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MODELING AND NUMERICAL SIMULATION OF WOOD TORREFACTION

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ABSTRACT

Torrefaction is a thermal treatment step in a relatively low temperature range of 210–240˚C, which aims to improve the dimensional stability and durability of wood. The weight loss kinetics for torrefaction of wood samples was studied using equipment specially conceived to measure mass losses during thermal treatment. Laboratory experiments were performed under nitrogen. A mathematical model for the kinetics of the thermodegradation process was used and validated. Measurements of temperature distribution and weight loss were performed sample of poplar wood during pyrolysis in an inert atmosphere at 230°C. The mathematical formulation describing the simultaneous heat and mass transfers requires coupled nonlinear partial differential equations. These unsteady-state mathematical model equations were solved numerically by the commercial package FEMLAB. A detailed discussion of the computational model and the solution algorithm is given. Once the validity of different assumptions of the model had been analyzed, the experimental results were compared with those calculated by the model. Acceptable agreement was achieved.

Key words: Heat treatment, modelling, reaction kinetics; thermo-degradation, wood

INTRODUCTION

Wood is commonly used as building and engineering material. Unprotected wood exposed to outdoor conditions undergoes a variety of degradation reactions induced by diverse factors such as light, moisture, heat, oxygen, pollutants (Evans *et al*. 1992). Moisture content promotes the fungal attack leading to sever destruction of wood. In the past, wood preservation has been carried out by chemical treatments, some of them including components that are poisonous for environment and human health. Nowadays, heat treatment of the wood by mild pyrolysis is used as an alternative to chemically impregnated wood materials when this latter one is not directly used in ground contact. It is an effective method to improve biological durability of wood (Shi *et al*. 2007). Wood heat treatment induces chemical modification and confers new properties as an improved dimensional stability (Mouras *et al*. 2002, Esteves *et al*. 2007, Esteves *et al*. 2007b) and better fungal resistance (Hakkou *et al.* 2006, Kamdem and Pizzi 2002). Chemical reactions involved during mild pyrolysis as well as final properties of the material depend strongly on the treatment temperature and process duration. During the heat treatment, wood is thermally decomposed at a slow rate (Repellin and Guyonnet 2005). The resulting anhydrous mass loss (ML) is representative for physical and chemical wood transformations and matches to the advancement of the heat treatment process.

Wood thermal degradation is a complex topic given that the material contains several fractions with different thermal behaviour.

Authors often distinguish a number of stages (Repellin and Guyonnet 2005, Nguila *et al.* 2009). A phase of elimination of some volatile compounds takes place at temperatures lower than 200 °C. For temperature range of 200–280 °C, hemicelluloses, lignin and cellulose are decomposed to give three products: gas, tar and char. Conferred properties of heat treated wood depend on the mass loss due to the thermodegradation (Weiland *et al.* 1998, Chaouch *et al.* 2010). Consequently, controlling the quality of the heat treated wood means to control precisely the mass loss during the treatment. Thus, the knowledge of the kinetic schemes of wood thermodegradation is required.

The aim of this work is to build up a kinetic model which could be applied to the industrial wood heat treatment processes, and make recommendations concerning the operating temperature and treatment duration in order to obtain a required mass loss. Because of the quantity and the complexity of degradation and polymerization reactions occurring in the wood during the heat treatment (Candelier *et al*. 2011), the concept is a simplified approximation of real phenomena. Wood thermodegradation is described using a two-stage, semi-global kinetic model. Numerous experiences of heat treatment at 210, 220 and 230 °C under nitrogen were carried out for Poplar wood species. The instantaneous mass loss and temperature were recorded. Experimental data were used to determine model parameters. Finally, a comparison between experimental data and numerical results was proposed.

1. MATERIAL AND METHODS

1.1. WOOD SAMPLE AND HEAT TREATEMENT PROCESS

Heat treatment is carried out on poplar (*Populus nigra*) wood panels of large sections, dried in a steam room at 105 °C until mass stabilization. Panel's dimensions are 25 x 11 x 2.5 cm^3 respectively in the longitudinal, tangential and radial directions.

