A One-Grid Framework for Pyrolysis of Porous Biomass Particles

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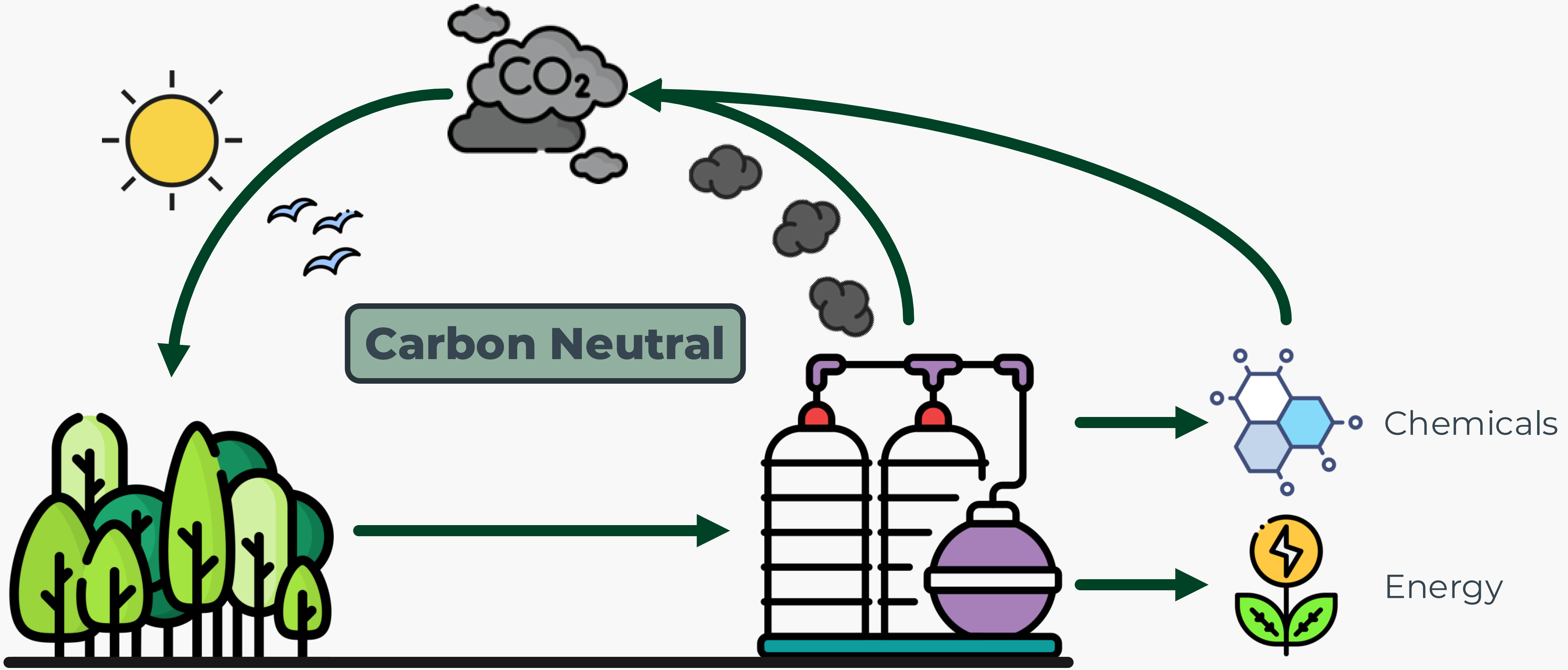
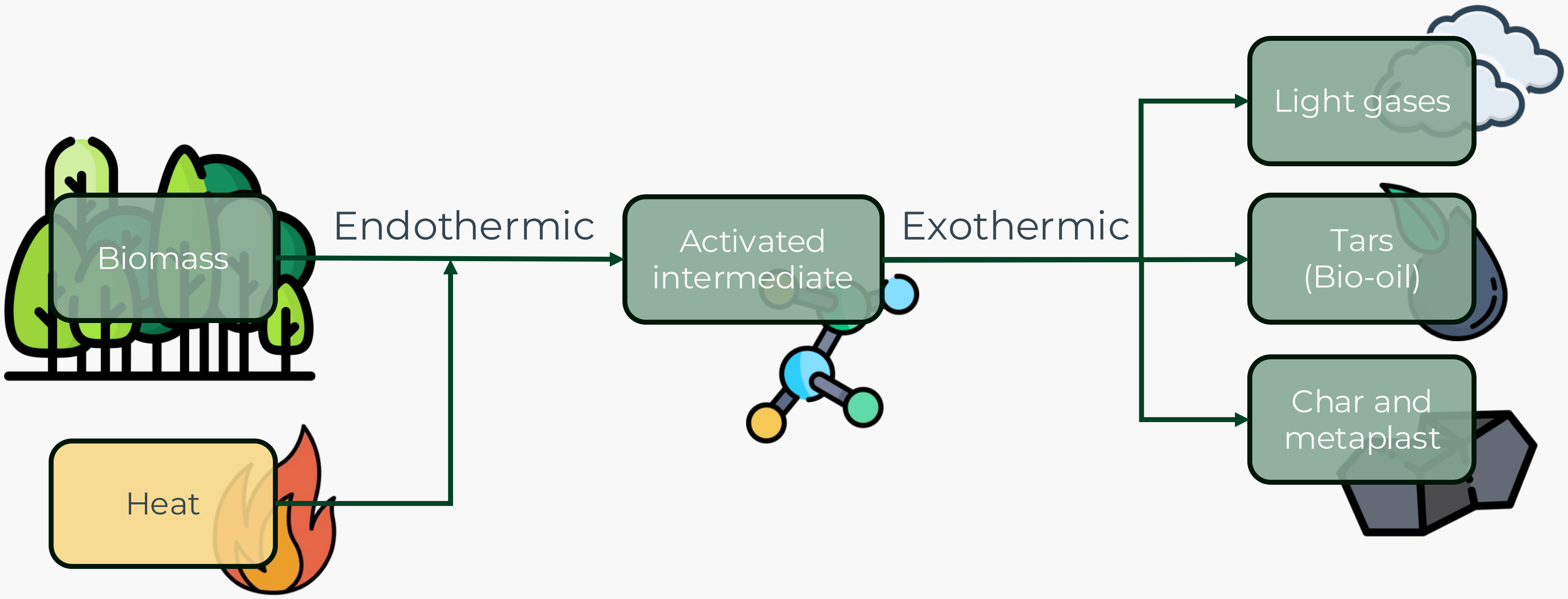
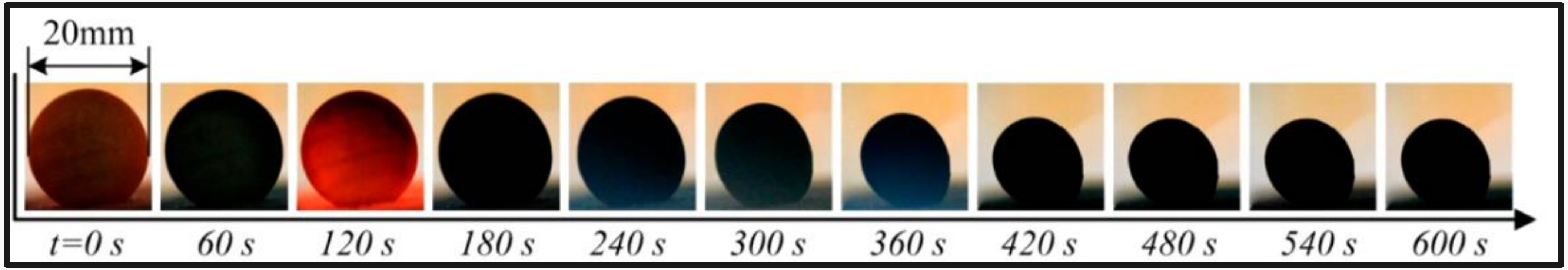
Towards a carbon neutral future



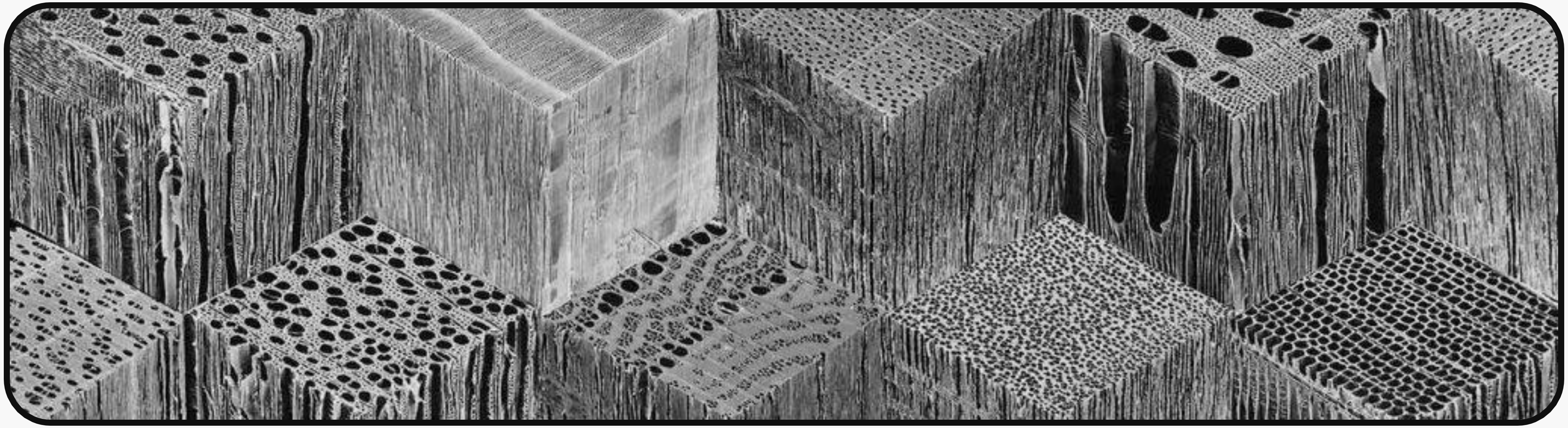
Understanding wood pyrolysis





Huang, Q. X., Wang, R. P., Li, W. J., Tang, Y. J., Chi, Y., & Yan, J. H. (2014). Modeling and experimental studies of the effects of volume shrinkage on the pyrolysis of waste wood sphere. *Energy & Fuels*, *28*(10), 6398–6406.

