ROLE OF THE COST FUNCTION

FOR MATERIAL PARAMETER ESTIMATION

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11. September 2020

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INTRODUCTION

Introduction

Topic: Inverse Modelling Of Bench-Scale Experiments

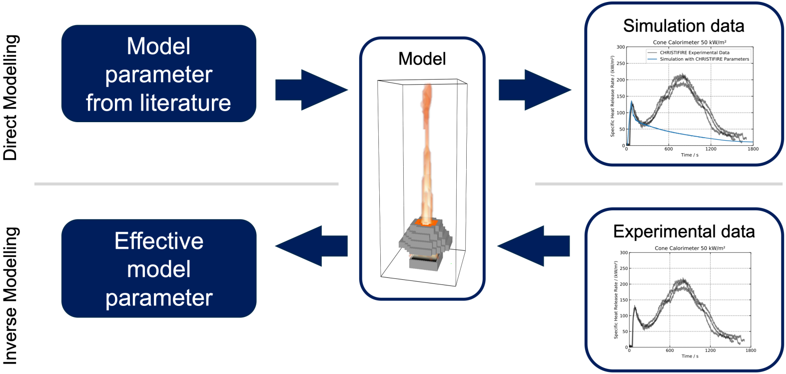
- estimates material parameters for pyrolysis simulation, e.g. to compute flame spread

Focus: Cost Function

- determines the deviation between target data and a model response, e.g. between experimental data and simulation results.

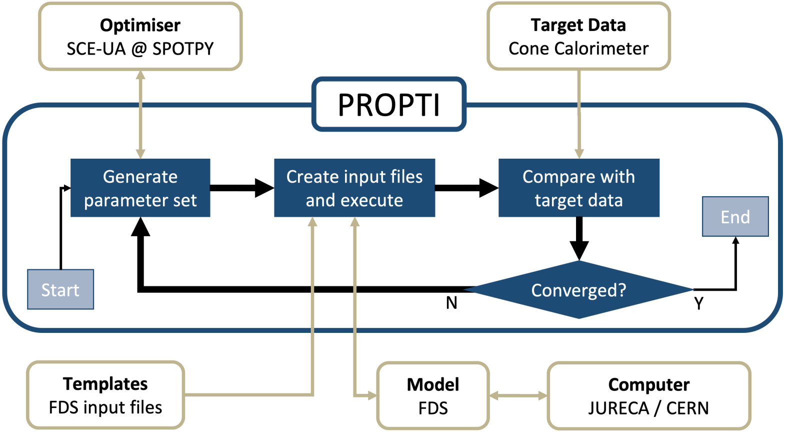
Several different cost functions are evaluated for estimating material parameter sets that allow the simulation of pyrolysation of solid polymers.

