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COMPARISON BETWEEN SIMPLE AND DETAILED KINETIC SCHEMES OF BIOMASS THERMAL DEGRADATION – TWO DIMENSIONAL CFD MODELLING OF PYROLYSIS OF ANISOTROPIC LARGE WOOD PARTICLES

Introduction and scope

Inhomogeneity of biomass composition and a lack of knowledge about the detailed influence of the process parameters causes a problem in the prediction of the pyrolysis outcome with appropriate accuracy. A better understanding of the biomass single particle behaviour during the pyrolysis process, with numerical models, would improve the prediction accuracy and in the future, increase the possibility of applying this biomass processing technology on a larger scale.

This work aimed to identify a kinetic model which will show the lowest discrepancy with the experimental data of pyrolysis of a porous single large wood particle. Kinetics were compared between simple competitive scheme and detailed schemes, represented by the improved Ranzi scheme and the Ranzi-Anca-Couce (RAC) scheme.

- All models were validated with experimental data of Bennadji et al. (2014)
- Particle's thermo-physical parameters were applied accordingly to Park et al. (2010). The exception was radial thermal conductivity of biomass, which was chosen to be 20% higher.
- Particle had cylindrical shape (Ø1.905cm x 4cm). Initial conditions: absolute solid density of 1500 kg/m3, the porosity of 0.68. Initial bio-composition (wt. %): 44.1 CELL, 21.8 HCE, 11.3 LIGC, 4.4 LIG-H, 18.4 LIG-O.
- A two dimensional, CFD model was built using the commercial software COMSOLTM v. 5.4. The domain was modelled as 2D-axisymmetric and was meshed into 1600 elements (20x80). Differential equations were discretized in the first order scheme.

Tab. 1. Models components gouverning equations and boundary conditions

Component		Gouverning equations	Boundary conditions
Mass	Solids	$\frac{\partial}{\partial t} < \rho_S >= \dot{\omega}_S$	$D_{eff} \nabla (< \rho_s >) \mid_{x=x_p} = 0$
	Gas compounds	$\frac{\partial}{\partial t} < \rho_i > + \nabla < u_G \rho_i >= \dot{\omega}_i$	$D_{eff} \nabla (< \rho_i >^G) \mid_{x=x_p} = h_m \left[\rho_{i,\infty} - < \rho_i >^G \mid_{x=x_p} \right]$
Momentum	Gases	$< u_G >= \frac{K_{G,eff}}{\mu_G} \nabla (< P_G >)$	$< P_G > \mid_{x=x_p} = P_\infty$
Energy	Total	$\frac{\partial T}{\partial t} \left(< \rho_S > C_{P,S} + \varepsilon_G < \rho_G >^G C_{P,G} \right) + \nabla T \left(\varepsilon_G \sum_{i=1}^{N} < u_i \rho_i > C_{P,i} \right) = \nabla \left(\lambda_{eff} \nabla T \right) + Q$	$\nabla \left(\lambda_{eff} \nabla T \right) \mid_{x=x_p} = h_T \left(T_{flow,\infty} - T \mid_{x=x_p} \right) + \sigma \omega \left(T_{wall}^4 - T^4 \mid_{x=x_p} \right)$

Kineic schemes

Simple - Shafizadeh's and Chin's (1978) competitive scheme; 3 reactions and 4 compounds. Biomass is not divided into bio-components and products are modelled as **lumped groups**: Gas (1:1 mixture of CO2 and CO), Tar (benzene) and Char (carbon)

Detailed models distinguish the biomass bio-components composition (lignin in 3 artificial forms), char is modelled as carbon and metaphase traps:

- **Ranzi** - The improved Ranzi model of fast pyrolysis (Deblagi et al. 2018); 25 reactions and 48 compounds
- **RAC** - The Ranzi-Anca-Course intermediate pyrolysis scheme (Anca-Couse et al. 2017); 24 reactions and 33 compounds (+5 parameters of charring)

