Numerical modeling of wood pyrolysis on OpenFOAM: prediction of gas speciation through detailed kinetic schemes

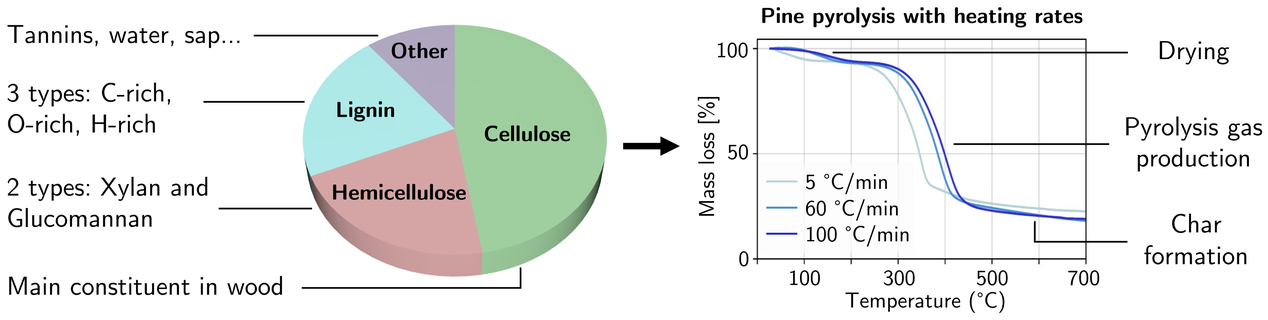
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Context

Wood pyrolysis: Thermal degradation of wood without oxygen. Can be used for energetic purposes, or to produce molecules of interest. Decomposition and products quantities depend on the composition and heating conditions:



PATO: (Porous material Analysis Toolbox based on OpenFOAM) [1] Models pyrolysis with parallel and simplified reactions. Does not capture the competitive nature of the reactions. Does not allow gas fraction prediction.

↳ **Objectives:** Implement competitive mechanisms from literature, building on previous work [2], and adapt them to experimental data for cellulose, xylan, lignin, and pine at different heating rates.

↳ **Strategy:** Ranzi's mechanism from 2017 [3] with the improvements added on cellulose [4]. Calibration and modification of the original mechanism to better fit the experimental results. Simulations of a small particle in TGA oven (set heating rate, homogeneous temperature).

Conservation equations

Mass conservation equations: [1,2,5]

$$\frac{\partial \epsilon_{s,i}\langle\rho_{s,i}\rangle^i}{\partial t} + \nabla\cdot\left(\epsilon_{s,i}\langle\rho_{s,i}\rangle^i\langle\boldsymbol{v_s}\rangle^s\right) = \sum_{i\in N_s} M_i\langle\pi_i\rangle \quad \text{Solid phase}$$

$$\frac{\partial \epsilon_g\langle\rho_g\rangle^g}{\partial t} + \nabla\cdot\left(\epsilon_g\langle\rho_g\rangle^g\langle\boldsymbol{v_g}\rangle^g\right) = -\sum_{i\in N_s} M_i\langle\pi_i\rangle \quad \text{Gas phase}$$

Accumulation — Transport — Rate of mass loss/prod

Momentum conservation equations:

$$\nabla\cdot\langle\underline{\underline{\boldsymbol{\sigma}}}\rangle^s = \mathbf{0} \quad \text{Solid phase}$$

$$\langle\boldsymbol{v_g}\rangle^g - \langle\boldsymbol{v_s}\rangle^s = \frac{-1}{\epsilon_g\langle\mu_g\rangle^g}\,\underline{\underline{K}}\cdot\nabla\langle p_g\rangle^g \quad \text{Gas phase}$$

Permeability

Energy conservation equation:

$$\frac{\partial\left(\langle\rho_t\rangle\langle e_t\rangle\right)}{\partial t} + \nabla\cdot\left(\epsilon_g\langle\rho_g\rangle^g\langle h_g\rangle^g\langle\boldsymbol{v_g}\rangle^g\right) = \nabla\cdot\left(\langle\underline{\underline{k}}\rangle\cdot\nabla\langle T\rangle\right) - \nabla\cdot\left(\sum_{i\in N_s}\epsilon_{s,i}\langle\rho_{s,i}\rangle^i\langle h_{s,i}\rangle^i\langle\boldsymbol{v_s}\rangle^s\right)$$