Wood species were thermally treated under nitrogen, by conduction between two metallic heating plates. The device was placed on a precision balance allowing the record of the dynamic mass loss and instantaneous temperature. Experimental apparatus was more precisely detailed in a previous work (Chaouch *et al.* 2010). The heat treatment consists of three successive thermal stability areas. First one is kept at 105°C in order to reach the anhydrous mass. The second one (165 °C) is useful for the thermal homogenization of the panel. The wood roasting was performed at 210, 220 and 230 °C.

1.2. MATHEMATICAL FORMULATION

Wood thermodegradation is a complex set of degradation and polymerization reactions giving several reaction products (Nguila *et al*. 2009, Weiland *et al*; 1998). Mathematical modeling of occurring coupled heat and mass transfers is a simplified approximation of real phenomena. Variety of methods based on the thermal analysis of polymer thermodegradation has been developed. An overview of required measurement, kinetic analysis of solid state reaction leading the determination of the reaction order and parameterization of the reaction rate, method's advantages and drawbacks has been proposed in the literature (Vyazovkin *et al.* 2011). Modeling of polymer thermodegradation is often based on global kinetics, since trying to represent full complexity of the process makes no sense. Global kinetics uses the key steps in the overall mass loss process. There is an ongoing debate concerning the determination of the kinetic parameters of the global reactions of wood pyrolysis (Di Blasi and Lanzetta 1997, Rousset *et al.* 2006, Grioui *et al.* 2006). Models available in the literature usually assume that kinetics of all the thermodegradation reactions obey an Arrhenius low defined by its kinetic constant and activation energy (Koufopanos *et al.* 1991, Di Blasi and Lanzetta 1997, Rousset *et al.* 2006, Grioui *et al.* 2006).

The following section is devoted to the mathematical formulation of coupled heat and mass transfers in wood porous media introducing heat effects due to the reactions of polymer decomposition, production of volatiles and non-degradable solid products. The sample thickness is very weak compared to the other dimension and modeling can be represented in 1D. The macroscopic conservation equation governing heat transfer phenomenon is given by:

$$\rho(t)\, Cp(T)\, \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda(T)\, \frac{\partial T}{\partial x} \right) + Hp\, \frac{\partial \rho(t)}{\partial t} \qquad \textbf{(1)}$$

Where: $\rho(t) = m(t)/V$ is the averaged anhydrous wood density, T is the local temperature; Hp is the global reaction enthalpy. The instantaneous sample weight $m(t)$. Mechanism adopted in this work is based on a two-stage, semi-global multi-reaction kinetic model of wood mild pyrolysis. Then, wood is assumed to be subdivided into three pseudo-components A_1, A_2, A_3, as it was previously done by (Grioui *et al.* 2006). Each pseudo-component is characterized by a specific kinetic law of decomposition and a mass fraction: $\alpha_1 = m_{A_1}/m_0$, $\alpha_2 = m_{A_2}/m_0$ and $\alpha_3 = m_{A_3}/m_0$ (m_{A_1}, m_{A_1} and m_{A_3} are the masses of pseudo constituents A_1, A_2, A_3 in the native wood and m_0 is the mass of the native anhydrous wood sample). At 165 °C occurs the elimination of some volatile wood compounds, the degradation of A_1 prevails giving a gaseous product G_1: $A_1 \xrightarrow{k_1} G_1$. At 210–230°C the thermo-degradation of A_2 leads to the production of a solid fraction C_2 and a gas product G_2: $A_2 \xrightarrow{k_2} \gamma_2\, C_2 + (1-\gamma_2) G_2$.

Mass fraction of non-degradable solid γ_2 depends on the operating temperature. With the assumption that kinetic of all involved reactions is described by a first order law, mass balance equations can be written:

$$\frac{\mathrm{d}\, m_{A_1}(t)}{\mathrm{d}\, t} = -k_1 m_{A_1}(t) \qquad \textbf{(2)}$$

$$\frac{\mathrm{d}\, m_{A_2}(t)}{\mathrm{d}\, t} = -k_2 m_{A_2}(t) \qquad \textbf{(3)}$$

$$\frac{\mathrm{d}\, m_{C_2}(t)}{\mathrm{d}\, t} = k_2\, \gamma_2\, m_{A_2}(t) \qquad \textbf{(4)}$$

