OPTIMIZATION *VIA* MACHINE LEARNING OF INTUMESCENT COATING FOR WOOD SUBSTRATES

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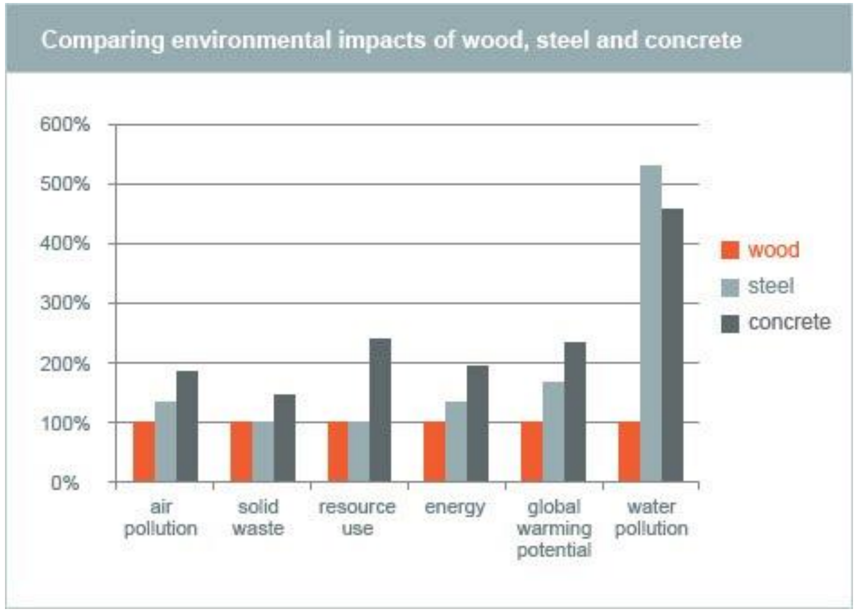
EDF, Chatou - 07/07/23

Introduction

Wood is more and more used in building applications

Low grey energy compared to traditional materials

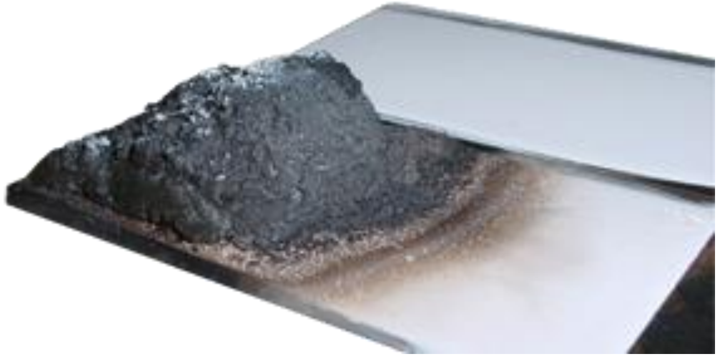


How to protect efficiently wood against fire ?

https://www.canfor.com/responsibility/why-wood/comparing-wood-and-non-renewable-materials

Our strategy

Intumescent coating efficient



Composition of the FR paint

weight Percentage (wt%)

0,35<	water	<0,45
0,10<	Emultex	<0,20
0,20<	APP	<0,30
0,05<	DIPER	<0,15
0,05<	MEL	<0,15
0	< Dio	<0,10

$$\sum_i x_i = 1$$

Design of Experiment (DoE): statistical approach

- High dimension ✗
- Multi-objective ✗
- Noisy observation ✗

machine learning guided optimization

Multi-Objective Bayesian Optimisation (MOBO)

Optimization of the chemical composition of an intumescent coating

Can we use AI for noisy observations ?

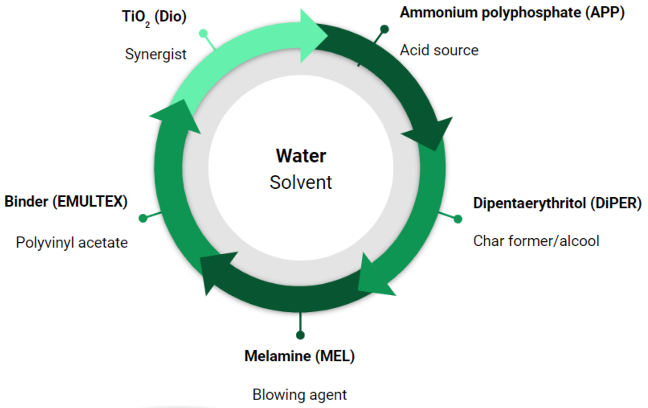
Can we optimise better and faster with AI ?

Weil, Edward D. "Fire-protective and flame-retardant coatings-A state-of-the-art review." Journal of fire sciences 29.3 (2011): 259-296.
Kotthoff, L., Wahab, H., & Johnson, P. (2021). Bayesian Optimization in Materials Science: A Survey. arXiv preprint arXiv:2108.00002.

Problem setup-Formulation

Inputs

weight percentage of each component ($\%wt$)



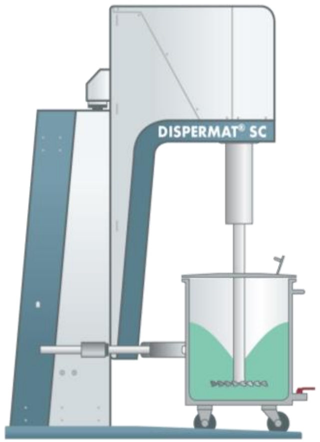
$$\sum_i x_i = 1$$

Inputs: 6 parameters

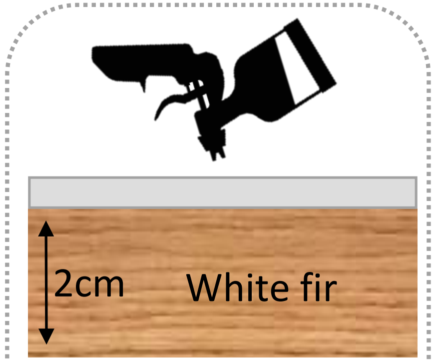
Preparation

1 → 2 → 3 → 4

1 Formulation Coating

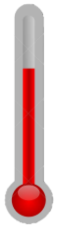


2 Application



Constant dry coating: 230g/m²

3 Conditionning



30°C

40%

5 days

4 Fire testing

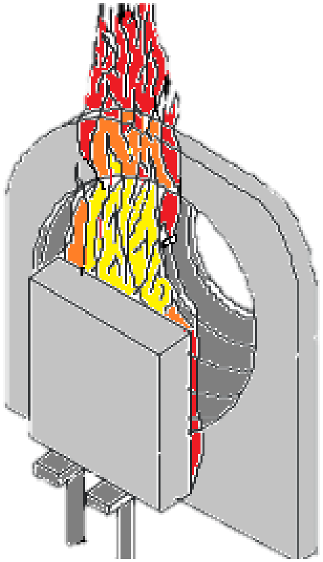
lab scale fire test

Problem setup-Fire performance

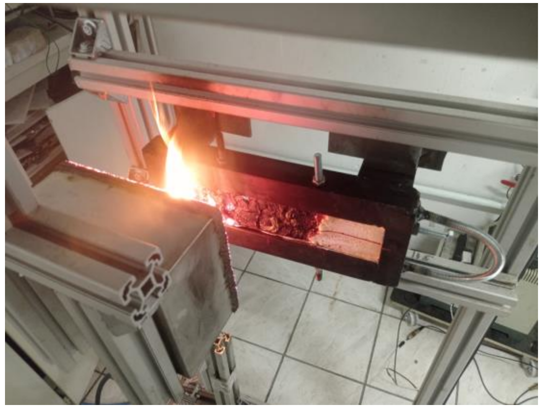
Outputs: 4 Fire Parameters (FP) to optimize

