Modeling Heat & Mass transfers in a porous material

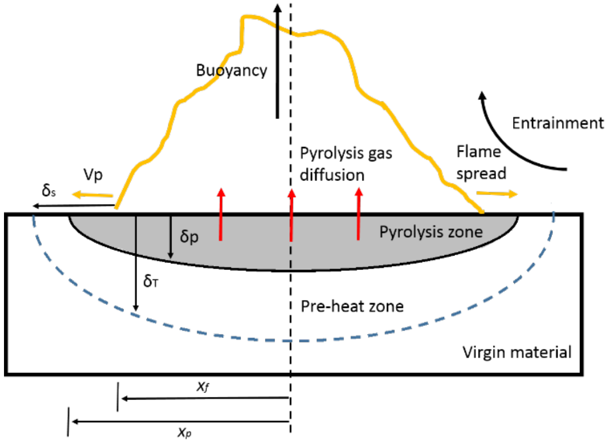
F.RICHARD*, X.QIN, B.BATIOT, J.COLOMBIANO (mimi),*
T. BENHASSI, T.ROGAUME
University of Poitiers
France

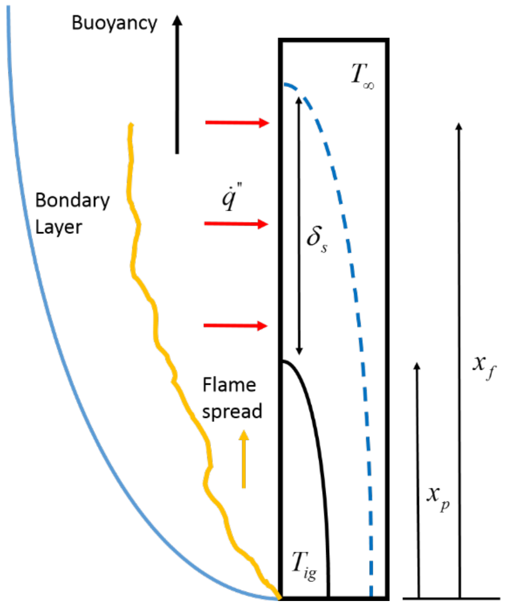
GDR « Feux »
IUSTI - Marseille
June, 6 – 7 2019

Flame spread over solid fuels

Fire dynamics involve complex physical and chemical phenomena often strongly coupled

- Combustion in the gas phase
- Heat & Mass transfer at interface
- Pyrolysis process in the condensed phase





