Progress on inverse pyrolysis modelling

with ensemble learning methods

Patrick Lauer

University of Wuppertal

lauer@uni-wuppertal.de

Content

What is pyrolysis?

Burning of solids can be separated in two phases:

- Thermochemical decomposition of solid material and phase change from solid to gas phase (Pyrolysis)
- Chemical reaction in the gas phase (Combustion)

To predict fire spread, we need to model burning of solids, hence pyrolysis.

Pyrolysis

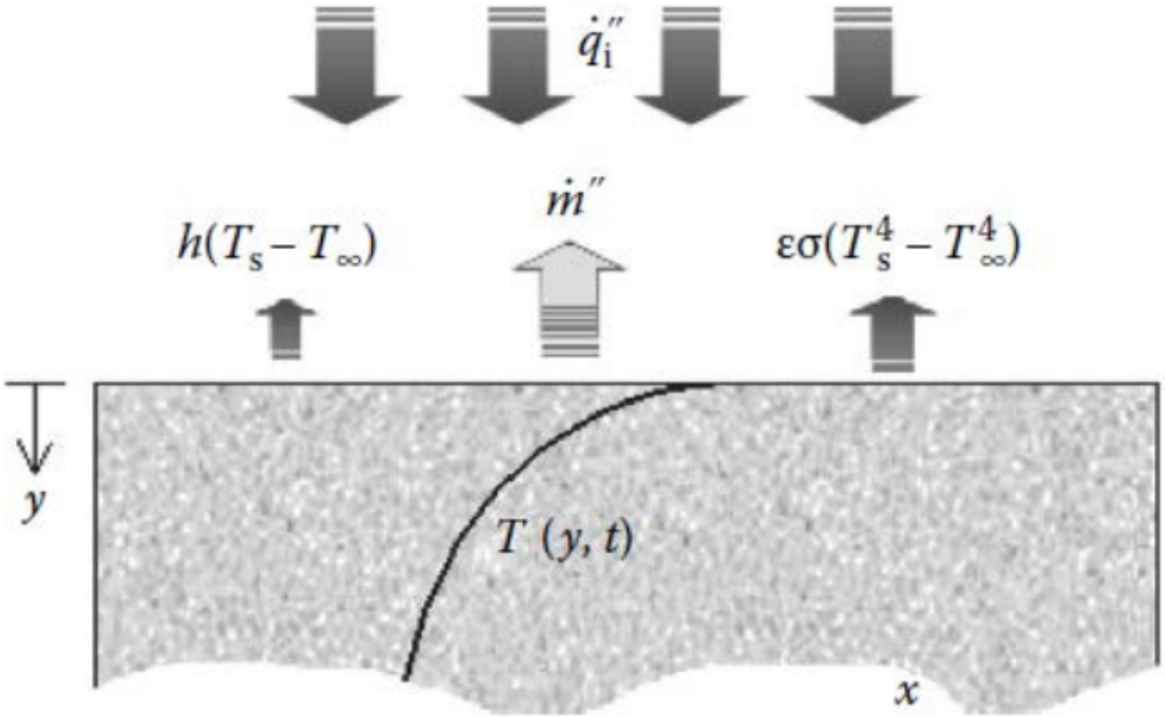

Figure 1. [Schematic of pyrolysis [12]]

How do we model pyrolysis?

Boundary condition

$$-k_{s,1}\frac{T_{s,1}^{n+1}-T_{s,0}^{n+1}}{\delta x_{\frac{1}{2}}}=\dot{q}_c''+\dot{q}_r'' \tag{1}$$

Heat conduction

$$\rho_s c_s\frac{\partial T_s}{\partial t}=\frac{\partial}{\partial x}(k_s\frac{\partial T_s}{\partial x})+\dot{q}_s''' \tag{2}$$

Reaction rate:

$$r=AY^n\cdot e^{-\frac{E_a}{RT}} \tag{3}$$

Parameter overview

Parameter	
Activation energie	E_a
Pre-exponential factor	A
Reaction order	n
Density	ρ
Conduction coefficient	k
Heat capacity	c

How do we get these parameters?