Challenges in wood modeling



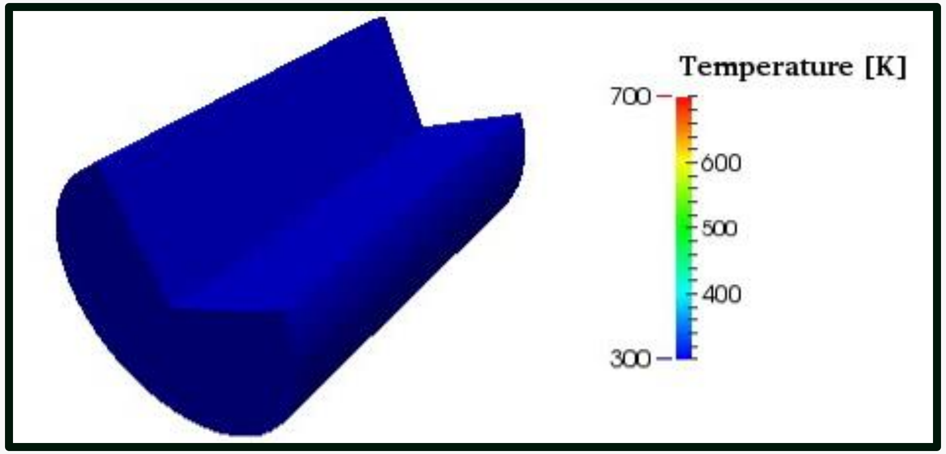
- Complex chemical kinetics
- Multiphase interactions
- Heat and mass transfer
- Anisotropy of wood properties
- Porous material
- Large uncertainties and variability

Wood Structure and Identification by H. A. Core, W. A. Côté and A. C. Day, Syracuse University Press, 1979.

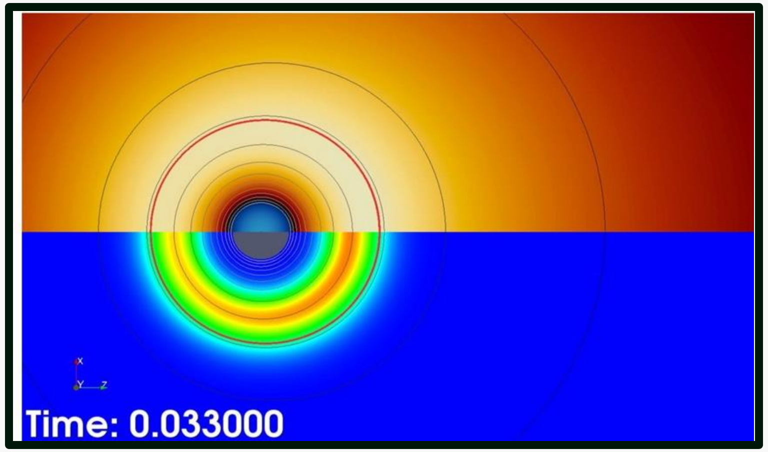
State of the art

Current models of reacting particles **either focus on one of two aspects**

Particle **shape and porosity changes**



External **gas combustion** of a **still spherical** or point **particle**

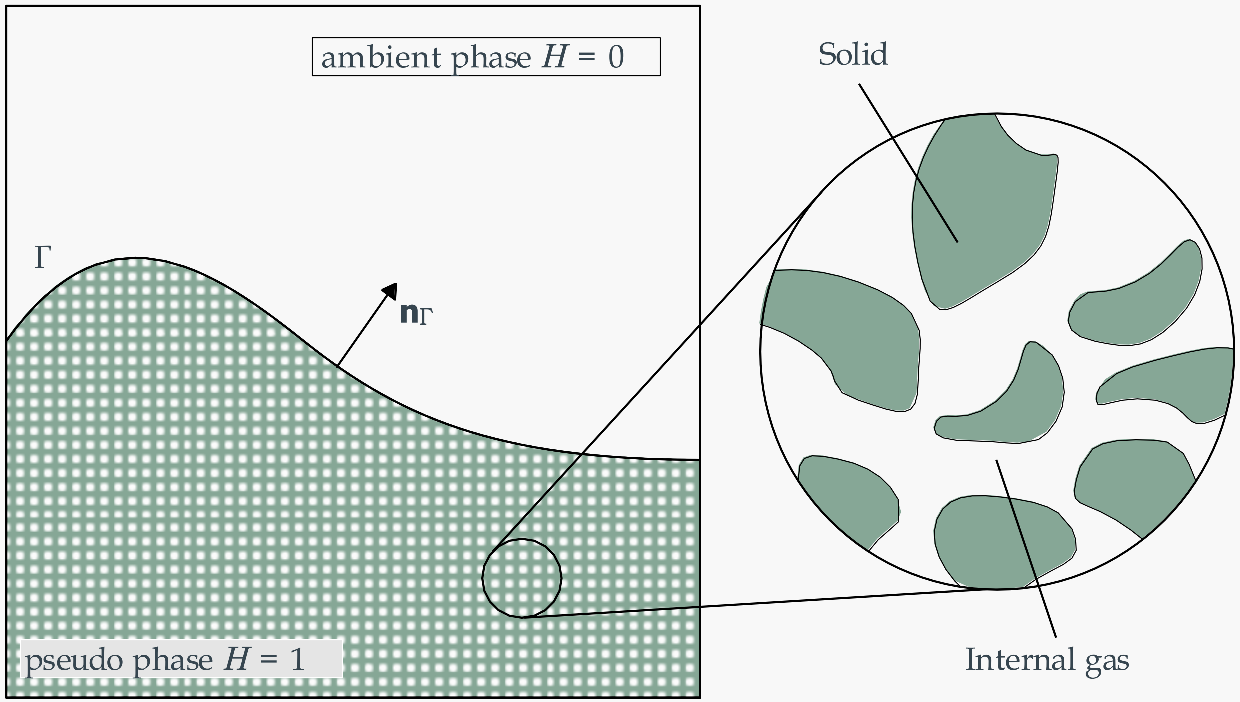


We want to be able to simulate both effects simultaneously

Gentile, G., Debiagi, P. E. A., Cuoci, A., Frassoldati, A., Ranzi, E., & Faravelli, T. (2017). A computational framework for the pyrolysis of anisotropic biomass particles. *Chemical Engineering Journal*, *321*,

Tufano, G., Stein, O., Kronenburg, A., Frassoldati, A., Faravelli, T., Deng, L., Kempf, A., Vascellari, M., & Hasse, C. (2016). Resolved flow simulation of pulverized coal particle devolatilization and ignition in air- and O2/CO2-atmospheres. *Fuel*, *186*, 285-292.

The particle scale



We avoid a sharp description of the pores interface and consider a whole **pseudo-phase** which includes both solid and fluid.

We define the **porosity** as:

$$\epsilon = {V_g}/{V_{tot}}$$

Properties are calculated as a function of the porosity:

$$\psi_m = \psi_G \epsilon + (1 - \epsilon)\psi_S$$

Chemical reactions can happen in the whole solid volume, no gas phase reactions (for now)

$$\Omega_i \left[{\mathrm{kg}}/{m_S^3 s} \right] = A\, e^{-\frac{E_a}{RT}}$$

OpenSMOKE++

For stiff ode chemistry integration, thermodynamic and transport properties

Cuoci, A., Frassoldati, A., Faravelli, T., & Ranzi, E. (2015). OpenSMOKE++: An object-oriented framework for the numerical modeling of reactive systems with detailed kinetic mechanisms. *Computer Physics Communications*, 192, 237-264

