Sensitivity Analysis of Input Parameters in Flame Spread Simulation

PhD Students' Seminar on Fire Safety Science

December 1, 2022 | Tássia Quaresma | Division Fire Dynamics - IAS 7

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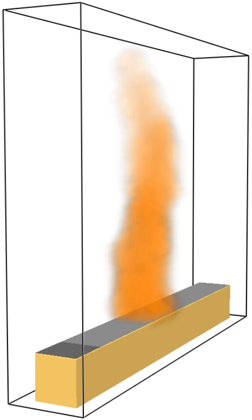
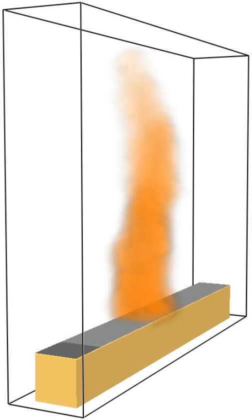
Flame spread modelling with the Fire Dynamics Simulator



Flame spread modelling with the Fire Dynamics Simulator

Simple pyrolysis models



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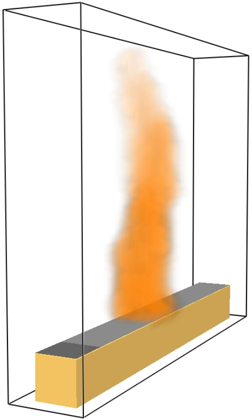

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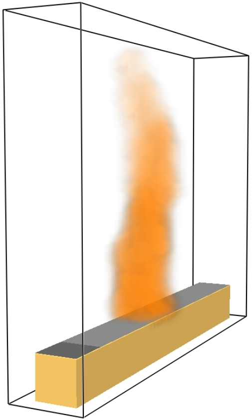

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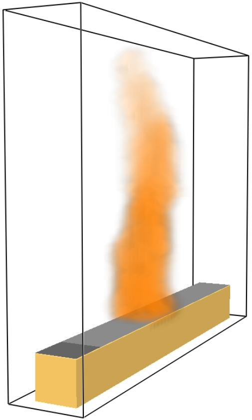

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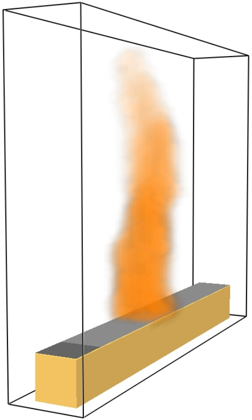

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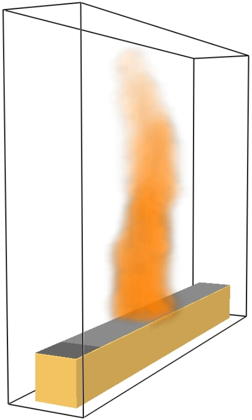

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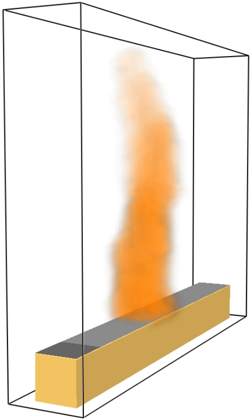

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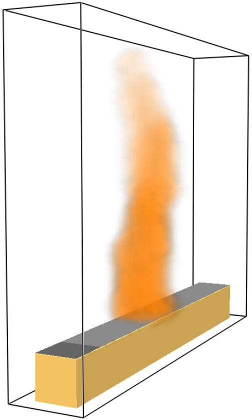

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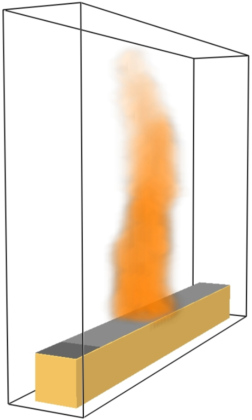
- Pyrolysis rates are given by the Arrhenius equation



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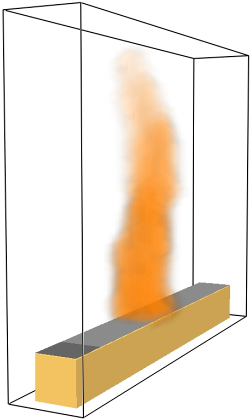


Complex pyrolysis models

- Heat release rate is calculated by the model itself
- Influence of material properties on heat transfer
- Pyrolysis rates are given by the Arrhenius equation
- *Require multiple input parameters!*