Inverse Modelling Process



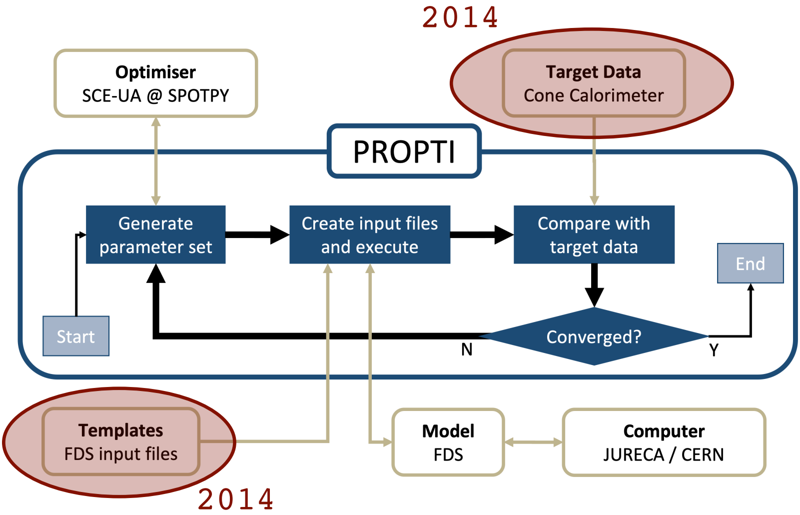
Inverse Modelling Process

Talks In The Past I



Inverse Modelling Process

Talks In The Past II



Inverse Modelling Process

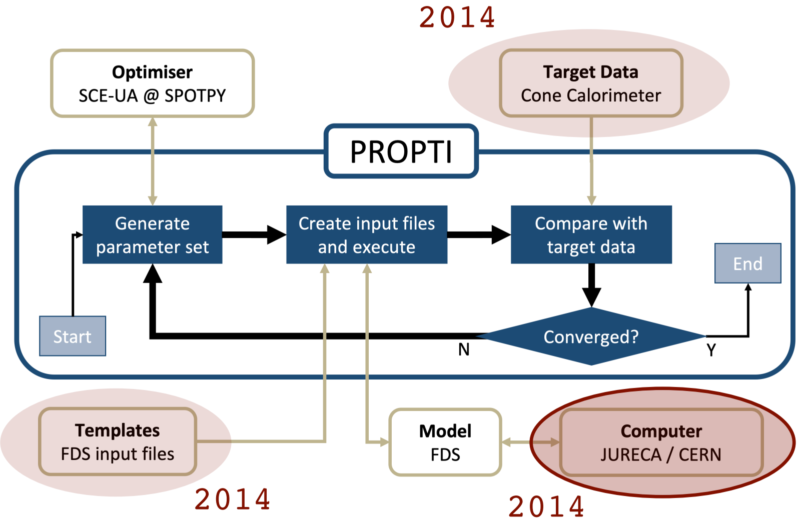
Talks In The Past III

Influence of Input Parameters on the Fire Simulation, FEMTC 2014

Trettin et al. [1]

Inverse Modelling Process

Talks In The Past IV



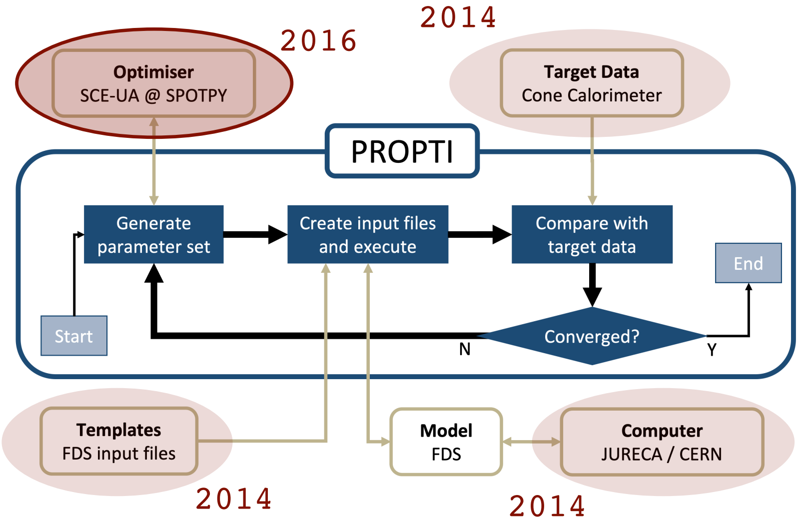
Inverse Modelling Process

Performance Analysis and Shared Memory Parallelization of FDS, FEMTC 2014

Arnold et al. [2]

Inverse Modelling Process

Talks In The Past IV

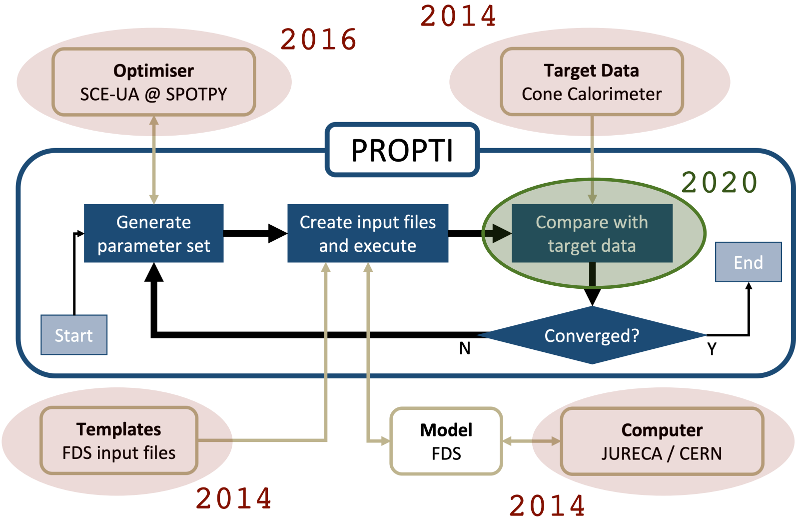


Performance Of Optimization Algorithms For Deriving Material Data From Bench Scale Tests, FEMTC 2016