Governing equations

One-field variable properties Navier-Stokes solution

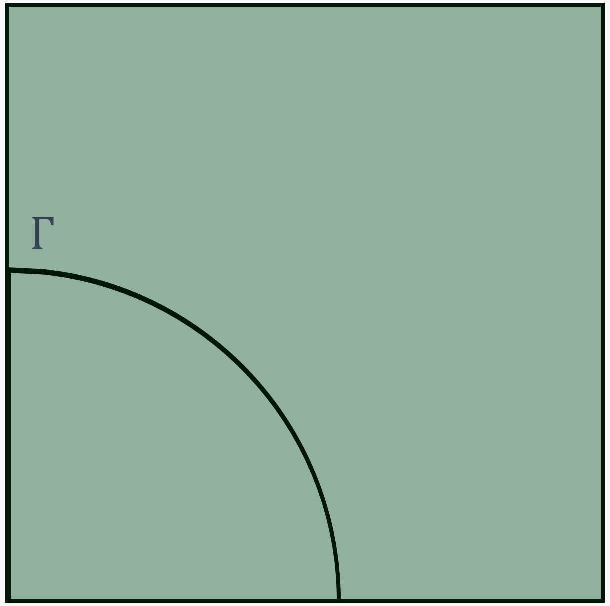
Effect of porous media

Chemical reactions

Darcy and Forchheimer contributions

$$\rho_G \left[\frac{\partial \boldsymbol{v}}{\partial t} + \nabla\left(\frac{\boldsymbol{v}\boldsymbol{v}}{\boldsymbol{\epsilon}}\right)\right] = -\nabla p + \nabla \cdot [\mu(\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T)] - \left[\frac{\mu\epsilon}{\boldsymbol{K}}\boldsymbol{v} + \frac{F\rho_G\epsilon}{\sqrt{\boldsymbol{K}}}|\boldsymbol{v}|\boldsymbol{v}\right] c$$

$$\nabla \cdot \boldsymbol{v} = (1-\epsilon)\dot{\Omega}\left[\frac{1}{\rho_g} - \frac{1}{\rho_s}\right] - \epsilon \frac{1}{\rho_g}\frac{D\rho_g}{Dt}$$



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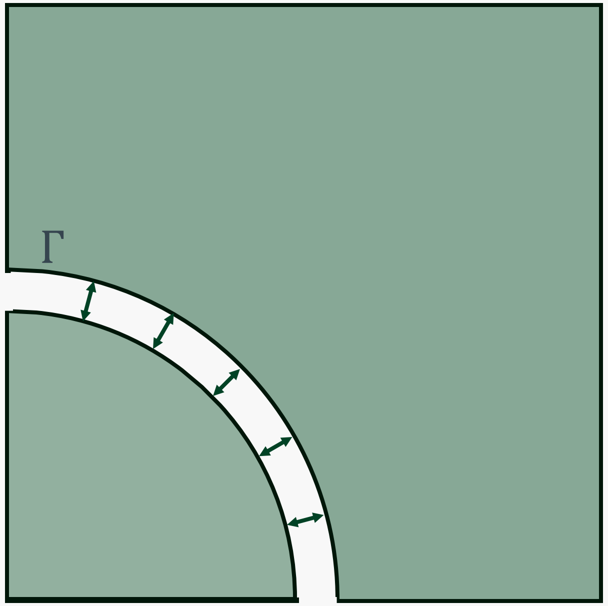
$$\nabla\cdot\boldsymbol{v}=(1-\epsilon)\dot{\Omega}\left[\frac{1}{\rho_g}-\frac{1}{\rho_s}\right]-\epsilon\frac{1}{\rho_g}\frac{D\rho_g}{Dt}$$



Two field species and energy equation

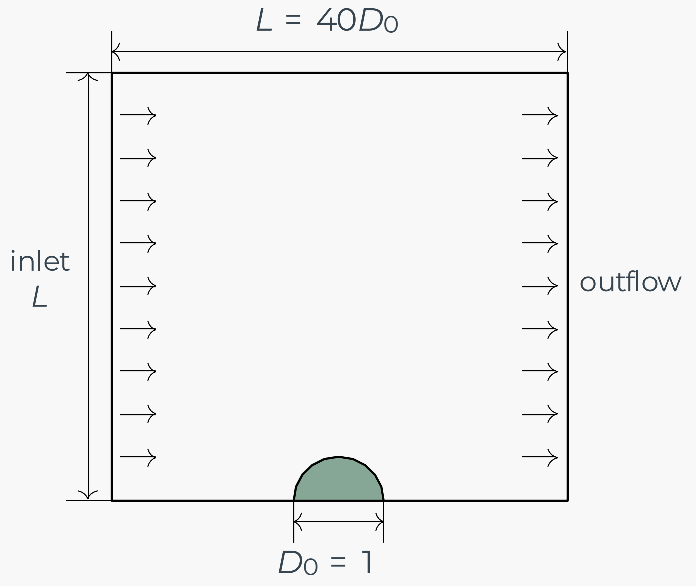
More accurate description of the interface temperature

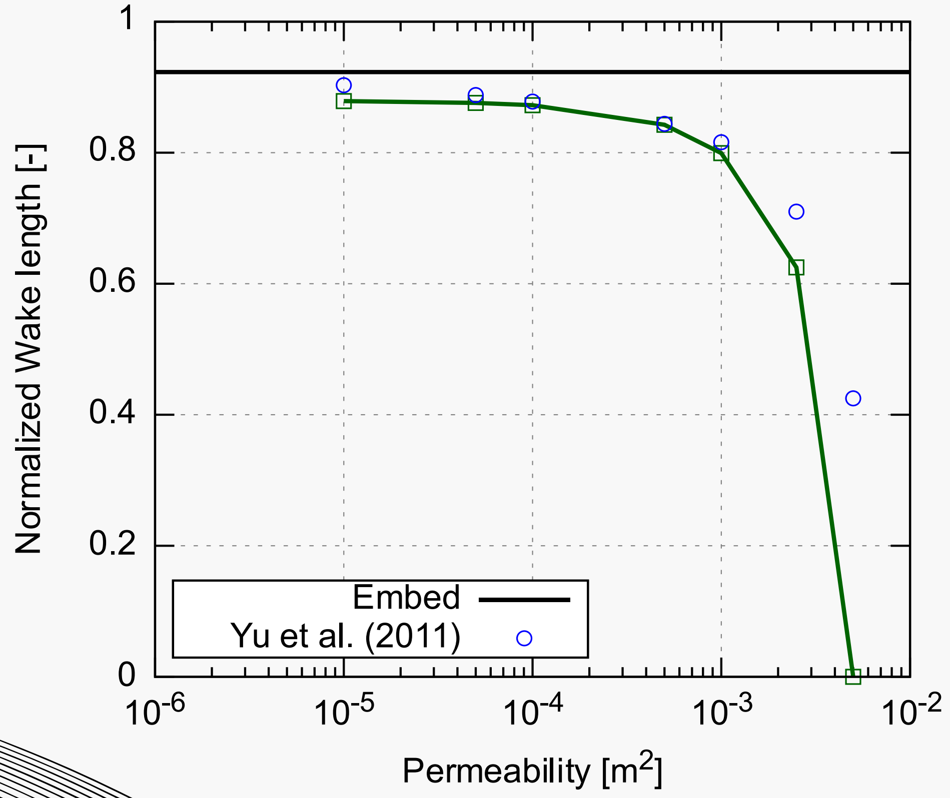
$$(\rho C_p)_m\frac{\partial T_m}{\partial t}+(\rho C_p)_g\boldsymbol{v}_g\cdot\nabla T_m=\nabla\cdot(\boldsymbol{\lambda}_m\nabla T_m)-\nabla T_m\cdot\left(\sum_{i=1}^{NGS}C_{p_i}j_{i,k}\right)+\dot{Q}+\epsilon\dot{Q}_k^r$$

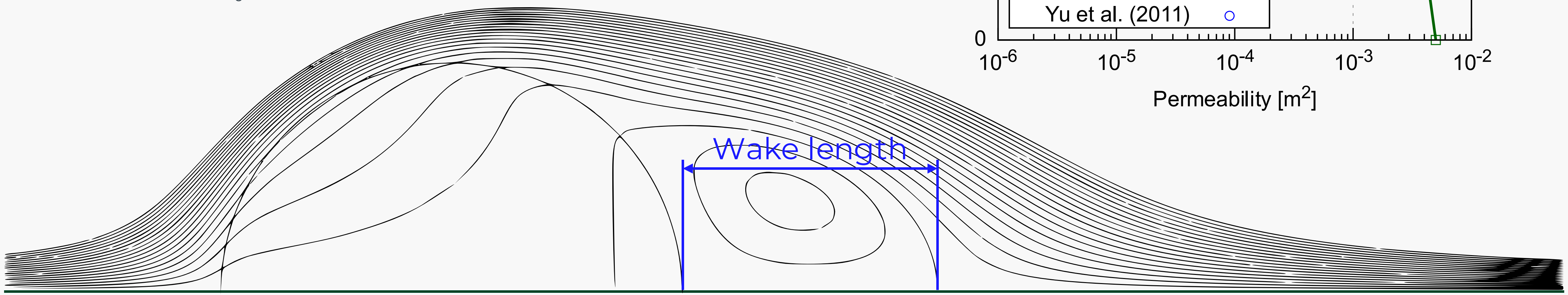
$$\frac{\partial(\omega_{i,k}\epsilon_k\rho_k)}{\partial t}+\nabla\cdot\left(\omega_{i,k}\rho_k(\boldsymbol{v}_k+\epsilon_k\boldsymbol{u}_m)\right)=-\nabla\cdot j_{i,k}+\epsilon_s\dot{\Omega}_{i,s}$$

Wake behind a porous cylinder

Non reacting case, laminar conditions Re = 20







An ill posed problem

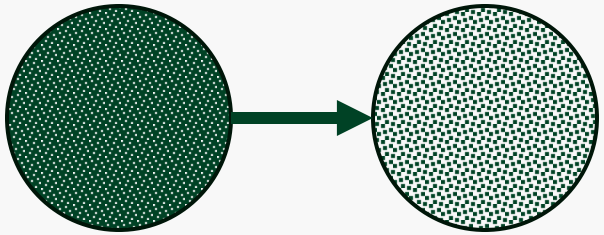
Conservation of solid mass

$$\frac{\partial M_s}{\partial t} = -\Omega V_S \rightarrow \cdots \rightarrow \qquad V_{tot}\boxed{\frac{\partial \epsilon}{\partial t}} + \epsilon \boxed{\frac{\partial V_{tot}}{\partial t}} = -\Omega \frac{\epsilon V_{tot}}{\rho_s}$$