A key feature in fire description

Predict the rate of flame spread (ROS) over solid fuels

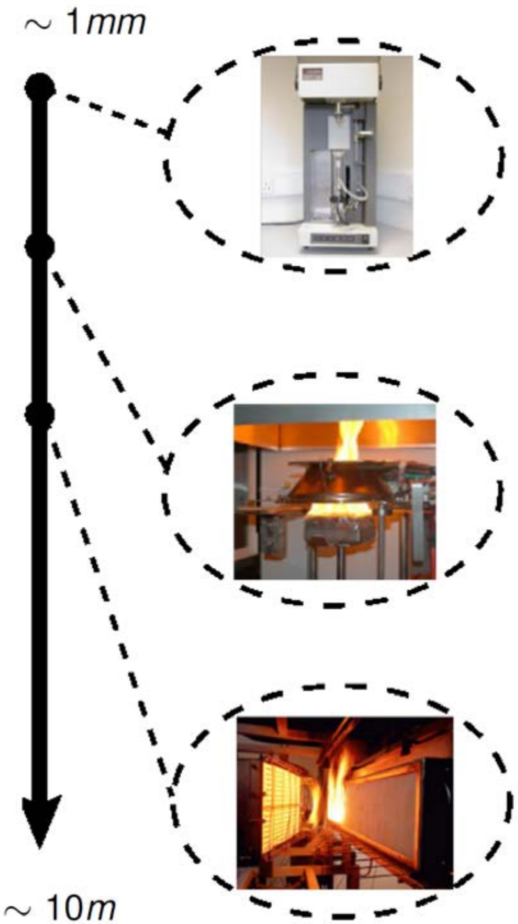
Scales separation

Properties extraction & Model validation

- Scales separation -

Flame spread : coupled problem

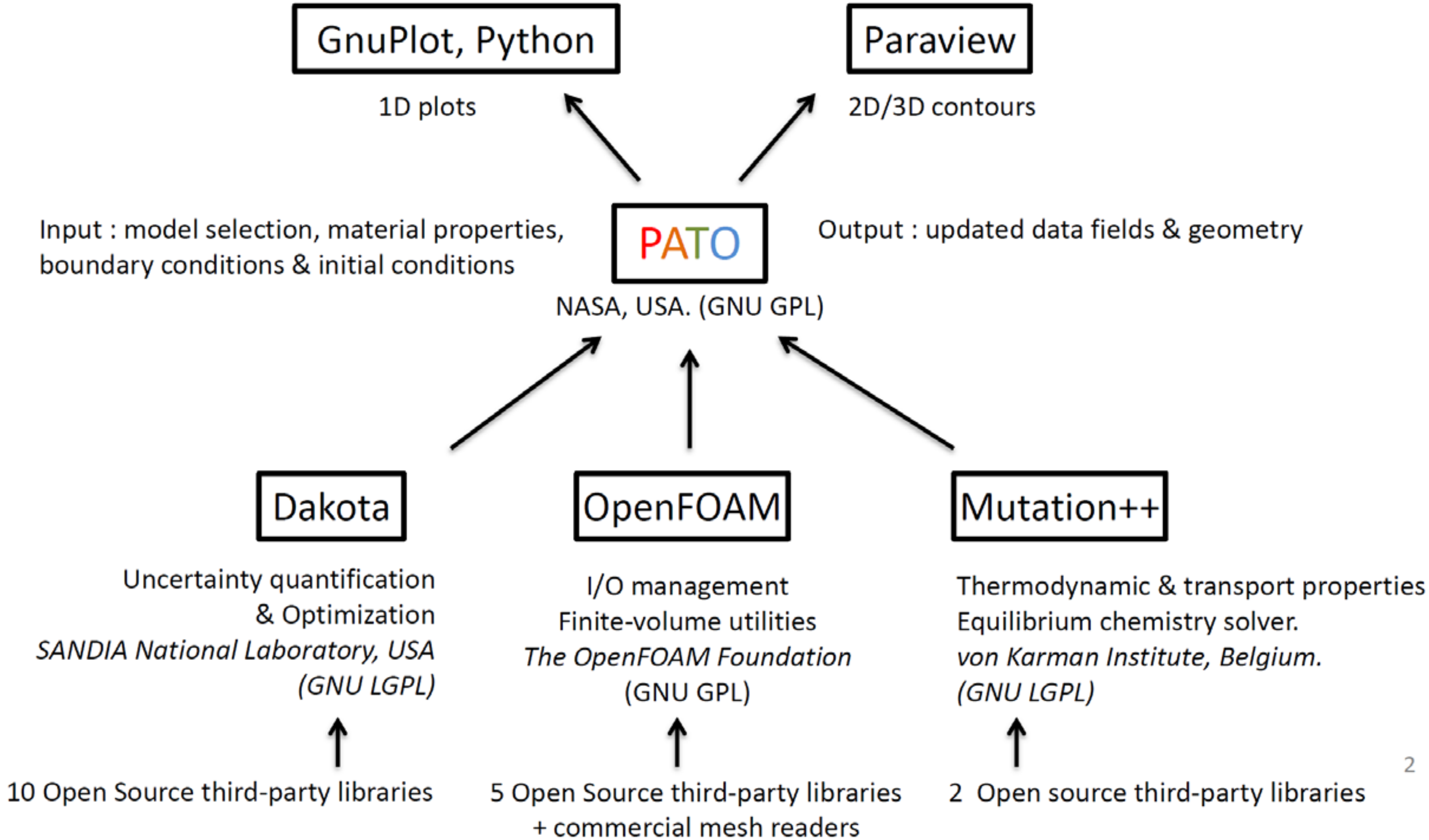
Separate effect validation



- ***TGA scale*** $(\sim 1\ mm)$
  - ✓ Controlled Heat & mass transfer
  - ✓ Chemical mechanism & kinetic properties extraction
- ***Cone calorimeter scale*** $(\sim 10\ cm)$
  - ✓ Add of heat & mass transfer model
  - ✓ Thermal properties extraction
- ***LIFT & radiant panel scale*** $(\sim 1\ m)$
  - ✓ Propagation of the pyrolysis front
  - ✓ Thermal properties extraction

Model

A flexible toolbox for Multiphase Porous Reactive Materials



Lachaud & al

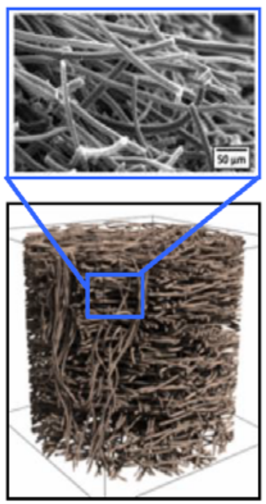
PATO

POROUS MATERIAL ANALYSIS TOOLBOX BASED ON OPENFOAM

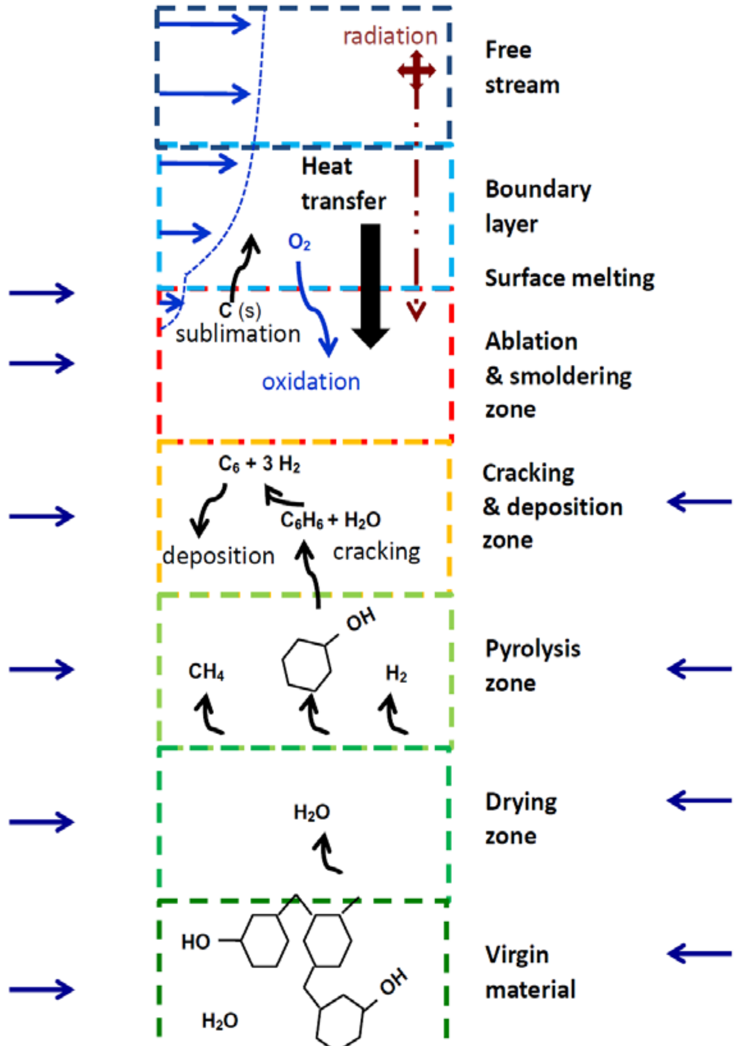
Model

A pragmatic generic model for porous reactive materials

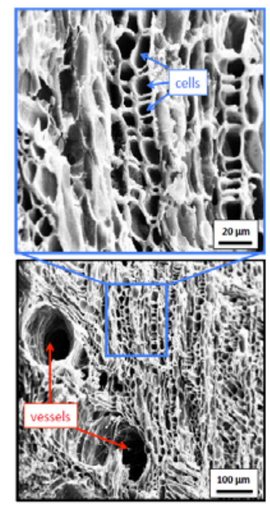
Thermal protection systems



Carbon fiber preform
(NASA/UC Berkeley)



Biomass pyrolysis



Charred wood
(University of New Caledonia)

Lachaud & al [5]

Model

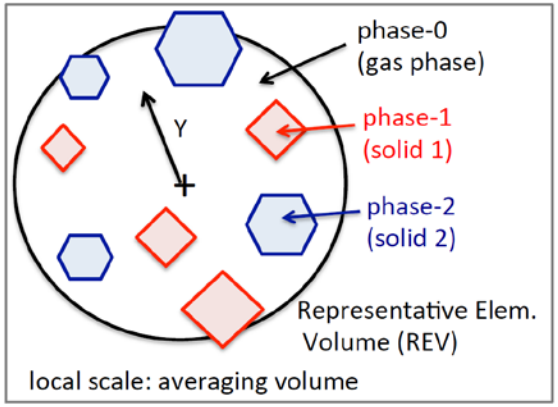
Hypotheses

- Multi-phase reactive material (Np solid phase)
- Multi-species reactive gas mixture (Ng gaseous species)
- Local thermal equilibrium : all the phases are locally at the same temperature
- Each solid phase can pyrolyze, vaporize, sublimate, and release species in the gas phase
- Each solid phase can react with the gas phase (e.g oxidation of a carbon phase)
- Gas phase chemistry can be in equilibrium, follow a finite rate mecganism, or be frozen

