Simulation of Wood Combustion in PATO Using a Detailed Pyrolysis Model Coupled to fireFoam

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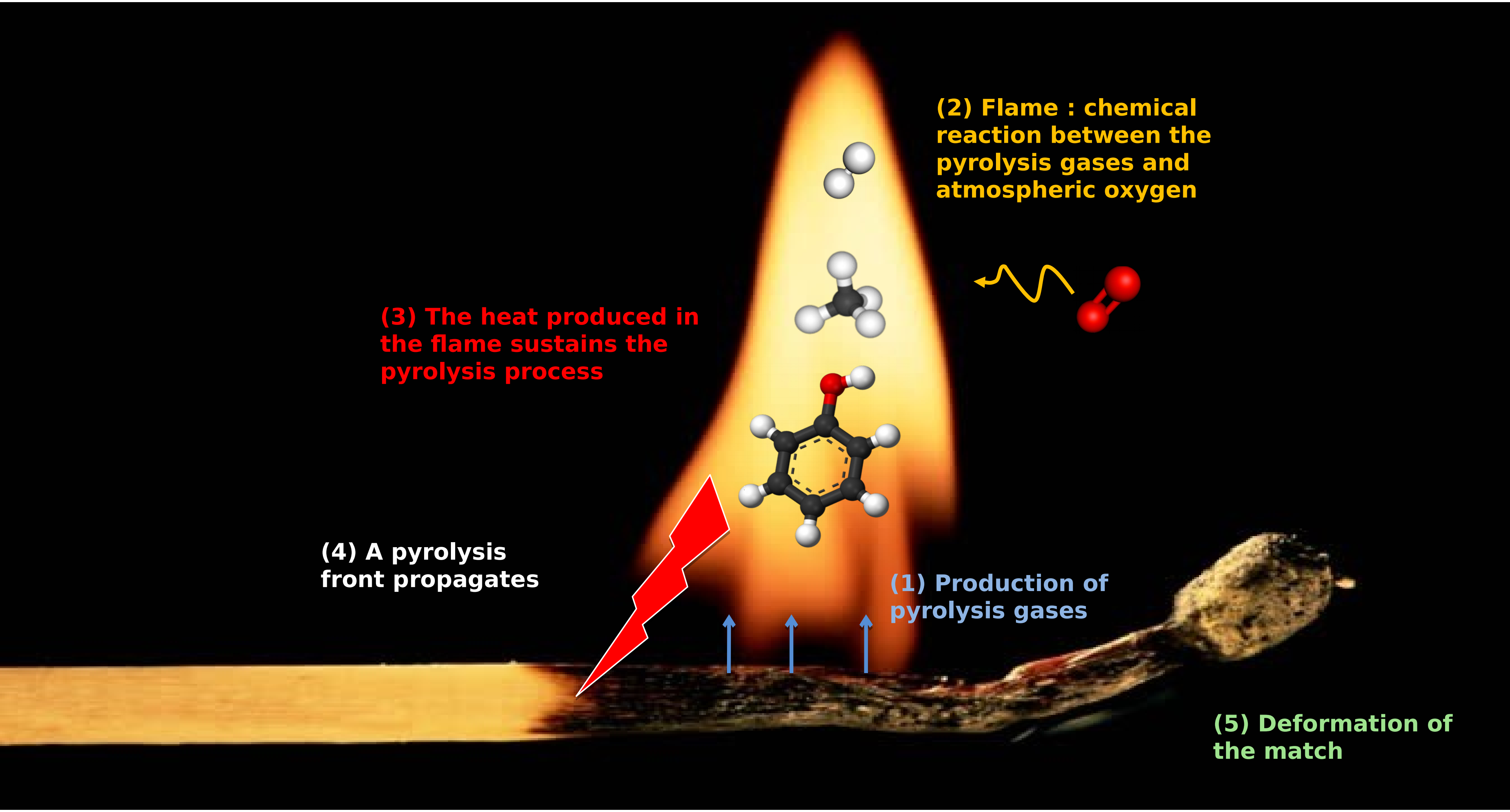
30e journées du GDR Feux 02 et 03 décembre 2021