2 unknowns with 1 equation

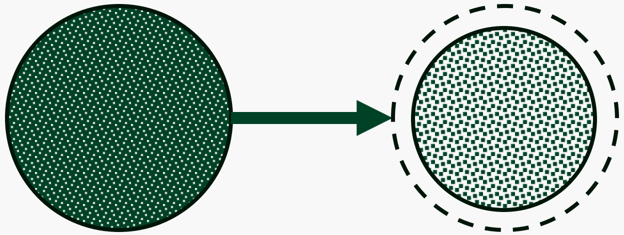
Only porosity variation

Uniform conversion model



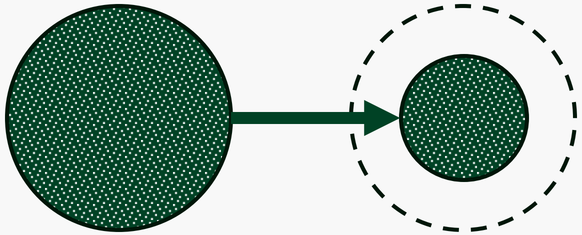
Reality is an in between situation

Both effects happened together



Only volume variation

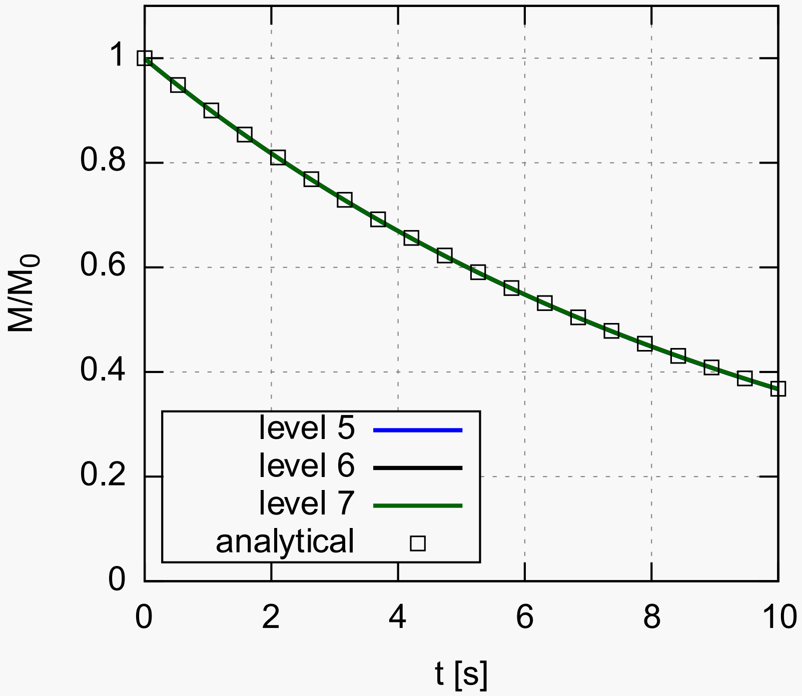
Shrinking particle model

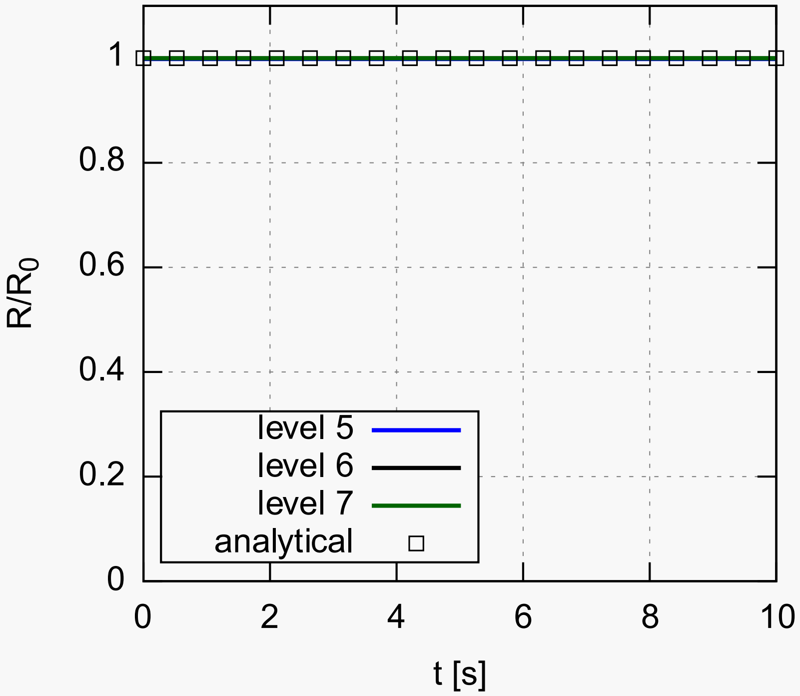


Porosity variation

$$V_{tot}\frac{\partial \epsilon}{\partial t} + \epsilon\frac{\partial V_{tot}}{\partial t} = -\Omega\frac{\epsilon V_{tot}}{\rho_s} \rightarrow \boxed{\frac{\partial \epsilon}{\partial t} = -\Omega\frac{\epsilon}{\rho_s}}$$

We solve the porosity equation in each cell





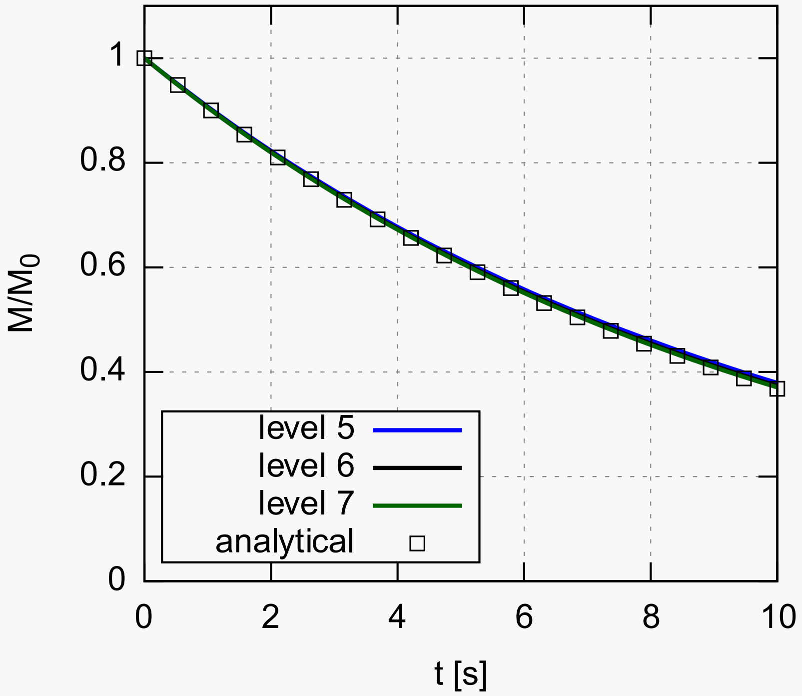
Volume variation

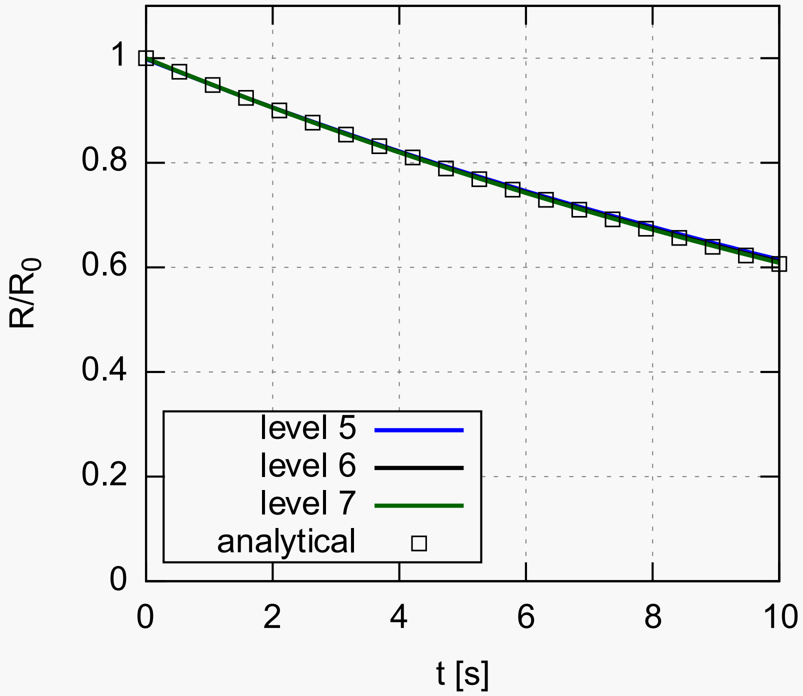
$$V_{tot}\frac{\partial \epsilon}{\partial t} + \epsilon \frac{\partial V_{tot}}{\partial t} = -\Omega \frac{\epsilon V_{tot}}{\rho_s} \rightarrow \frac{\partial V_{tot}}{\partial t} = -\Omega \frac{V_{tot}}{\rho_s}$$

How to connect Ω and $\boldsymbol{u}_m$?

