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Lattice Boltzmann Simulation of the Carbonization of Wood Particle

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***Abstract*—**A numerical study based on the Lattice Boltzmann Method (LBM) is proposed to solve one, two and three dimensional heat and mass transfer for isothermal carbonization of thick wood particles. To check the validity of the proposed model, computational 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 thermal boundary conditions, on the evolution of the local temperature and the mass distributions of the wood particle during carbonization.

***Keywords*—**Lattice Boltzmann Method, pyrolysis conduction, carbonization, Heat and mass transfer.

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/m^2). 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 this work is to apply the lattice Boltzmann method to the resolution of the wood carbonization problem. 1D, 2D and 3D models with different thermal boundary conditions are studied for modeling the wood carbonization.

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The thermal properties of wood are considered to be linear functions of the local temperature and have been estimated from literature data. The model is used to study the effect of reactor temperature and thermal boundary conditions, on the evolution of the local temperature and the mass distributions of the wood particle during carbonization.

A. Physical Model

The physical models considered here are represented in Figs. 1 (a)-(c).

Fig. 1 (a) shows the one dimensional wood particle model. A cylindrical dried wood particle is placed in a reactor at constant temperature (T_R). 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.

Fig. 1 (b) shows the two dimensional wood particle models. 2D square geometry is used; the south surface is kept isothermal at the reactor temperature (T_R), the other surfaces are adiabatic.

Fig. 1 (c) shows the three dimensional wood particle models. 3D cubical geometry is used; the south surface is adiabatic, the other surfaces are kept isothermal at the reactor temperature (T_R).

For the three models studied, the following carbonization reaction scheme, developed recently by the authors [18] is used here:

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

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

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

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

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:

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

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

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

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

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

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

where

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

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:

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

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

$$\rho = \nu_1\rho_{\mathrm{A_1}} + \nu_2(\rho_{\mathrm{A_2}} + \rho_{\mathrm{C_2}}) + \nu_3(\rho_{\mathrm{A_3}} + \rho_{\mathrm{B}} + \rho_{\mathrm{C_3}}) \tag{14}$$

where S is the power generated by the exothermic reaction of the wood decomposition, ρ is the wood density and $\nu_{i=1,2,3}$ are the mass fraction, its values are reported in [18]. Thermophysical 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:

***For 1D model*:**

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

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

where *h* represents the global heat transfer coefficient these values are reported in Table III.

***For 2D model*:**

The side surfaces: $\left.\dfrac{\partial T}{\partial x}\right|_{y=0,L} = 0$

The north surface: $\left.\dfrac{\partial T}{\partial y}\right|_{x=L} = 0$

The south surface: $T(x, y=0) = T_R$

***For 3D model*:**

The side surfaces: $T = T_R$

The top surface: $T = T_R$

The bottom surface: $\left.\dfrac{\partial T}{\partial y}\right|_{x=0} = 0$

C. Lattice Boltzmann Simulation

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

$$\frac{\partial f_i(\vec{r},t)}{\partial t} + \vec{e}_i.\nabla f_i(\vec{r},t) = -\frac{1}{\tau}\left[f_i(\vec{r},t) - f^{eq}{}_i(\vec{r},t)\right] \quad i = 1...m \tag{15}$$

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:

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

The temperature is obtained after summing f_i overall direction:

$$\mathrm{T}(\vec{r},t)=\sum_{i=1,m} f_i(\vec{r},t) \tag{17}$$

To process (22), an equilibrium distribution function is required, which for a conduction-radiation problem is given by:

$$f^{eq}{}_i(\vec{r},t)=\mathrm{w}_i\mathrm{T}(\vec{r},t) \tag{18}$$

To account for the source term, the energy equation in the LBM formulation, (22) is modified to:

$$f_i(\vec{r}+\vec{e}_i\Delta t,\ t+\Delta t)=f_i(\vec{r},t)-\frac{1}{\tau}\left[f_i(\vec{r},t)-f^{eq}{}_i(\vec{r},t)\right]-\frac{\Delta t\,\mathrm{w}_i}{\rho(\vec{r},t)c_{Pw}(\vec{r},t)}S(\vec{r},t) \tag{19}$$

***For 1D model*:**

For 1D model, D1Q2 uniform lattices are used, the relaxation time τ for the D1Q2 lattice is computed from:

$$\tau=\frac{\lambda_w}{|\vec{e}_i|^2\rho c_{pw}}+\frac{\Delta t}{2} \tag{20}$$

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

$$e_1=\frac{\Delta r}{\Delta t}\qquad e_2=-\frac{\Delta r}{\Delta t} \tag{21}$$

$$\mathrm{w}_1=\mathrm{w}_2=\frac{1}{2} \tag{22}$$

***For 2D model*:**

For 2D model, D2Q9 uniform lattices are used, the relaxation time τ for the D2Q9 lattice is computed from:

$$\tau=\frac{3\lambda_w}{|\vec{e}_i|^2\rho c_{pw}}+\frac{\Delta t}{2} \tag{23}$$

For this lattice, the 9 velocities and their corresponding weights are given by:

$$e_{1,3}=(\pm1,0)\frac{\Delta r}{\Delta t},\ e_{2,4}=(0,\pm1)\frac{\Delta r}{\Delta t},\quad e_{5,8}=(\pm1,\pm1)\frac{\Delta r}{\Delta t},\ e_9=(0,0) \tag{24}$$

$$\mathrm{w}_{1,4}=\frac{1}{9},\ \mathrm{w}_{5,8}=\frac{1}{36},\ \mathrm{w}_9=\frac{4}{9} \tag{25}$$