The Burning of a Match



(2) Flame : chemical reaction between the pyrolysis gases and atmospheric oxygen

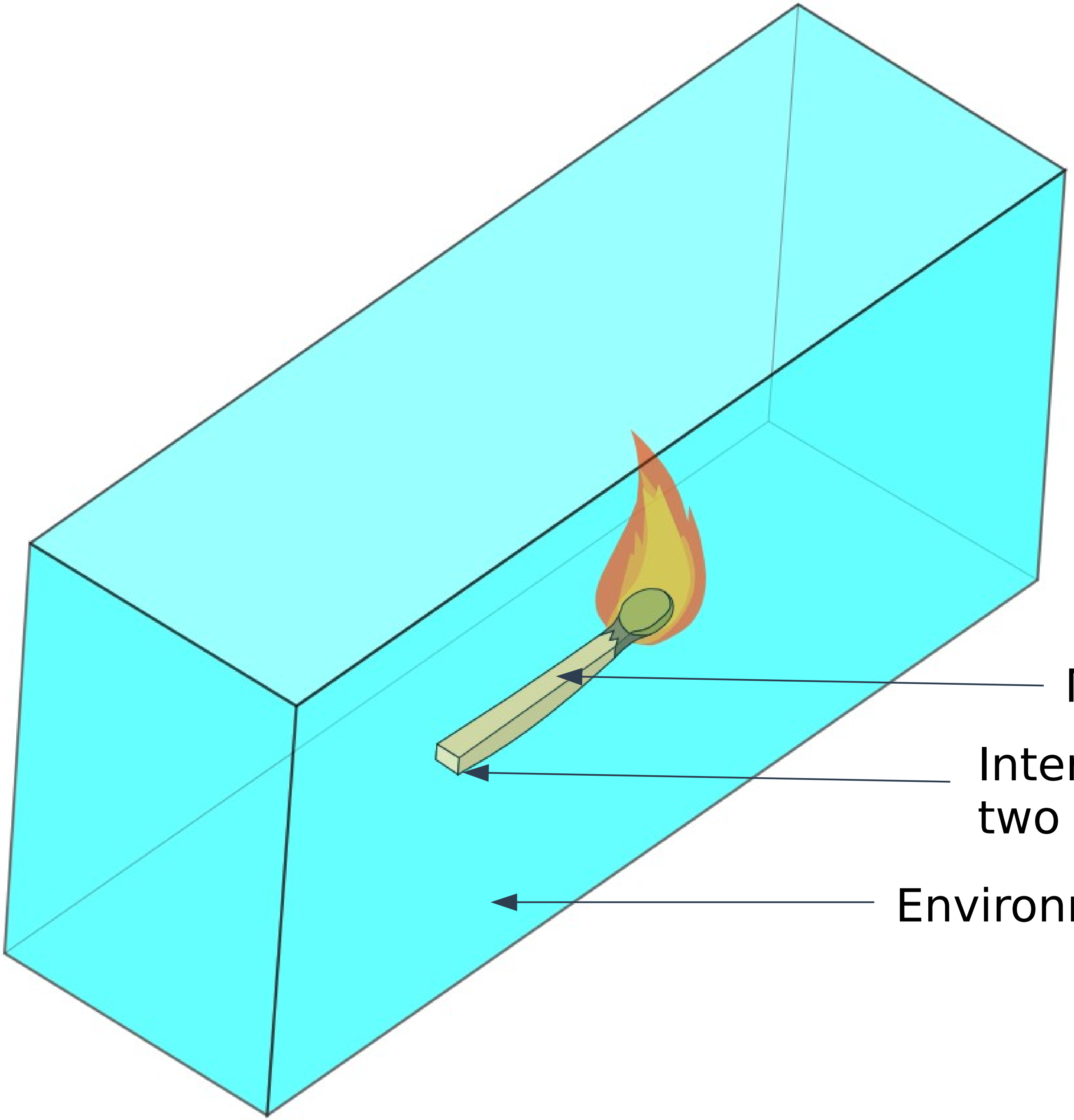
(3) The heat produced in the flame sustains the pyrolysis process