Accumulation — Gas transport — Conduction — Solid transport

Chemical reaction modeling

Chemical kinetic equations:

The general form of a chemical mechanism composed of N_s species S_i and N_r reactions:

$$\sum_{i\in N_s}\nu_{i,r}^f S_i \underset{k_r^b}{\overset{k_r^f}{\rightleftharpoons}} \sum_{i\in N_s}\nu_{i,r}^b S_i \quad \forall r\in N_r$$

The total mass production rate for a species i due to all reactions considered is given by:

$$\langle\pi_i\rangle = \sum_{r\in N_r}\left[\left(\nu_{i,r}^f - \nu_{i,r}^b\right)\left(k_r^f\prod_{i\in N_s}\langle X_i\rangle^{m_{i,r}^f} - k_r^b\prod_{i\in N_s}\langle X_i\rangle^{m_{i,r}^b}\right)\right]$$

Mass prod/loss rate

With the Arrhenius law:

$$k_r^f = \mathcal{A}_r\langle T\rangle^n\exp\left(\frac{-\mathcal{E}_r}{R\langle T\rangle}\right)$$

With the species molar fraction:

$$\begin{cases}\langle X_i\rangle = \varepsilon_i\langle\rho_i\rangle^i / M_i\\ \langle X_i\rangle = \langle\rho_g\rangle^g\langle y_i\rangle^g / M_i\end{cases}$$

[1,2,5]

Chemical mechanism:

Wood

- Cellulose → Volatiles + Char + Gases $_{trapped}$
- Active Cellulose → Volatiles + Char + Gases $_{trapped}$ / Sugars + Gases $_{trapped}$
- Hemicelluloses → Hem 1 + Hem 2
- Hem 1 → Volatiles + Char + Gases $_{trapped}$
- Hem 2 → Furans + Gases $_{trapped}$ / Volatiles + Char + Gases $_{trapped}$
- Lig-C → Volatiles + Char + Gases $_{trapped}$ + Lig-CC → Volatiles + Char + Gases $_{trapped}$
- Lig-H → Volatiles + Gases $_{trapped}$ + Lig-OH
- Lig-O → Volatiles + Gases $_{trapped}$ + Lig-OH
- Volatiles + Char + Lig + Gases $_{trapped}$ → Volatiles + Gases $_{trapped}$ + Phenols / Volatiles + Char + Gases $_{trapped}$ / Volatiles + Char + Gases $_{trapped}$
- Extractives → Volatiles + Gases $_{trapped}$ + Char

[3,4]