Horizontal MLC

Vertical MLC



CFE 1/3 scale



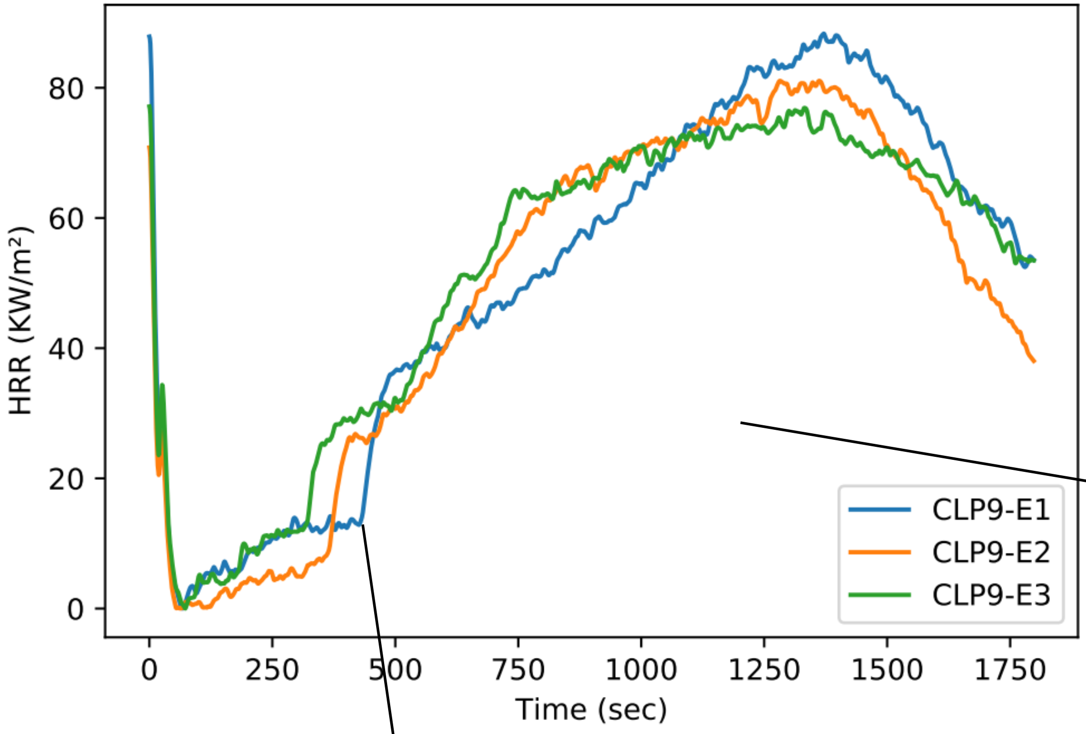
FP1. Total heat rate released (THR)
FP2. Time of ignition (ti)

FP3. Median of the mass loss rate

FP4. Distance of degradation

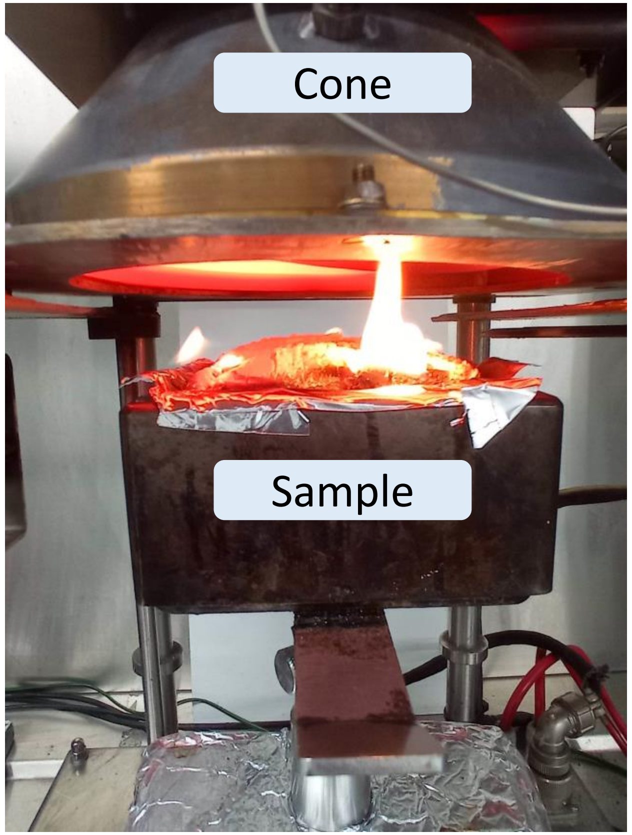
Horizontal Mass Loss Cone (MLC)

- Heat flux density: 50 kW/m²
- Test time: 30 min
- Measurement of the heat released: Thermopile



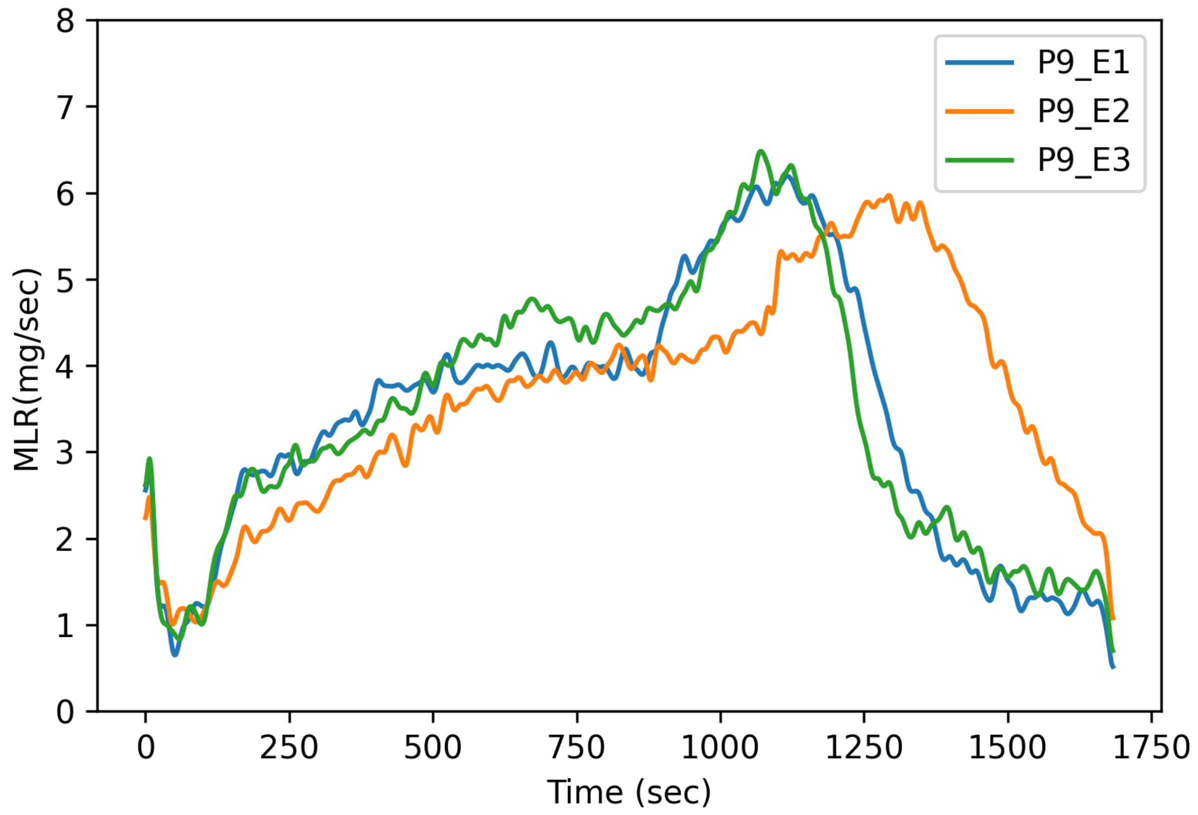
Area under the curve = Total Heat Released (THR - FP1)