(4) A pyrolysis front propagates

(1) Production of pyrolysis gases

(5) Deformation of the match

Numerical Problem



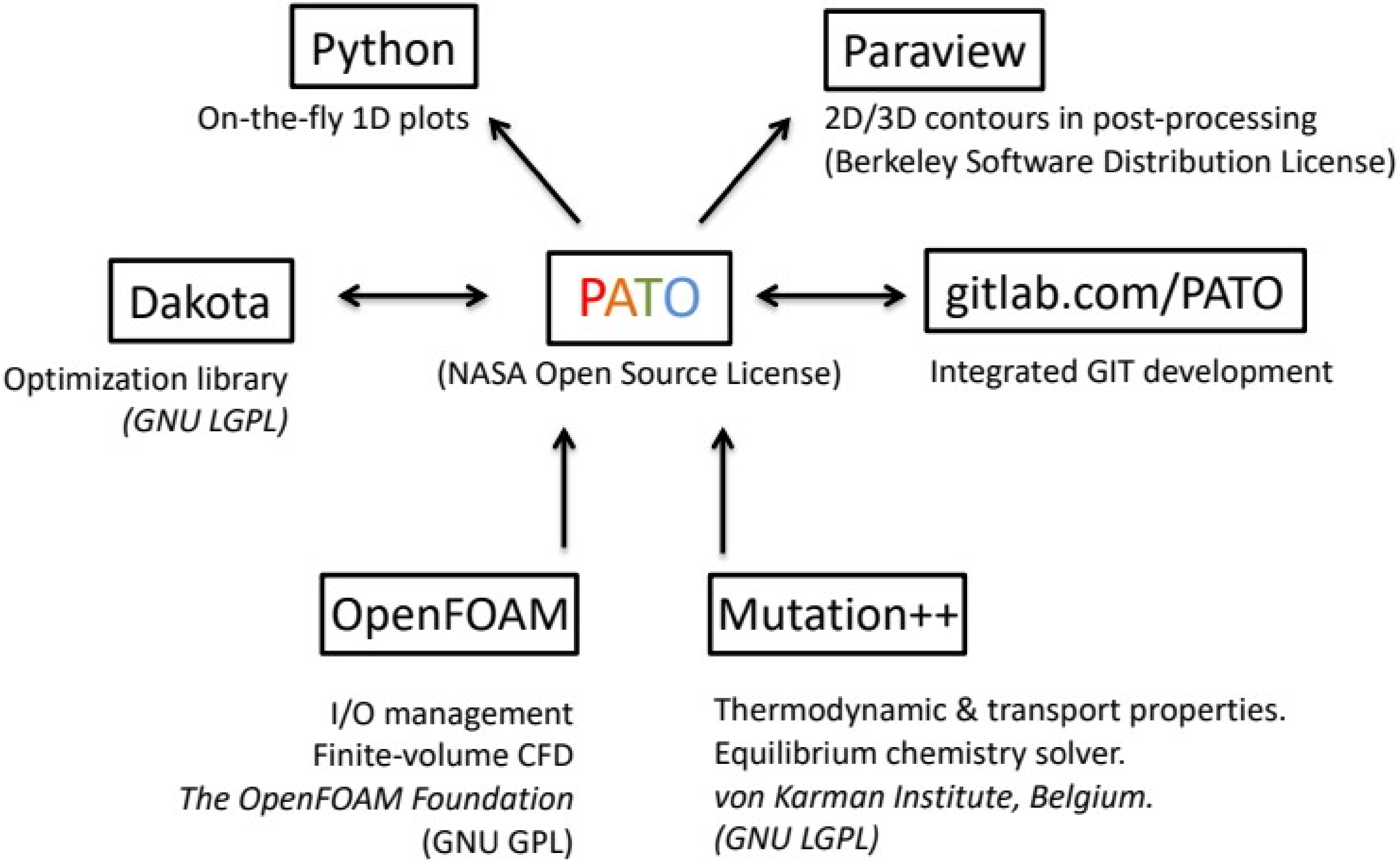
Material region

Interface between the two regions

Environment region

PATO

POROUS MATERIAL ANALYSIS TOOLBOX BASED ON OPENFOAM



Python

On-the-fly 1D plots

Paraview

2D/3D contours in post-processing
(Berkeley Software Distribution License)

Dakota

Optimization library
(GNU LGPL)

PATO

(NASA Open Source License)

gitlab.com/PATO

Integrated GIT development

OpenFOAM

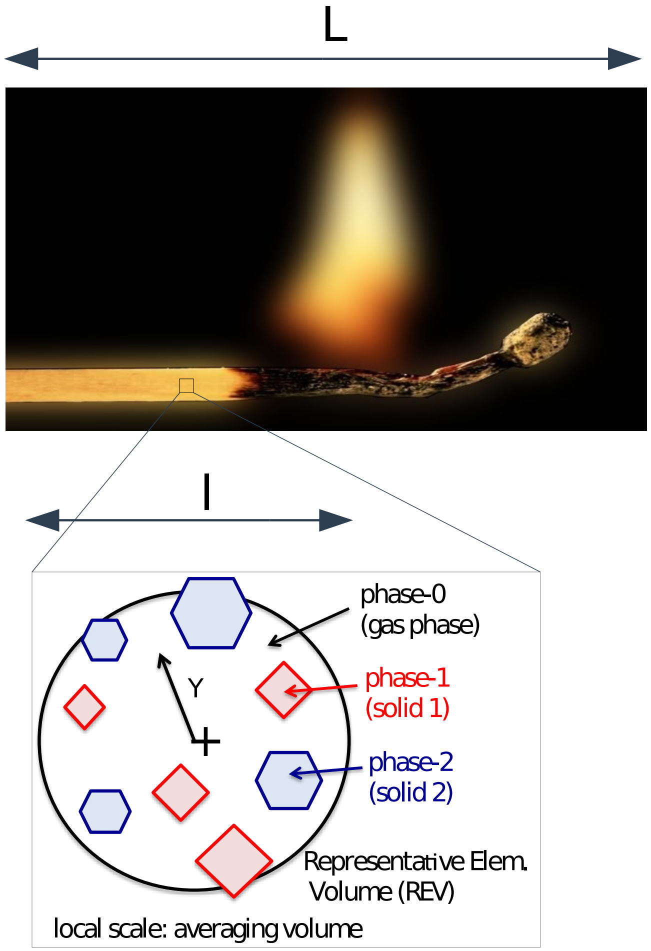
I/O management
Finite-volume CFD
The OpenFOAM Foundation
(GNU GPL)

Mutation++

Thermodynamic & transport properties.
Equilibrium chemistry solver.
von Karman Institute, Belgium.
(GNU LGPL)

https://pato.ac/

Material Region



$$\boxed{L \gg l}$$

Averaged effective properties e.g. density

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

volume fraction intrinsic phase density

Mass conservation

- For each solid phase

$$\partial_t(\epsilon_i\rho_i) = -\Pi_i - \Omega_i^h$$

density pyrolysis heterogeneous reactions

- For the gas phase

$$\partial_t(\epsilon_g\rho_g) + \partial_{\mathbf{x}}\cdot(\epsilon_g\rho_g\mathbf{v_g}) = -\sum_i \partial_t(\epsilon_i\rho_i)$$

density convection exchange with solid phases

Species conservation

$$\partial_t(\epsilon_g\rho_g y_i) + \partial_{\mathbf{x}}\cdot(\epsilon_g\rho_g y_i\mathbf{v_g}) + \partial_{\mathbf{x}}\cdot\mathcal{F}_i = \pi_i + \epsilon_g\omega_i\mathcal{M}_i,\ \forall\, i \in N_g^s$$

species mass fractions convection diffusion pyrolysis by species chemistry source terms gaseous species