Input parameters

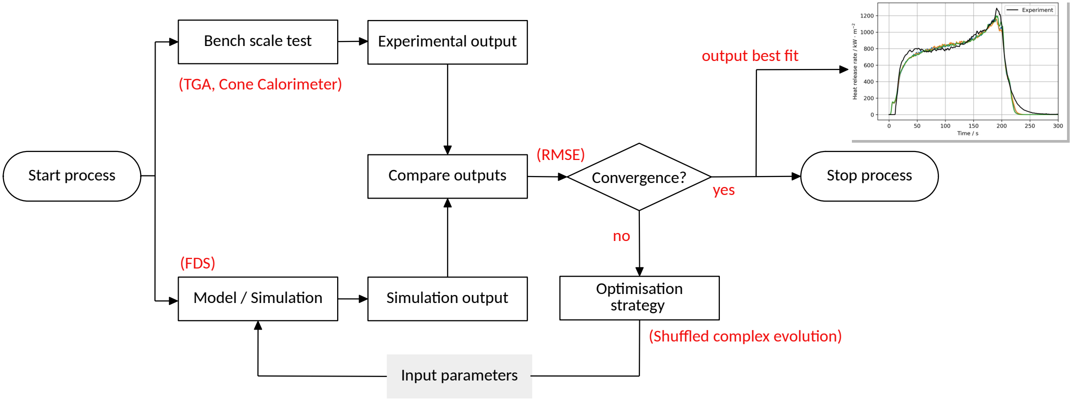
- Kinetic parameters:
  - pre-exponential factor
  - energy of reaction
  - heat of reaction
- Material properties:
  - emissivity
  - specific heat
  - thermal conductivity
  - absorption coefficient
  - (...)

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

$$\dot{q}_{s,c}'''(x) = -\rho_s(0) \sum_{\alpha=1}^{N_m} \sum_{\beta=1}^{N_{r,\alpha}} r_{\alpha\beta}(x)\, H_{r,\alpha\beta}$$

$$r_{\alpha\beta}(x) = \left(\frac{\rho_{s,\alpha}(x)}{\rho_s(0)} \right)^{n_{\alpha\beta}} A_{\alpha\beta} \exp\left(-\frac{E_{\alpha\beta}}{RT_s(x)} \right)$$

Inverse modelling and optimisation

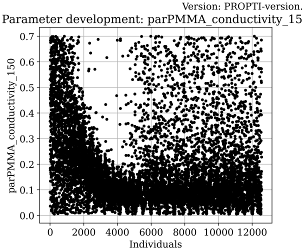


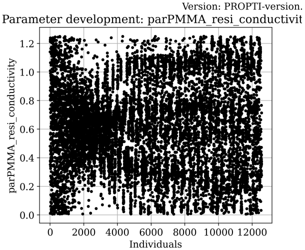
Adapted from: Lauer et al., 2016.

Inverse modelling and optimisation

Some issues

- Computationally expensive
- Estimation of multiple input parameters
- Sensitivity to input parameters is often unknown
- Large uncertainty in less important parameters
- Uncertainty is carried over to the validation step (flame spread setup)





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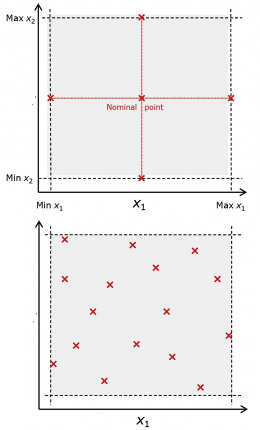
Sensitivity analysis (SA)

How is the model's *output* influenced by the model's *inputs*?

- Local SA
  - based on varying one parameter at a time;
  - cannot effectively explore a multi-dimensional space;
  - interactions among input factors cannot be detected;
  - only valid for linear models.

- Global SA
  - any approach that is based on moving the factors together;
  - explore efficiently the multi-dimensional space;
  - capable of detecting interactions among factors;
  - valid for non-linear models.



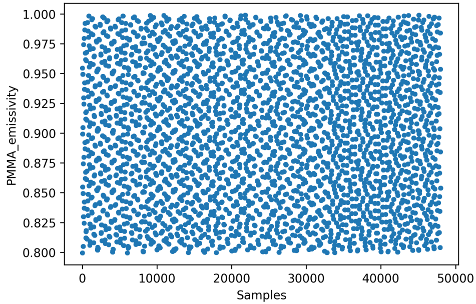
Adapted from: Saltelli et al., 2019.