Time to ignition (ti – FP2)

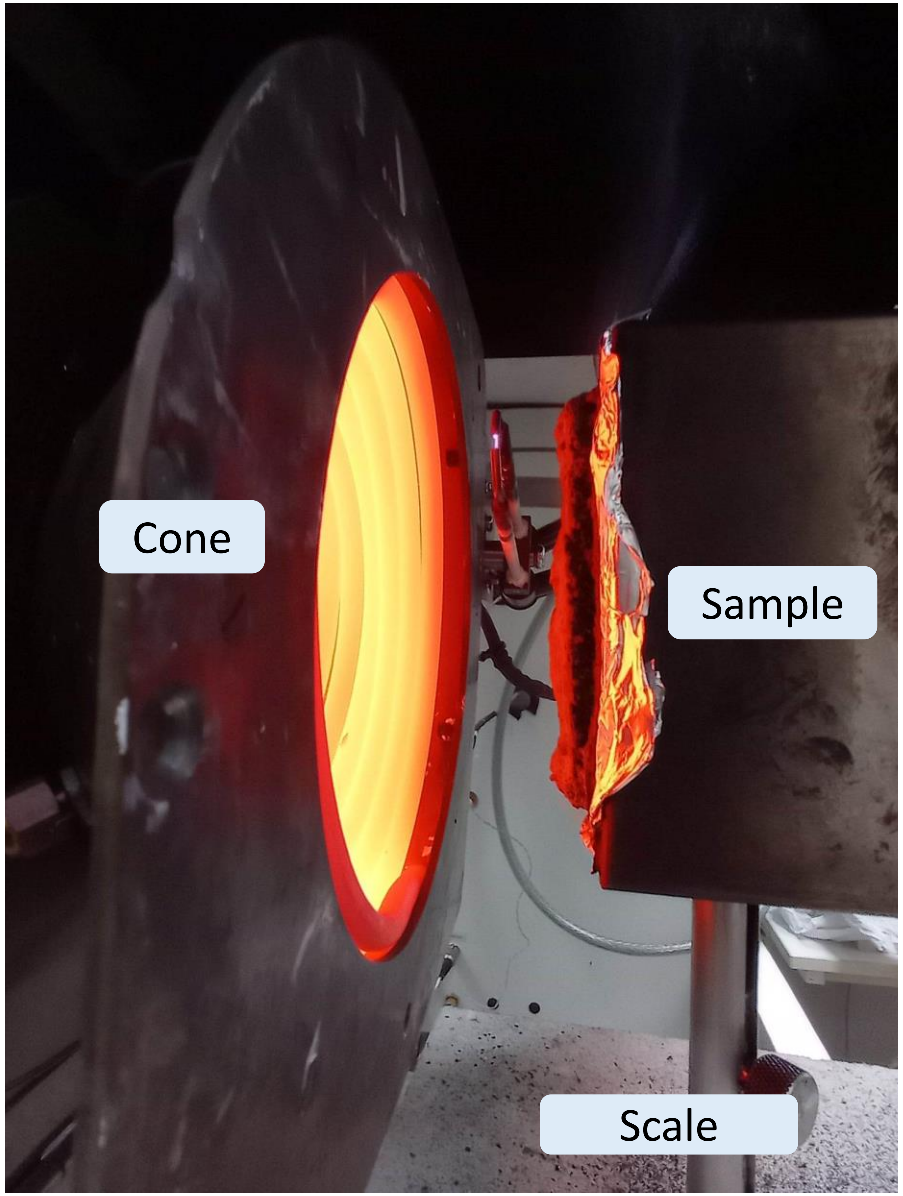


Vertical Mass Loss Cone (MLC)

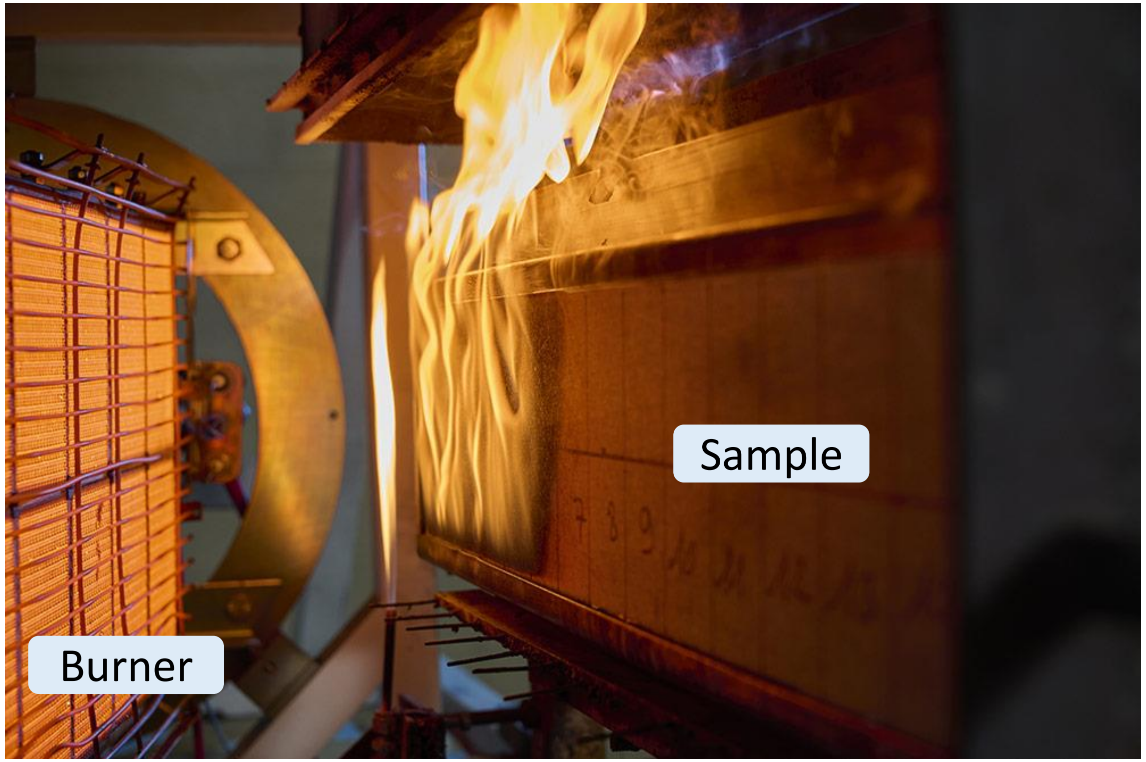
- Heat flux density: 50 kW/m²
- Test time: 30 min

