A New Algorithm for Solving Isothermal Carbonization of Wood Particle

Ahmed Mahmoudi, Imen Mejri, Mohamed A. Abbassi, Ahmed Omri

Abstract—A new algorithm based on the lattice Boltzmann method (LBM) is proposed as a potential solver for one-dimensional heat and mass transfer for isothermal carbonization of wood particles. To check the validity of this algorithm, the LBM results have been compared with the published data and a good agreement is obtained. Then, the model is used to study the effect of reactor temperature and particle size on the evolution of the local temperature and mass loss inside the wood particle.

Keywords—Lattice Boltzmann Method, pyrolysis, conduction, carbonization.

I. INTRODUCTION

WOOD carbonization is a promising route for production of charcoal as well as gaseous fuels. However, experimental results show that the thermal decomposition of the material wood is an unpredictable and complex process. Particularly, the complexity of some phenomena during the carbonization of thick wood particles, such as heat and mass transfer within the wood, chemical reactions and mechanical deformations, and the absence of detailed information about the chemical kinetics and the evolution of the thermal properties of wood in the different stages of decomposition from the virgin wood up to the charcoal constitute a major problem to the development of relevant models of carbonization. Salazar et al. [1]–[3] studied the influence of the size and shape of the wood particles on the pyrolysis mechanisms. According to these authors, the thermal decomposition of wood results in three parallel reactions of first order, corresponding respectively to the decomposition of hemicellulose, cellulose and lignin. The reactions rate is described by an Arrhenius formalism, whose kinetic parameters are determined experimentally. This model gave satisfaction only for wood particles whose diameters are lower than 20mm. Koufopanos et al. [4] defined a model in which they coupled conduction heat transfer with chemical kinetics. They concluded that the reactions heat can be represented by endothermic or exothermic values according to the conversion rate. The model predictions show a good agreement with experimental data relevant to a diameter of 20mm. Di Blasi and Russo [5], [6] proposed a model based on three primary

reactions and two secondary reactions that follow the formalism of Arrhenius. Also, the model takes into account conduction, convection and radiation heat transfer. The validation of this model with the experimental data of Lee et al. [7] relevant to a diameter of 25mm shows good predictions only for short reaction times. Gronli [8] developed a transient mono-dimensional model for the simulation of humid wood drying and pyrolysis. This model is based on a wood decomposition scheme including three parallel reactions leading to simultaneous production of gas, tar and charcoal and takes into account interactions between mass, momentum and heat transfer in the porous structure of the wood. The model leads to the study of the effect of the wood particle diameter ($1 \leq d \leq 100$mm) and the intensity of the heating flux ($50 \leq \Phi \leq 200$kWm²) on the temperature profile and the production rate of different products. The predictions of this model are in good agreement with their experimental data. Larfeldt et al. [9] have modified the mono-dimensional model of Melaaen [10] to take into account the structural changes during pyrolysis of the wood. In comparison with the experimental data, the results of the modified model show an important reduction of pyrolysis time. Peters and Bruch [11] have developed a numerical study similar to that of Gronli [8] that was positively validated experimentally. Abbassi et al. [12] investigated into pyrolysis of biomass both experimentally and numerically. The reactor was divided into three zones that were treated as perfectly stirred reactors. Tar as a major product of pyrolysis was assumed to crack into methane CH_4, carbon monoxide CO, carbon dioxide CO_2 and hydrogen H_2, determined by an Arrhenius expression. The model was validated with measurements and was used to control plant operation. Rattea et al. [13] predicted pyrolysis of wood waste by a model approach developed earlier by Peters [14] and proved that this approach may also be employed to large wood particles. The latter approach has also been used by Sadhukhan et al. [15] for large wood particles and they emphasised that intra-particle convection is important. Dupont et al. [16] performed biomass pyrolysis also in an entrained flow reactor under high temperatures from 1073 to 1273K and high heat fluxes (10–100kW/m²). Their experimental results were compared to predictions of the kinetic mechanism of Ranzi et al. [17] and encouraged design and understanding of industrial gasifiers.