***For 3D model*:**

For 3D model, D3Q19 uniform lattices are used, the relaxation time τ for the D3Q19 lattice is computed from:

$$\tau=\frac{3\lambda_w}{|\vec{e}_i|^2\rho c_{pw}}+\frac{\Delta t}{2} \tag{26}$$

For this lattice, the 19 velocities and their corresponding weights are given by:

$$e_{1,2}=(\pm1,0,0)\frac{\Delta r}{\Delta t},\ e_{3,4}=(0,\pm1,0)\frac{\Delta r}{\Delta t},e_{5,6}=(0,0,\pm1)\frac{\Delta r}{\Delta t},\quad e_{7,10}=(\pm1,\pm1,0)\frac{\Delta r}{\Delta t},e_{11,14}=(0,\pm1,\pm1)\frac{\Delta r}{\Delta t},\quad e_{15,18}=(0,\pm1,\pm1)\frac{\Delta r}{\Delta t},\ e_{19}=(0,0,0) \tag{27}$$

$$\mathrm{w}_{1,6}=\frac{2}{36},\ \mathrm{w}_{7,18}=\frac{1}{36},\ \mathrm{w}_{19}=\frac{12}{36} \tag{28}$$

D. Solution Procedure in the LBM

After dividing the medium into a finite number of lattices, the algorithm for solving the carbonization of thick wood particles using the LBM is as follows:

1. Given the initial temperature field, compute $f_i(\vec{r},0)$
2. For the Kth iteration, at the time level *t*
   - a. Compute $T(\vec{r},t)$
   - b. Compute $f^{eq}{}_i(\vec{r},t)$
   - c. Compute the source term *S*
   - d. Compute the thermal diffusivity
   - e. Compute the relaxation time
   - f. Compute $f_i(\vec{r}+\vec{e}_i\Delta t,\ t+\Delta t)$
   - g. apply the boundary conditions
   - h. Check for convergence, if converged, go to 3. Else go to 2a.
3. Terminate the process when the desired time level or the steady state is reached. Else go to step 2

II. RESULTS AND DISCUSSION

A. One Dimensional Model

In order to validate the present LBM algorithm, we compared our results with the experimental results of Koufopanos et al. [4] (Figs. 2 (a)-(c)) for isothermal carbonization at reactor temperatures of T_R = 623 and 673K, the proposed model is applied to carbonization of a cylindrical wood particle of $d=20\times10^{-3}m$ diameter and $\rho_w=650\ \mathrm{kg\ m^{-3}}$ density. Fig. 2 (a) compares the local temperature evolution at the axis of the wood particle to the experimental data of Koufopanos et al. [4] corresponding to a reactor temperature T_R = 623K. This figure shows that the model describes correctly the temperature profile at the axis of the particle. Fig. 2 (b) presents a comparison of the temperature profiles at $r = d/4$ inside the wood particle carbonized isothermally at a reactor temperature of 673K. This figure shows that the model results are in good agreement with the experimental data. Fig. 2 (c) compares the residual density evolution of the wood particle. Also this figure shows there is a good agreement between the experimental and the numerical results.

B. Two Dimensional Model

Two dimensional wood particle models is studied; the south surface is kept isothermal at the reactor temperature (T_R = 623K), the other surfaces are adiabatic. Fig. 3 shows the temperature and the density profile for wood conversions (dry wood basis) of 5%, 15%, 30%, 60% and 65%. The temperature profile determines the activity of the pyrolysis reactions. The regions where wood density is high, indicates that the wood has not yet reacted in this region. Initially only the bottom of the wood particle reacted, through time, pyrolysis diffuses inside the wood particle with the temperature diffusion. The area where the wood is in the reacting process is the hottest area. The pyrolysis reaction is endothermic; the hot area temperature may exceed the reactor temperature.

C. Three Dimensional Model

Three dimensional wood particle models is studied; the bottom surface is kept adiabatic, the other surfaces are isothermals at the reactor temperature (T_R = 623K). Figs. 4 and 5 show the temperature and the density profile in the xy plane at z = L / 4, L / 2 and 3L / 4. For the planes (z = L / 4, L / 2 and 3L / 4), pyrolysis is favored next to hot side surface. For the plane (z = 3L / 4), the pyrolysis and temperature diffusion is more intense than the two other planes. This can clearly be seen in Fig. 6.