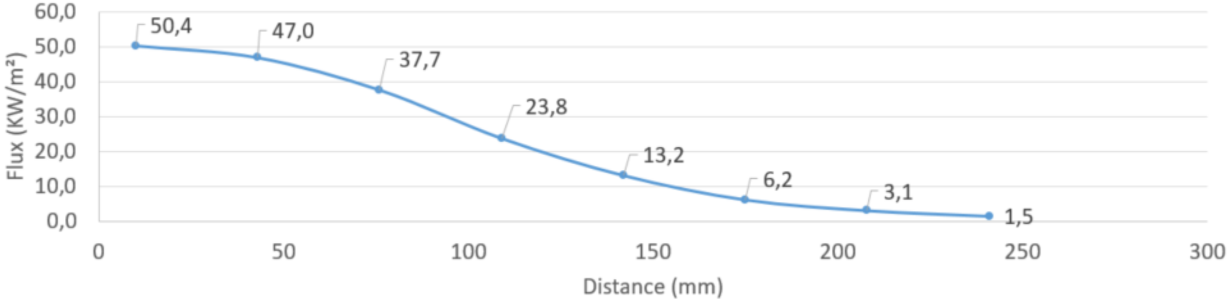


- Median of the mass loss rate (FP4)



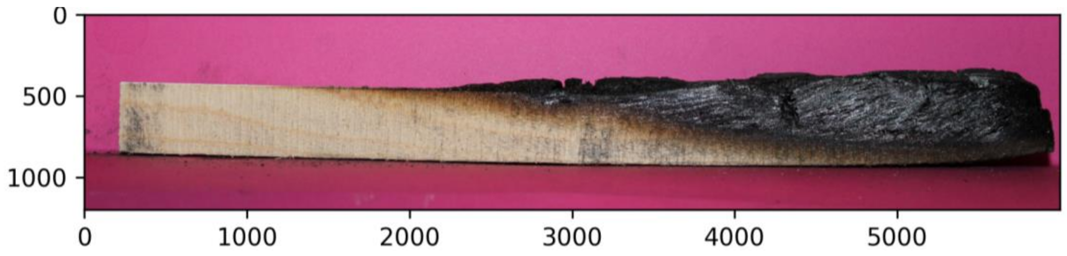
Critical heat flux at extinguishment (CFE)-1/3 scale



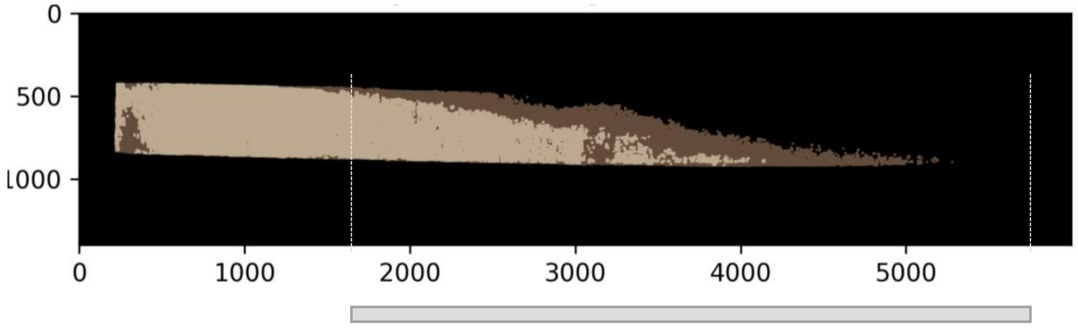


Machine learning algorithm (K-means clustering) = Image segmentation

Input



Output

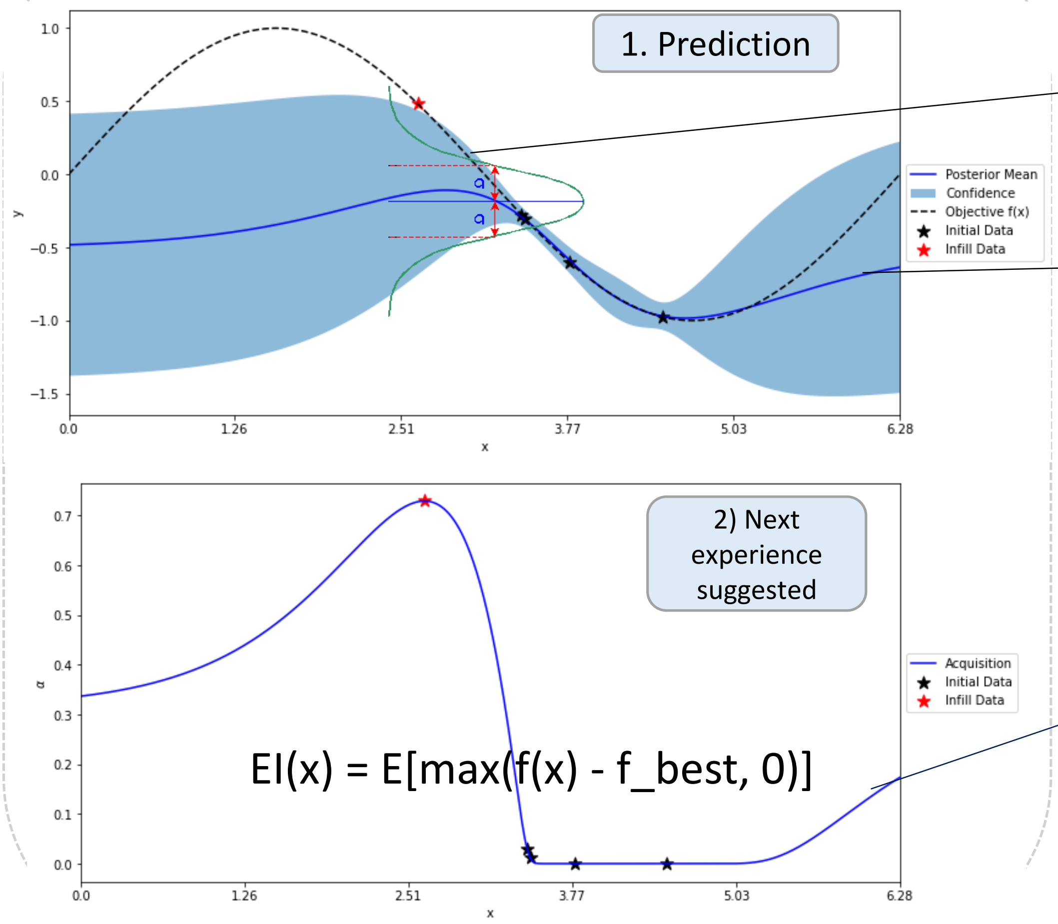


Distance of degradation (FP4)

What is Bayesian Optimization (BO)? 1D example

Maximisation of
$$y = f(x)$$

Iteration n°0



EI(x) = E[max(f(x) - f_best, 0)]

Unknown function to optimise

Prediction with Gaussian process (GP)

