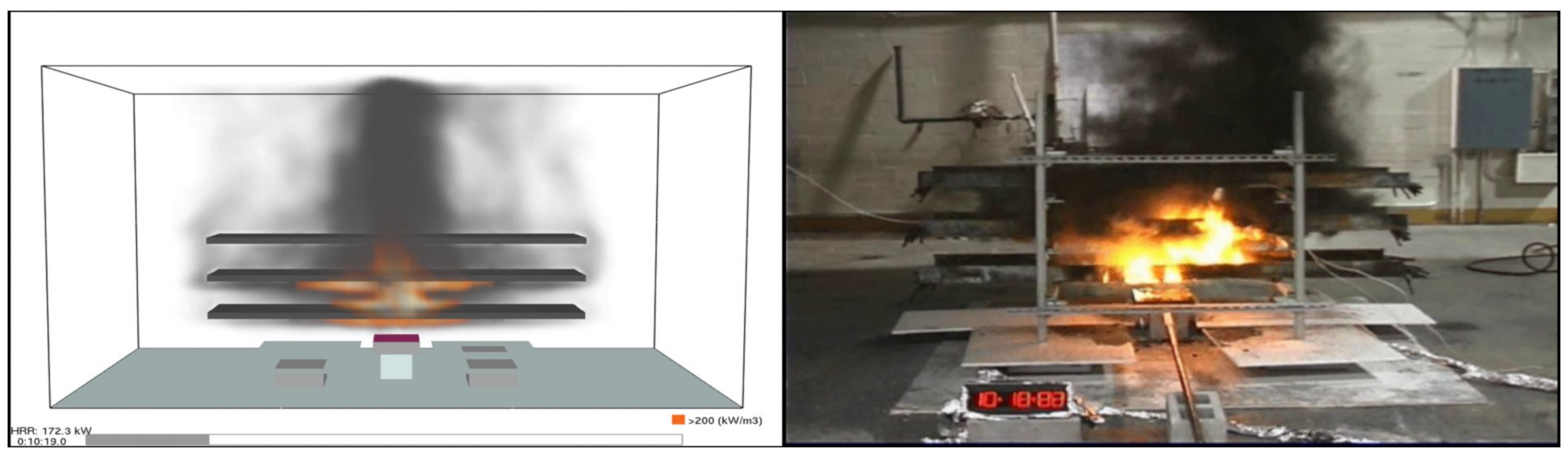


Fig. 3: Comparison of cable tray model [5] and experiment [3]

[1]: Arnold et al. "Propti–a generalised inverse modelling framework." Journal of Physics: Conference Series. Vol. 1107. No. 3. IOP Publishing, 2018.

[2]: Lauer et al. "Role of the Cost Function for Material Parameter Estimation" Fire and Evacuation Modeling Technical Conference, September 2020.

[3]: McGrattan et al. "Cable Heat Release, Ignition, and Spread in Tray Installations during Fire (CHRISTIFIRE): Phase 1 – Horizontal Trays. Contractor Report", NUREG/CR-7010. Office of Nuclear Regulatory Research, July 2012.

[4]: McGrattan et al. Fire Dynamics Simulator (FDS), National Institute of Standards and Technology

[5]: Hehnen et al. "Numerical Fire Spread Simulation Based on Material Pyrolysis - An Application to the CHRISTIFIRE Phase 1 Horizontal Cable Tray Tests" Fire, 2020, 3.