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AI-Based Material Parameter Prediction from Cone Calorimeter Measurements

Swathikrishna Punnoli Valayanad[1] **and Lukas Arnold**[1,2]

[1]Chair of Computational Civil Engineering, University of Wuppertal, Germany
[2]Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

E-mail: punnolivalayanad@uni-wuppertal.de, arnold@uni-wuppertal.de

Abstract.

In pyrolysis simulation, methods such as inverse modelling are used to determine the material parameters from small-scale experiments. This often requires significant computational resources due to its iterative nature. This study investigates an artificial intelligence (AI)-based alternative approach, that can give instantaneous predictions for material parameters once trained. A dataset based on Fire Dynamics Simulator (FDS) simulation of a cone calorimeter experiment is used for training these AI models. Different AI models are trained to predict polymethyl methacrylate's thermo-physical parameters using heat release rate (HRR) curves as input. AI models including Random Forest, 1D-convolution, and Recurrent Neural Networks showed the ability to predict the material parameters accurately with low mean squared error on the test dataset. These models were also able to recreate the HRR curves in FDS using their predictions, following the trend of the experimental HRR curve closely. Expanding the dataset to include materials with different behaviours and modelling different experiments could give these AI models broader applicability. However, FDS version dependence is a limitation for the AI models explored here because they were trained on a simulation-based dataset. Looking at the results, AI models in general can be used to predict material parameters required for pyrolysis modelling, potentially saving time and effort or, at the very least, used to complement the existing inverse modelling approaches.

1. Introduction

Pyrolysis modelling is an important part of fire spread simulations because it accounts for a detailed and accurate representation of the complex thermal and chemical processes involved in fire propagation. One way to determine material parameters required for pyrolysis modelling is based on inverse modelling. Currently, data from small-scale experiments like thermogravimetric analysis (TGA), micro-combustion calorimetry (MCC), or cone calorimetry, are used to indirectly determine the parameters' values. However, such traditional methods are resource intensive and require large computational effort to find parameters for each material that needs to be modelled. In contrast, AI-based methods present a good alternative because once computational effort is invested in training the AI models on a comprehensive dataset, parameters of multiple materials can be predicted instantaneously when needed.

In this context, Lauer et al. [1] have proposed a supervised machine learning approach that employs extremely randomised trees as a pre-trained surrogate model for inverse modelling of pyrolysis kinetics. Recent research has also explored the application of different AI methods in pyrolysis modelling for various materials, for example, biomass [2] and pine needles [3]. Leveraging these insights, the goal of the current work is to investigate the feasibility of using existing machine learning models to estimate thermo-physical parameters from the HRR curves

obtained via cone calorimetry of polymethyl methacrylate (PMMA). This study builds up on the existing research on inverse modelling [4] and sensitivity analysis [5] on material parameters for flame spread.

2. Methodology

2.1. AI Models

The AI models investigated in this study range from classical machine learning models like Random Forest to more complex deep learning models. The following section provides a brief introduction to the AI models used in this study.

Random Forest (RF): The Random Forest model [6] is an ensemble of Decision Trees (DT), each based on different samples of the dataset. Each DT comprises of roots and branches leading to leaf nodes. The data is split starting from the roots into smaller decision-making nodes, with each decision aimed at minimising the variation between actual and predicted values. The final prediction by the RF model is made by averaging the predictions of individual trees. RF is one of the classic machine learning models used for prediction tasks.

Fully Connected Neural Networks (FCNN): A Fully Connected Neural Network [7] is a basic type of Artificial Neural Network, also known as a dense neural network because each neuron in one layer is connected to every neuron in the next layer. The general architecture of FCNN includes an input layer, hidden layers with non-linearity, and an output layer. The number of neurons in the hidden layers is adjusted according to the complexity of the task. The simplicity and straightforward architecture of this model make it worth exploring in the context of this study.

One-Dimensional CNN (1D-CNN): The 1D-CNN [7, 8] is a type of neural network designed to learn important temporal features from sequential or time series data and processes one-dimensional data. The core of this network is the convolution layers that apply filters designed to capture temporal behaviours to the input time series to produce a feature map. Pooling layers, which reduce dimensionality, and fully connected layers at the end to make predictions, are also essential components of this model. The ability to recognise patterns regardless of time shifts in the input time series, makes this model ideal for this investigation.

Recurrent Neural Network (RNN): RNNs [7, 9] are designed specifically for sequential data like time series. RNNs focus on using information from previous steps to influence the output of the current step, effectively 'remembering' features learned from past inputs across different layers. Each RNN unit combines input from a specific time step with a hidden state vector from previous step to generate a new hidden state for the current step.