The aim of the present study is to develop a numerical algorithm to predict heat and mass transfer during the carbonization of wood particle. The algorithm is based on the LBM which to the knowledge of the authors, is applied at the first time to carbonization of wood particle. The proposed model takes into account the heat and mass transfer and
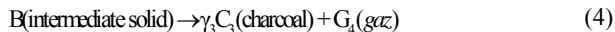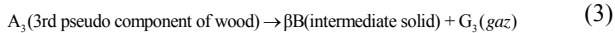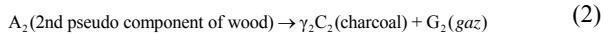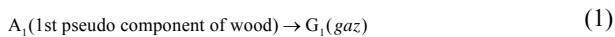
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chemical kinetics simultaneously. The thermal properties of wood are considered to be linear functions of the local temperature and have been estimated from literature data. The carbonization process has been described by a kinetic scheme based on a two stage semi-global kinetic model. The model is used to study the effect of reactor temperature and particle size on the evolution of the local temperature and mass loss inside the wood particle

A. Physical Model

Fig. 1 shows the physical model for the considered problem, a cylindrical dried wood particle is placed in a reactor at constant temperature (TR). The heat transfer at the particle surface takes place essentially by convection and radiation. As the temperature increases at the surface, heat diffuses inside the wood by conduction. The following carbonization reaction scheme, developed recently by the authors [18], is used here:

$$A_1(\text{1st pseudo component of wood}) \rightarrow G_1(gaz) \tag{1}$$

$$A_2(\text{2nd pseudo component of wood}) \rightarrow \gamma_2 C_2(\text{charcoal}) + G_2(gaz) \tag{2}$$

$$A_3(\text{3rd pseudo component of wood}) \rightarrow \beta B(\text{intermediate solid}) + G_3(gaz) \tag{3}$$

$$B(\text{intermediate solid}) \rightarrow \gamma_3 C_3(\text{charcoal}) + G_4(gaz) \tag{4}$$

By assuming that the kinetics is described by the first order laws of Arrhenius for the four reactions, the mass balance of the solid and slightly volatile components A_1, A_2, A_3, C_2, B and C_3, can be written, respectively:

$$\frac{\partial \rho_{A_1}}{\partial t} = -k_1 \rho_{A_1} \tag{5}$$

$$\frac{\partial \rho_{A_2}}{\partial t} = -k_2 \rho_{A_2} \tag{6}$$

$$\frac{\partial \rho_{A_3}}{\partial t} = -k_3 \rho_{A_3} \tag{7}$$

$$\frac{\partial \rho_{C_2}}{\partial t} = \gamma_2 k_2 \rho_{A_2} \tag{8}$$

$$\frac{\partial \rho_B}{\partial t} = \beta k_3 \rho_{A_3} - k_4 \rho_B \tag{9}$$

$$\frac{\partial \rho_{C_3}}{\partial t} = \gamma_3 k_4 \rho_B \tag{10}$$

where

$$k_i = k_{0i} \exp(E_{ai}/RT) \quad \text{for } i = 1, 2, 3 \text{ and } 4 \tag{11}$$

The activation energies E_{ai} and pre-exponential coefficients k_{0i} are given in Table I and γ_2, β and γ_3 are defined by experimental correlations in [18].

B. Formulation: Energy Equation

The energy equation for a control volume during carbonization is:

$$\rho c_{pw} \frac{\partial T}{\partial t} = \vec{\nabla}.\left(\lambda_w \vec{\nabla} T\right) + S \tag{12}$$

$$S = (k_1 \rho_{A_1} + k_2 \rho_{A_2} + k_3 \rho_{A_3})\Delta H + k_4 \rho_B \Delta H_4 \tag{13}$$

$$\rho = v_1 \rho_{A_1} + v_2(\rho_{A_2} + \rho_{C_2}) + v_3(\rho_{A_3} + \rho_B + \rho_{C_3}) \tag{14}$$

where S is the power generated by the exothermic reaction of the wood decomposition, ρ is the wood density and $v_{i=1,2,3}$ are the mass fraction, its values are reported in [18]. Thermo-physical properties of wood vary linearly with the local temperature and are estimated from relations published in the literature. These relations are given in Table II.

For resolution of (12), the following boundary conditions are considered:

At particle axis:
$$\left.\frac{\partial T}{\partial r}\right|_{r=0} = 0$$
$$\tag{15}$$

At the surface:
$$\left.\frac{\partial T}{\partial r}\right|_{r=d/2} = -\frac{h}{\lambda_w}\left(T_R - T(r=d/2,t)\right)$$

where h represents the global heat transfer coefficient these values are reported in Table III. The mass and energy conservation equations constitute a coupled nonlinear partial differential equations system that can be solved simultaneously by the LBM.