Lauer et al. [3]

Inverse Modelling Process

Todays Talk



MATERIALS AND METHODS

MATERIALS AND METHODS

Inverse Modelling Process

Simulation Setup

Data Source

- Material: black poly methyl methacrylate (PMMA)
- Experimental Data:
  - Thermogravimetrical Analysis (TGA)
    - Heating rates: 1 K/min, 10 K/min and 50 K/min
    - Atmosphere: Nitrogen
    - Sample mass: 4–7 mg
    - Sample geometry: Powdered
  - Controlled Atmosphere Pyrolysis Apparatus II (CAPA II)
    - Heat flux: 25 kW/m^2, 60 kW/m^2
    - Atmosphere: Nitrogen
    - Sample dimension: Diameter: 0.07 m, Thickness: 0.0058 m
- Source: Measurement and Computation of Fire Phenomena (MaCFP): Condensed Phase Material Database [4]

Simulation Setup

Reaction Kinetics

- Estimated from TGA experimental data
- Obtained with inverse modelling
- Parameters: reaction kinetics (Arrhenius model)
- Target: 3 different heating rates
- Simulated with pyrolysis model of FDS
- Modelled with two independent reactions
- Estimation process not covered in this talk [5]

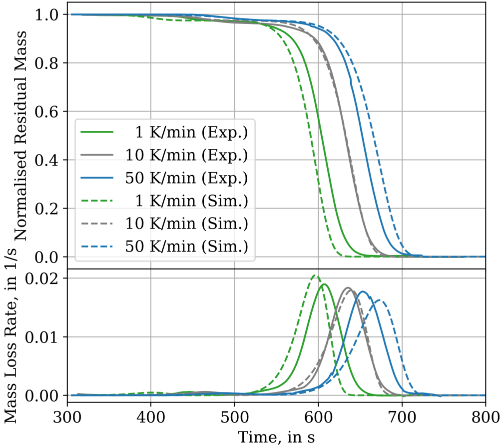


Figure 1: Comparison between TGA experiments by UMET [4] (Exp.) and the best parameter set of the IMP run that determined the reaction kinetics parameters (Sim.).

Simulation Setup

Thermophysical Properties

- Estimated from CAPA II experimental data
- Obtained with inverse modelling
- Parameters: thermophysical parameters (density, emissivity, conductivity, specific heat capacity)
- Target: $25\,\mathrm{kW/m^2}$ heat flux
- Validation: $60\,\mathrm{kW/m^2}$ heat flux
- Pyrolysis model of FDS
- Reaction kinetics from TGA (see above)
- Calculation conducted with three different cost functions
- 25 repetitions of each IMP setup for evaluation of robustness

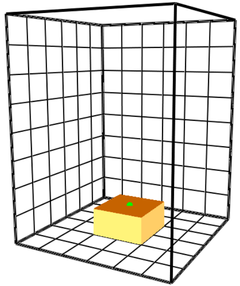


Figure 2: Simplified FDS simulation setup of the CAPA II, based on [5].

Simulation Setup

Software

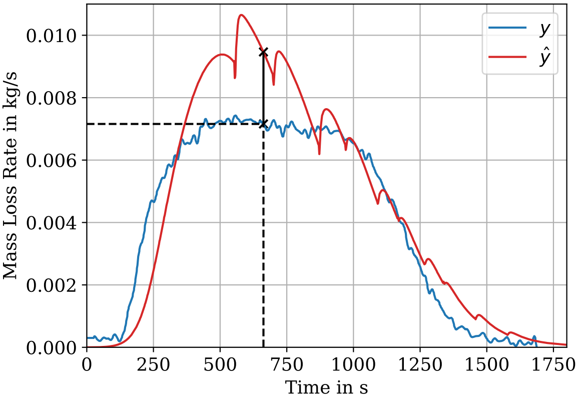
- Pyrolysis Model: Fire Dynamics Simulator [6]
- Inverse Modelling Framework: PROPTI [5, 7]