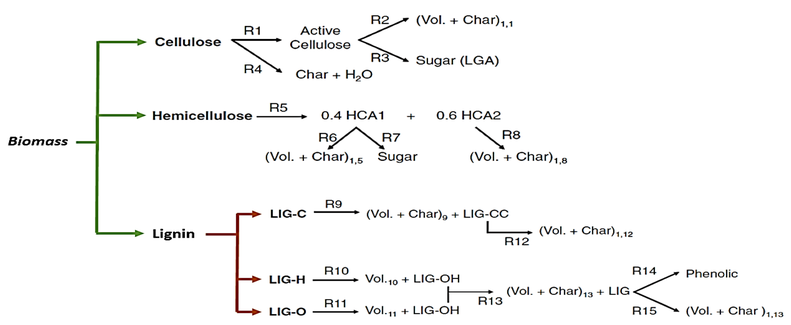

Fig. 1. The Ranzi fast pyrolysis scheme

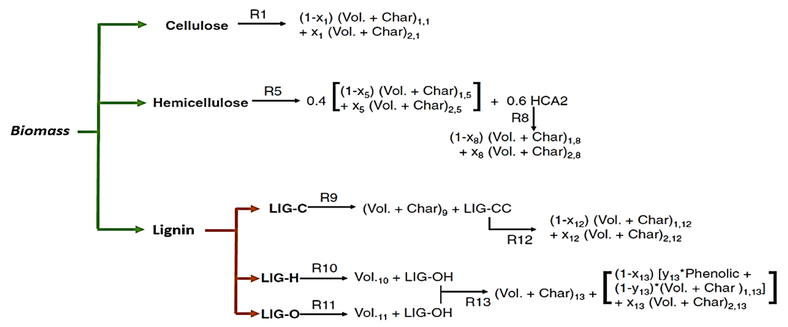

Fig. 2. The Ranzi-Anca-Couse (RAC) intermediate pyrolysis scheme

Center Temperature and products yield

- All models agree well with experimental data, but the RAC model was the best; Simple (R2=0.965), Ranzi (R2=0.965) and RAC (R2=0.995)
- Only detailed models were able to predict the temperature peak between 350-500s. The RAC model predicts the peak most accurately.
- Models predict the products yields with good accuracy (5-10% differenced deviation).
- The Ranzi model gives a better prediction of yields of all products in comparison to the RAC model.

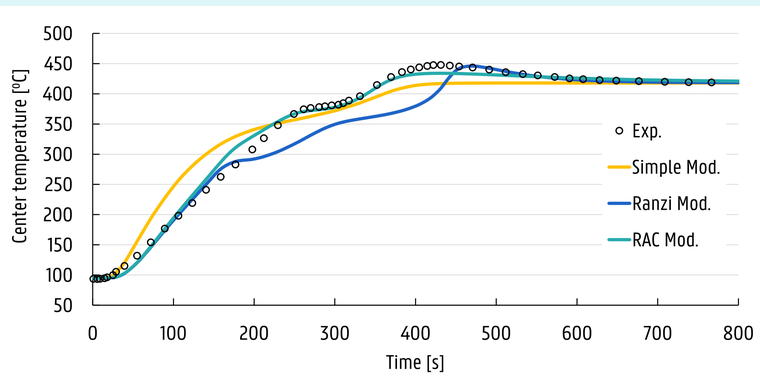

Fig.3. Temperature center simulations results against experimental data from Bennadji et al. (2014)

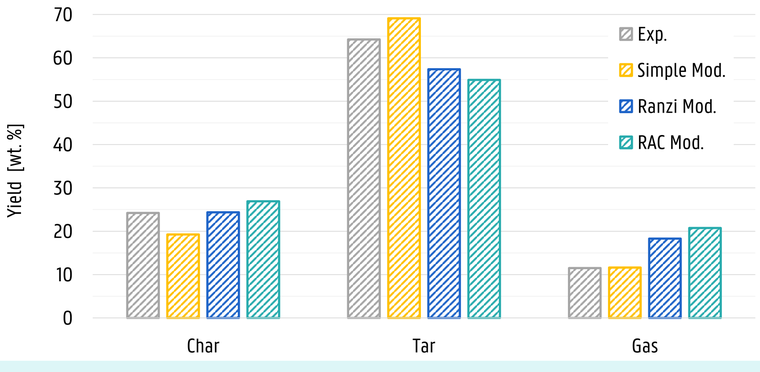

Fig. 4 . Products yields simulations results against experimental data from Bennadji et al. (2014)

Boundary gases outflow

- On Fig. 5 shows simulation results of boundary gases outflow from the particle for the Ranzi and the RAC kinetic scheme
- The Simple model was not taken into account (lumped groups of products)
- Both models show moderate agreement with experimental data for the outflow of the CO_2 and CO, over-predicting its formation n first 200s of process
- Both models strongly over-predicts the formation of the methane in the first 300s; the RAC model perform better at the end of conversion
- The Ranzi model show better agreement for the prediction of the methanol formation
- For the formaldehyde and acetic acid, the Ranzi model strongly under-predicts its formation, in opposition to the RAC model which shows good agreement with experimental data