Averaged effective properties, e.g density :

$$\rho = \epsilon_g \rho_g + \sum_{i \in [1,N_p]} \epsilon_i \rho_i = \sum_{i \in [0,N_p]} \epsilon_i \rho_i$$

volume fraction — intrinsic density



Lachaud & al

TGA scale

Thermogravimetric analysis TGA

Mesure mass of sample as a function of temperture

Experimental conditions

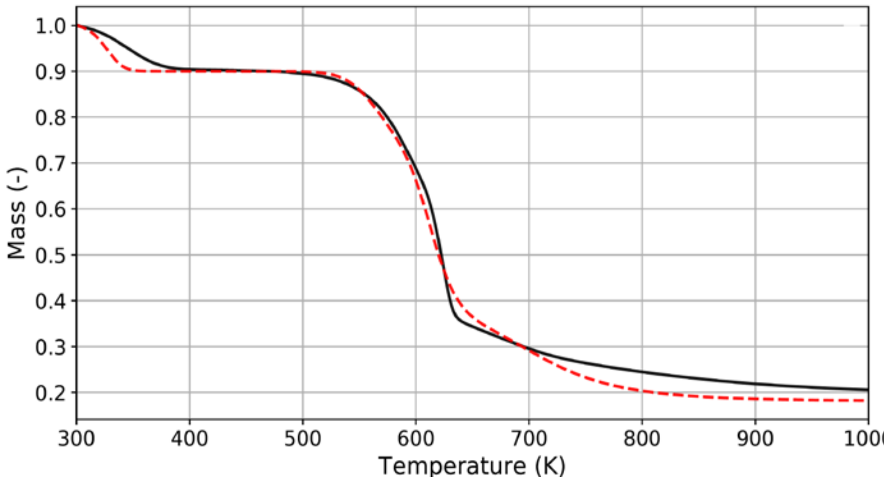
- Sample weight $(\sim 10mg)$
- Non isothermal tests $(\beta \in [5,50]°C/\min)$
- Atmosphere $(O_2 \in [0,21]\%vol)$

Properties extraction : PATO / DAKOTA

JEGA library (SOGA, MOGA)

$$\begin{cases} cellulose \rightarrow \nu_{cell} char + \nu_{1,gas} gas \\ hemicellulose \rightarrow \nu_{hemi} char + \nu_{2,gas} gas \\ lignin \rightarrow \nu_{lign} char + \nu_{3,gas} gas \end{cases}$$

Douglas Fir

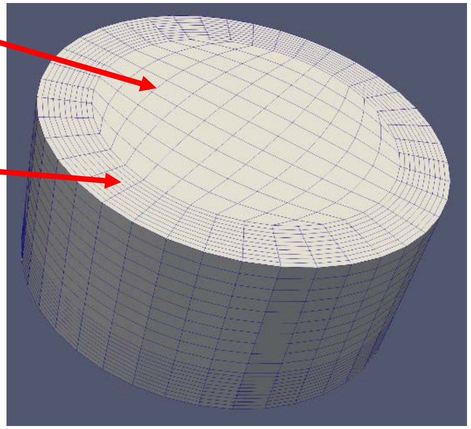


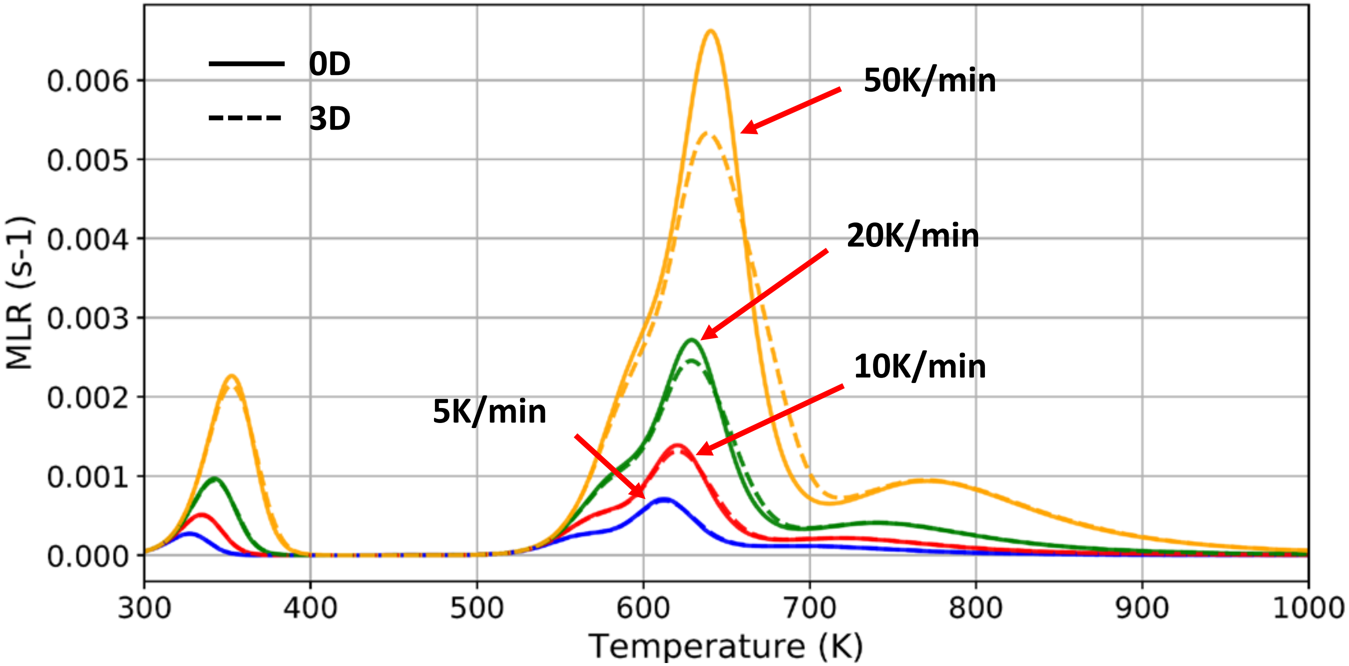
TGA scale : 0D / 3D simulations

0D Arrhenius model

$$
\begin{cases}
virgin \rightarrow v_c char + v_g gas \\
\dfrac{d\alpha_i}{dt} = A\exp\left(-\dfrac{E_a}{RT}\right)(1-\alpha_i)^n \\
T = T_0 + \beta t
\end{cases}
$$