Where, $m_{A_1}(t)$, $m_{A_2}(t)$ and $m_{C_2}(t)$ are the instantaneous mass of the constituents A_1, A_2 and C_2; k_1 and k_2 are the reaction rate constants obeying an Arrhenius low: $k_1 = k_{01} \exp\left(-\frac{Ea_1}{RT} \right)$, $k_2 = k_{02} \exp\left(-\frac{Ea_2}{RT} \right)$. k_{01} and k_{02} are the pre-exponential factors; Ea_1 and Ea_2 are the activation energies of global thermo degradation reactions of pseudo constituents A_1 and A_2. Instantaneous total sample mass is $m(t) = m_{A_A}(t) + m_{A_2}(t) + m_{A_3}(t) + m_{C_2}(t)$.

The resolution of the Eq. (1-4) requires the determination of 8 parameters: pre-exponential factors k_{01}, k_{02}, and activation energies Ea_1, Ea_2, mass fraction fractions α_1, α_2 and γ_2; reaction enthalpy *Hp* of the global process. Kinetics parameters have been derived numerically.

The mass loss is calculated by the formula: $ML = \left(m_0 - m(t)\right)/m_0$.

Governing equations are solved numerically with the commercial package Femlab 2.0. The mesh convergence was verified with refined mesh sizes. Time step of 360 s, 1866 nodes and 8080 elements mesh size were considered to be appropriate.

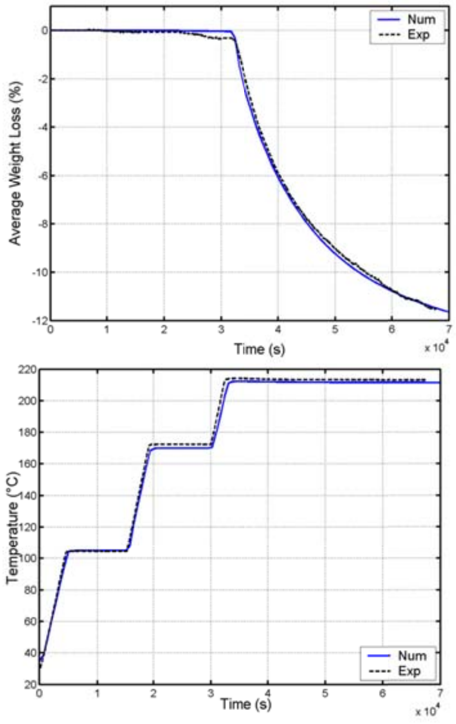
The kinetic parameters obtained with this method are given in Table 1:

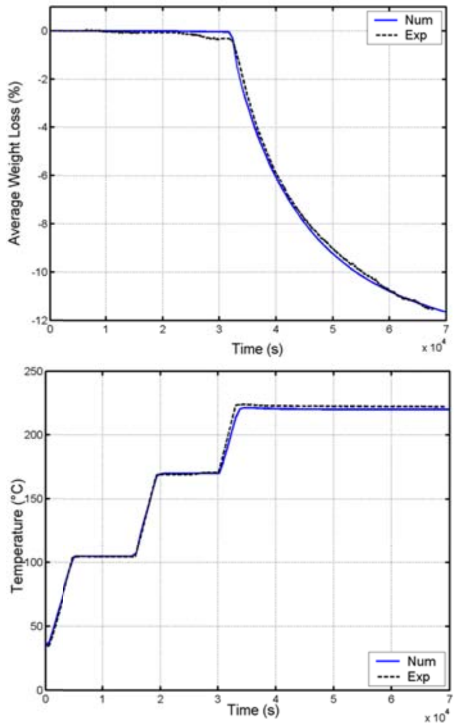
Table 1: Kinetic parameters used in the numerical simulation for the poplar.