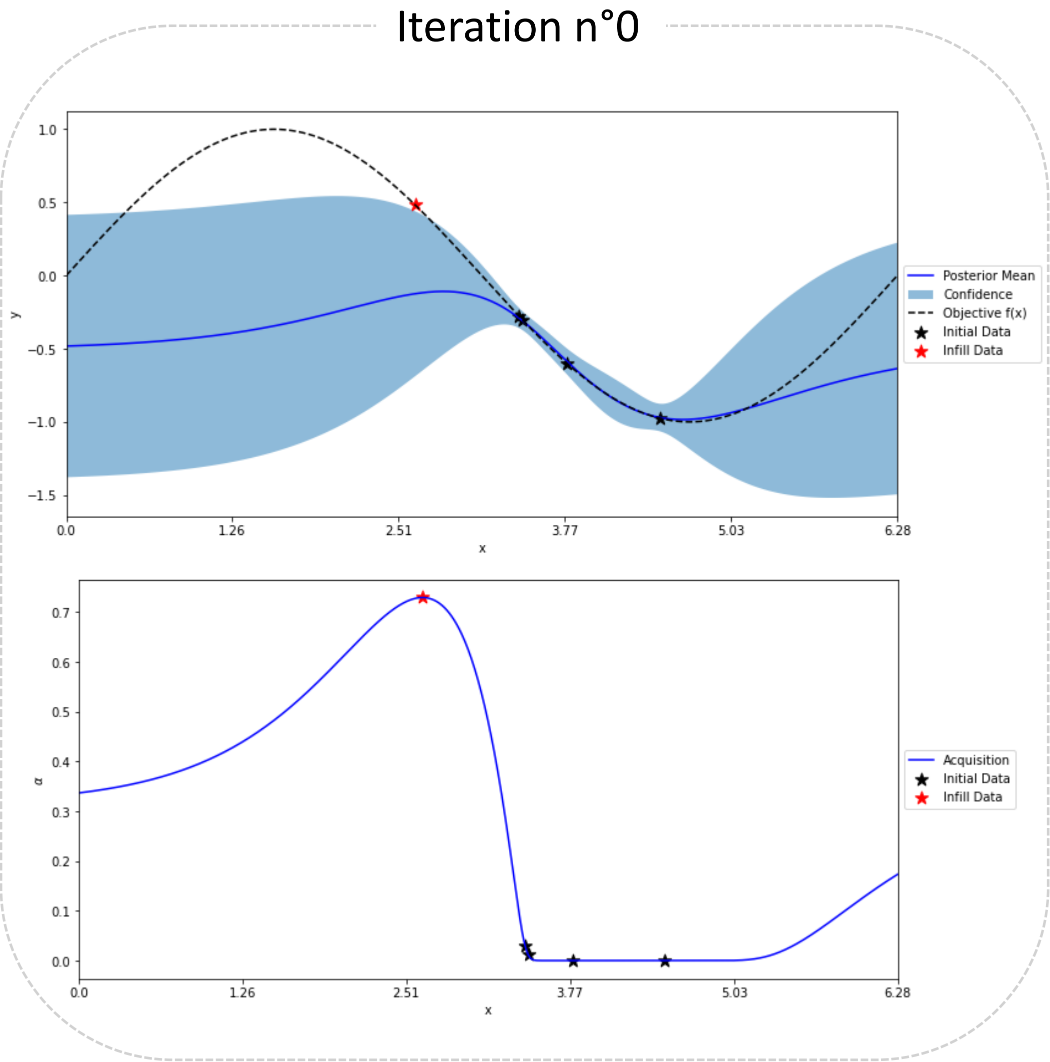
Acquisition function = Expected Improvement (EI)

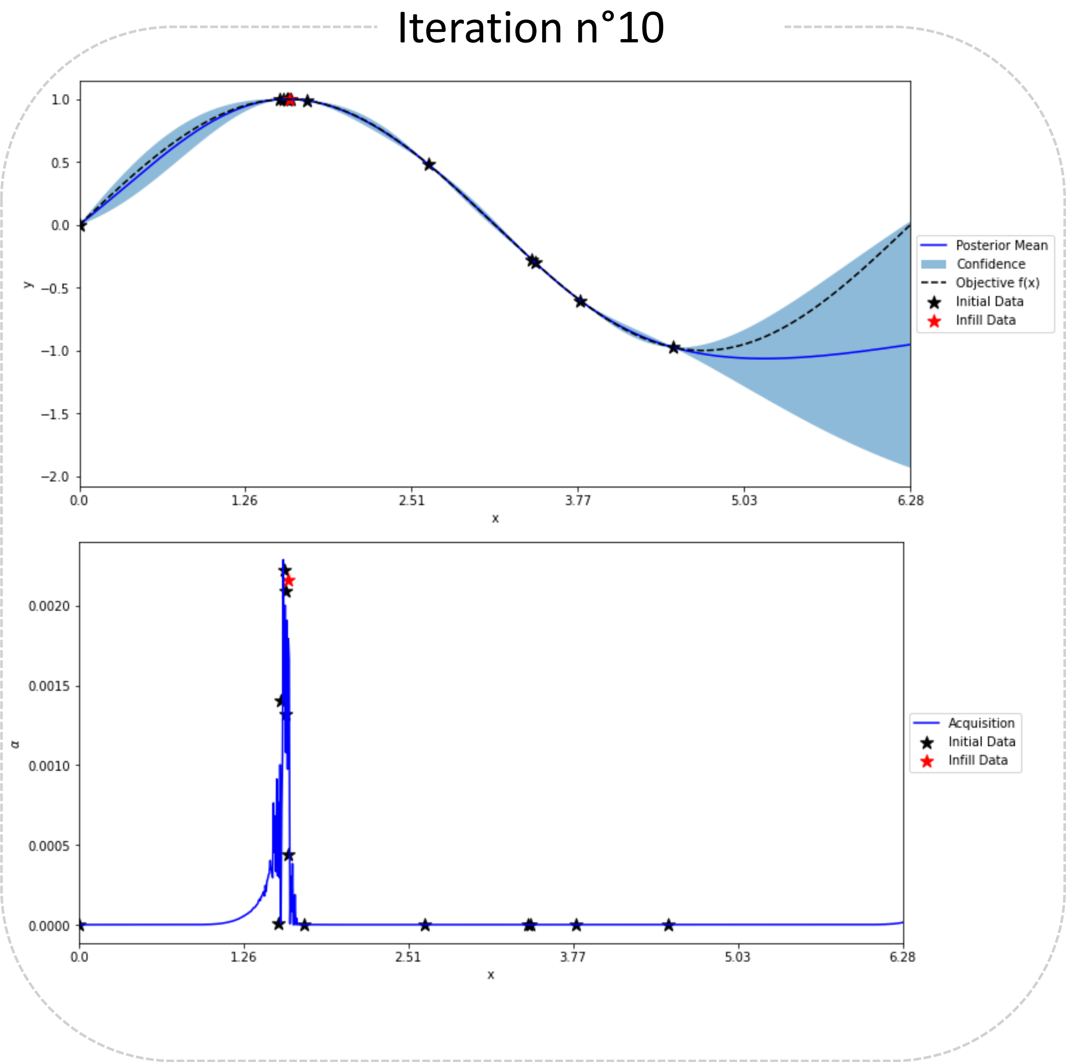
- x is the candidate point
- f(x) is the estimated value at point x
- f_best is the best value observed so far
- E[.] represents the expectation over the distribution of f(x)

Take away

- Maximisation of a black box function by an active loop
- Maximise the knowledge behind each point
- Efficient for noisy and costly evaluation