Momentum conservation

$$\mathbf{v_g} = -\frac{1}{\epsilon_g}\left(\frac{1}{\mu}\underline{\underline{\mathbf{K}}} + \frac{1}{p}\underline{\underline{\beta}}\right)\cdot\partial_{\mathbf{x}}p$$

gas velocity Darcy Klinkenberg

Energy conservation

- solid

$$\sum_{i=1}^{N_p}[(\epsilon_i\rho_i C_{p,i})\partial_t T_s] + \sum_{i=1}^{N_p} h_i\partial_t(\epsilon_i\rho_i) = \partial_x\cdot(\underline{\underline{K_s}}\cdot\partial_x T_s) + h_v(T_g - T_s)$$

- gas

$$(\epsilon_g\rho_g C_{p,g})\partial_t T_g - \partial_t(\epsilon_g p) + \sum_{j=1}^{N_g}[h_j\partial_t(\epsilon_j\rho_j y_j) + \partial_x\cdot Q_j] + \partial_x\cdot(\epsilon_g\rho_g h_g\boldsymbol{v_g}) = \partial_x\cdot(\underline{\underline{K_g}}\cdot\partial_x T_g) + h_v(T_s - T_g)$$

energy pressure term species effective diffusion convection diffusion/viscous dissipation convective heat transfer

Solid deformation

$$\partial_t(\rho\,\partial_t\mathbf{D}) = \partial_{\mathbf{x}}\cdot\underline{\underline{\sigma}} + \rho\mathbf{f}$$

displacement stress tensor body forces

Inside the Environment: fireFoam

Navier-Stokes equations with LES filtering and Favre mean variables

$$\bar{\Phi} \equiv \frac{1}{T}\int_T \Phi(t)dt$$

$$\tilde{\Phi} \equiv \frac{\overline{\rho\Phi}}{\bar{\rho}}$$

Mass conservation

$$\partial_t(\bar{\rho})+\nabla\cdot(\bar{\rho}\tilde{\mathbf{u}})=0$$

density velocity

Momentum conservation

position

$$\partial_t(\bar{\rho}\tilde{\mathbf{u}})+\nabla\cdot(\bar{\rho}\tilde{\mathbf{u}}\tilde{\mathbf{u}})=-\nabla\bar{p}_m-(\boldsymbol{g}\cdot\boldsymbol{x})\nabla\bar{\rho}+\nabla\cdot[\mu_{eff}(\nabla\tilde{\mathbf{u}}+(\nabla\tilde{\mathbf{u}})^T-\frac{2}{3}(\nabla\cdot\tilde{\mathbf{u}})\boldsymbol{I})]$$

modified pressure effective viscosity

gravity

$$\bar{p}_m=\bar{p}-\bar{\rho}\boldsymbol{g}\cdot\boldsymbol{x}$$

thermodynamic pressure

$$\mu_{eff}=\mu_{sgs}+\mu$$

sub-grid viscosity

dynamic viscosity

Species transport equations

$$\partial_t(\bar{\rho}\tilde{Y}_i)+\nabla\cdot(\bar{\rho}\tilde{\mathbf{u}}\tilde{Y}_i)=\nabla\cdot(\bar{\rho}D_{eff}\nabla\tilde{Y}_i)+\bar{w}_i$$

i-th specie mass fraction effective mass diffusivity

rate of production of a specie

Energy conservation

$$\partial_t(\rho\tilde{h}_s)+\nabla\cdot(\rho\tilde{\mathbf{u}}\tilde{h}_s)=\partial_t\bar{p}+\tilde{\mathbf{u}}\cdot\nabla p+\nabla\cdot(\rho\alpha_{eff}\nabla\tilde{h}_s)+\bar{Q}_c-\nabla\cdot\bar{\boldsymbol{q}}_{\boldsymbol{R}}$$

Effective thermal diffusivity

sensible enthalpy

heat generated by combustion

thermal radiation flux

Ideal gas

$$\bar{\rho}=\frac{\bar{p}M}{R\tilde{T}}$$

Molar weight

temperature

$$M=[\frac{\sum_{i=1}^{N}\tilde{Y}_i}{M_i}]^{-1}$$

$$\tilde{h}_s=\sum_{i=1}^{N}\tilde{Y}_i h_{s,i}(\tilde{T})$$

$$\tilde{h}_{s,i}(\tilde{T})=h_{s,i}^{ref}+\int_{T^{ref}}^{T}C_{P,i}^{0}dT$$

constant-pressure speficif heat

JANAF model

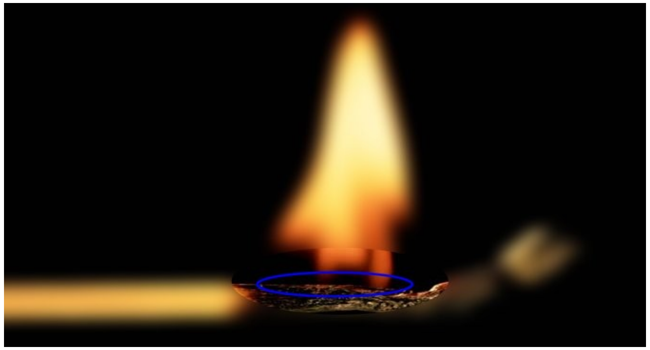
$$C_{P,i}^{0}=R[\frac{a_1}{T^2}+\frac{a_2}{T}+a_3+a_4T+a_5T^2+a_6T^3+a_7T^4]$$