α_1	α_2	**E_{a1} [kJ.mol^{-1}]**	**E_{a2} [kJ.mol^{-1}]**	**k_{01} [s^{-1}]**	**k_{02} [s^{-1}]**	γ	**Hp [kJ.mol^{-1}]**
0.08	0.12	118.5	119.0	4.10^{7}	6.10^{8}	0.07	123.0

2. RESULTS AND DISCUSSION

2.1. SIMULATION OF THE TRATEMENT TEMPERATURE EFFECT





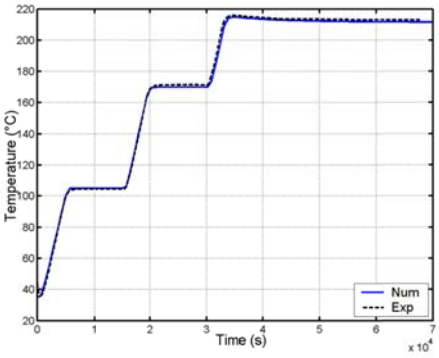


Figure 1: Time evolution of average weight loss, surface temperature, center temperature: 1 °C.min^{-1}, T_{max}=210 °C.

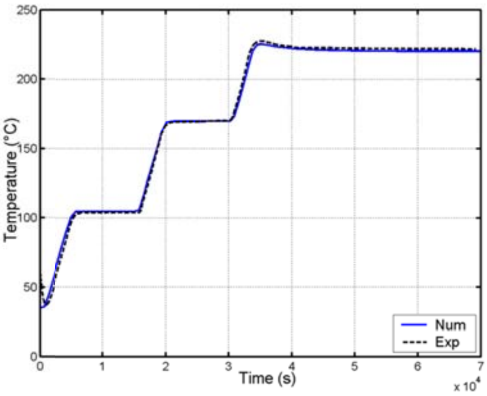
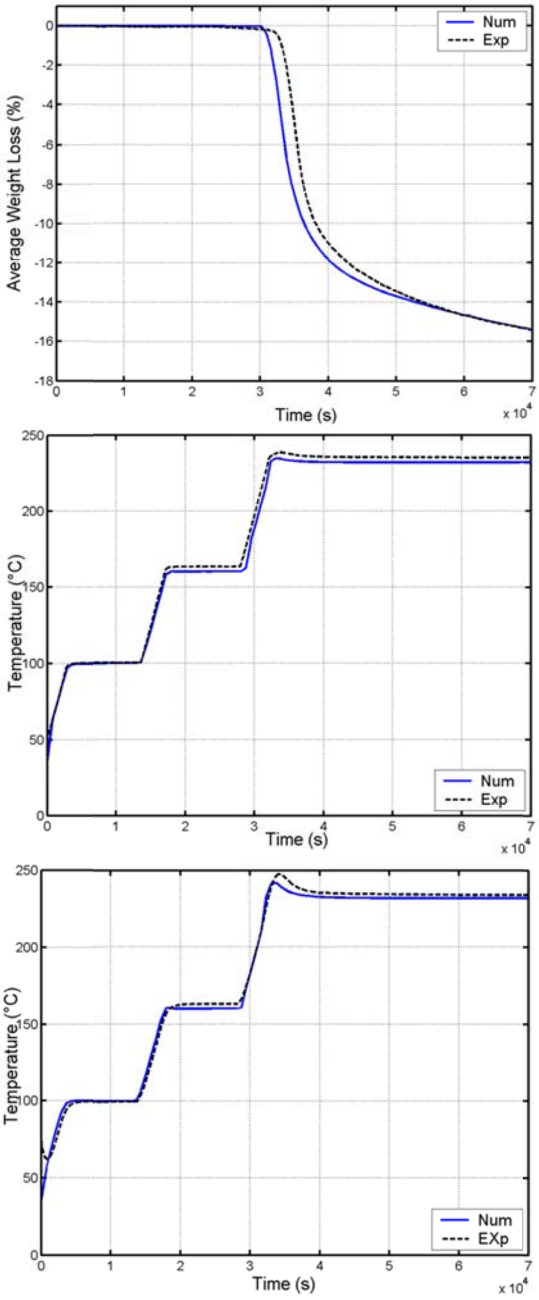


Figure 2: Time evolution of average weight loss, surface temperature, center temperature: 1 °C.min^{-1}, T_{max}=220 °C.