Sobol sensitivity indices: a global SA method

- Measure sensitivity by determining how much the uncertainty (variance) in the output could be reduced if a given x_i parameter could be fixed
  - $S1_{x_i}$: measures the effect on the output when x_i is varied alone (main effect)
  - $S2_{x_i,x_j}$: measures the effect of varying x_i and x_j simultaneously (interaction effects between x_i and x_j)
  - ST_{x_i}: measures the total effect of x_i on the output, as the sum of x_i main effect and all interaction effects, providing a broad picture of model behaviour
- Sensitivity indices are computed to every input parameter
- The indices vary from 0 to 1. The greater the index is to 1, the larger is its importance

Sobol sensitivity indices: a global SA method

- For the calculation of the sensitivity indices, a large number of simulations need to be conducted
- An accordingly large number of samples of input parameters need to be created out of their sampling ranges
- Sampling method is based on the Sobol sequence
- Variables are assumed to be uniformly distributed
- The sample ranges were defined as 15% of variation around the best parameter set coming from the optimisation
- Python library: SALib



Input parameters, their sampling ranges and units

	Parameters	Ranges	Units
1	Emissivity	[0.799 ; 0.999]	-
2	Absorption coefficient	[6782 ; 9176]	m^{-1}
3	Refractive index	[2.426 ; 3.281]	-
4	Conductivity at 150°C	[0.322 ; 0.436]	$W \cdot m^{-1} \cdot K^{-1}$
5	Conductivity at 480°C	[0.021 ; 0.028]	$W \cdot m^{-1} \cdot K^{-1}$
6	Conductivity at 800°C	[3.687 ; 4.988]	$W \cdot m^{-1} \cdot K^{-1}$
7	Specific heat at 150°C	[0.658 ; 0.890]	$kJ \cdot kg^{-1} \cdot K^{-1}$
8	Specific heat at 480°C	[3.237 ; 4.380]	$kJ \cdot kg^{-1} \cdot K^{-1}$
9	Specific heat at 800°C	[6.183 ; 8.366]	$kJ \cdot kg^{-1} \cdot K^{-1}$
10	Residue emissivity	[0.469 ; 0.635]	-
11	Residue conductivity	[3.833 ; 5.186]	$W \cdot m^{-1} \cdot K^{-1}$
12	Residue specific heat	[5.009 ; 6.777]	$kJ \cdot kg^{-1} \cdot K^{-1}$
13	Backing emissivity	[0.375 ; 0.507]	-
14	Backing conductivity	[2.047 ; 2.769]	$W \cdot m^{-1} \cdot K^{-1}$
15	Backing specific heat	[3.457 ; 4.677]	$kJ \cdot kg^{-1} \cdot K^{-1}$

Running multiple simulations

Emissivity
Absorption coefficient
Refractive index

Conductivity at 150 °C
Conductivity at 480 °C
Conductivity at 800 °C

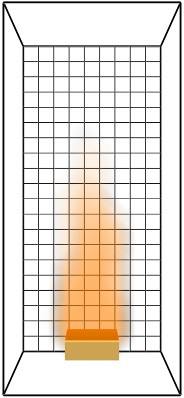
Specific heat at 150 °C
Specific heat at 480 °C
Specific heat at 800 °C