Sutherland model

$$\mu=\frac{C_1T^{3/2}}{T+C_2}$$

+ Combustion model ($\bar{Q}_C$)
+ Turbulence model ($\mu_{sgs}, \alpha_{sgs}, D_{sgs}$)
+ Radiation model ($\boldsymbol{q}_{\boldsymbol{R}}$)

Interface between the 2 Regions



f = environment
g = material

Velocity

$$\tilde{\boldsymbol{u}}_f = \boldsymbol{u}_g$$

Pressure

$$\bar{p}_f = p_g$$

Species concentration (y)

- if flux from the environment to the material

$$y_{i,g} = \widetilde{y_{i,f}}$$

- if flux from the material to the environment

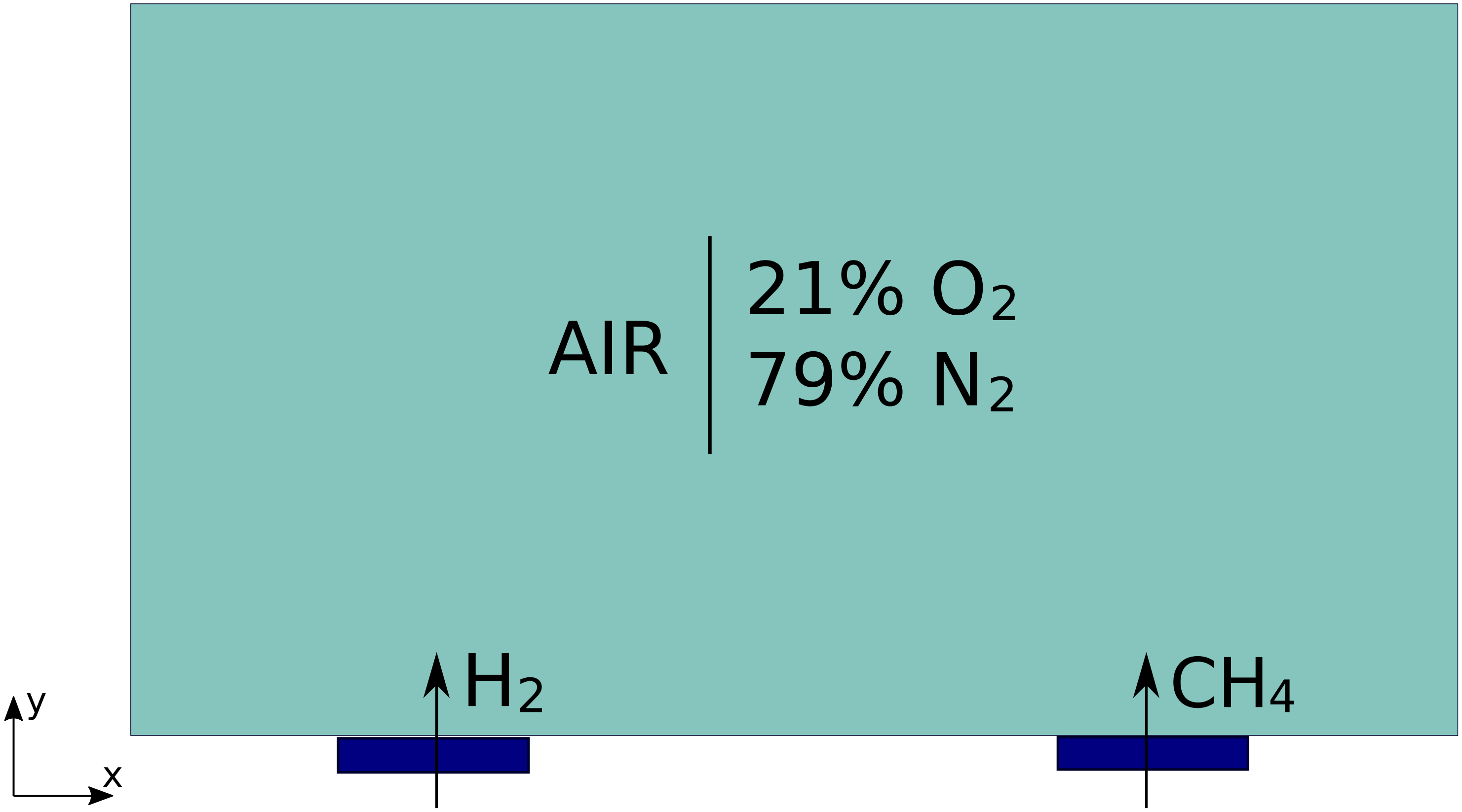
$$\widetilde{y_{i,f}} = y_{i,g}$$

Temperature

$$\tilde{T}_f = T_g$$

$$k_f \nabla \tilde{T}_f = k_g \nabla T_g$$

Two Combustion Reactions

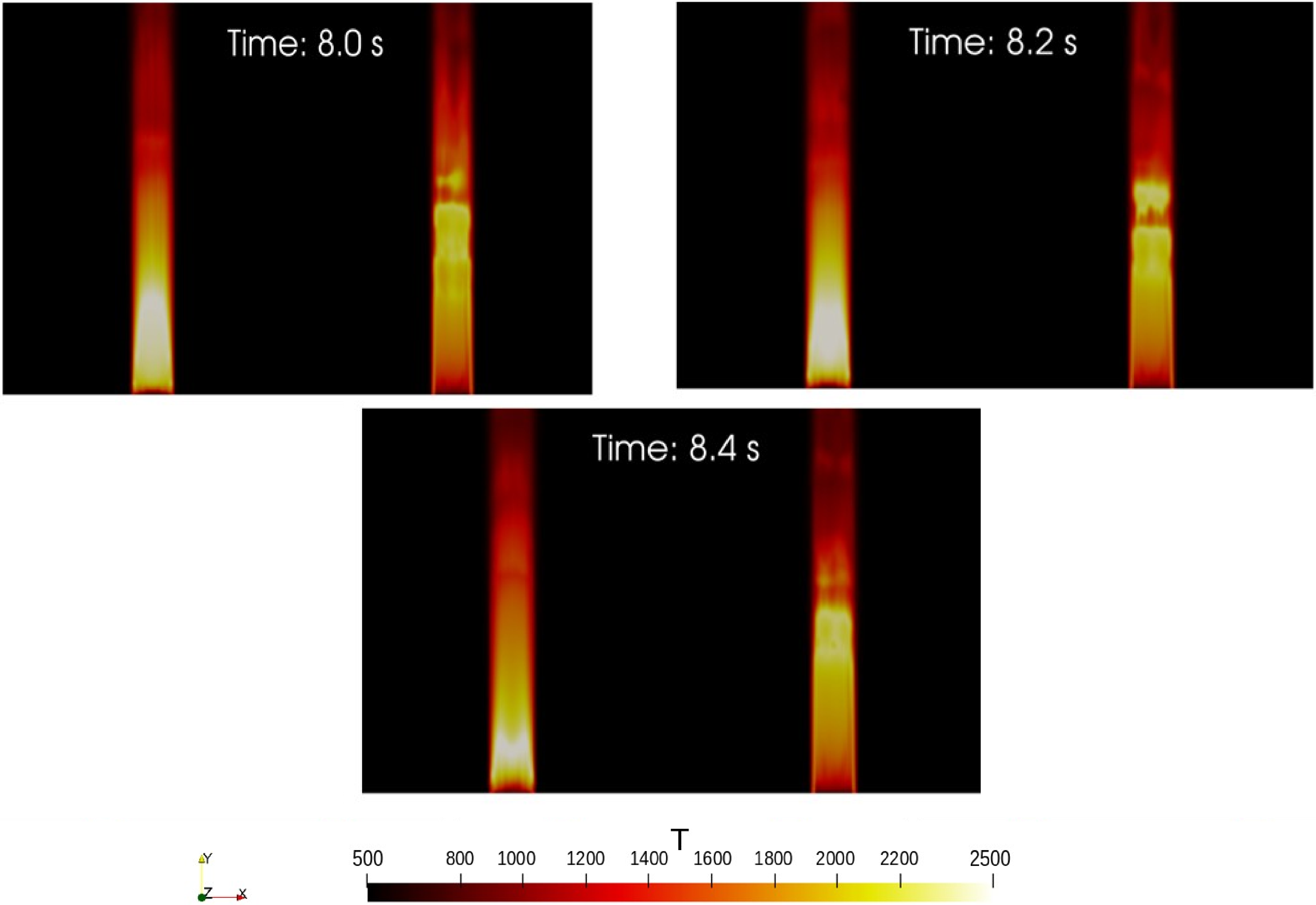


Combustion reactions

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

$2H_2 + O_2 \rightarrow 2H_2O$

Results


Time: 8.0 s
Time: 8.2 s
Time: 8.4 s
T
500
800
1000
1200
1400
1600
1800
2000
2200
2500
Y
Z
X