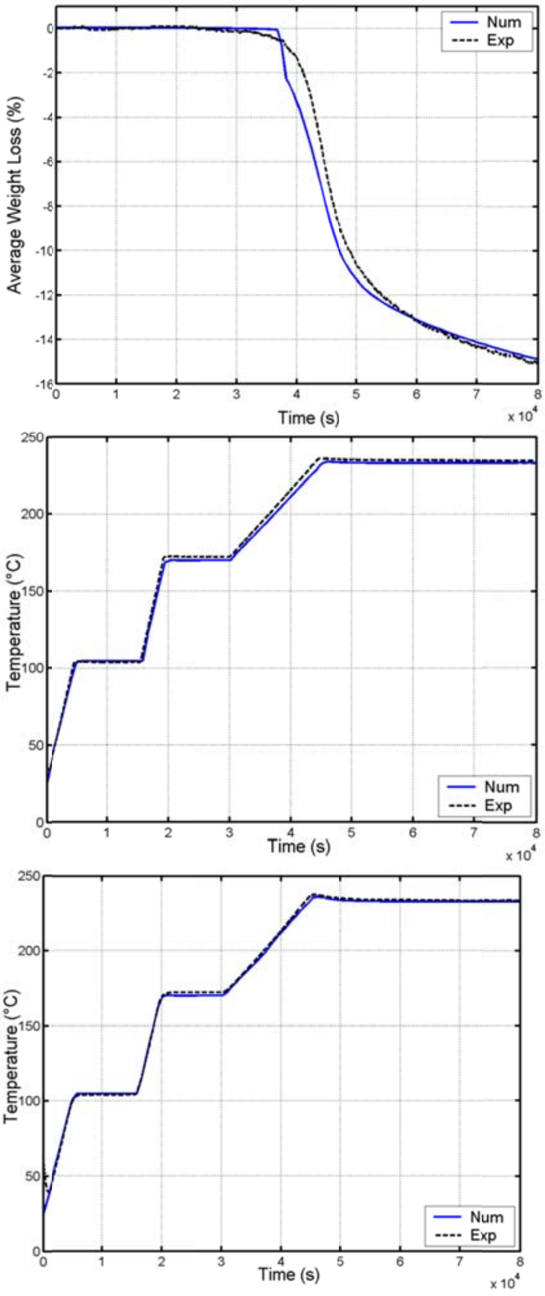


Figure 3: Time evolution of average weight loss, surface temperature, center temperature: 1 °C.min^{-1}, T$_{max}$= 230 °C.

Figure 4: Time evolution of average weight loss, surface temperature, center temperature: 0.25 °C.min^{-1}, T$_{max}$=230 °C.

The effect of the heat treatment temperature of on the anhydrous weight loss has been investigated. Three experiences with poplar wood have been carried out during 20 hours under heat treatment temperature respectively 210 °C, 220 °C and 230 °C. The heat treated rate has been fixed to 1 °C.min^{-1}. Experimental and numerical results are shown on Fig. 1–3. It can be observed that the increase of the treatment temperature enhances the mass loss. A good agreement is observed between the experience and the numerical simulation.