Velocity potential

$$\begin{cases} \nabla \cdot (\nabla \boldsymbol{\phi}) = \dfrac{\Omega}{\rho_s} \\ \boldsymbol{u}_{\mathrm{m}} = -\nabla \boldsymbol{\phi} \end{cases}$$

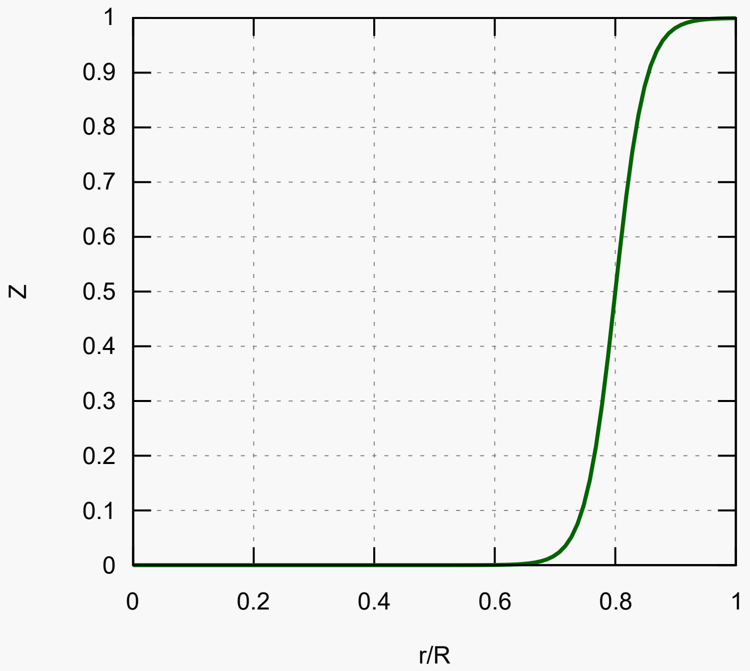


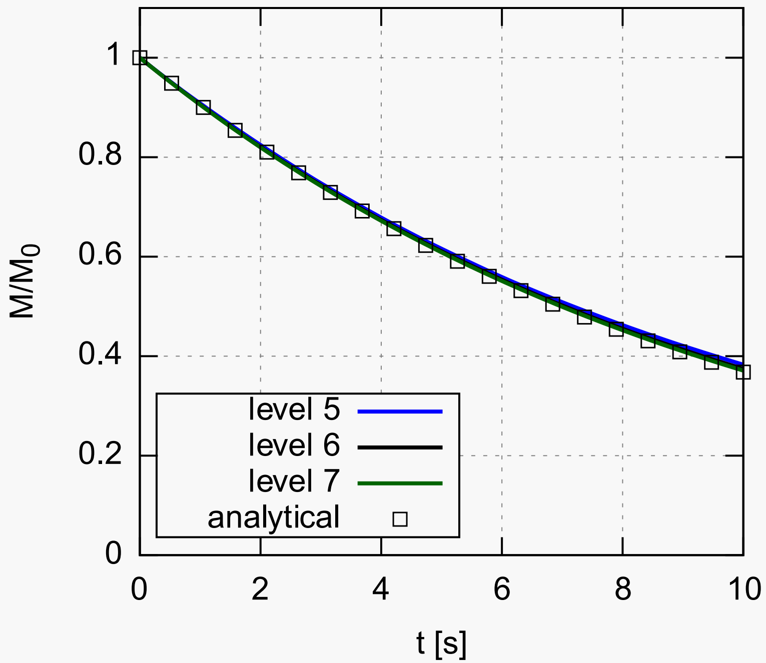


Reality is an in between situation

We **split** the contribution of Ω to account for both effects

$$\frac{\partial V_{tot}}{\partial t} = -\frac{\Omega V_{tot}}{\rho_s} Z, \qquad \frac{\partial \epsilon}{\partial t} = -\frac{\Omega \epsilon}{\rho_s}(1 - Z)$$

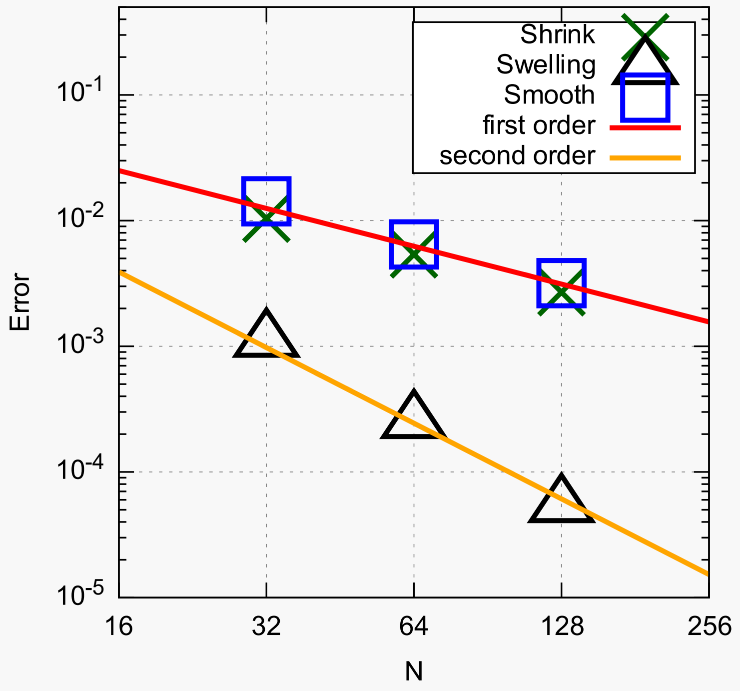




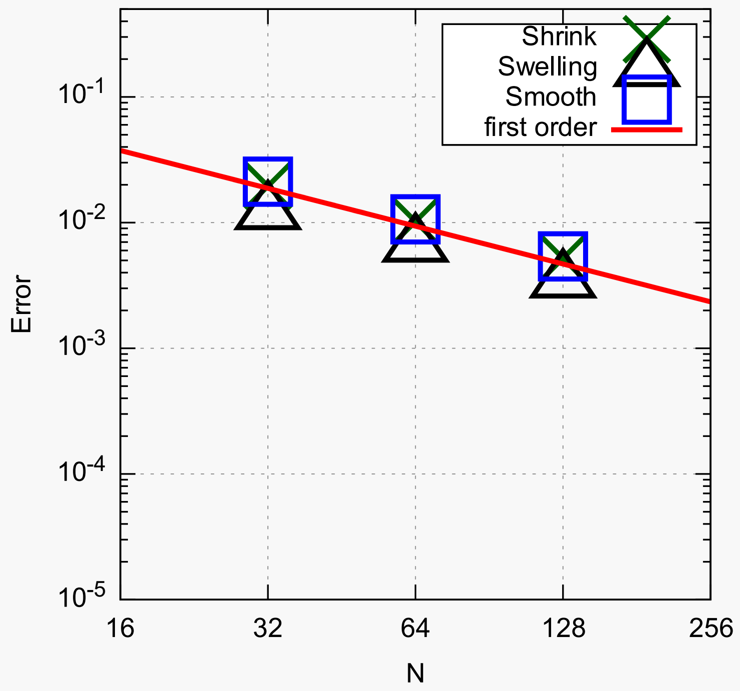
Ideally Z should be a function of the physics of the problem, for example: $Z = {}^{\Omega}/_{\max(\Omega)}$