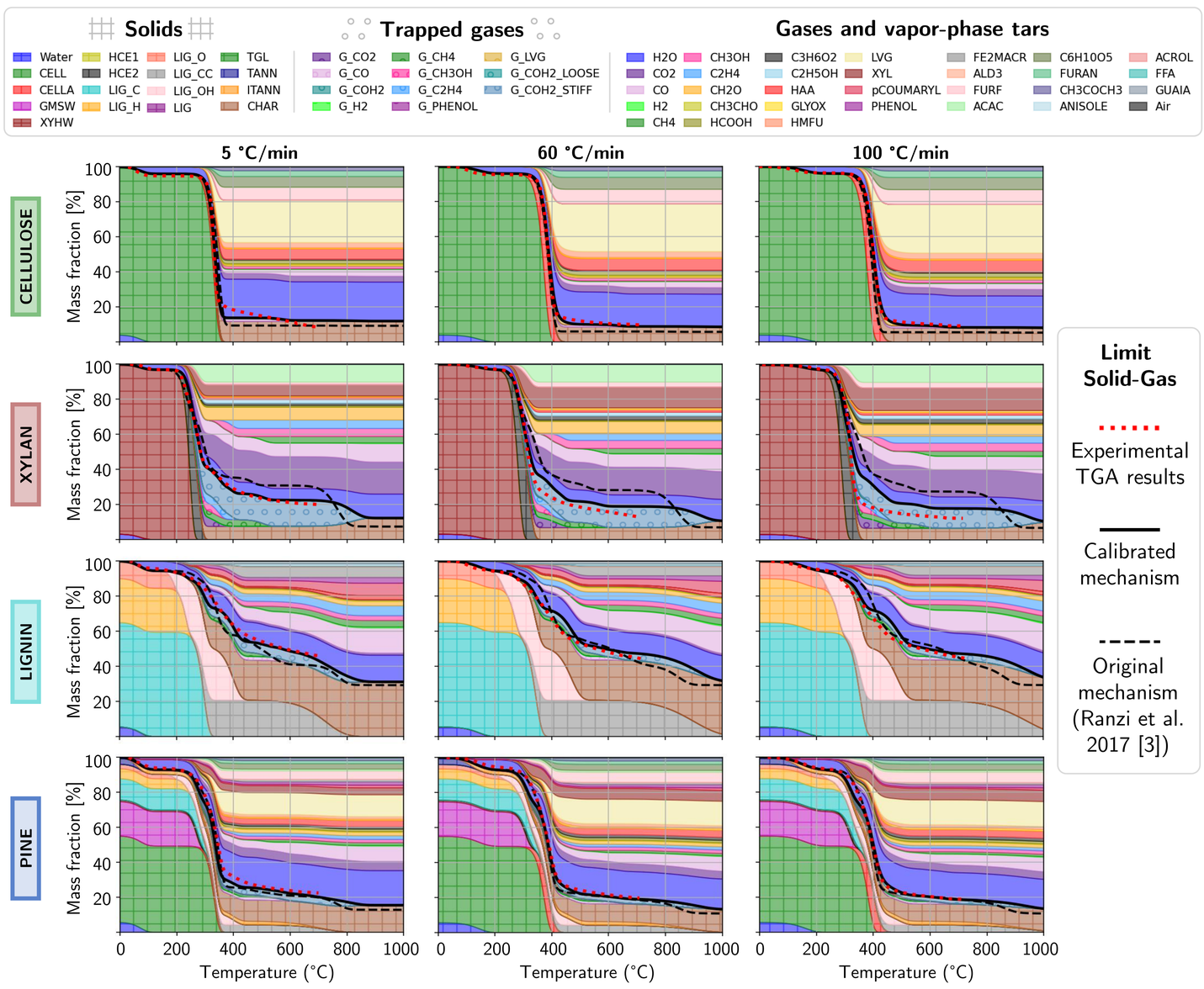
* Gases $_{trapped}$ are gaseous intermediates trapped in the solid matrix

Gases $_{trapped}$ → Volatiles / Volatiles + Char

Results

The following graphs show the evolution of mass fractions during pyrolysis for different wood components at three heating rates. The initial solid fraction (hatched) decreases with temperature as new species are formed: intermediate solids, trapped gases (circle markers) that are subsequently released from the solid matrix, and finally gases and non-condensed tars (solid colors).

NB: Although pine hemicellulose is mainly composed of glucomannans, xylan was used as a model compound because no suitably pure glucomannan was commercially available.



Implementation of competitive mechanism allows tracking the evolution of 50+ species during pyrolysis, showing heating rate effects on product distribution. Calibration and adaptation of the original mechanism improve the prediction of solid evolution.

Can you spot it? The original mechanism parameters have been chosen to better represent wood pyrolysis, whereas this work has been calibrated on the individual components !

Conclusions & Perspectives

New developments:

- Competitive mechanisms were successfully implemented and validated against benchmark software in 0D configurations to verify the chemistry.
- The energy equation was validated in a 0D test case against an analytical solution.
- 1D and 2D-axisymmetric simulations can now be coupled with the solid deformation solver recently developed [5]. Simulation times range from a few seconds to a few minutes.
- The mechanism was adapted to improve agreement with experimental solid residue evolution as a function of temperature.
- The Arrhenius parameters (E, A, and n) were chosen to remain consistent with values reported in the literature and in a previous study [6].

The next steps:

- The mechanism could still be improved to better reproduce experimental gas production and species evolution.
- Interactions between biomass components may delay their decomposition; additional reactions could be introduced to account for this phenomenon.

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