2.2. SIMULATION OF THE HEATING RATE EFFECT

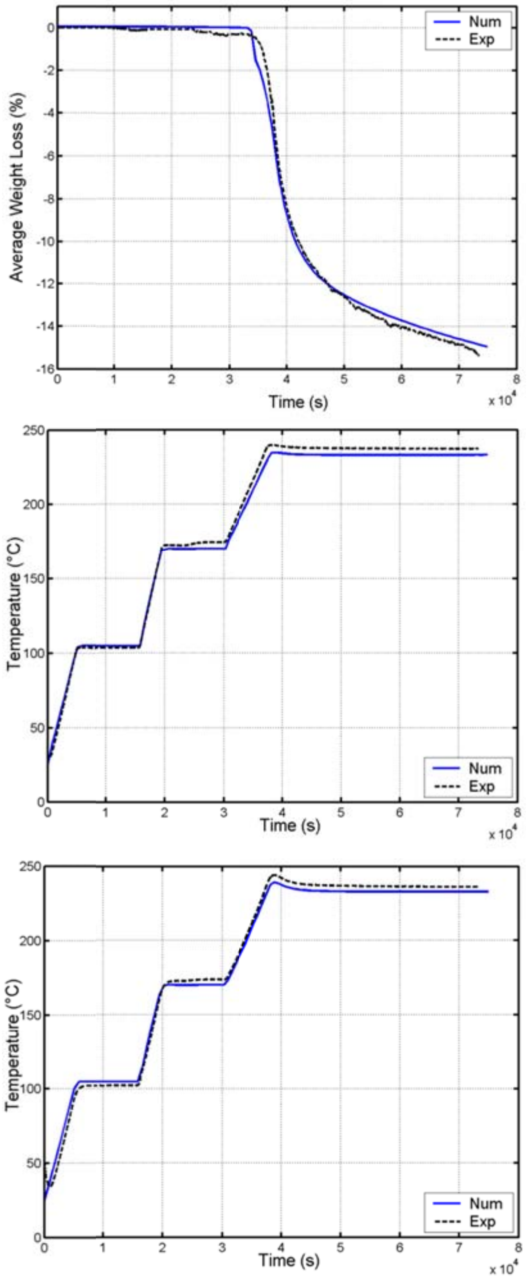


Figure 5: Time evolution of average weight loss,

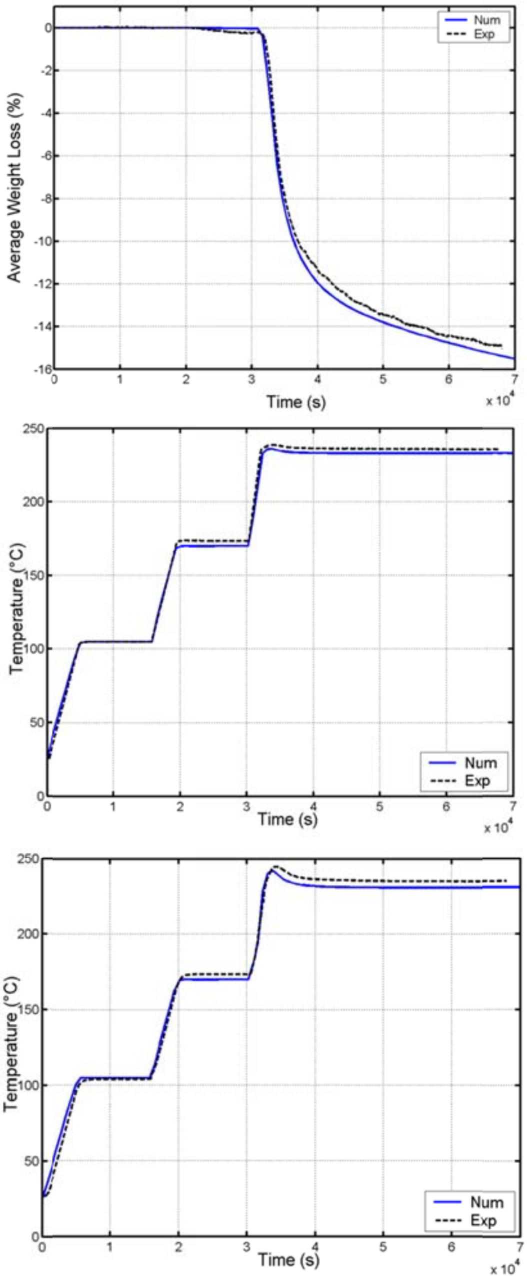


Figure 6: Time evolution of average weight loss,

surface temperature, center temperature: 0.5 °C.min^{-1}, T$_{max}$=230 °C.

surface temperature, center temperature: 2 °C.min^{-1}, T$_{max}$=230 °C.

The study has been performed on the poplar wood, under treatment temperature 230°C and for different temperature rates, respectively 0.25, 0.5, 1 and 2 °C.min^{-1}. Results are shown on Fig. 3-5.

CONCLUSION

Wood thermodegradation kinetics was investigated. A semi global multi constituents' mathematical model was proposed and validated. This model allows the simulation of temperature profiles and average mass loss. The Femlab software was used to solve the system of partial differential equations. The comparison between numerical results and experimental data shows a reasonable agreement. This model can be used in the design of industrial pyrolysis installations. However the determination of the kinetic parameters for each wood species is required.

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