2.2. Dataset

For training and evaluating the AI models, a dataset of 131,072 material parameter sets and corresponding HRR curves generated by FDS simulations are used. These simulations were initially conducted for a sensitivity analysis (SA) on a simplified cone calorimeter setup by Quaresma et al.[5]. The PMMA model [4] used for simulations consists of multiple parallel reactions that release a surrogate fuel and about one mass percent of the sample as inert residue. Here, pyrolysis kinetic parameters are fixed, and only thermo-physical parameters are varied. Fifteen material parameters were adjusted around the optimal set from [4]. The cone calorimeter experiment data used here, provided by Aalto University and available in the MaCFP database [10], involves black cast PMMA samples with 10 cm edges and 6 mm thickness exposed to a 65 $\mathrm{kW\,m^{-2}}$ radiative heat flux. Further details about the simulations and material parameters are available in the original study [5]. The Aalto experimental HRR curve and the best-fitting simulated HRR curve are shown in Figure 3. All simulations used FDS version FDS6.7.6-810-ge59f90f-HEAD [11].

In this study, the thermo-physical parameters that are the input to the FDS simulations are the output of the AI model and the corresponding HRR curves generated by the FDS simulations are the input. The training dataset, characterised by a large number of simulations and a bounded sample space of parameters, provides a good starting point for investigating the feasibility of using AI-based models for predicting the material parameters in a more general context.

2.3. Pre-processing and Data Split

Before the simulation data can be used for training, both the HRR curves and the thermo-physical parameters undergo some pre-processing. Given the wide variation in simulation times, the HRR curves are interpolated to 100 data points for the sake of uniformity. Linear interpolation is chosen for a balance between standardisation and maintaining the general trend of the HRR curve. As for the material parameters, since the values for each parameter are sampled from different ranges, min-max scaling is employed to normalise the values.

The study is conducted in two parts: first, where all of the simulated HRR curves are used to train the AI models (131,072 simulations), and second, where only HRR curves that are closer to the experimental range are selected, i.e., HRR curves lasting up to 300 seconds are selected (90,045 simulations). Then for the training of the AI models, the resulting dataset is split into training, validation, and test datasets with 80:10:10 ratios respectively.

2.4. AI Model Training and Evaluation

AI models are adapted to meet this study's requirements and implemented using Scikit-learn's built-in RF (RandomForestRegressor) [12] and PyTorch [13] for other deep learning models. The mean squared error (MSE) metric is employed to assess the models' performance throughout the training phase. Hyperparameter tuning here involves grid search across batch sizes (16, 32, 64, 128, 256) and learning rates (0.01, 0.001, 0.0001) for deep learning models, and across 100 to 500 estimators for Random Forest. Additional model-specific hyperparameters are detailed in Table 1. Default settings are used for unspecified hyperparameters.

Table 1: AI Models and Specific Hyperparameters Considered During Training

AI Model	**Model Specific Hyperparameters**
RF	Estimators: 100 to 500 (increments of 50)
FCNN	Hidden layer: [64, 32, 16], [64, 32, 32, 16], [128, 64, 32, 16]
1D-CNN	Number of convolution layers: 2
RNN	Number of RNN layers: 1, 2, 3; Hidden size: 64,128

For further evaluation of AI-models' ability to generalise, the predicted parameters by each of the trained AI-model is used as input to a FDS cone calorimeter simulation. The HRR curves generated from these simulations are then compared with both the experimental HRR curve and the best fit-simulation HRR curve. The whole process of training and evaluation is illustrated in Figure 1.

3. Results and Discussions

After training, the best-performing model from each of the four types of AI model is selected based on the MSE of predictions on the test dataset. These test-MSE values for the AI models, trained on both the complete dataset and a reduced version of it, are presented in Table 3. The low MSE values for all AI models on the test dataset suggests they are performing well. It can also be observed that, in general, for all AI models except RNN, the test-MSE values