Find parameters with small scale experiments and mathematical fitting, scale up to parts and devices

Usual experiments:

- Thermogravimetrical analysis
- Cone calorimeter
- Micro combustion calorimeter
- ...

Approaches

- Forwad fitting
  - Basic graphical fitting [5, 6, 10]
  - Advanced automated fitting [3]
- Inverse modeling [11]
  - Optimization algorithms [1, 8]
  - Machine learning

History of my presentations at PhD seminar

- Optimization algorithms in fire simulation (Geneva, 2017)
- Progress on using optimization algorithms in fire simulation (Wuppertal, 2017)
- No more hacks and workarounds? – Get your data processing straight with a little help from your friends (Berlin, 2018)

New approach

Machine Learning (supervised)

- Neural networks
- Ensemble learning
- Stochastic regression
- ...

Supervised learning concept

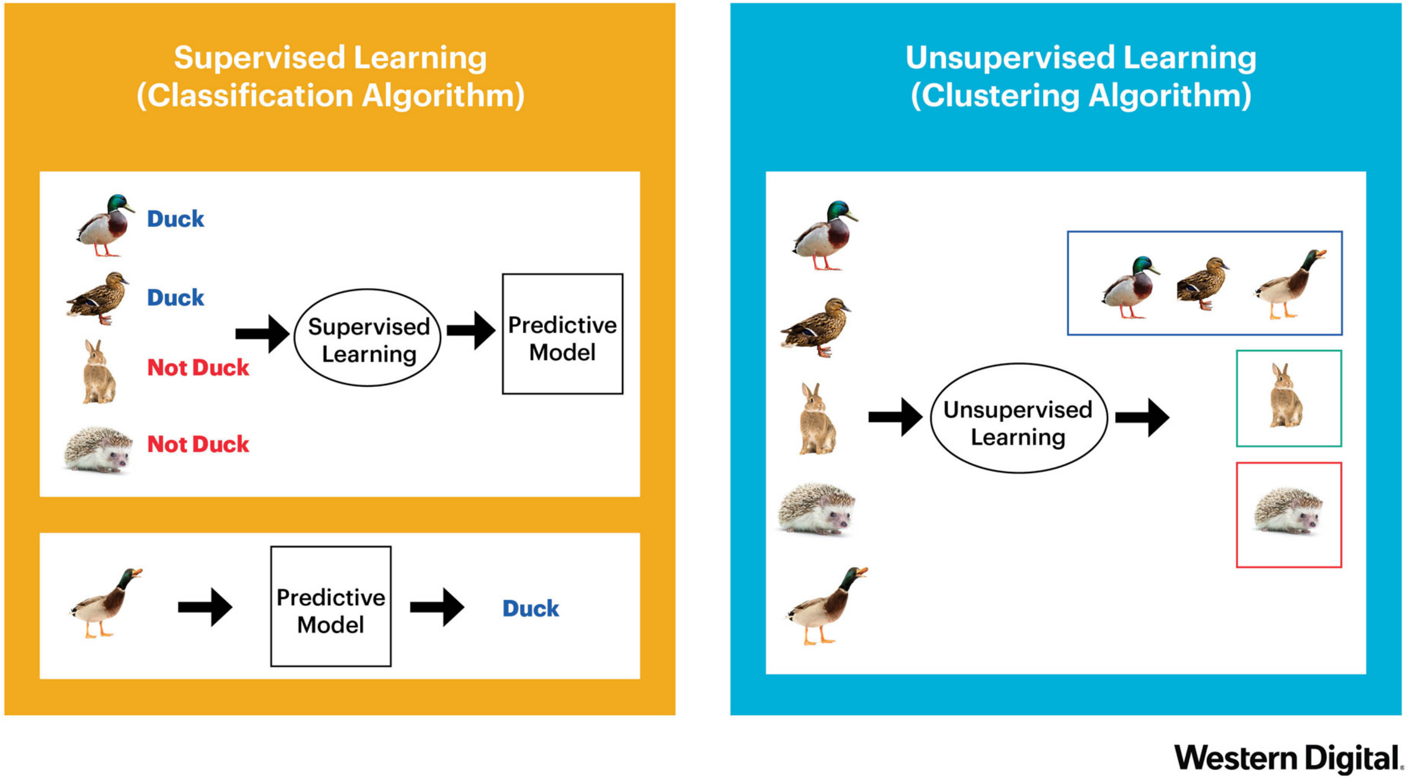

Figure 2. Supervised vs. unsupervised learning (https://blog.westerndigital.com/machine-learning-pipeline-object-storage/)