Convergence of mass conservation

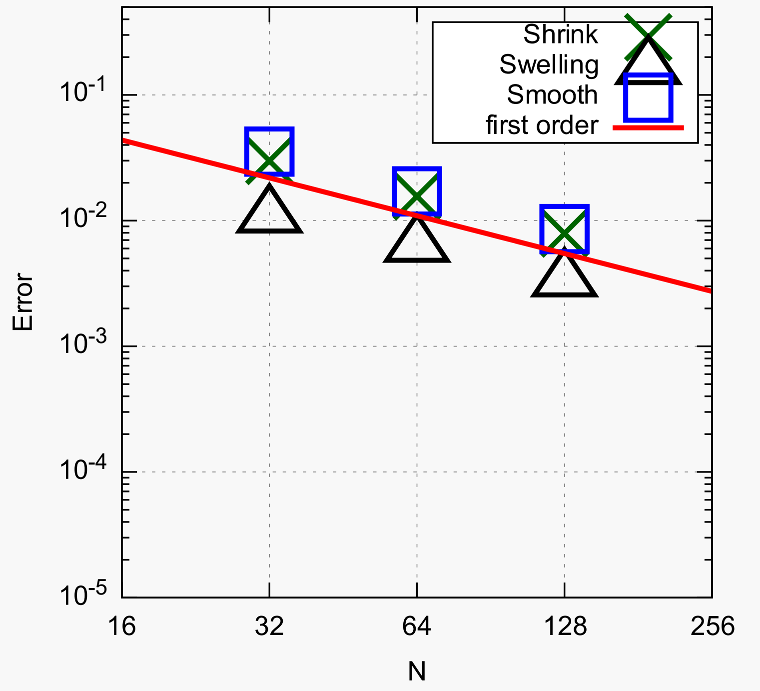
Error in solid mass



Error in gas mass

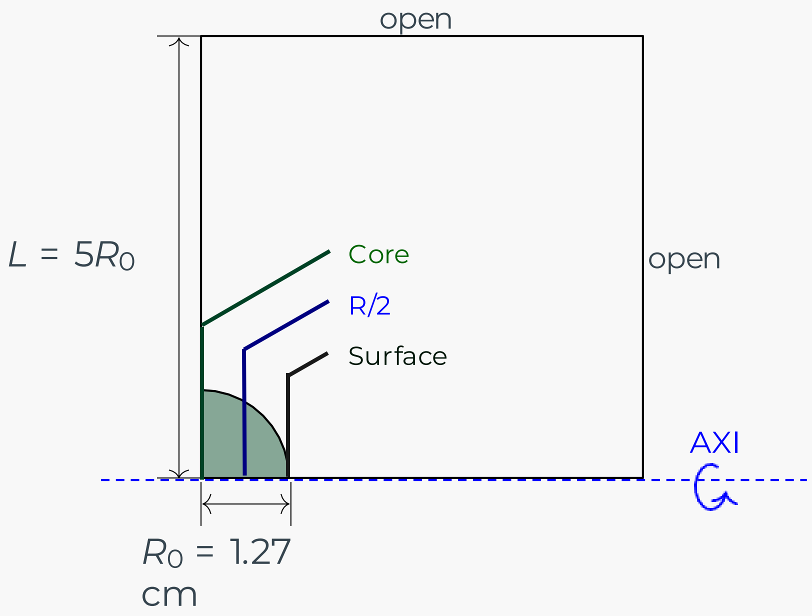


Error in total mass



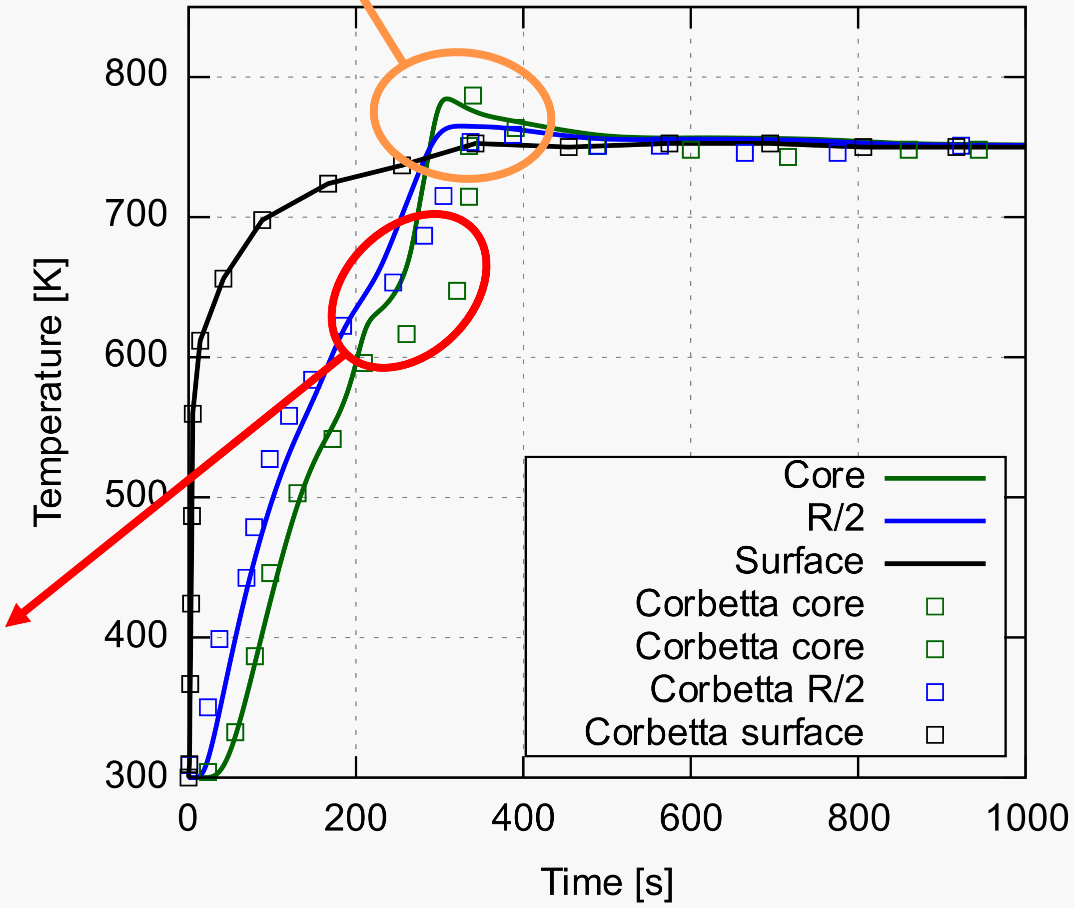
Internal phase validation

- Heating of a reacting spherical wood particle
- Data from Corbetta et al
- Imposed surface temperature profile



Exothermic charrification reactions

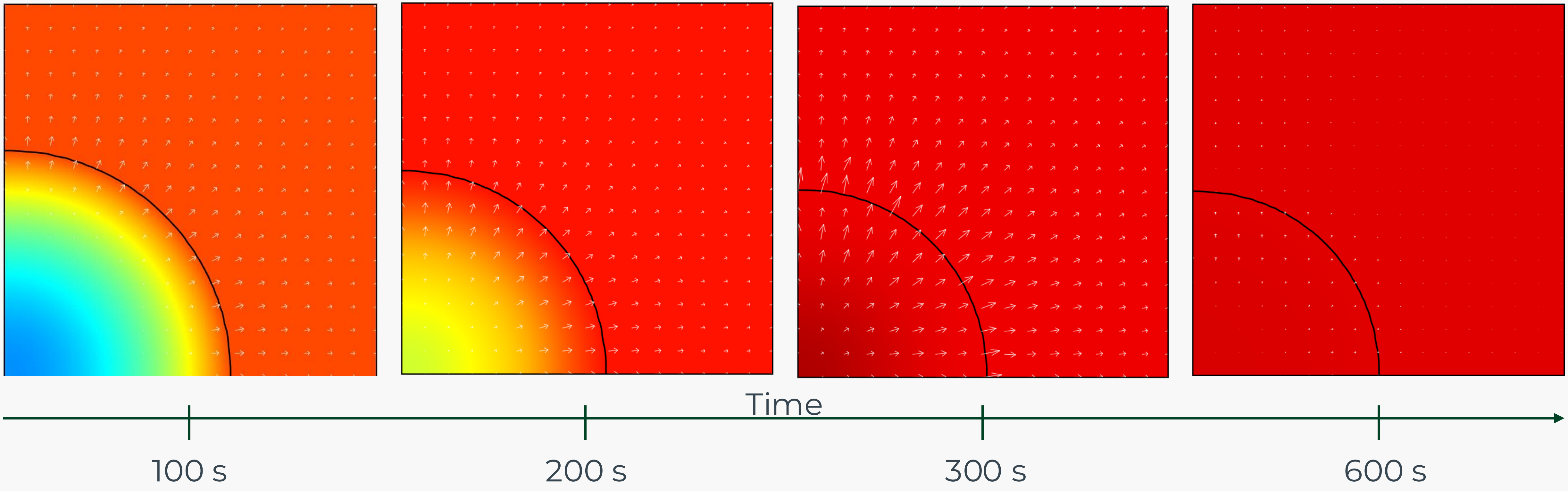
Endothermic degradation reactions



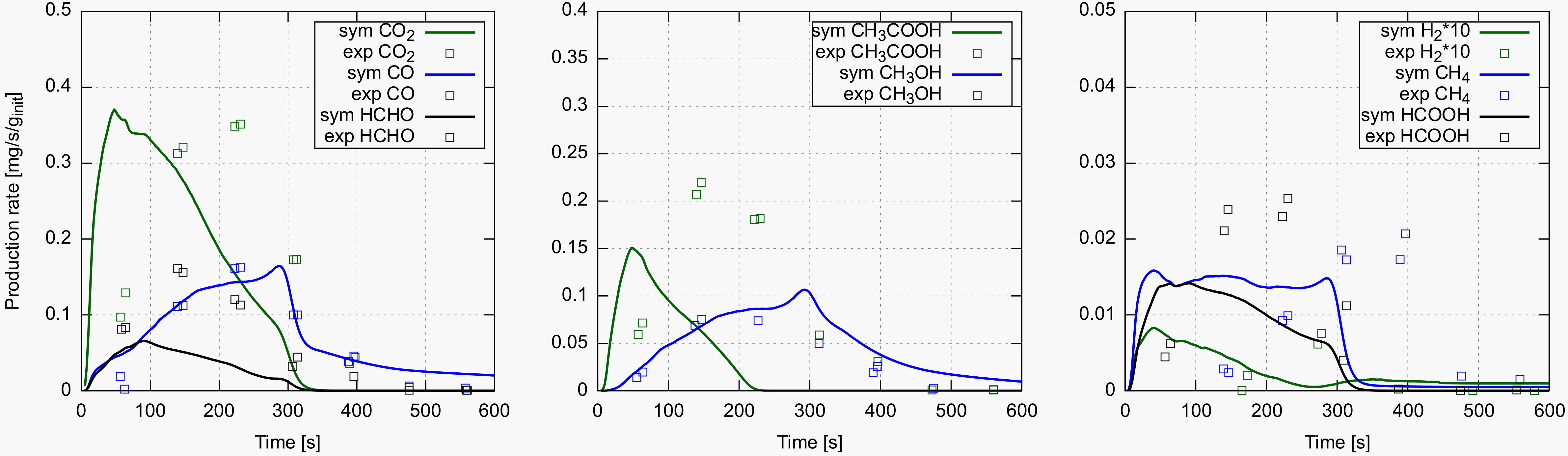
Corbetta, M., Frassoldati, A., Bennadji, H., Smith, K., Serapiglia, M. J., Gauthier, G., Melkior, T., Ranzi, E., & Fisher, E. M. (2014). Pyrolysis of Centimeter-Scale woody Biomass particles: kinetic modeling and experimental validation. Energy & Fuels, 28(6), 3884–3898.