Combustion of a Wood Log

Pyrolysis reactions

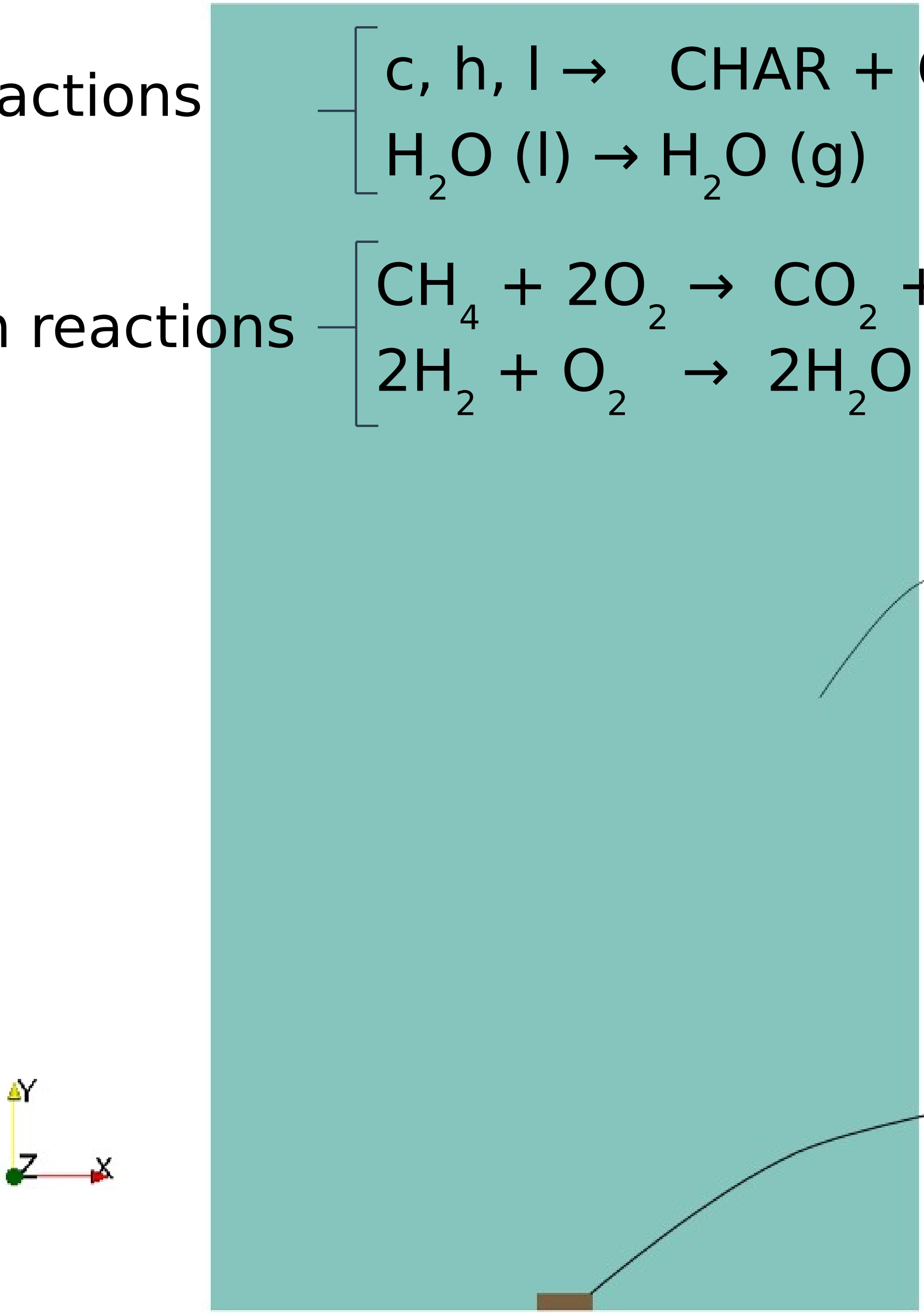
$$\mathrm{c,\ h,\ l} \rightarrow \mathrm{CHAR} + CH_4 + N_2 + H_2 + CO_2 + CO$$