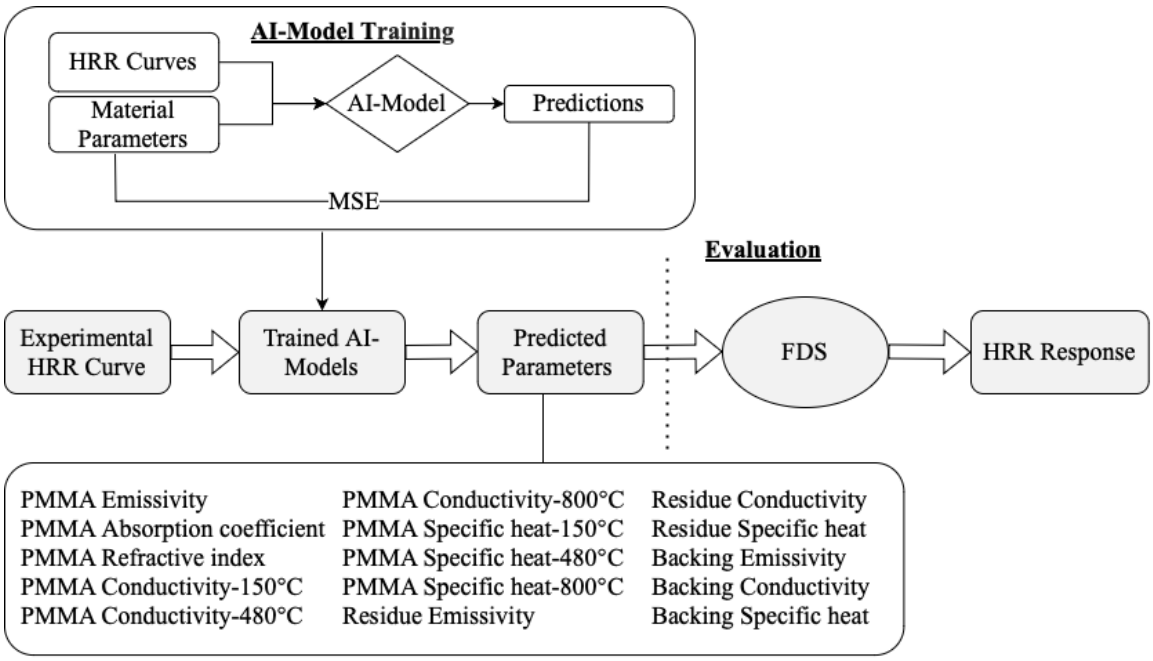


Figure 1: Training and Evaluation Process of AI Models

improve (i.e. reduce) when trained with HRR curves that more closely align with the range of this particular cone calorimeter experiment. This improvement is likely because the selection of samples closer to the experiment removed outliers that did not contribute and could have acted as noise to the models' ability to predict. Among the AI models, the RF model consistently shows the lowest test-MSE values in both cases.

Table 2: Mean Squared Error (MSE) Values of Top-Performing AI Models on the Test Dataset

AI Models	RF	FCNN	RNN	1D-CNN
Trained on complete dataset	0.0294	0.0529	0.0489	0.0438
Trained on reduced dataset	0.0288	0.0506	0.0507	0.0380

Further analysis of the distribution between actual and predicted values across different models for the test dataset reveals that AI models prioritise the optimisation of certain parameters over others. For instance, Figure 2 shows the normalised distribution of predicted values with respect to actual values of the 1D-CNN model trained on a reduced dataset. For some parameters such as PMMA emissivity, conductivity at 150 °C, specific heat at 150 °C and 480 °C, and emissivity of the residue, the predictions form a close cluster around the line of perfect prediction. However, for other parameters like PMMA specific heat at 800 °C or backing emissivity, the larger spread of predicted values suggests that the model struggles to predict these values accurately. This could be because the AI model is unable to capture the underlying relationships. Considering the fact that the complete decomposition of the PMMA sample occurs below 500 °C in the simulation, its specific heat at 800 °C is not significant. It is interesting to observe that this is reflected in the importance the AI models place on predicting this value.

In addition to looking at the test-MSE error, each model is further evaluated by using its predictions as input parameters for FDS simulations. The resulting HRR curves are then

compared to reference simulation from inverse modelling and the experiment. These HRR curves are shown in Figure 3. As it can be seen from both the plots, all models except for the FCNN follow the general trend of the experimental HRR curve. 1D-CNN, Random forest and RNN models can generalise well enough to capture the trend of experimental curve very closely. This demonstrates that these AI models are capable of finding correlations between HRR curves and material parameters, as well as some understanding of the underlying process of FDS simulations.