Method

- Train a model to predict reaction kinetic parameters with given reaction rate
- Case study: mockup TGA experiment with constant heating rate
- All data used is randomly generated with the pyrolysis model

Method II

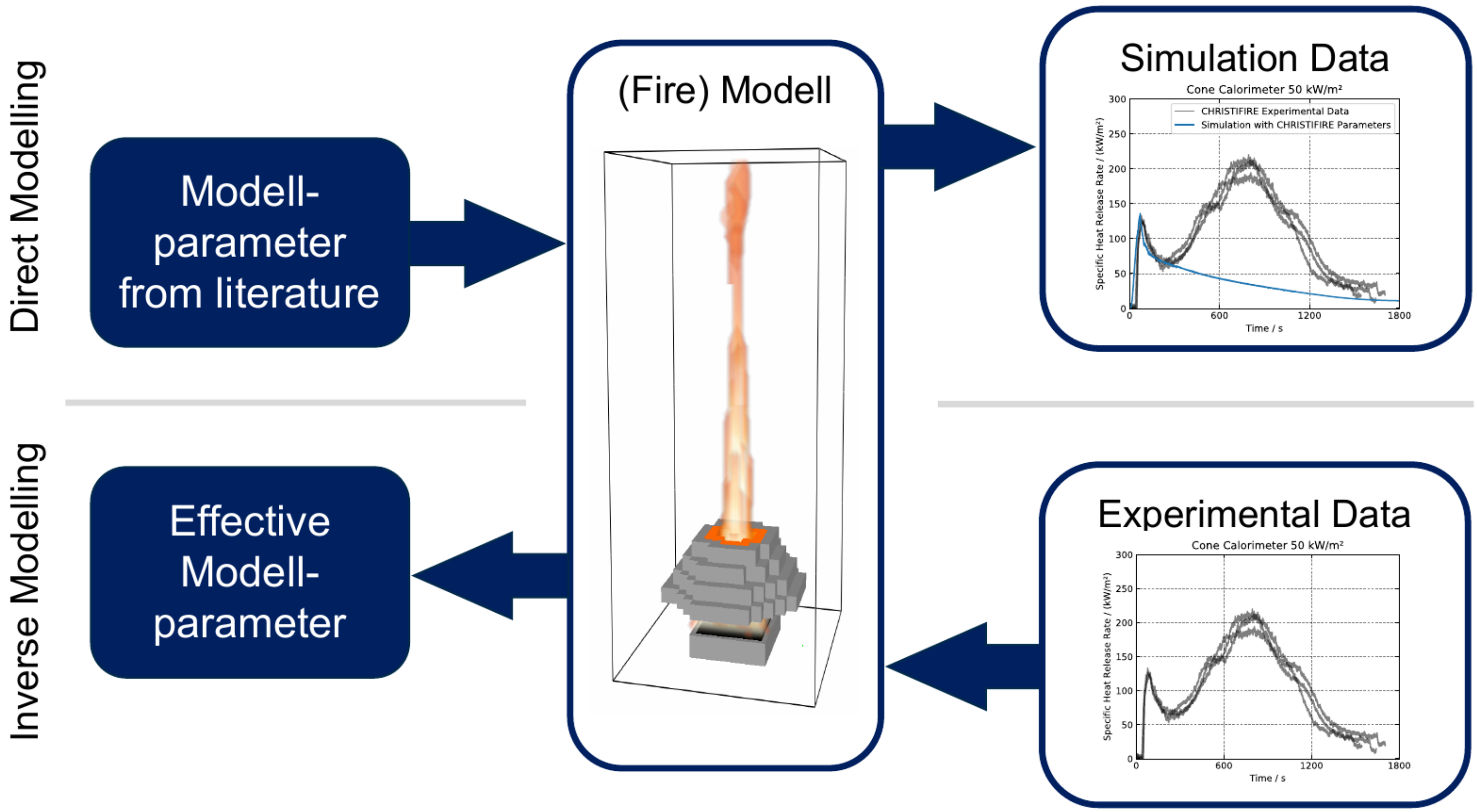

Figure 3. Invers modelling then

Method III

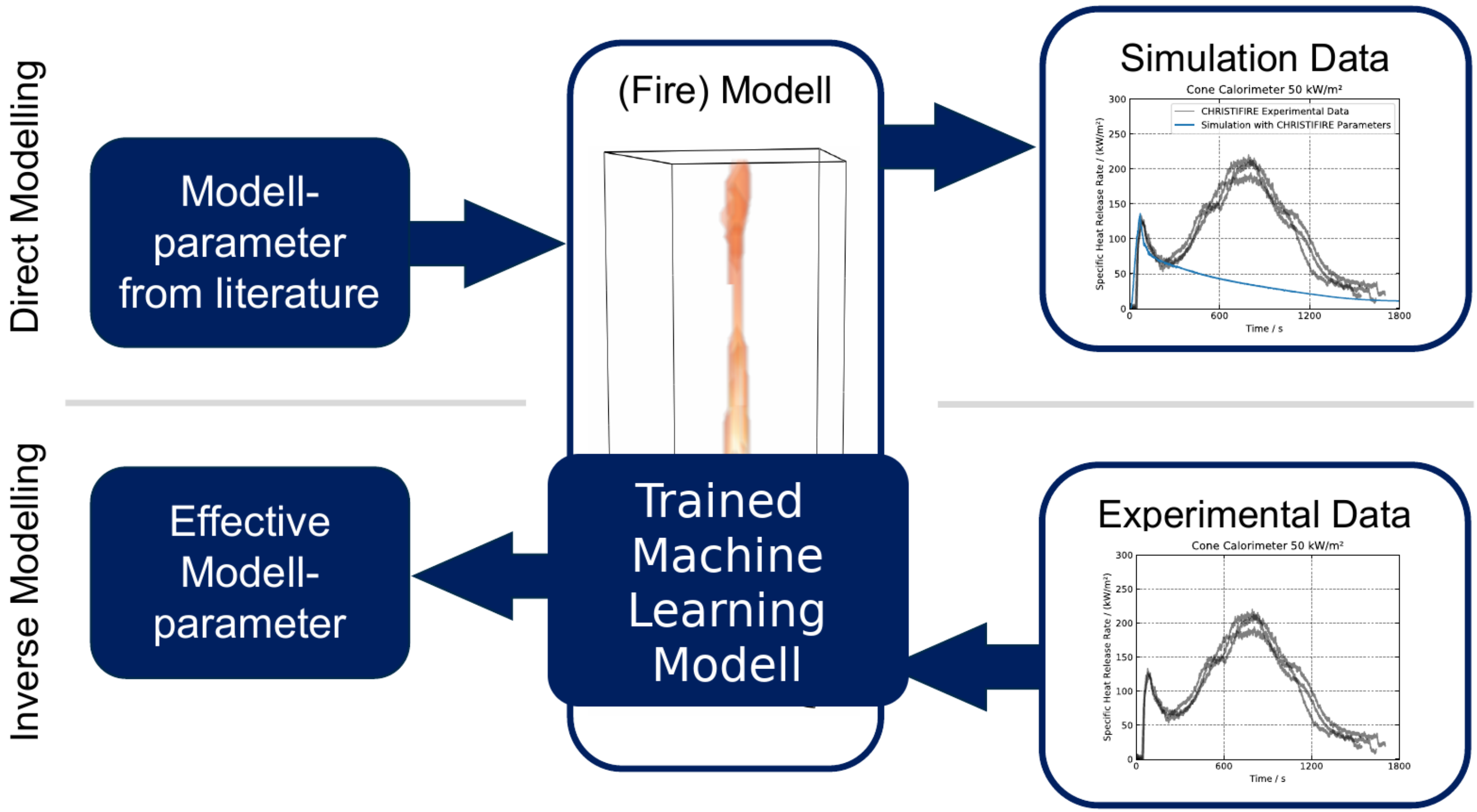

Figure 4. Invers modelling now

Process

1. Generating sample data set with the regarding model
    - Samples for 1, 2 and 3 reactions, with 3 heating rates applied each
    - Up to 500k samples generated, with $r(T)$ and A_n, E_n