C. Lattice Boltzmann Simulation

The discrete Boltzmann Equation with Bhatanagar-Gross-Krook (BGK) approximation is given by [19]:

$$\frac{\partial f_i(\vec{r},t)}{\partial t} + \vec{e}_i.\nabla f_i(\vec{r},t) = -\frac{1}{\tau}\left[f_i(\vec{r},t) - f^{eq}_i(\vec{r},t)\right] \quad i = 1...m \tag{16}$$

where f_i is the particle distribution function denoting the number of particles at the lattice node $\vec{r}$ and time t moving in direction i with velocity $\vec{e}_i$ along the lattice $\Delta r = e_i \Delta t$ connecting the neighbors, m is the number of directions, τ is the relaxation time, and f^{eq}_i is the equilibrium distribution function.

After discretization, (15) is written as:

$$f_i(\vec{r} + \vec{e}_i \Delta t, \; t + \Delta t) = f_i(\vec{r},t) - \frac{1}{\tau}\left[f_i(\vec{r},t) - f^{eq}_i(\vec{r},t)\right] \tag{17}$$

The temperature is obtained after summing f_i overall direction:

$$T(\vec{r},t) = \sum_{i=1,m} f_i(\vec{r},t) \tag{18}$$

To process (17), an equilibrium distribution function is required, which for a conduction-radiation problem is given by:

$$f^{eq}{}_i(\vec{r},t) = w_i T(\vec{r},t) \qquad (19)$$

To account for the source term, the energy equation in the LBM formulation, (17) is modified to:

$$f_i(\vec{r}+\vec{e}_i \Delta t,\ t+\Delta t) = f_i(\vec{r},t) - \frac{1}{\tau}\left[f_i(\vec{r},t) - f^{eq}{}_i(\vec{r},t)\right]$$
$$-\frac{\Delta t\ w_i}{\rho(\vec{r},t)c_{P_w}(\vec{r},t)}S(\vec{r},t) \qquad (20)$$

The relaxation time τ for the D1Q2 lattice is computed from:

$$\tau = \frac{\lambda_w}{\left|\vec{e}_i\right|^2 \rho c_{pw}} + \frac{\Delta t}{2} \qquad (21)$$

For this lattice, the two velocities e_1 and e_2, and their corresponding weights w_1 and w_2 are given by:

$$e_1 = \frac{\Delta r}{\Delta t} \qquad e_2 = -\frac{\Delta r}{\Delta t} \qquad (22)$$

$$w_1 = w_2 = \frac{1}{2} \qquad (23)$$

II. RESULTS AND DISCUSSION

In order to check on the accuracy of the numerical technique employed for the solution of the considered problem, the present numerical code was validated with the published experimental results (Figs. 2 (a)-(c)) of Koufopanos et al. [4] for isothermal carbonization of a cylindrical wood particle of $d = 20 \times 10^{-3} m$ diameter and $\rho_w = 650$ kg m^{-3} density at reactor temperatures of T_R = 623 and 673 K.

Fig. 2 (a) shows the local temperature evolution at the axis of the wood particle at reactor temperature T_R = 623 K. the results show that the model describes correctly the temperature profile at the axis of the particle. Fig. 2 (b) shows

the local temperature evolution at $r = d/4$ at reactor temperature of 673 K. An excellent agreement is found. Fig. 2 (c) shows the residual density evolution of the wood particle. An excellent agreement is also found.

The present LBM algorithm is also validated with the numerical results of Grioui et al. [20] (Figs. 3 (a)-(c)) obtained by the finite difference method using an implicit scheme, for isothermal carbonization of a cylindrical olive wood particle of $d = 20 \times 10^{-3} m$ diameter and $\rho_w = 879$ kg m^{-3} density at reactor temperatures of T_R = 623K,

Fig. 3 (a) shows the local temperature evolution at the surface of the wood particle. Figs. 3 (b) and (c) show the local residual density evolution respectively at the axis and at the surface of the wood particle. Figs. 3 (a)-(c) shows that the LBM numerical results are in good agreement with the numerical results of Grioui et al. [20].