3D mesh





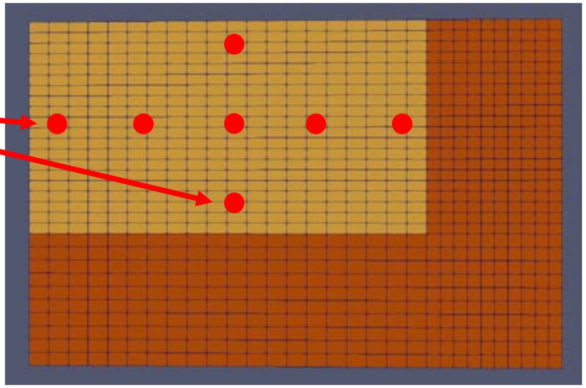
TGA scale : 0D / 3D simulations

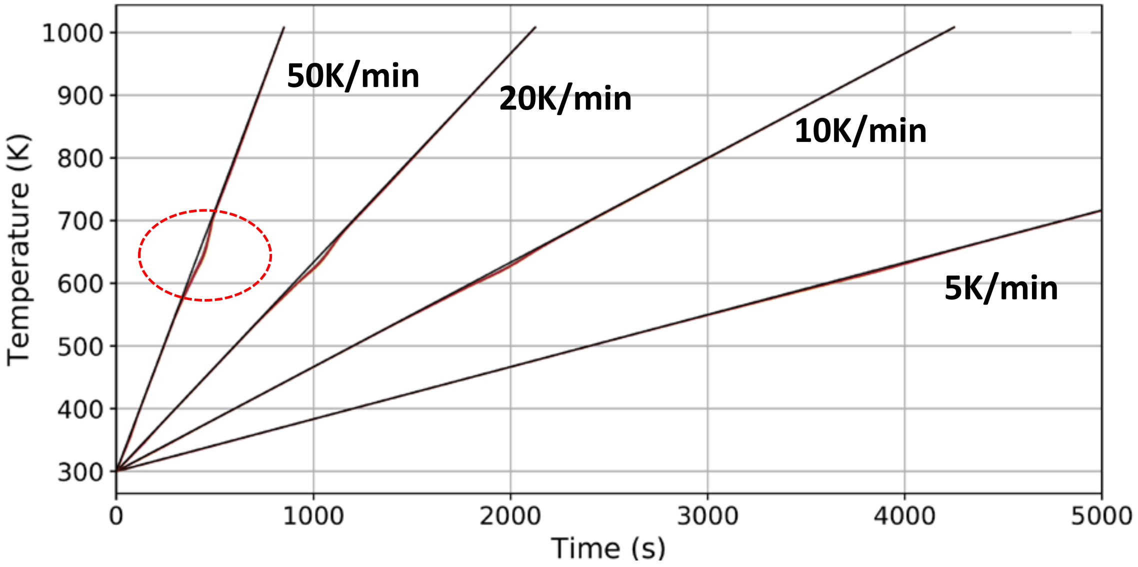
0D Arrhenius model

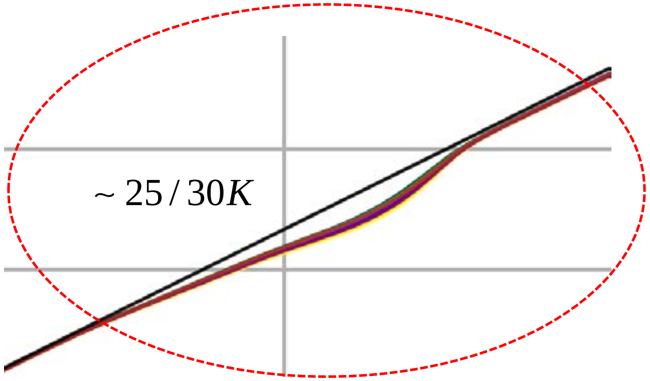
$$\begin{cases} virgin \rightarrow \nu_c char + \nu_g gas \\ \dfrac{d\alpha_i}{dt} = A\exp\left(-\dfrac{E_a}{RT}\right)(1-\alpha_i)^n \\ T = T_0 + \beta t \end{cases}$$

3D mesh

Temperatures







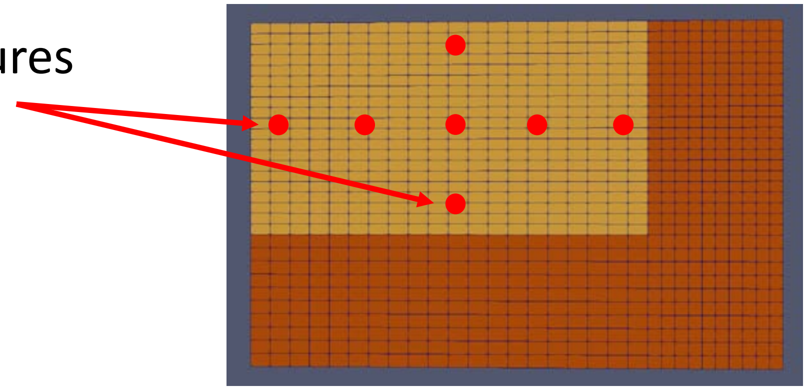
TGA scale : 0D / 3D simulations

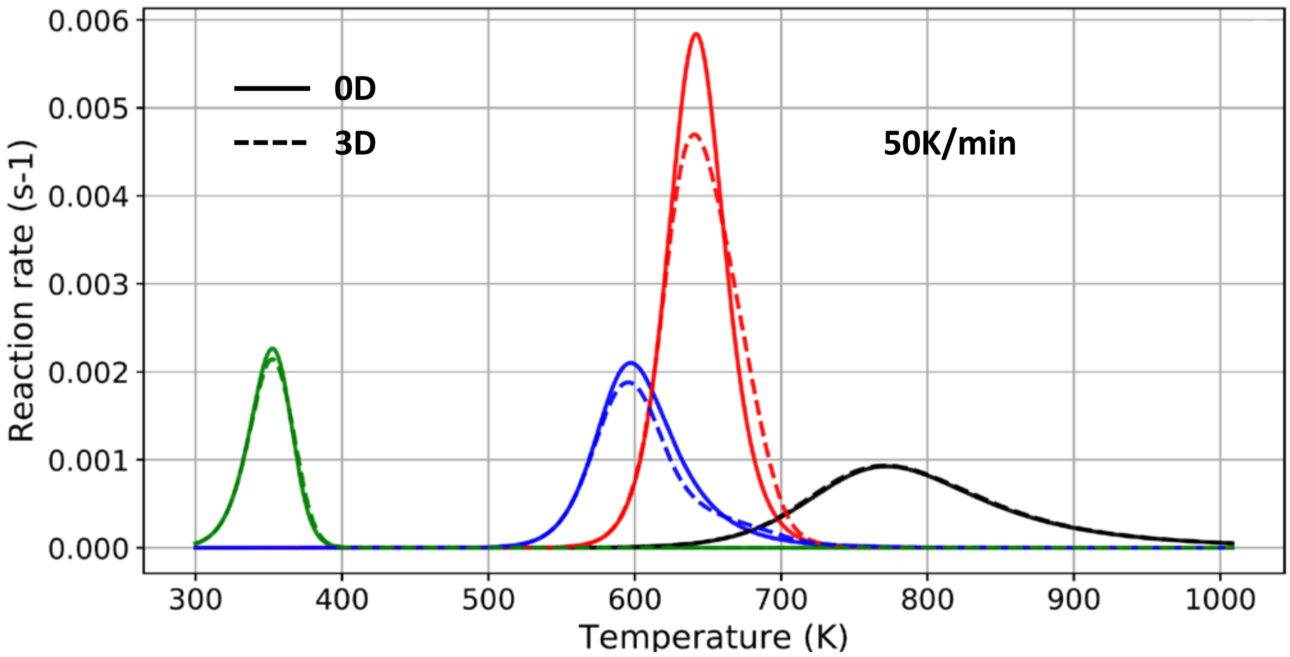
0D Arrhenius model

$$\begin{cases} virgin \rightarrow \nu_c char + \nu_g gas \\ \dfrac{d\alpha_i}{dt} = A\exp\left(-\dfrac{E_a}{RT}\right)(1-\alpha_i)^n \\ T = T_0 + \beta t \end{cases}$$