Residue conductivity
Residue emissivity
Residue specific heat

Backing conductivity
Backing emissivity
Backing specific heat

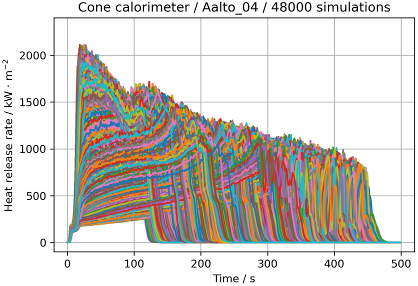
Input parameters

→ 48,000 samples



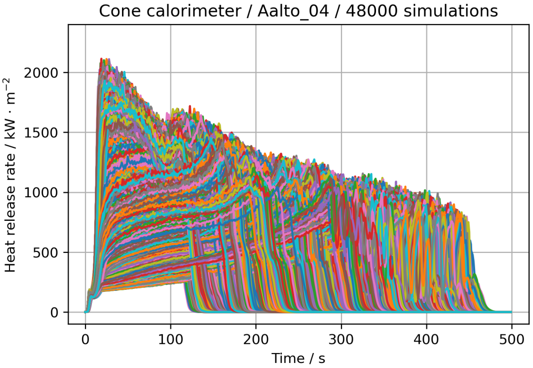
Cone calorimeter setup

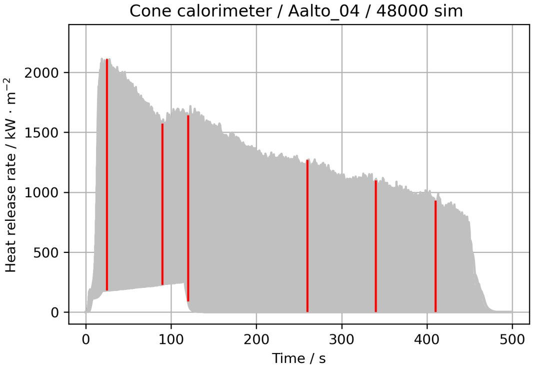
→



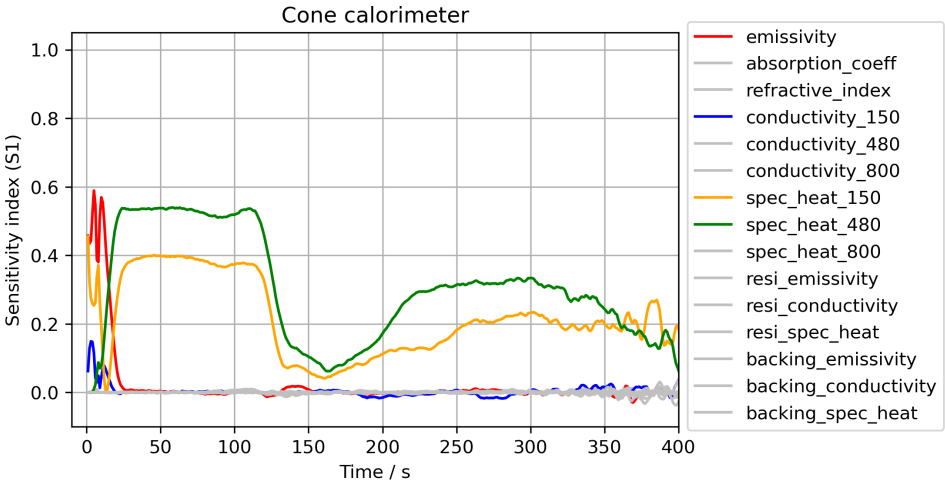
48,000 simulations

Analysis of outputs: every point in time

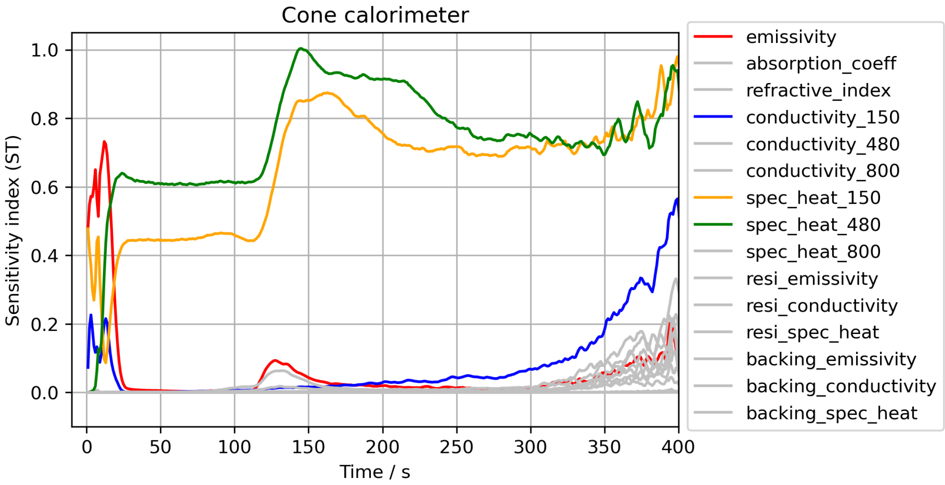




Sobol sensitivity indices: S1



Sobol sensitivity indices: ST



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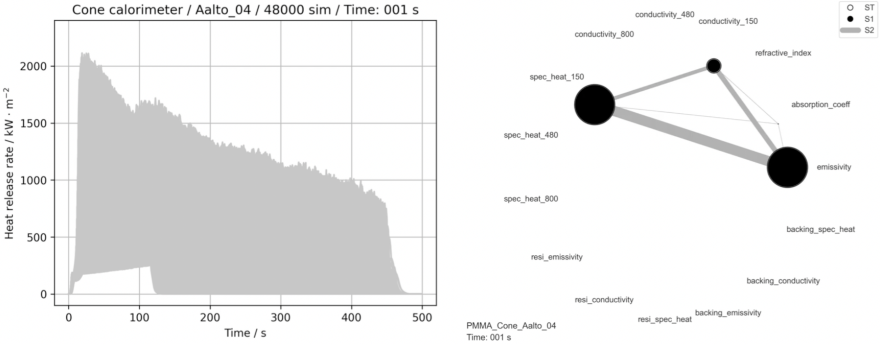
Video: sensitivity indices over time



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- Sensitivities can depend on the chosen sampling ranges, broader ranges should be considered in future analyses
- The SA method is now to be applied on a flame spread setup, so the results can be compared with the ones in the cone

Thank you!

Questions?

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