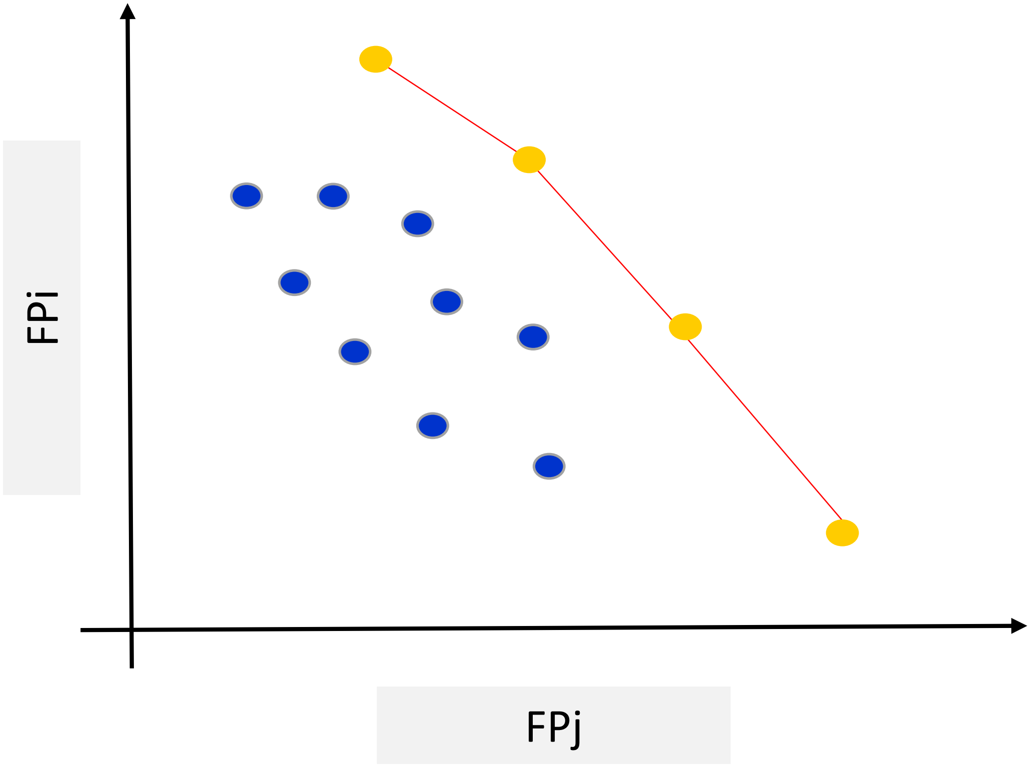
What is Bayesian Optimization (BO)? 1D example y = f(x)

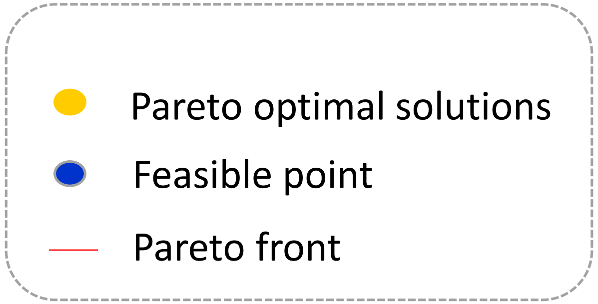




Multi-objective optimization (MOBO) – Pareto front

The goal in MOBO is to learn the Pareto front





Take away

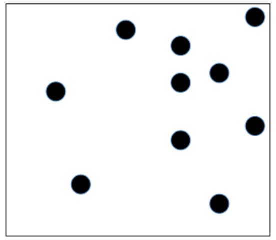
- multi-objective optimization = no single best solution
- Pareto optimal solutions = trade off between objectives

Multi-Objective Bayesian Optimisation - pipeline

1 → **1,5**

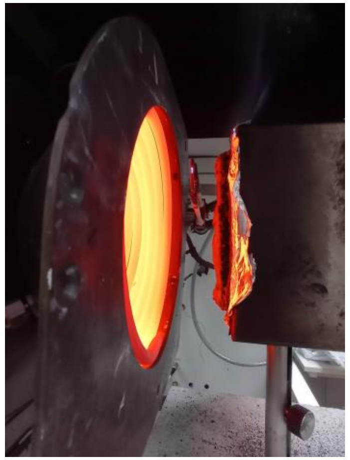
Initial sampling

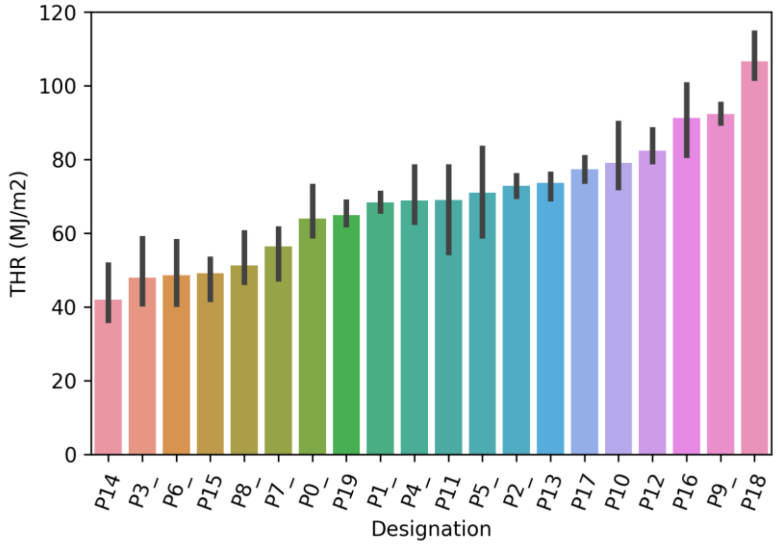
20 paint formulations Randomly chosen

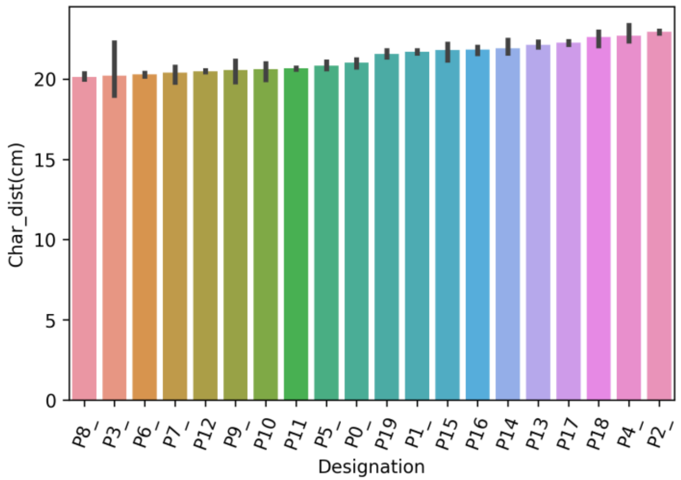


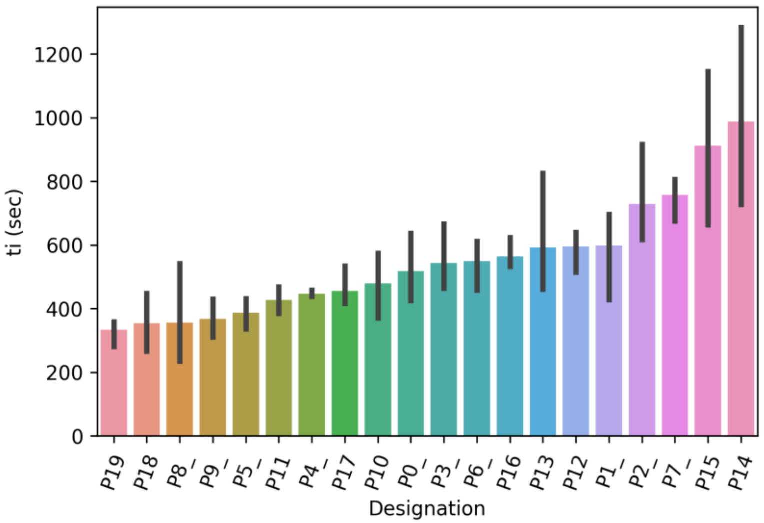
Experimental data

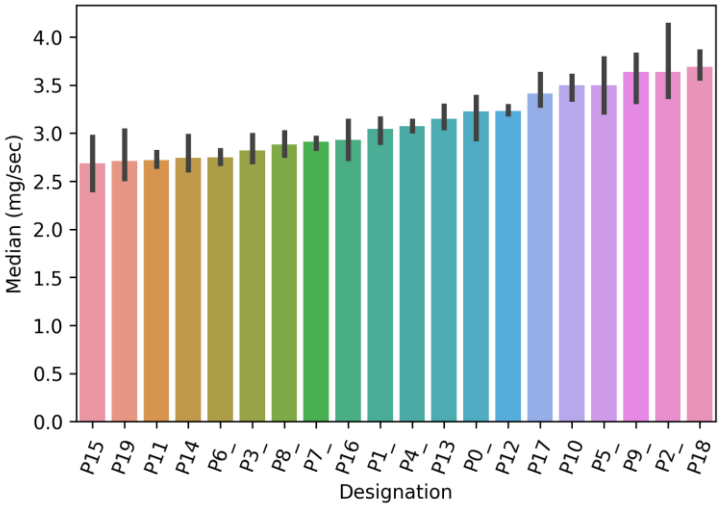
Fire performance evaluation











Multi-Objective Bayesian Optimisation - pipeline

1 → **1,5** → **2** → **3** → **4**

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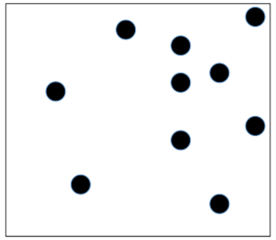