3D mesh

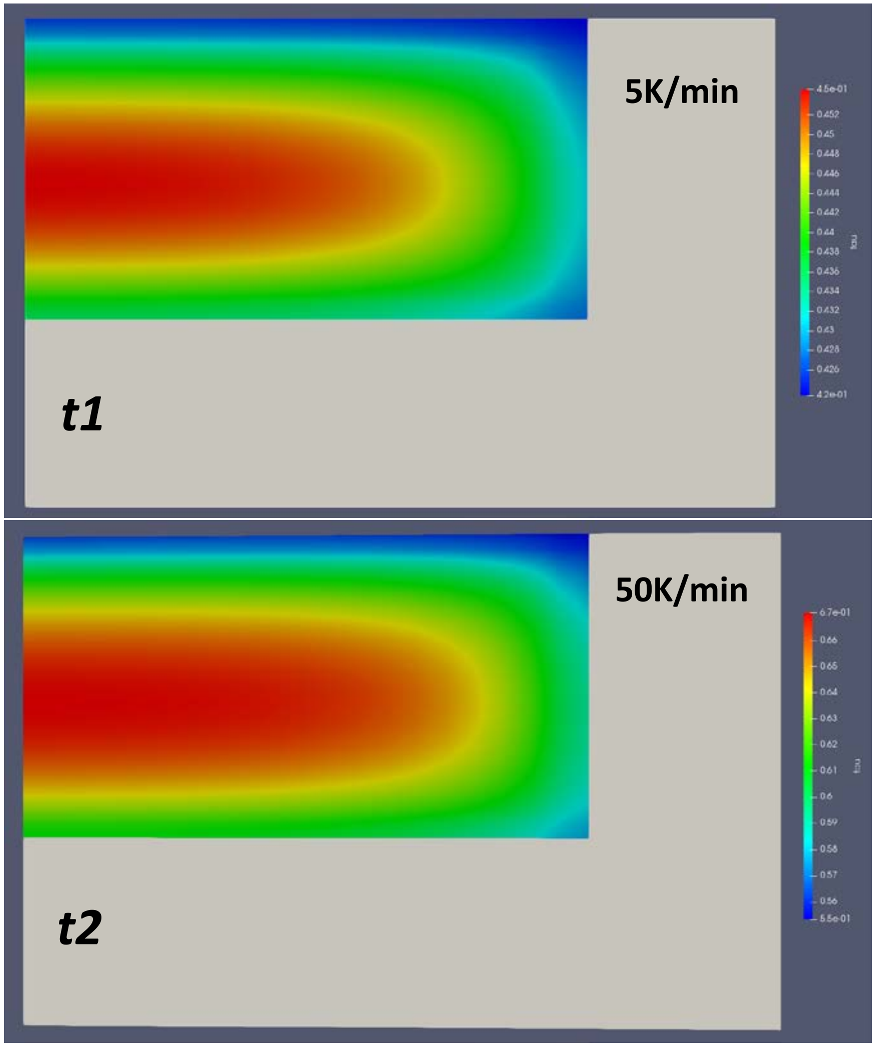
Temperatures

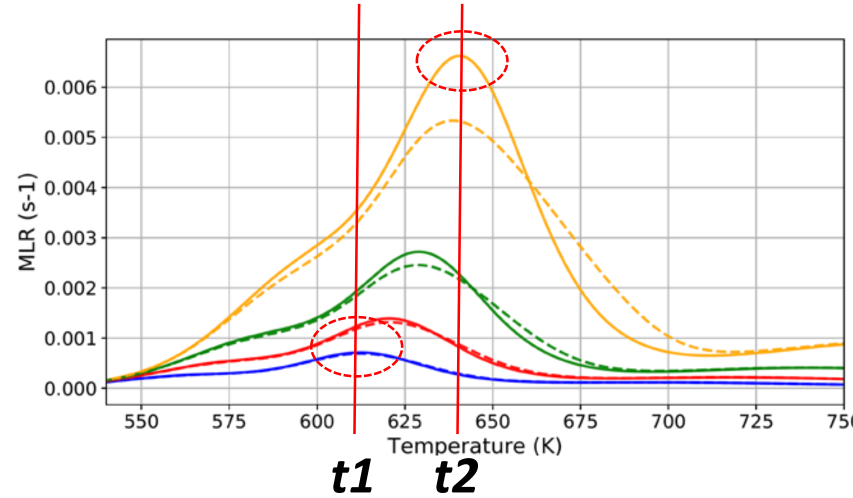




TGA scale : 0D / 3D simulations

Total reaction rate



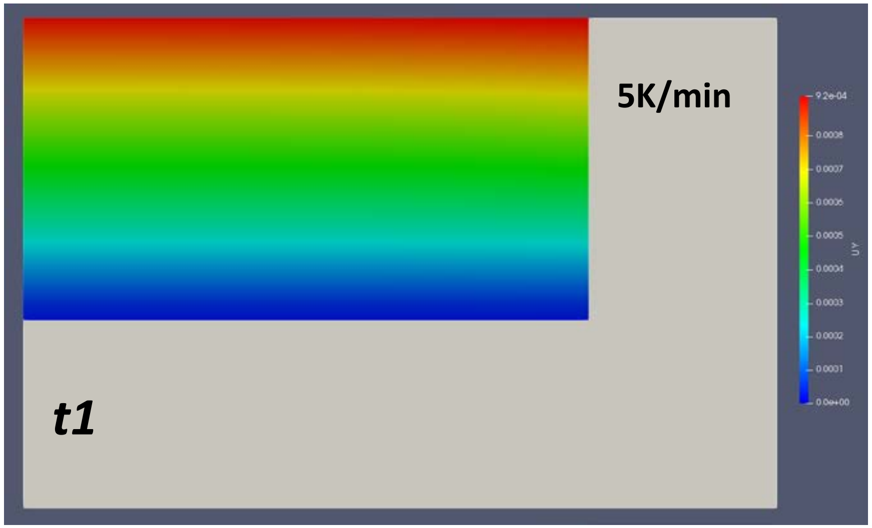


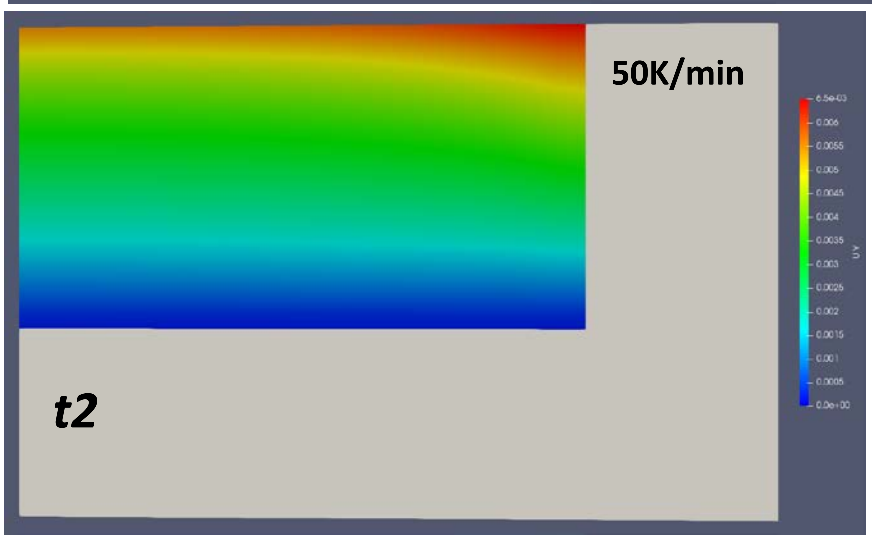
Spatial gradient :