MATERIALS AND METHODS

Evaluation Methods

Cost Function

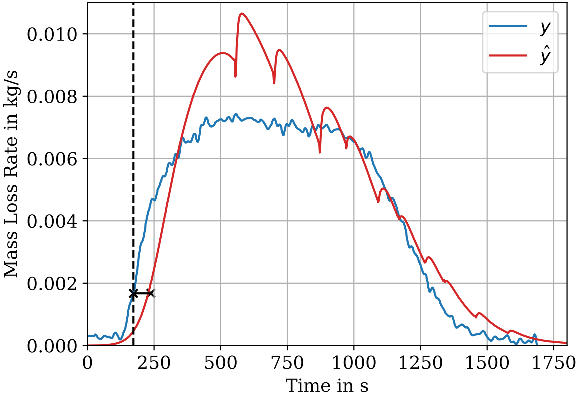
Single Point



$$\mathrm{NRSE} = \frac{|\hat{y}_t - y_t|}{y_t} \tag{1}$$

Cost Function

Threshold

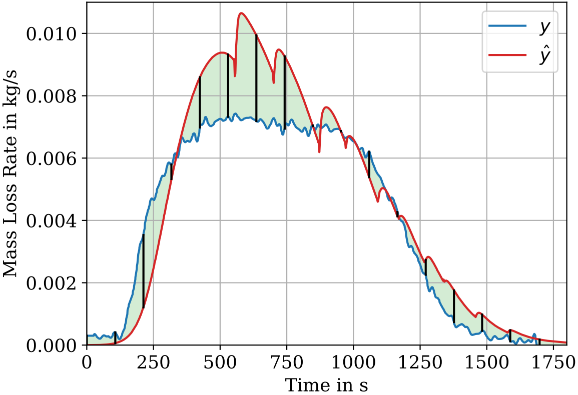


$$\mathrm{THR}_{min} = \min\left\{|\{t|\hat{y}(t) > y(t_0)\} - t_0|, \max\{|t_{min} - t_0|, |t_{max} - t_0|\}\right\}/t_0 \quad (2)$$

$$\mathrm{THR}_{max} = \min\left\{|\{t|\hat{y}(t) < y(t_0)\} - t_0|, \max\{|t_{min} - t_0|, |t_{max} - t_0|\}\right\}/t_0 \quad (3)$$

Cost Function

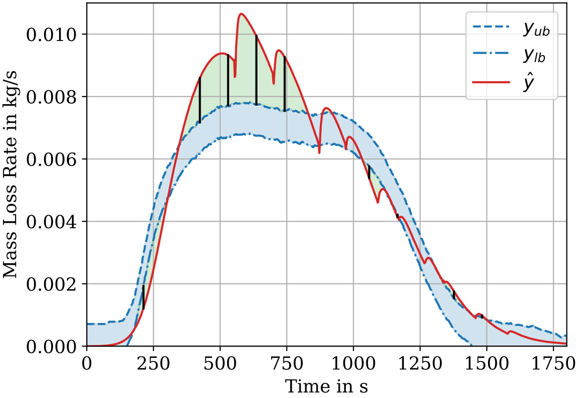
RMSE



$$\text{RMSE} = \frac{1}{y_N \sqrt{n_y}} \sqrt{\sum_{t=1}^{n_y} (\Delta y_t)^2} \text{ with } \Delta y = \hat{y}_t - y_t \tag{4}$$

Cost Function

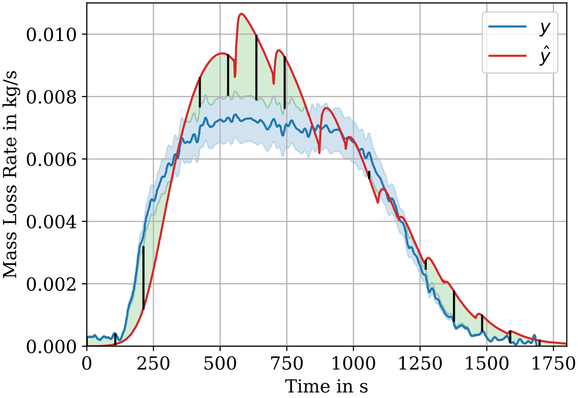
RMSE BANDS



$$\text{RMSE} = \frac{1}{y_N\sqrt{T}}\sqrt{\sum_{t=1}^{T}(\Delta y_t)^2} \text{ with } \Delta y = \begin{cases} 0 & y_{t,lb} \leqslant \hat{y} \leqslant y_{t,ub} \\ \hat{y}_t - y_{t,lb} & \hat{y}_t < y_{t,lb} \\ \hat{y}_t - y_{t,ub} & \hat{y}_t > y_{t,ub} \end{cases} \tag{5}$$