$$H_2O\ (l) \rightarrow H_2O\ (g)$$

Combustion reactions

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

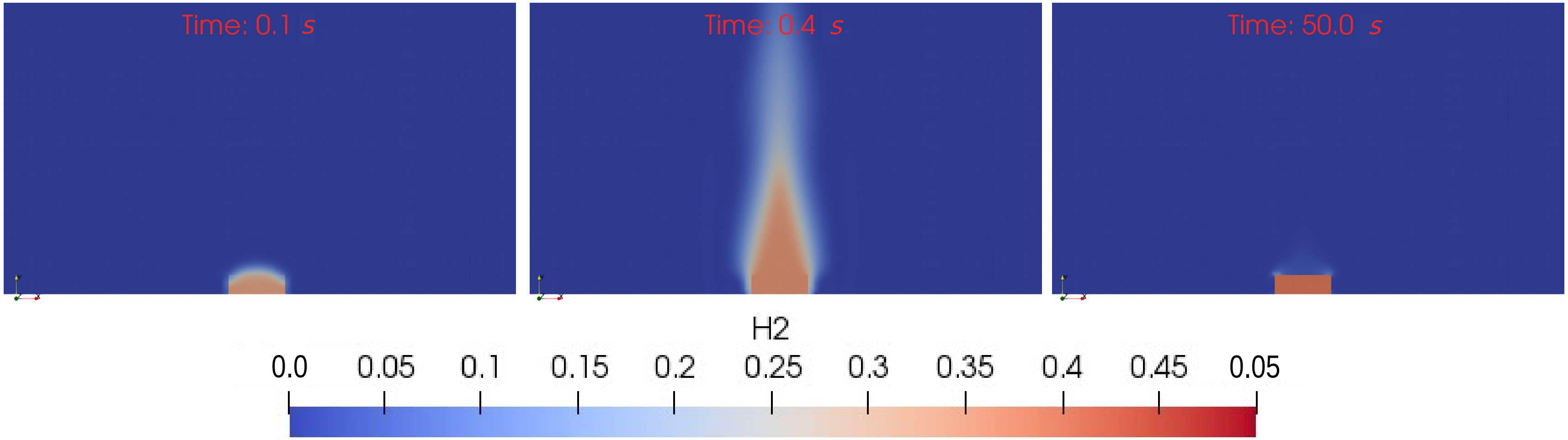
$$2H_2 + O_2 \rightarrow 2H_2O$$

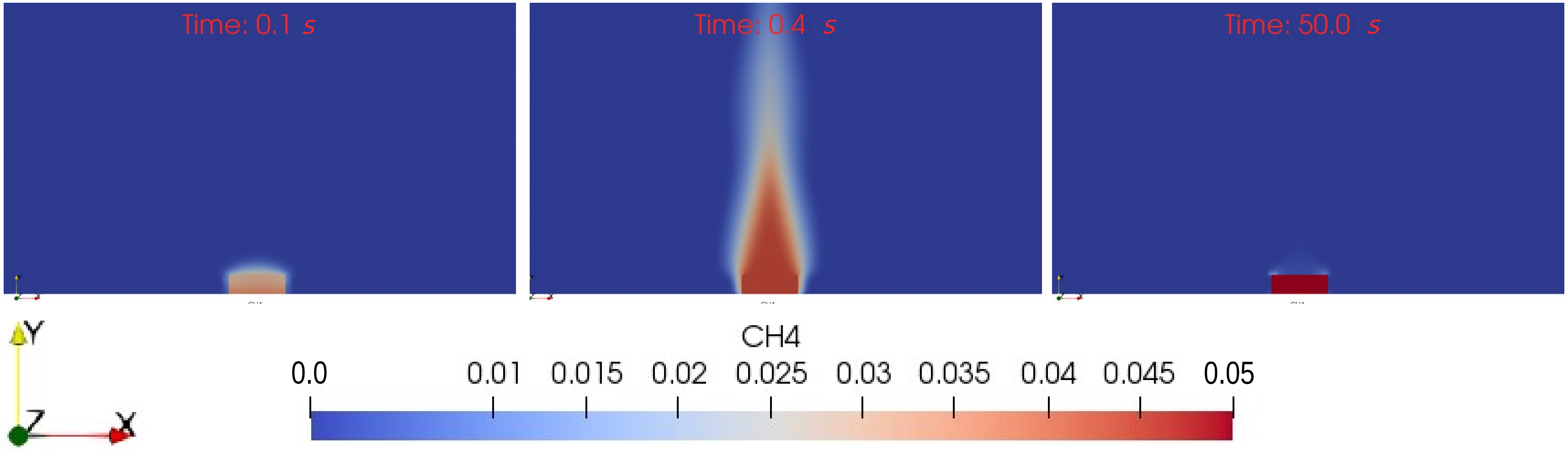


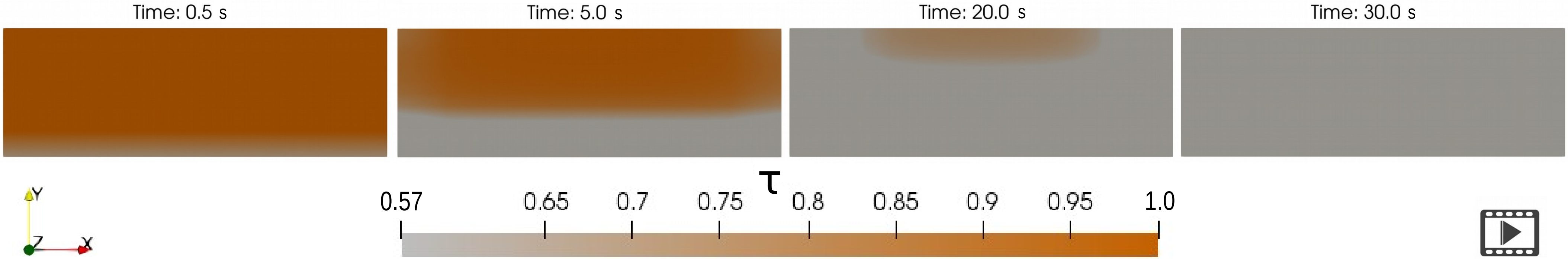
air
- 29% O_2
- 71% N_2

wood (ε_w=0.5)
- 28% hemicellulose
- 18% lignin
- 44% cellulose
- 10% water

Results


Time: 0.1 s
Time: 0.4 s
Time: 50.0 s
H2
0.0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.05


Time: 0.1 s
Time: 0.4 s
Time: 50.0 s
Y
Z
X
CH4
0.0
0.01
0.015
0.02
0.025
0.03
0.035
0.04
0.045
0.05


Time: 0.5 s
Time: 5.0 s
Time: 20.0 s
Time: 30.0 s
Y
Z
X
τ
0.57
0.65
0.7
0.75
0.8
0.85
0.9
0.95
1.0

Conclusion & Future Work

Main Goal

Define a numerical tool to deal with this multi-physical problem.

Numerical tool

PATO: detailed porous material solver coupled to several OpenFoam flow solvers, including FireFoam

A First Application

Numerical simulation of a log combustion.

Future Works

- Extend the application by considering solid deformation;
- Extend the application to 3D;
- Apply the solver to the Burning of the match;

THANK YOU

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