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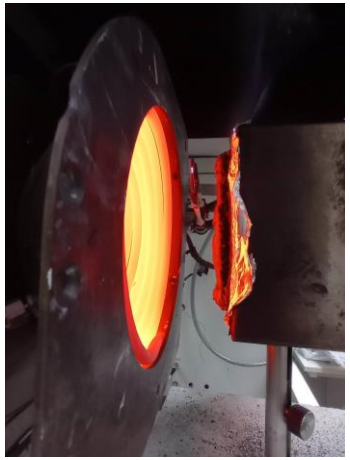
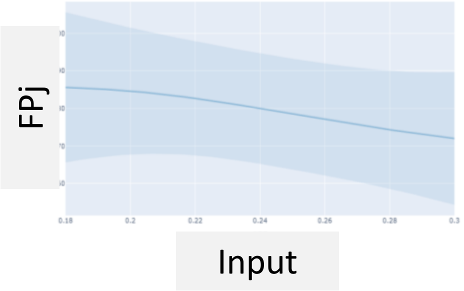
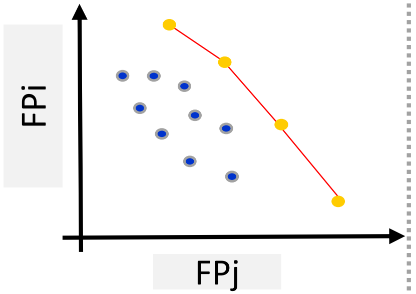


Model training

Fit Gaussian processes for each objective



Pareto front prediction

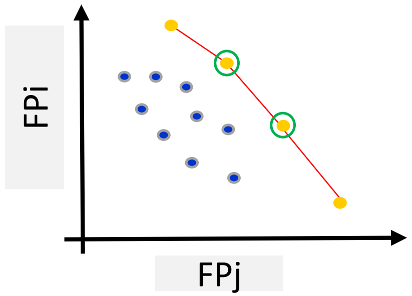


Pareto front

Observations

Next experience

Selected points



Batch of formulation to evaluate next

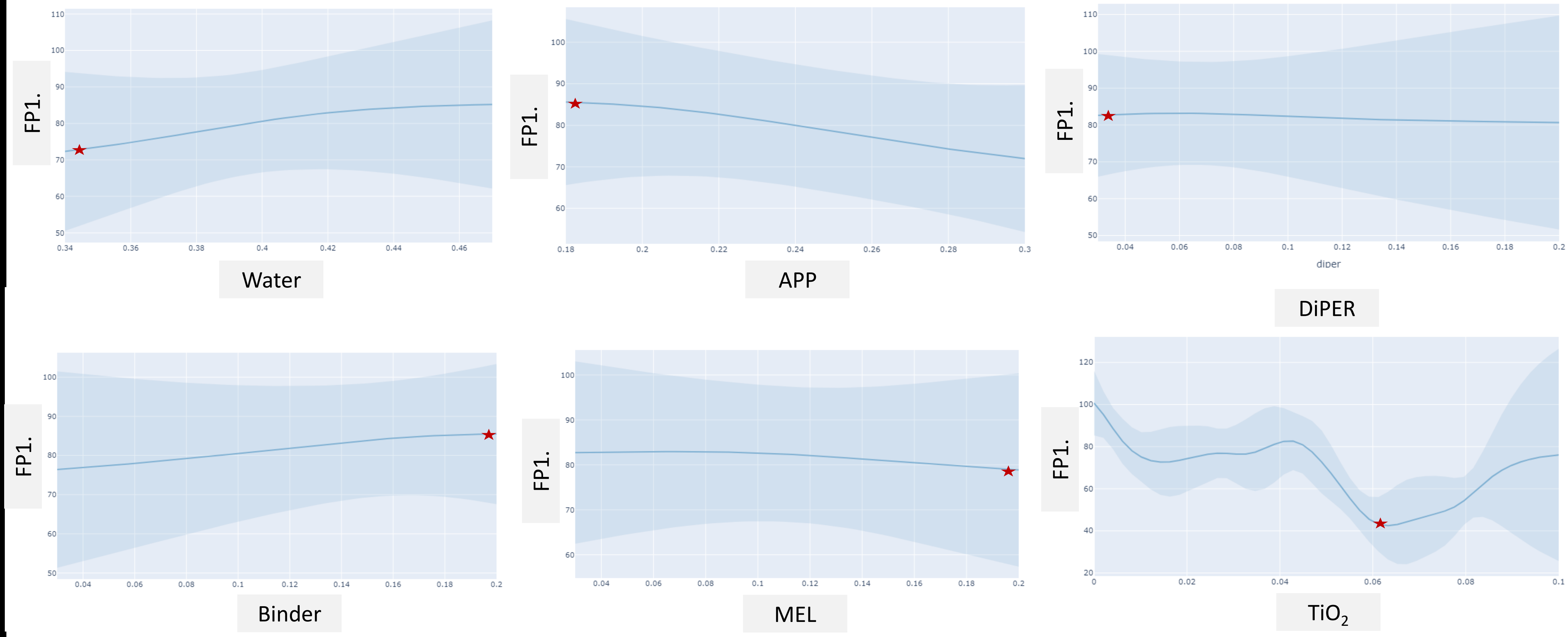
Active learning loop (work in process)

Prediction of the model

facebook/Ax

Adaptive Experimentation Platform

python



★ Next formulation to evaluate

Aim of the active loop

- Reduce the uncertainty
- Learn the pareto front

Conclusion

- Simple intumescent coating as a case study
- The performance of the coating is evaluate 4 Fire Parameters performed by 3 fire tests under 6 input parameters
- Multi objective Bayesian optimization (MOBO) has been chosen to find the optimum configuration of the paint (pareto front) and minimize the number of trials

Outlooks

- This framework applicable on other substrates ?
- Generalisation of the segmentation methodology for the measurement of degradation front in different materials