Cost Function

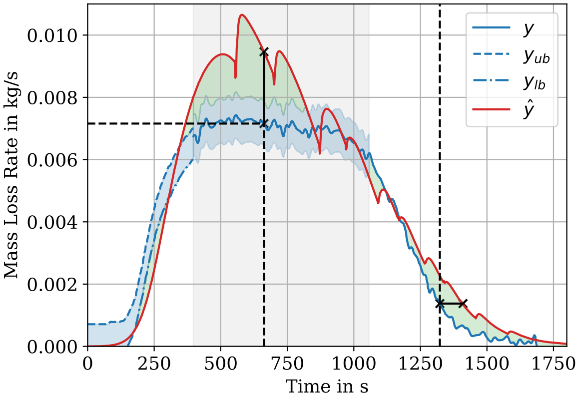
RMSE RANGE



$$\text{RMSE} = \frac{1}{y_N\sqrt{T}}\sqrt{\sum_{t=1}^{T}(\Delta y_t)^2} \text{ with } \Delta y = \begin{cases} 0 & (1-r)y_t \leqslant \hat{y} \leqslant (1+r)y_t \\ \hat{y}_t - (1-r)y_t & \hat{y}_t < (1-r)y_t \\ \hat{y}_t - (1+r)y_t & \hat{y}_t > (1+r)y_t \end{cases} \tag{6}$$

Cost Function

Combination



$$E = \sum_{i=0}^{I} (w_i \cdot \mathrm{RMSE}_i) + \sum_{j=0}^{J} (w_j \cdot \mathrm{THR}_j) + \sum_{k=0}^{K} (w_k \cdot \mathrm{NRSE}_k) \tag{7}$$

Evaluation

Evaluated Cost Functions

- RMSE: mean experimental data
- RMSE RANGE: $\pm 5\,\%$ of experimental data
- RMSE BAND: uncertainty band provided with the experimental data

Thermophysical Properties

Estimation with 25 kW/m^2 case

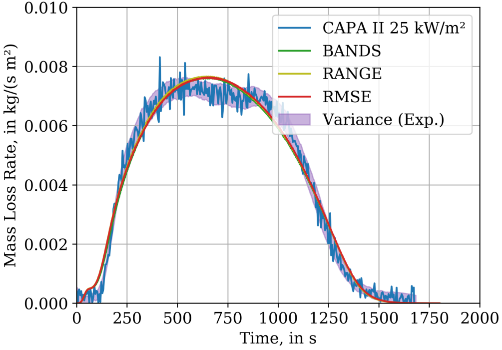


Figure 3: Comparison between CAPA II experiment [4] and the best parameter sets of the IMP runs with different cost functions.

Thermophysical Properties

Validation with 60 kW/m^2 case

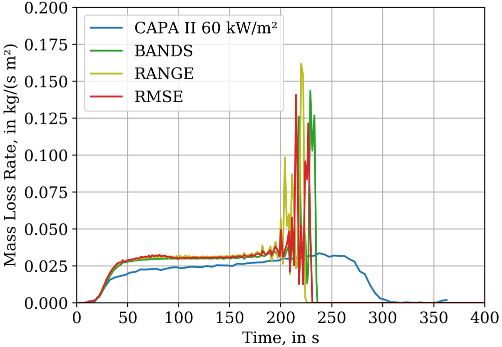


Figure 4: Comparison between CAPA II experiment [4] and the best parameter sets of the IMP runs with different cost functions as validation cases.

Thermophysical Properties

Estimated Parameters

	RMSE			RANGE			BANDS		
	best	mean	σ	best	mean	σ	best	mean	σ
fit	0.0892	0.0897	0.0002	0.0838	0.0846	0.0004	0.0417	0.0421	0.0002
ρ_a	1201.3	1204.5	1.3	1200.5	1205.0	3.1	1194.8	1196.0	0.8
$_a$	0.1083	0.1133	0.0021	0.1075	0.1125	0.0037	0.1160	0.1213	0.0030
$c_{p,a}$	2.6037	2.7065	0.0241	2.5920	2.6909	0.0268	2.6575	2.6986	0.0167
ϵ_a	0.9298	0.9694	0.0109	0.9322	0.9656	0.0139	0.9451	0.9691	0.0110
Δh	669.2	704.3	12.3	676.6	703.0	14.7	675.2	709.1	16.3

Robustness

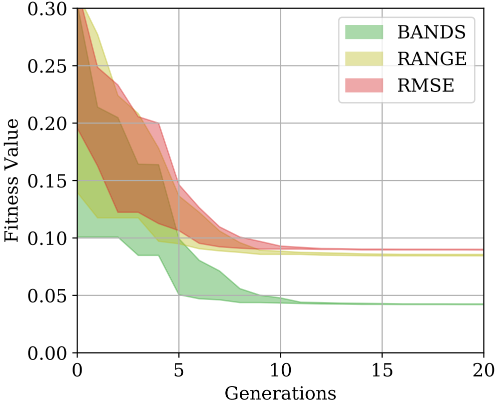


Figure 5: Cumulative minimum areas for the three cost functions over 25 repeated IMP runs for each cost function. Note: The individual plots are not directly comparable due to their different cost functions.