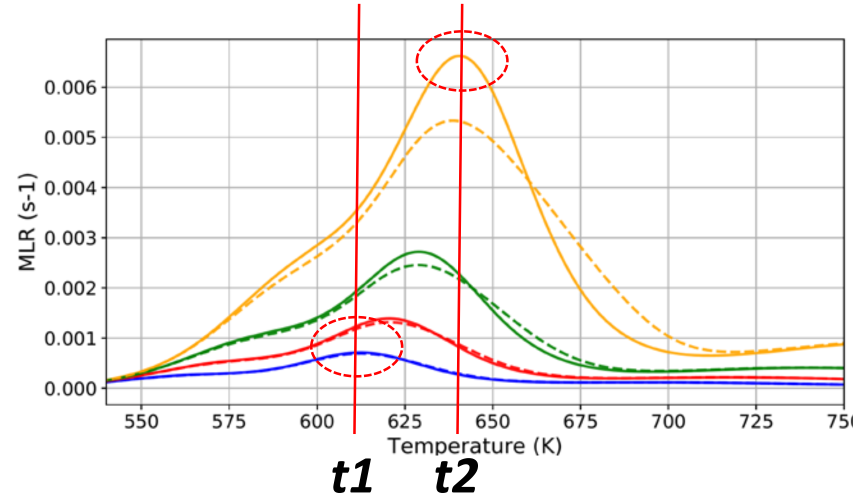
- ~ 3% à 5K/min
- ~ 12% à 50K/min

TGA scale : 0D / 3D simulations

Axial velocity





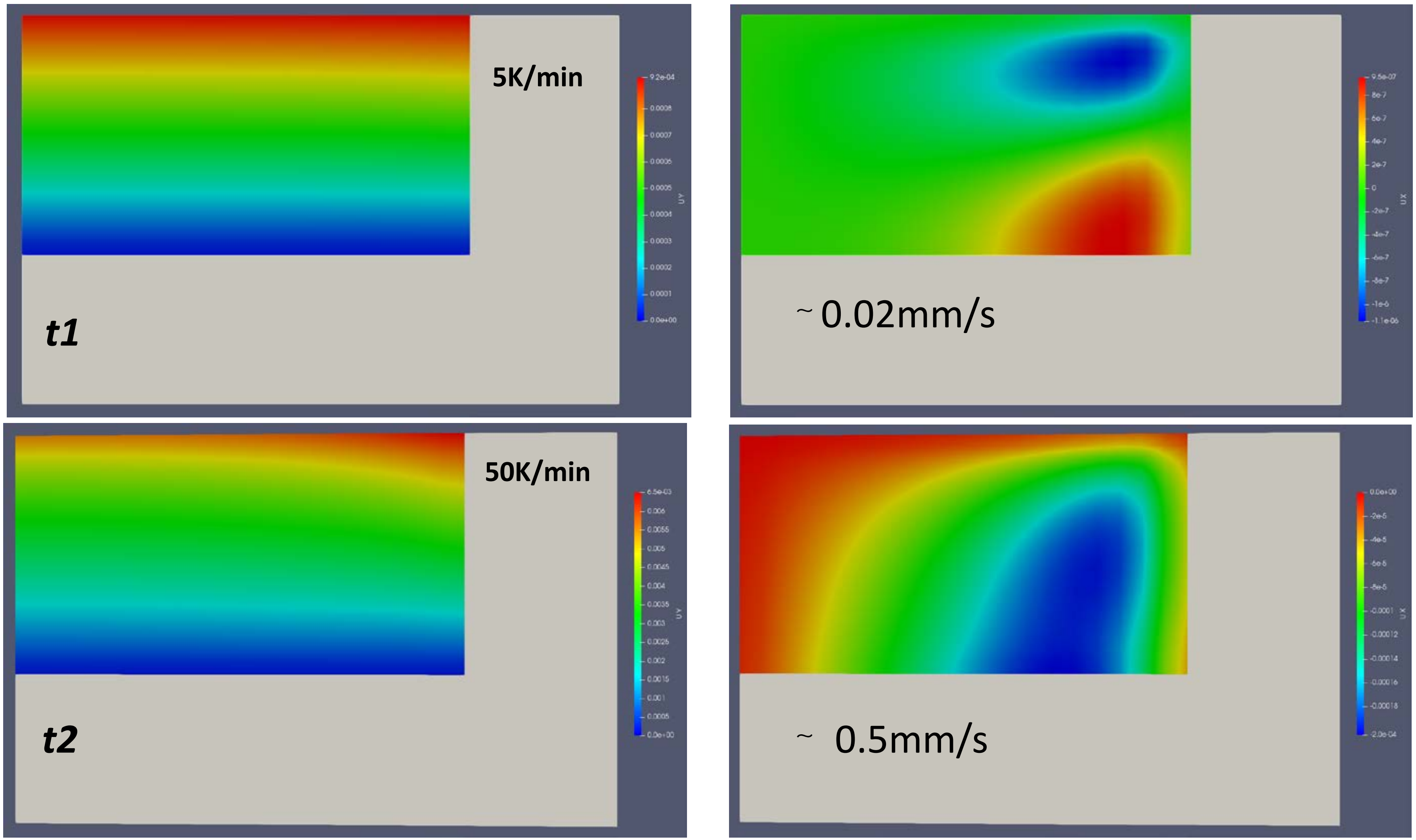


Spatial gradient :