Based on the aforementioned comparisons, the developed code is reliable for studying wood particle carbonization. To test the LBM algorithm for different operating conditions, Figs. 4 and 5 show respectively the effect of the reactor temperature T_R and the wood particle size d on the evolution of the heat and mass transfer mechanisms during the carbonization of a cylindrical olive wood particle $(\rho_w = 879 \text{ kg m}^{-3})$. The obtained results showed that the developed algorithm predicts correctly the dependency of the carbonization process of the considered parameters.

III. CONCLUSION

A new algorithm for solving one-dimensional heat and mass transfer for isothermal carbonization of wood particles has been developed. The algorithm is based on the lattice Boltzmann method (LBM). Results of the carbonization of wood particle have been obtained and compared to the published results; the good agreement between the lattice Boltzmann results and published results shows that the proposed model is able to predict correctly the physical phenomena of carbonization.

TABLE I
KINETICS DATA OF WOOD CARBONIZATION [18]

Reaction rate $k_i(s^{-1})$	Activation energy $E_{ai}(\text{kJmol}^{-1})$	Pre-exponential constant $k_{0i}(s^{-1})$
k_1	105.89	3.5×10^7
k_2	106.78	3.72×10^6
k_3	169.56	7.23×10^{11}
k_4	51.04	3.4×10^{-1}

TABLE II
THERMOPHYSICAL PROPERTIES OF WOOD [20]

Thermal conductivity of wood $(\mathrm{Wm^{-1}K^{-1}})$	$\lambda_w = 0.13 + 3 \times 10^{-4} \times (T - 273)$
Specific heat of wood $(\mathrm{JKg^{-1}K^{-1}})$	$c_{pw} = 1112 + 4.85 \times (T - 273)$
Heat of reaction (1,2,3) $(\mathrm{JKg^{-1}})$	$\Delta H_4 = 42 \times 10^3$
Heat of reaction (4) $(\mathrm{JKg^{-1}})$	$\Delta H = 100 \times 10^3$

TABLE III
GLOBAL HEAT TRANSFER COEFFICIENT FOR DIFFERENT REACTOR TEMPERATURES [20]

Reactor temperature T_R (K)	Global heat transfer coefficient $h\,(\mathrm{Wm^{-2}K^{-1}})$
623	50
673	61

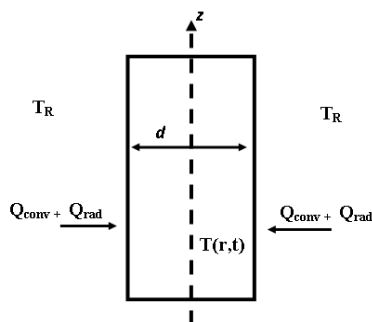Fig. 1 Physical model of isothermal carbonization of a cylindrical wood particle

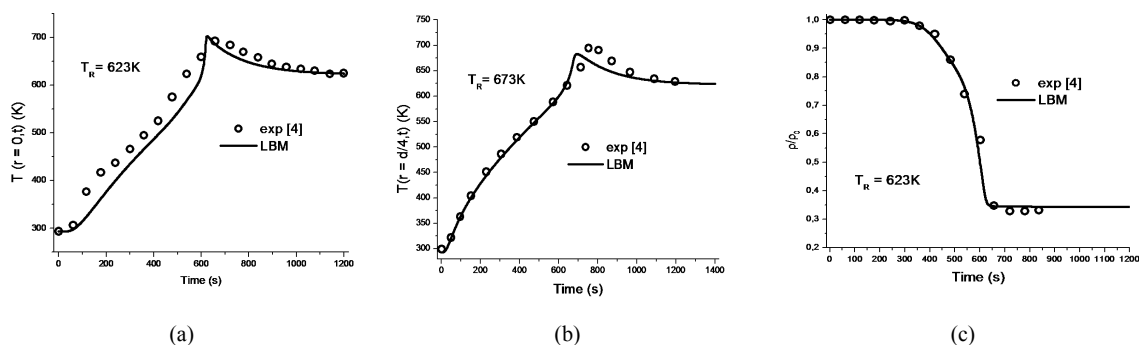(a)   (b)   (c)

Fig. 2 Validation of the (a) temperature profile at the axis of the wood particle (b) temperature profile at r = d/4 (c) residual density evolution with experimental data of Koufopanos et al. [4].