2. Splitting data set in two independent sets (75 % training data set and 25 % validation data set)

Process II

3. Train model with training data set
    - Input: $r(T)_{train}$
    - Output: $A_{n,train}$, $E_{n,train}$
    - Model adopts to transform input to output
4. Validate trained model by feeding $r(T)_{prescribed}$ of validation data set and check for expected outcome

Process III

5. Recalculate $r(T)_{predicted}$ with A_n, E_n, calculate RMSE between $r(T)_{validation}$ and $r(T)_{predicted}$

Process IV

6. Evaluate
7. Repeat with different algorithms and different hyperparameter settings

Results

- Results for predicting kinetic parameters for 2 reactions with 3 heating rates tested
- Different algorithms with different hyperparameter settings
  - AdaBoost (ADA) [4], Extra Trees (ET) [7], Random Forests (RF)[2], Stochastic Gradient Descent (SGD) [9]
- Sample size 100k...500k (total)
- Total generated inverse models: 1900

Results II

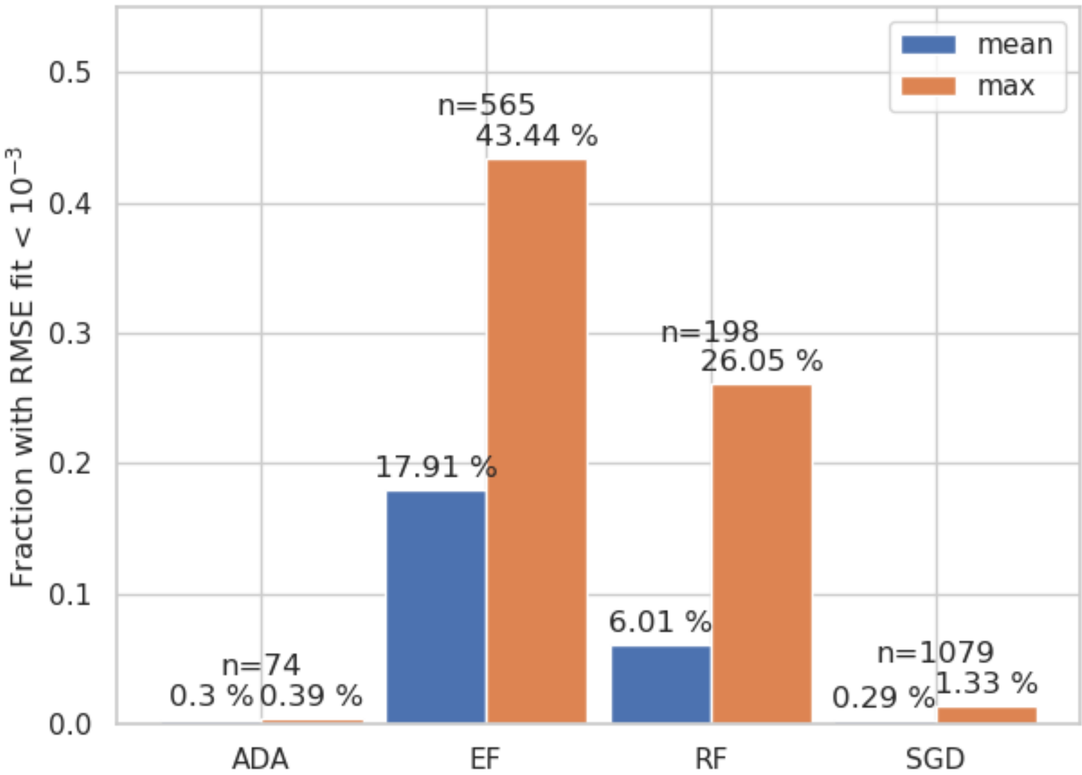

Figure 5. Model results with RMSE fit < 10^{-3} for 2 reactions with 3 heating rates