- ~ 1mm/s à 5K/min
- ~ 7mm/s à 50K/min

TGA scale : 0D / 3D simulations

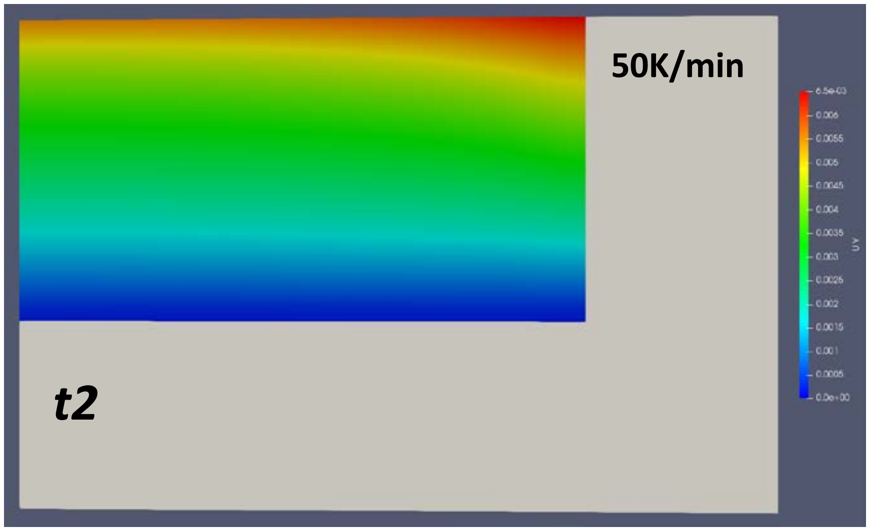
Axial velocity | **Radial velocity**

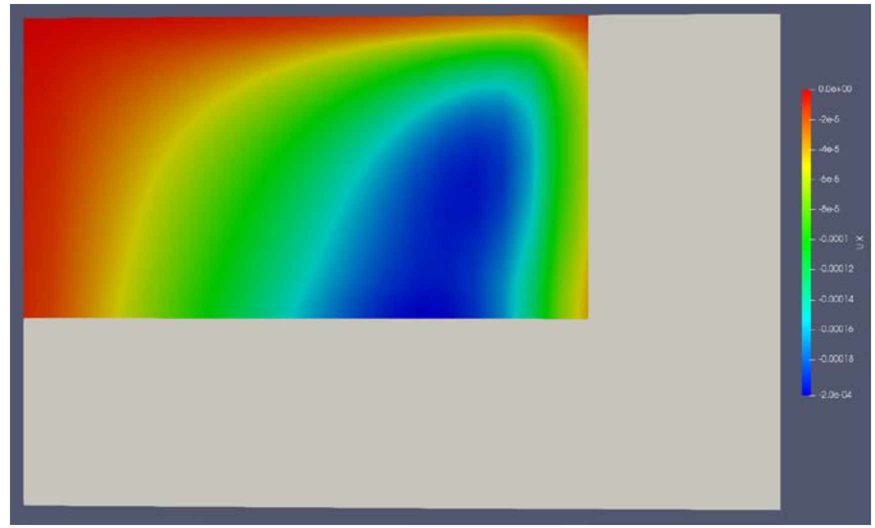


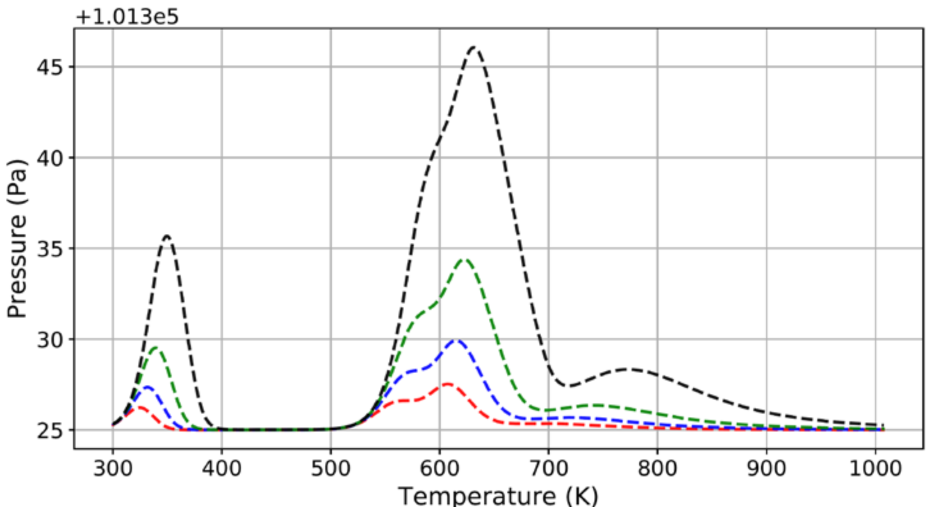
TGA scale : 0D / 3D simulations

Axial velocity

Radial velocity





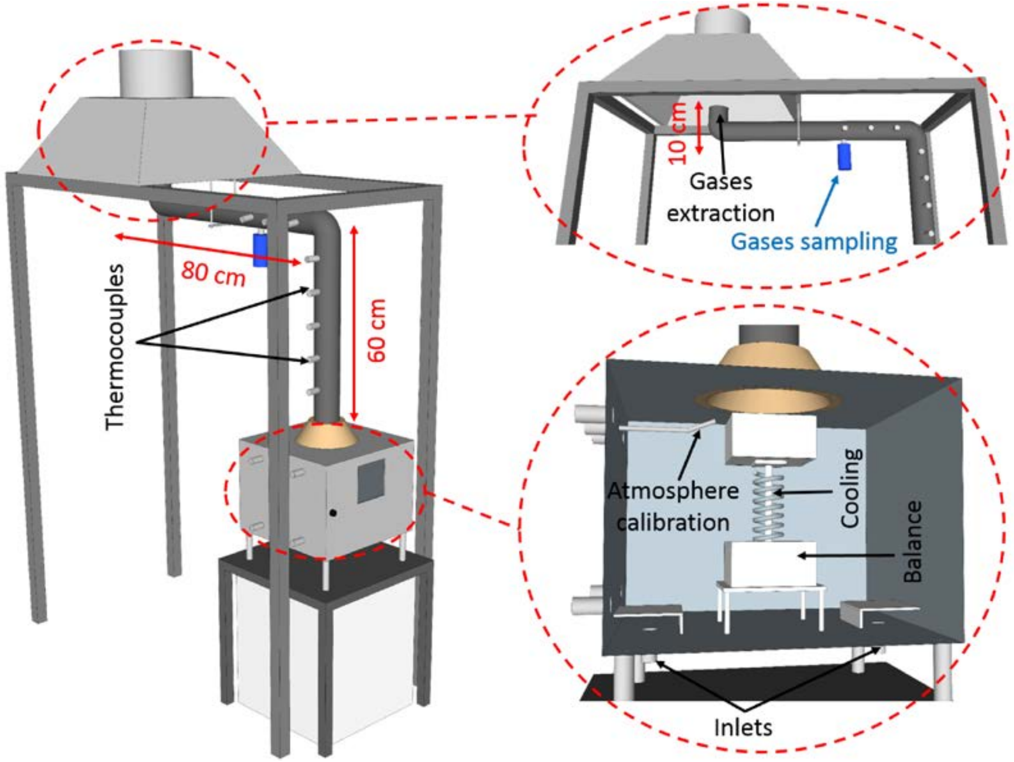


Cone calorimeter scale

Cone calorimeter analysis

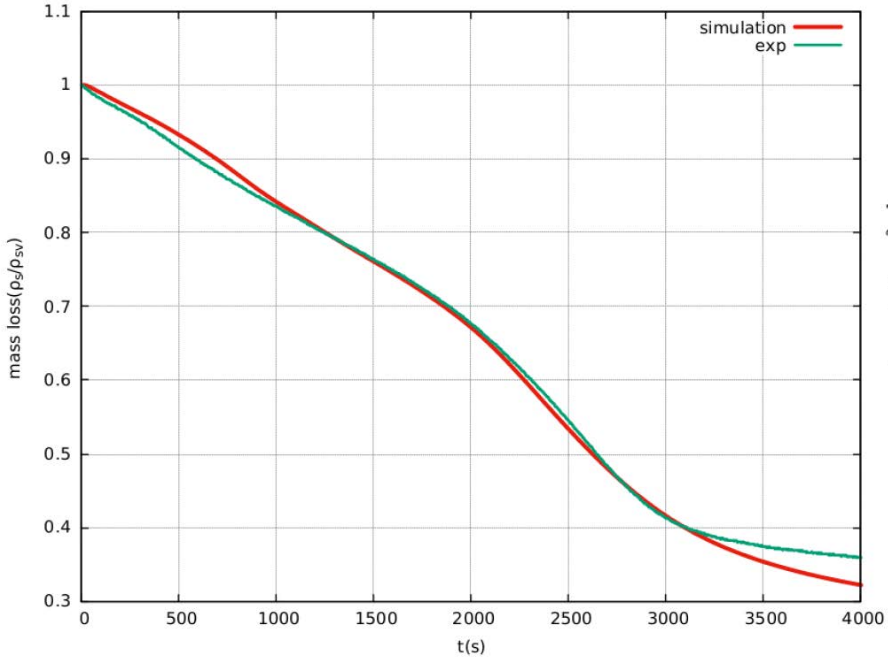
Experimental conditions

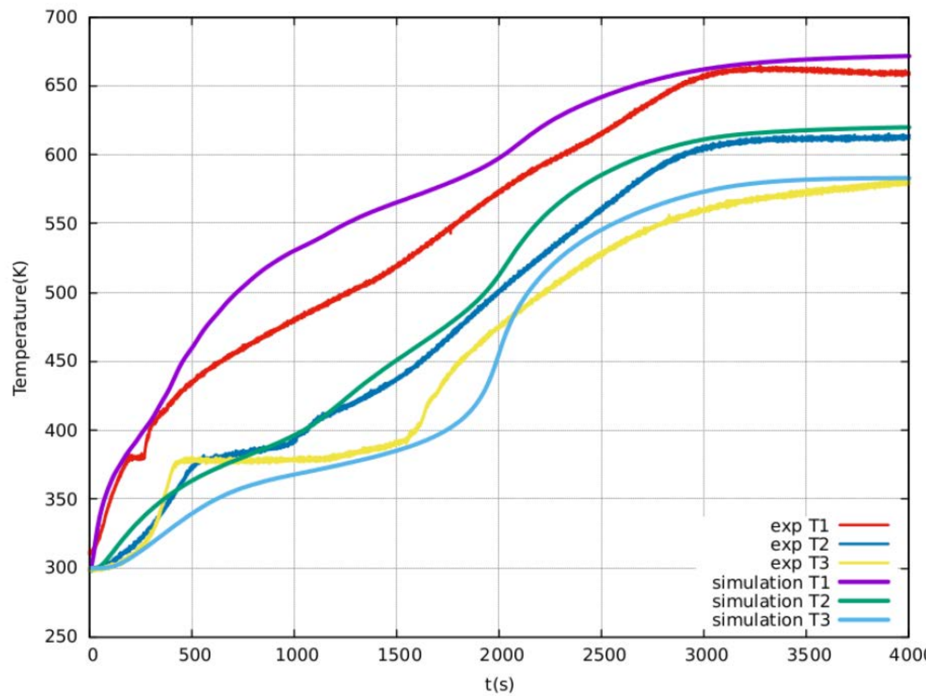
- Heat fluxes $\left(Q \in [0,50]\,\mathrm{kW/m^2}\right)$
- Atmospheres $\left(O_2 \in [1,21]\%vol\right)$