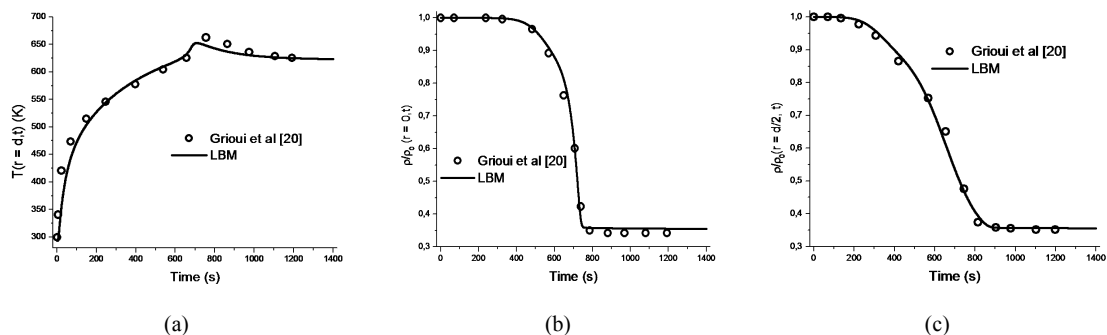(a)   (b)   (c)

Fig. 3 Validation of the (a) temperature profile at the surface of the wood particle (b) residual density evolution at the axis of the wood particle (c) residual density evolution at r = d/2 with numerical data of Grioui et al. [20]
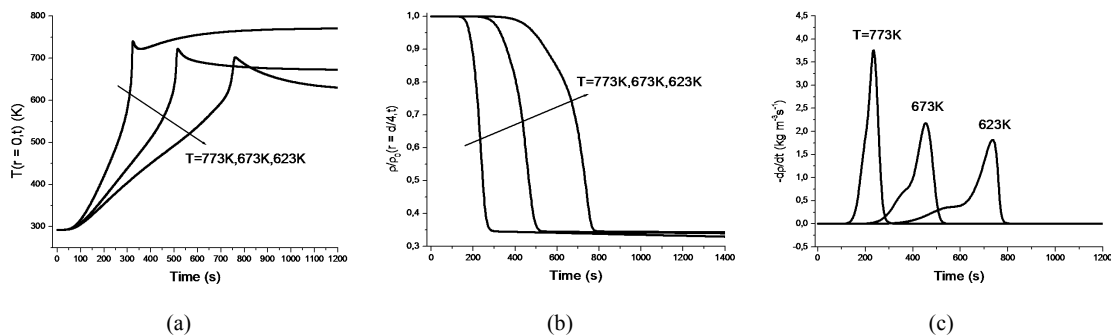
Fig. 4 Effect of the reactor temperature on the (a) temperature profile (b) residual density (c) density loss rate
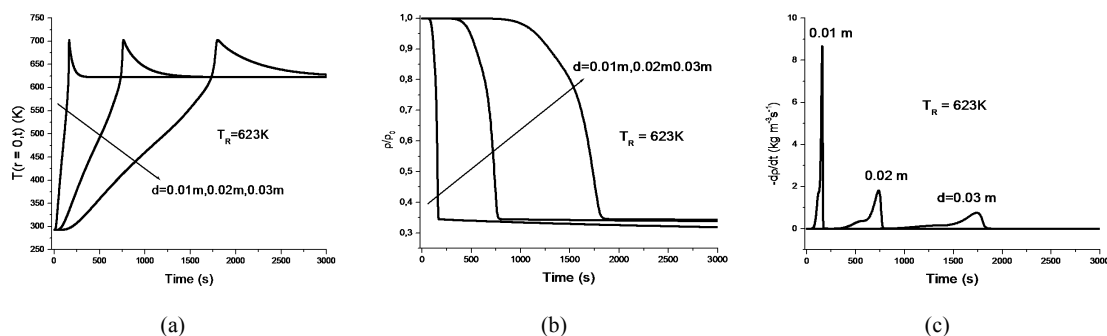

Fig. 5 Effect of the wood particle size on the (a) temperature profile (b) residual density (c) density loss rate

REFERENCES

[1] M.A. Connor and C.M. Salazar "the pyrolysis of wood at at low heating rates", In: *Proc forest products research international achievements and the future. Carbon from biomass*, pp. 5-12. 1985

[2] C.M .Salazar. PhD thesis, University of Melbourne, Australia, 1987.