Results III

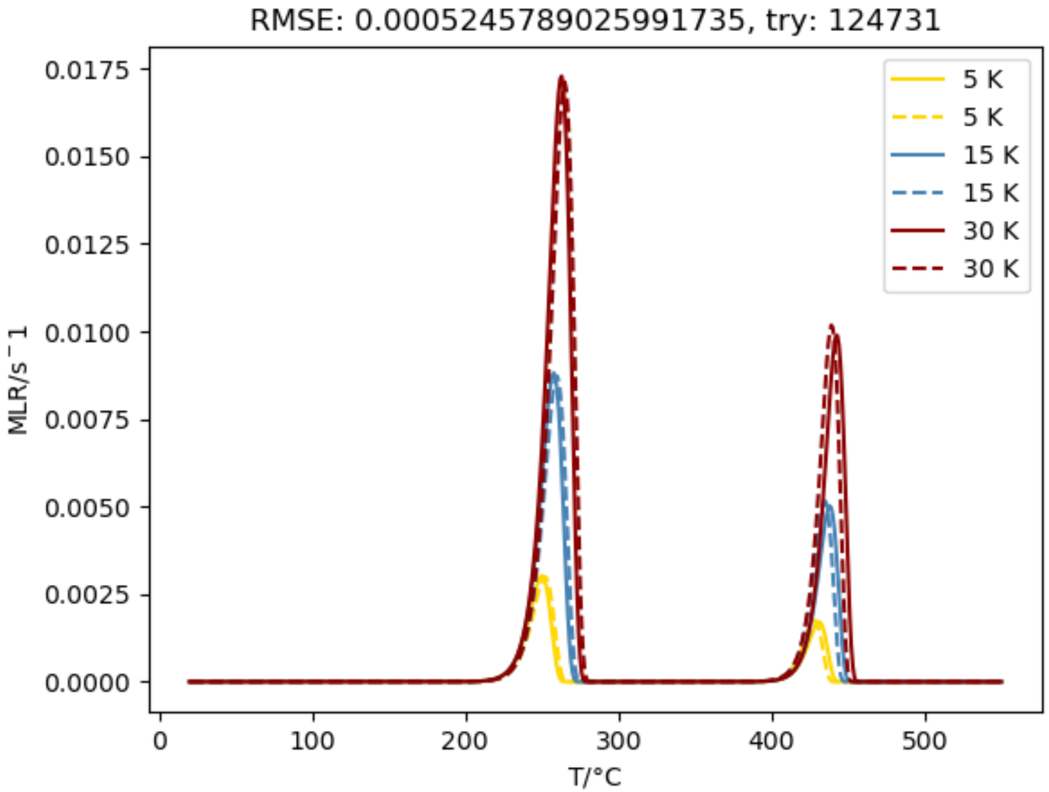

Figure 6. Random example with ET

Advantages over other methods

- Trained model is fast (instant result)
- Trained model is portabel
- Results are pretty good (by now in 43 % of presented case)
  - better for 1 reaction
  - worse for 3 reactions
- If no perfect fit was found, it is at least a good starting point for other methods

Disadvantages over other methods

- Generating samples is costly
- Training a model is costly
- Results are only good in 43 % of presented case

What is ET?

- Extremely randomized trees (Extra trees) is a tree based ensemble method and a modified variant of random forest
- Uses randomized, uncorrelated decision trees
- Efficient for big data sets
- Fast training

Outlook

- Couple with Heat conduction
- Use larger sample data sets
- Try with different Pyrolysis models
- Validate with real data
- Compare to other machine learning models

References

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