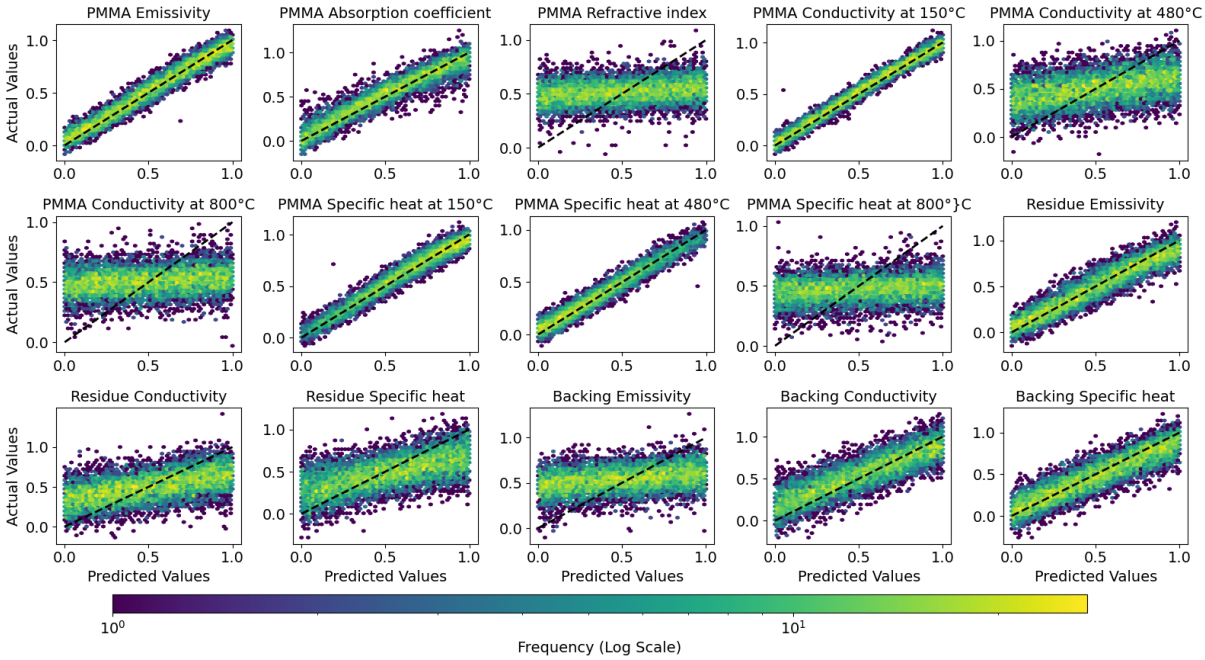
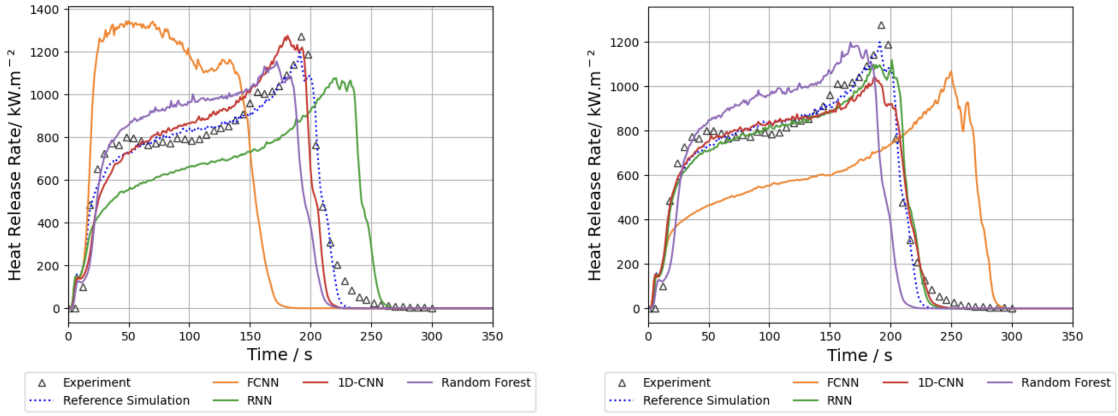


Figure 2: Distribution of Actual vs. Predicted Values for all Material Parameters by 1D-CNN Model Trained on a Reduced Dataset



(a) Trained on Complete Dataset (b) Trained on Reduced Dataset

Figure 3: HRR Curves from AI Model Predictions vs. Experimental and Reference Simulations

Conclusion

This study is a preliminary investigation into using different AI models for predicting thermo-physical parameters from a given HRR curve. It shows promising results for parameter

values in the vicinity of PMMA. The RF, RNN and 1D-CNN models succeed in capturing the general trends in the HRR by identifying the relationship between the input HRR and output predictions. An interesting observation from the results is that AI models do not treat all parameters equally. This suggests that it would be insightful to select parameters that AI models predict well and also investigate the importance of certain parameters and train the models accordingly.

This study focused solely on one material and relevant cone calorimeter experiment. However, considering the viability of using AI models to predict parameters, expanding the training dataset with different kinds of materials and evaluating the results against different experiments is promising. The study also explored only a few types of AI models and a limited number of variations in their architecture. More fine-tuning and different methods for feature selection are expected to lead to better results. A limitation to consider is that since the training data is generated by FDS simulations, the performance of the AI models and further validations will depend on the FDS version. Nonetheless, considering all observed points, AI-based models can be an effective method for obtaining instantaneous parameter predictions or can be at least used as preconditioner for existing inverse modelling approaches.

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