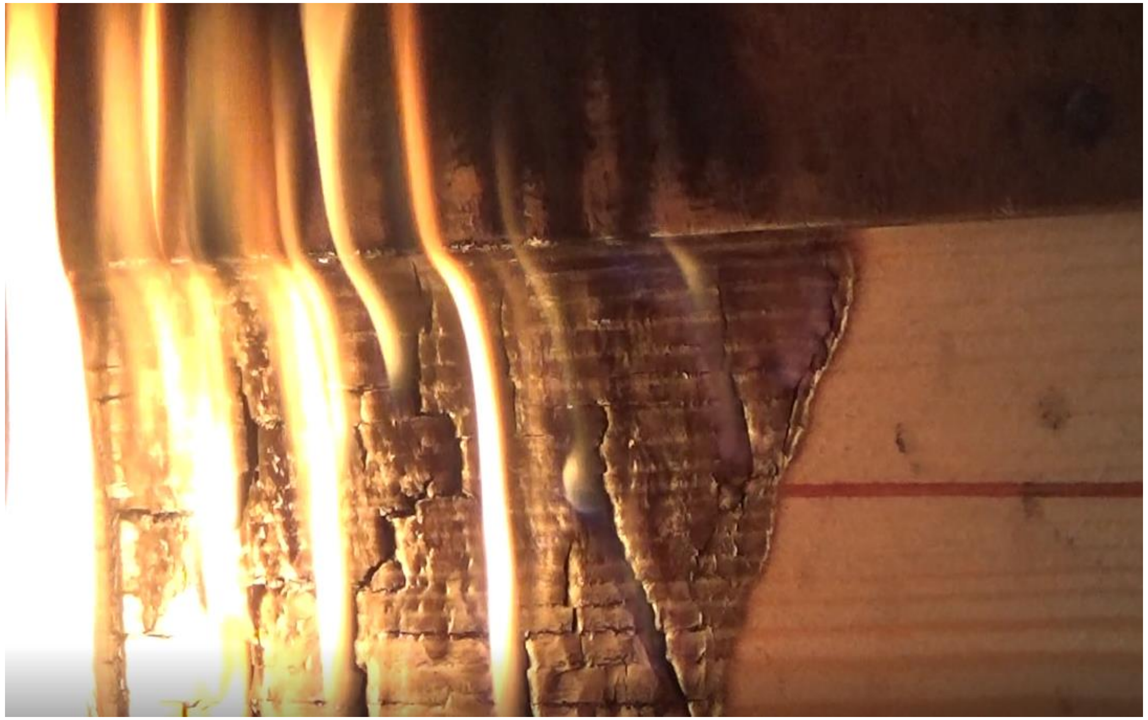
Open Science

GitHub

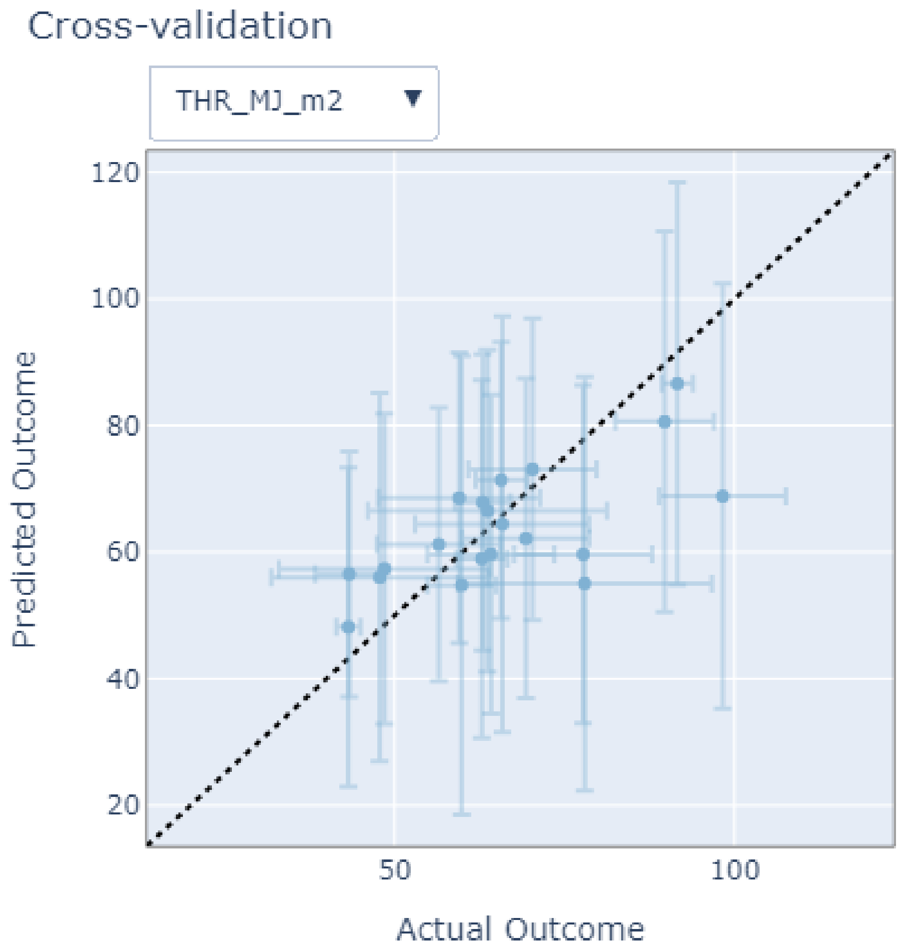
https://github.com/Eric-verret

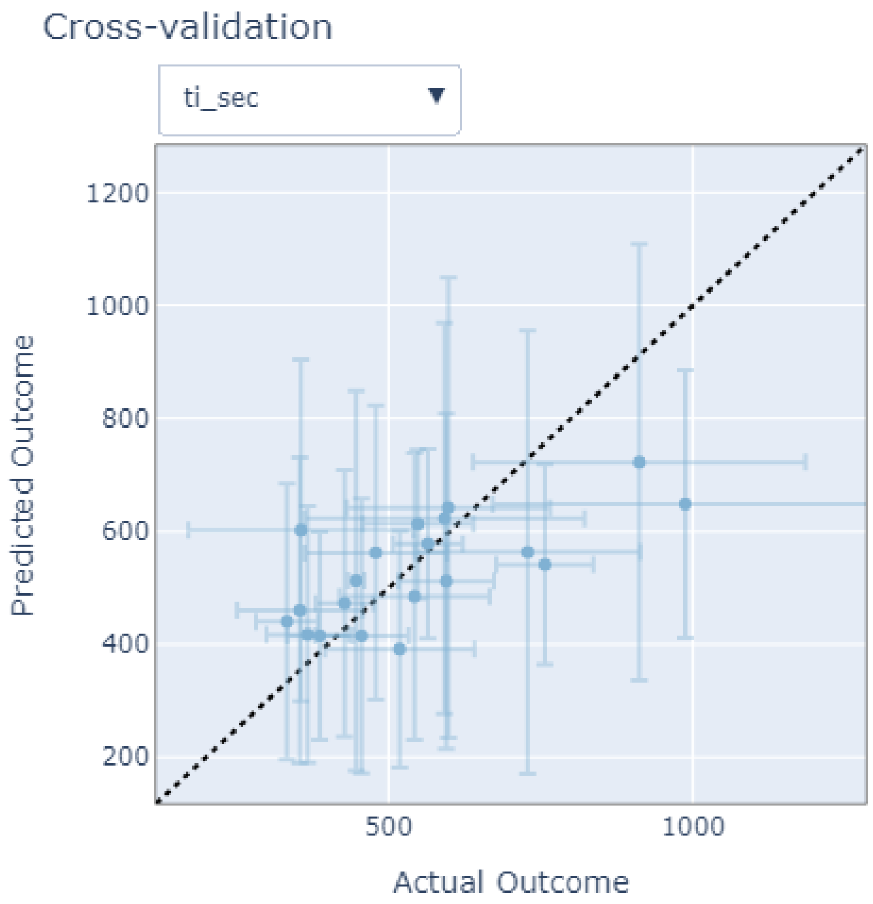
Stay tuned !

Thank you for your attention !



Evaluation of the performance of the model-





facebook/**Ax**

Adaptive Experimentation Platform

Metric	THR	Ti
Mean absolute percentage error (MAPE)	13%	17%
Coefficient of determination (R^2)	0,57	0,42
Fisher exact test p	0,011	0,011