[3] M.A Connor and C.M Salazar "Factors influencing the decomposition processes in wood particles during low temperature pyrolysis", In: Bridgwater AV, Kuester JL, editors. *Proc research in thermochemical biomass conversion*. Londre, UK: Elsevier Applied Science Publisher, pp. 164–78, 1988

[4] C.A .Koufopanos, N. Papayannakos, G. Maschio and A. Lucchesi. "Modelling of the pyrolysis of biomass particles. Studies on kinetics thermal and heat transfer effects", *Can J Chem Eng*, pp. 907–915. 1991.

[5] C. Di Blasi and G. Russo. "Modeling of transport phenomena and kinetics of biomass pyrolysis", In: Bridgwater AV, editor. *Proc advances in thermochemical biomass conversion. Glasgow*, UK: Blackie Academic & Professional Publishers. pp. 906–921, 1994.

[6] C. Di Blasi. "A transient, two dimensional model of biomass pyrolysis", In: Bridgwater AV, Boocock DGB, editors. *Proc developments in thermochemical biomass conversion. Glasgow*, UK: Blackie Academic & Professional Pub .pp.147–160, 1997

[7] C.K .Lee, R.F Chaiken and J.M. Singer. "Charring pyrolysis of wood in fires by laser simulations" In: 16th Int symp on combustion. pp. 1459–1470, 1976.

[8] M.A. Gronli. PhD thesis, Norwegian University of science and Technology, Norway, 1996.

[9] J. Larfeldt, B. Leckner and M.C. Melaaen. "Modeling and measurement of pyrolysis of large wood particles", *Fuel*. pp.1637–1643, 2000

[10] M.C. Melaaen. "Numerical analysis of heat and mass transfer in drying and pyrolysis of porous media", *Numer Heat Transfer Part A*. 29, pp.331–355, 1996

[11] B. Peters and Ch. Bruch. "Drying and pyrolysis of wood particles: exprements and simulation", *J Anal Appl Pyrol*, pp.1–18.2002

[12] M.A. Abbassi, N. Grioui, K. Halouani, A. Zoulalian, B. Zeghmati. "A practical approach for modelling and control of biomass pyrolysis pilot plant with heat recovery from combustion of pyrolysis products". *Fuel Process Technol*, 90, pp.1278–1285, 2009.

[13] J. Rattea, F. Mariasb, J. Vaxelaireb and P. Bernada. "Mathematical modelling of slow pyrolysis of a particle of treated wood waste". *J Hazard Mater*. pp.1023–1040. 2009

[14] N, Peters. "Flame calculations with reduced mechanisms – an outline". In: Peters N, Rogg B, editors. Reduced kinetic mechanisms for applications in combustion systems. *Lecture notes in physics*. New York: Springer-Verlag, Berlin, pp. 3–14,1993

[15] A.K. Sadhukhan, P. Gupta and R.K. Saha. "Modelling of pyrolysis of large wood particles". *Bioresour Technol*, pp.3134–3139, 2009.

[16] C. Dupont, L. Chena, J. Cancesa, J.M. Commandre, A. Cuocic, S. Pieruccic, et al. ''Biomass pyrolysis: kinetic modelling and experimental validation under high temperature and flash heating rate conditions''. *J Anal Appl Pyrolysis* , pp.260–267, 2009.

[17] E. Ranzi, A. Cuoci, T. Faravelli, A. Frassoldati, G. Migliavacca, S.Pierucci, et al. ''Chemical kinetics of biomass pyrolysis''. *Energy Fuels*, pp.4292–4300, 2008.

[18] N. Grioui, K. Halouani, A. Zoulalian, F. Halouani. ''Thermogravimetric analysis and kinetics modeling of isothermal carbonization of olive wood in inert atmosphere'', *Thermochim Acta*. pp. 23–30, 2006.

[19] S. Succi. *The lattice Boltzmann method for fluid dynamics and beyond*. New York: Oxford University Press; 2001

[20] N. Grioui, K. Halouani, A. Zoulalian, F. Halouani. ''Thermochemical modeling of isothermal carbonization of thick wood particle – Effect of reactor temperature and wood particle size'', *Energy Conversion and Management*, pp. 927–936, 2007.