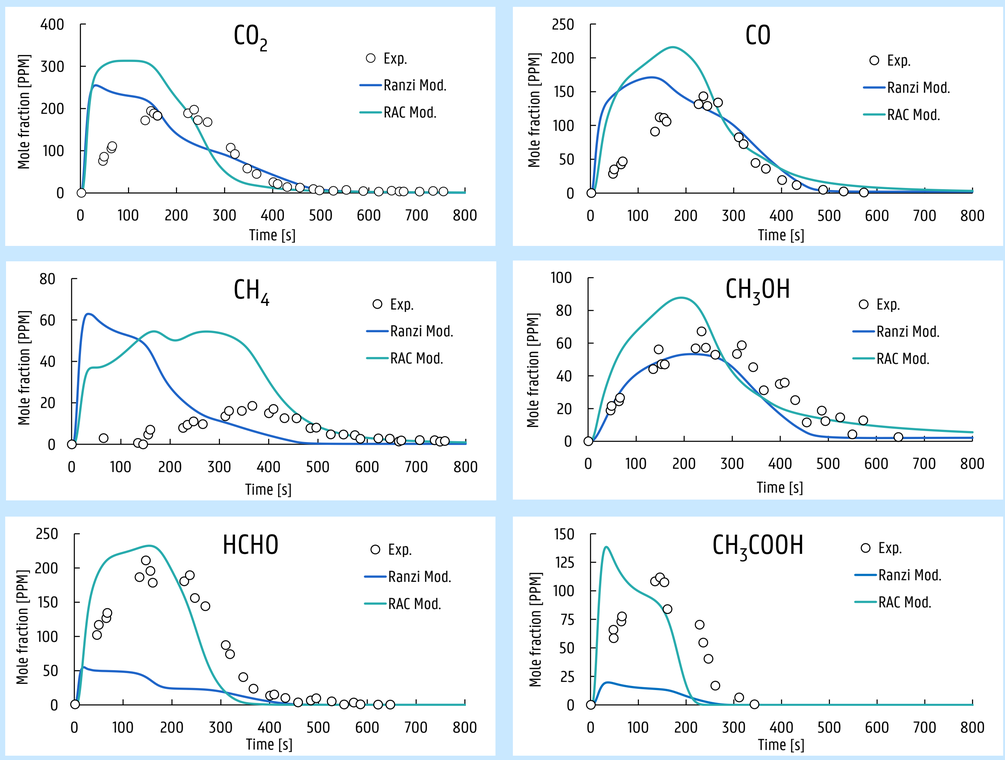

Fig. 5. Boundary gases outflow in function of time simulations results against experimental data from Bennadji et al. (2014)

Thermal effects of the reactions

- The thermal effects of the specific reaction contained in the Ranzi and the RAC scheme
- The Ranzi model shows more extreme changes in the thermal effects compared to the RAC scheme
- The existence of extreme changes in thermal effect cause problems with the model's simulation stability and hinder the model from achieving the convergence

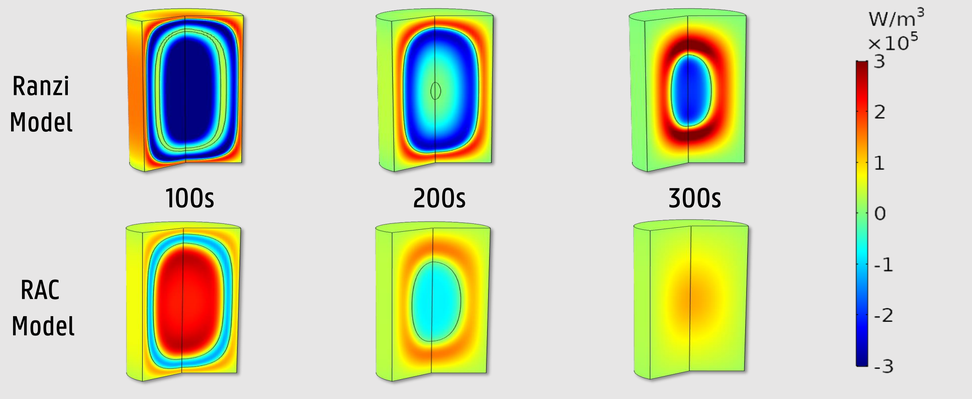

Fig. 6. Results of particle's reactions thermal effect at different time (shown as 3D axisymmetric)

Conclusions

Detailed models show better agreement with experimental data than a simple kinetic scheme and are able to predict the composition of the vapours produced during the pyrolysis of the large wood particle.

Between two detailed models, the RAC kinetic scheme performs better than Ranzi model in terms of the center temperature, gas composition, and its implementation do not introduce significant model instability during the simulation.

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