Temperature snapshots

Temperature [K]



Species released



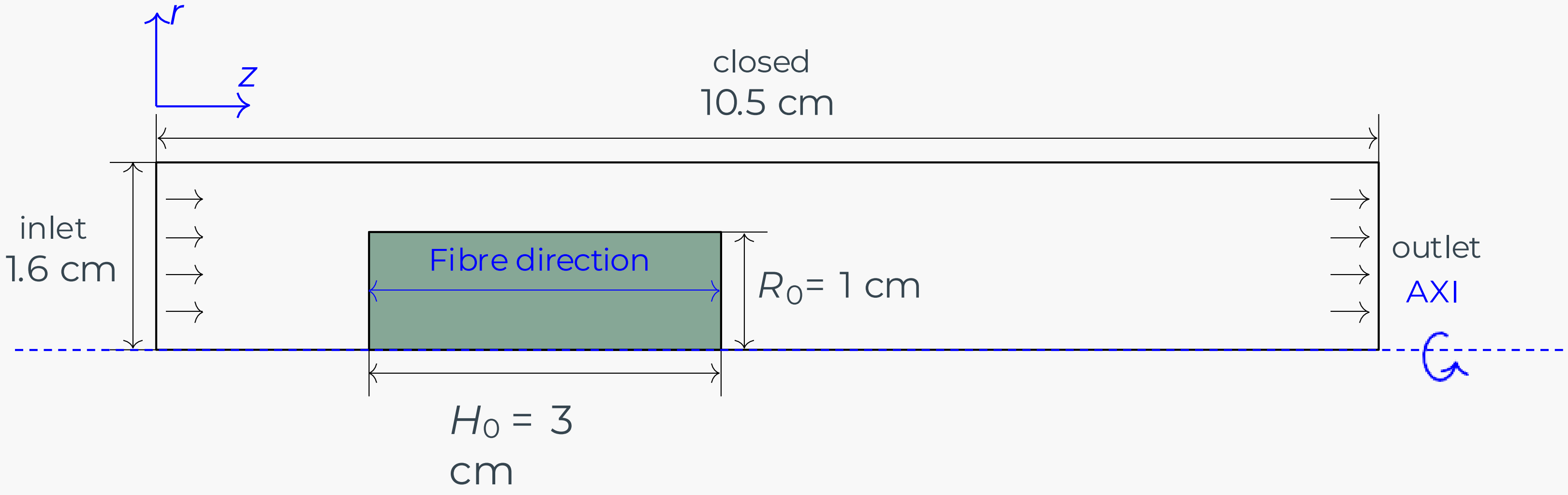
Results are strongly influenced by the kinetic mechanism

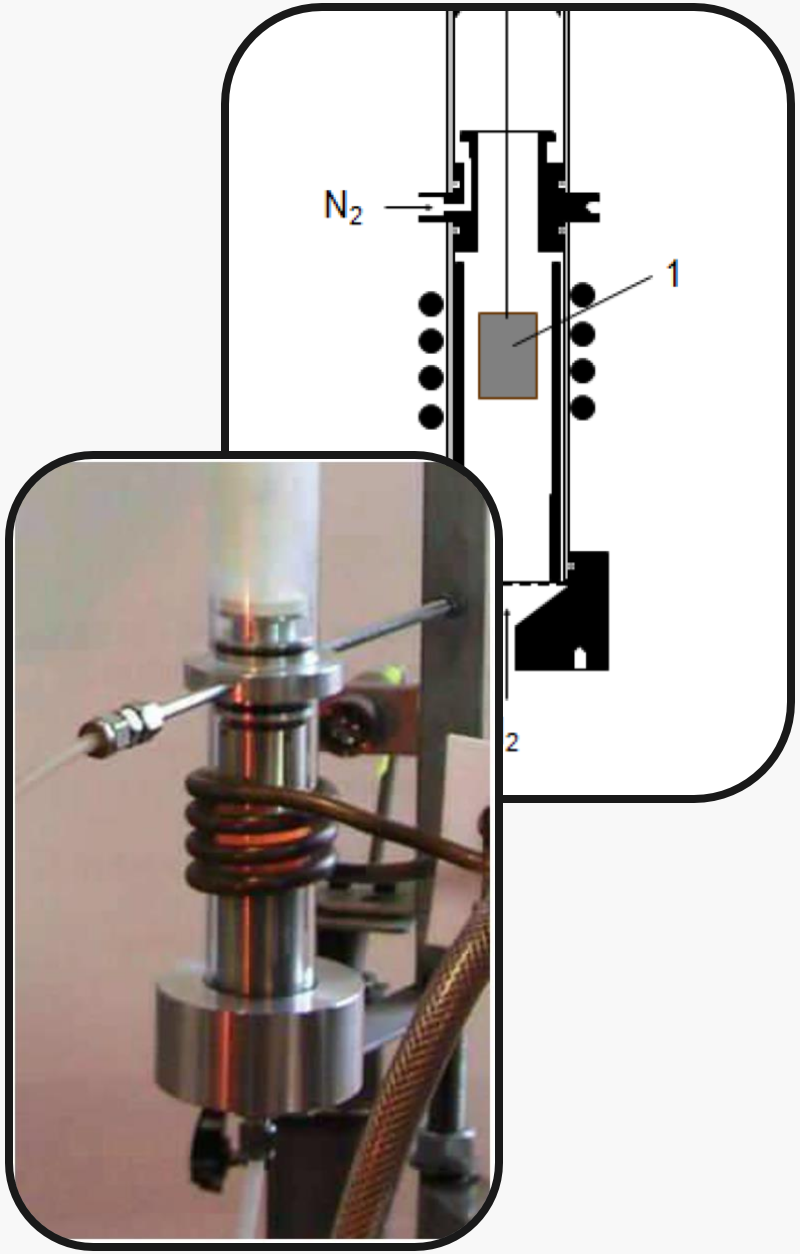
Good agreement in terms of:

+ Order of magnitude
+ Released time

Anisotropic cylinder in flow

Data from G. Gauthier
Thermal conductivity is higher along the fibres

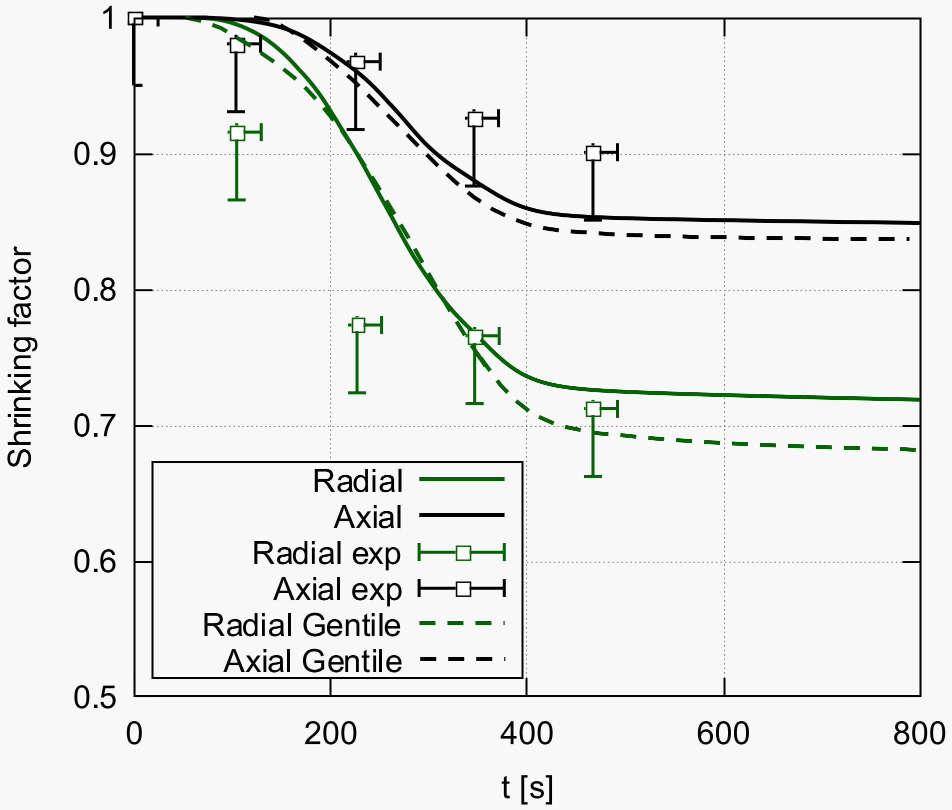


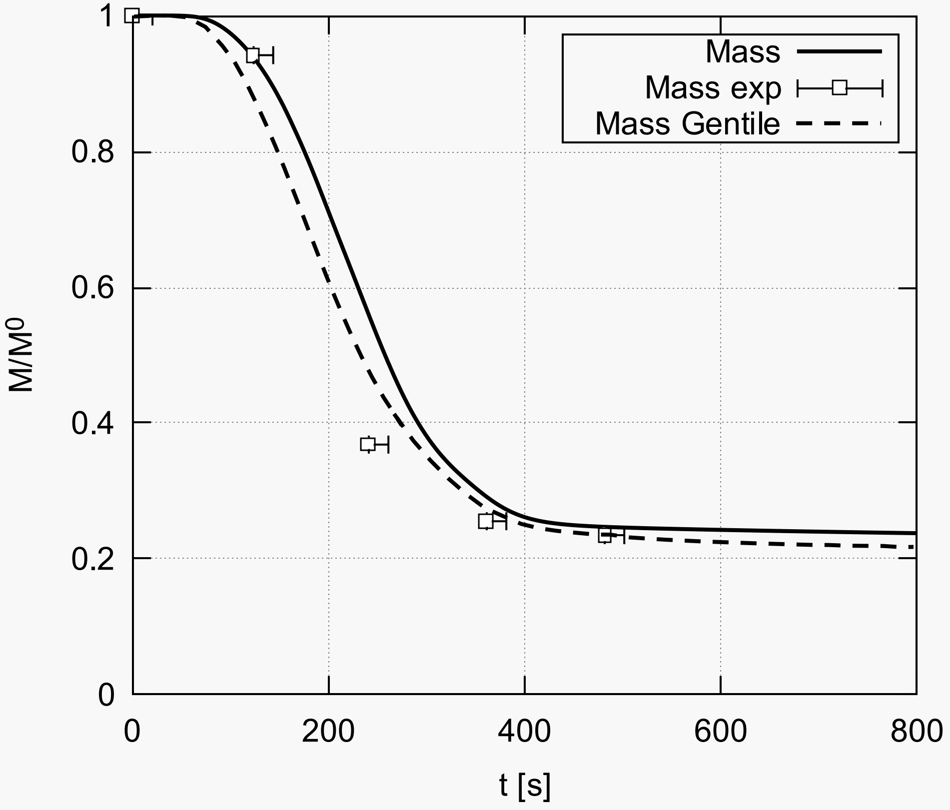


G. Gauthier, Syntesis of Second Generation Biofuels: Study of Pyrolysis of Centimeter-Scale Wood Particles at High Temperature, Univerisite de Toulouse, 2013.

Anisotropic cylinder in flow

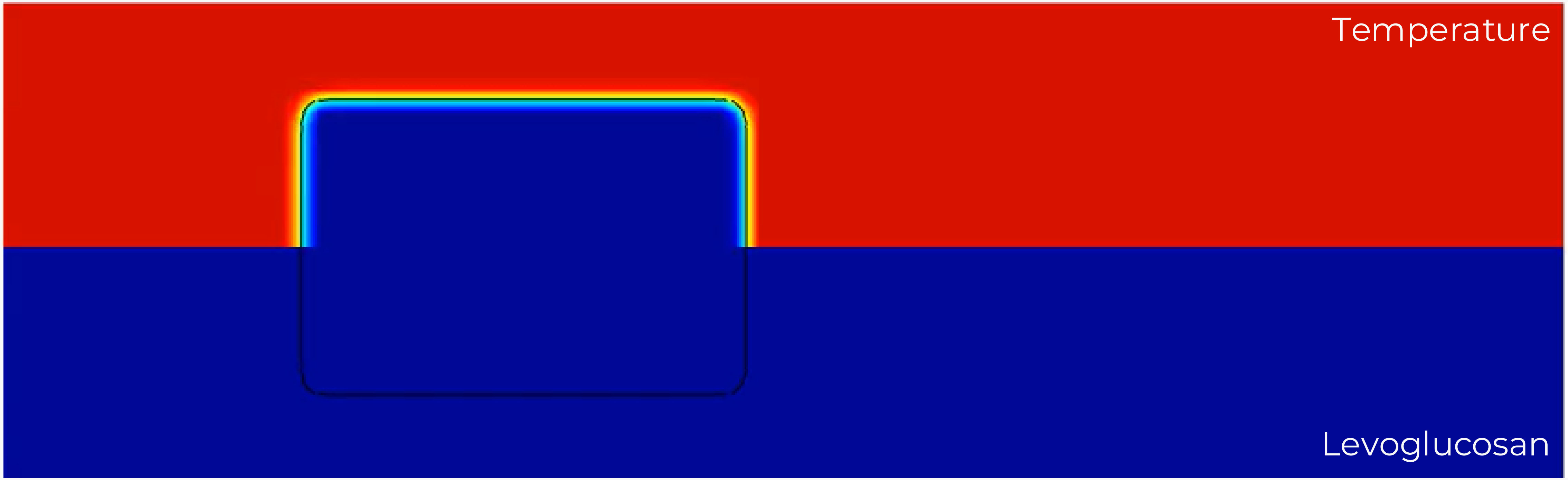
Additional comparison with Gentile et al results: **NO NEED FOR CORRELATIONS**



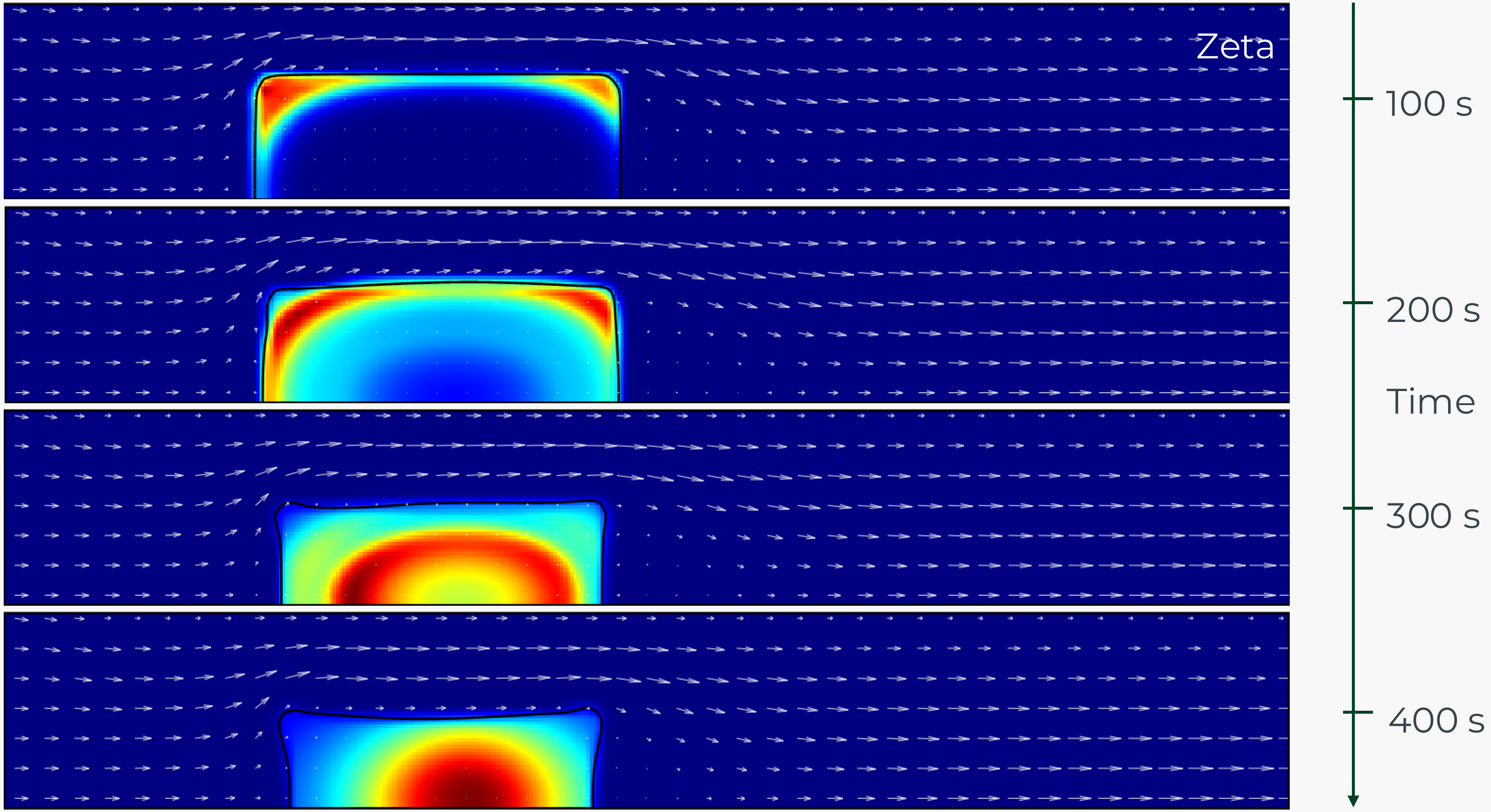


Gentile, G., Debiagi, P. E. A., Cuoci, A., Frassoldati, A., Ranzi, E., & Faravelli, T. (2017). A computational framework for the pyrolysis of anisotropic biomass particles. Chemical Engineering Journal, 321, 458-473.

Anisotropic cylinder in flow



Propagation of the shrinking region



Summary

- VoF and Chemical reaction coupling
- Solution of both internal and external phases
- Both changes in porosity and shape
- Anisotropic properties

Future works

Already done for droplets!
Check out Edoardo Cipriano's presentation

- More validation
- Gas-phase reactions
- Combustion
- Chemistry reduction methods

Thank you for your attention!

Are there any questions?

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