DISCUSSION

Discussion

Specific Case I

Different cost functions are investigated with respect to their performance in finding material parameter sets.

For the chosen example case here, none of the different cost functions significantly outperforms any of the others.

The best parameter sets within each cost function group, as well as across these groups, show nearly the same simulation response.

Looking at the cumulative minimum of the fitness values, none of the discussed cost functions stands out in terms of how fast they converge to their respective minimum.

Thus, no useful statement as to how fast convergence is reached can be made here.

Discussion

Specific Case II

For a larger number of optimisation parameters this behaviour might be different.

Larger sampling limits for the individual parameters might have a stronger effect on the convergence when choosing different cost functions.

Experiments were conducted in an inert atmosphere and in the simulations the gas phase reactions were neglected. This could contribute to an oversimplified modelling of the involved processes, leading to a more trivial case.

Discussion

Generic Considerations

A cost function that uses an area as a target, provides means to incorporate the uncertainty observed in the experiments.

RMSE requires exact matches of the data points, while slight variations in the other cases could still fall inside the target area. BANDS and RANGE could be useful to account for variance that is encountered when repeating a single experiment multiple times and allow for its representation during the IMP.

The ability to combine cost functions in different ways allows to target multiple values, like heat release rate or surface temperature, and their unique features, like heat release peaks on different experimental setups (e.g. different heat fluxes or gas atmospheres), as these may be of crucial importance for the real-scale applications, especially for flame spread modelling.

Conclusion

Two newly implemented cost functions were evaluated against a commonly used cost function.

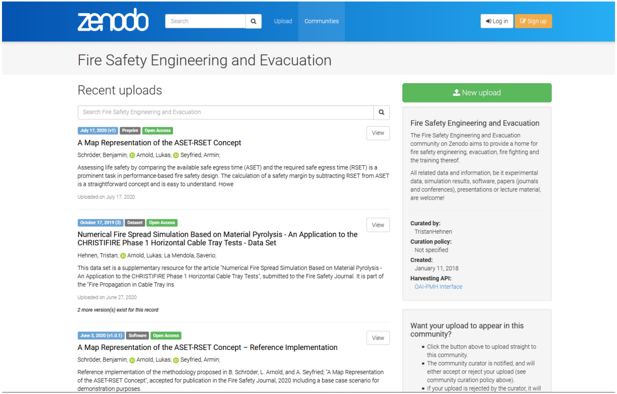
They compare the modelled data against an area, not a data series.

No significant difference in performance, robustness and results was observed for the investigated case.

Still, this is useful to take experimental uncertainty into account.

It might also provide an advantage in performance, robustness and results in more complex cases.

Zenodo Fire Safety Community



https://zenodo.org/communities/fire-safety-engineering-and-evacuation https://zenodo.org/record/1438349

Data set repository

https://zenodo.org/record/3987799

Fin

Thank you very much for your attention!

References

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[4] Randall McDermott and Isaac Leveton (Editors). Measurement and Computation of Fire Phenomena (MaCFP): Condensed Phase Material Database, 11 2019. URL `https://github.com/MaCFP/matl-db`. Commit: `7335c4470ec2cb0327ac0fe8386ecfeee6b3c6b1`.

[5] Lukas Arnold, Tristan Hehnen, Patrick Lauer, Corinna Trettin, and Ashish Vinayak. Application cases of inverse modelling with the propti framework. *Fire Safety Journal*, page 102835, 2019. ISSN 0379-7112. doi: https://doi.org/10.1016/j.firesaf.2019.102835. URL `www.sciencedirect.com/science/article/pii/S0379711219300438`.

[6] Kevin McGrattan, Simo Hostikka, Jason Floyd, Randall McDermott, and Marcos Vanella. *Fire Dynamics Simulator User's Guide, version 6.7.4*, 3 2020.

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