- Inlet flow rate $\left([120,160]\,l/\min\right)$



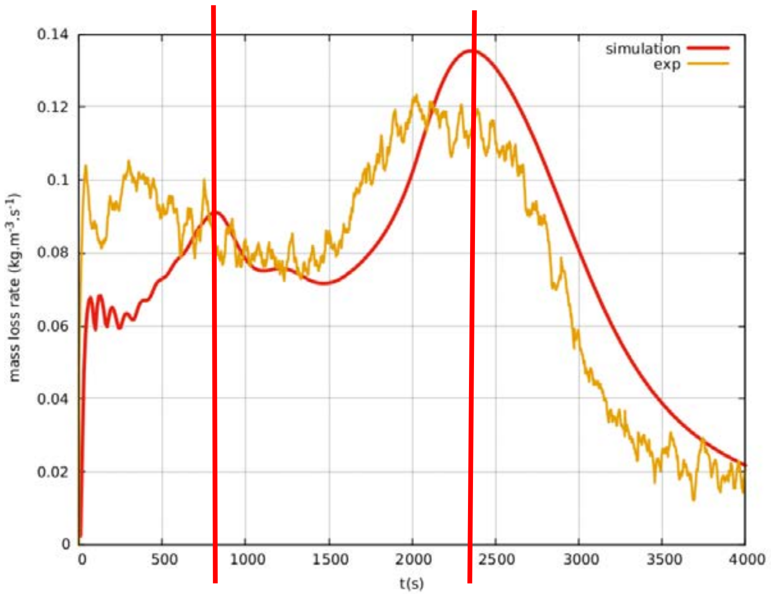
Cone calorimeter scale

Conditions : N2, 20 kW/m2





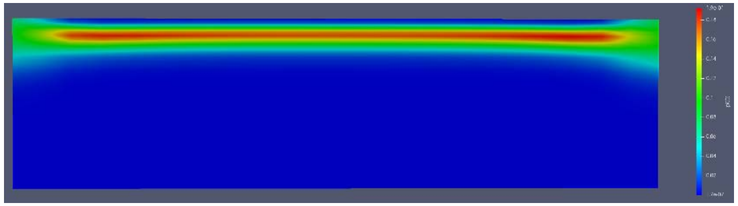
Cone calorimeter scale



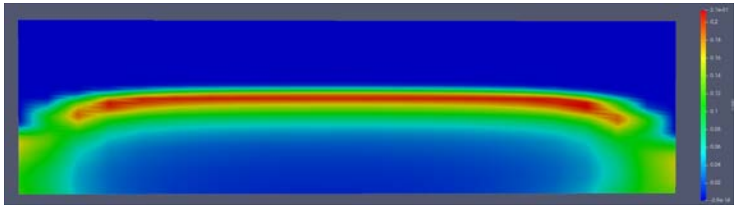
t1=800s ***t2=2400s***

- Pyrolysis front evolves in 3D (space dependant)
- Pyrolysis front depends on boundary conditions
- Dynamic of pyrolysis front is unsteady

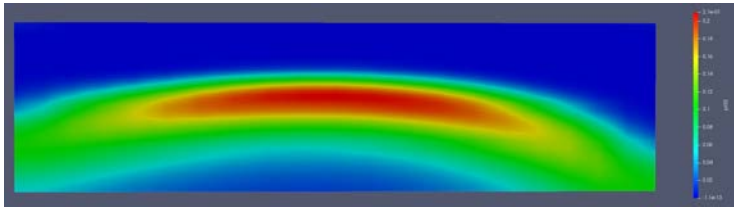
Pyrolysis front at t=800s



Water evaporation front at t=800s



Pyrolysis front at t=2400s



Thank you