Fig. 6 shows the temperature and the density profile in the zx plane at y = L / 2 for wood conversions (dry wood basis) of 5%, 15%, 30%, 60% and 65%. Fig. 6 shows that the Temperature diffuses through the sides, also by the top surface to the inside of the wood particle. The pyrolysis is promoted near the hot surfaces.

III. CONCLUSION

A numerical study based on the lattice Boltzmann method (LBM) for solving one, two and three dimensional heat and mass transfer for isothermal carbonization of thick wood particles has been developed. For one dimensional model, the results of the carbonization of wood particle have been obtained and compared to the published results; a good agreement is found. The lattice Boltzmann method is able to predict correctly the physical phenomena of carbonization.

TABLE I
KINETICS DATA OF WOOD CARBONIZATION [18]

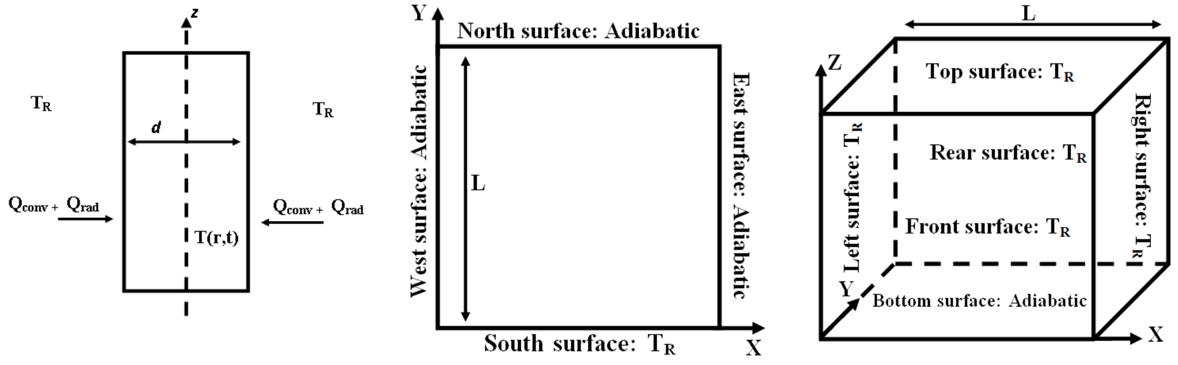
Reaction rate $k_i(s^{-1})$	Activation energy $E_{ai}(\mathrm{kJmol}^{-1})$	Pre-exponential constant $k_{0i}(s^{-1})$
k_1	105.89	3.5×10^{7}
k_2	106.78	3.72×10^{6}
k_3	169.56	7.23×10^{11}
k_4	51.04	3.4×10^{-1}

TABLE II
THERMOPHYSICAL PROPERTIES OF WOOD [20]

Thermal conductivity of wood $(\mathrm{Wm^{-1}K^{-1}})$	$\lambda_w = 0.13 + 3\times10^{-4}\times(T-273)$
Specific heat of wood $(\mathrm{JKg^{-1}K^{-1}})$	$c_{pw} = 1112 + 4.85\times(T-273)$
Heat of reaction (1,2,3) $(\mathrm{JKg^{-1}})$	$\Delta H_4 = 42\times10^{3}$
Heat of reaction (4) $(\mathrm{JKg^{-1}})$	$\Delta H = 100\times10^{3}$

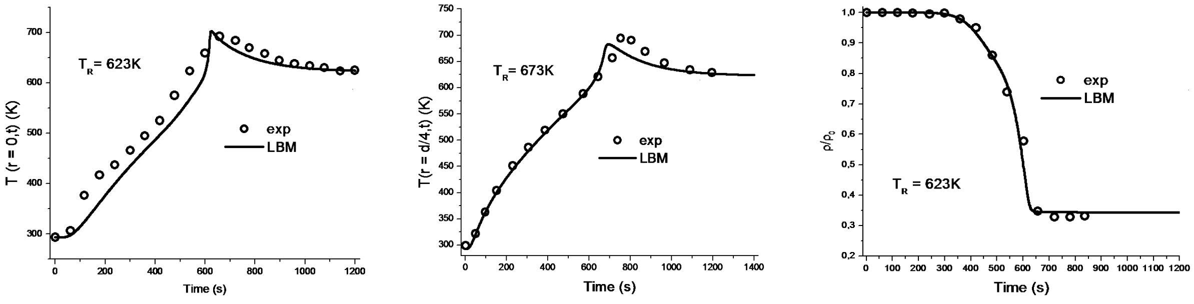
TABLE III
GLOBAL HEAT TRANSFER COEFFICIENT FOR DIFFERENT REACTOR TEMPERATURES [20]

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



(a) (b) (c)

Fig. 1 Physical model of (a) 1D (b) 2D (C) 3D isothermal carbonization of 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 [4]

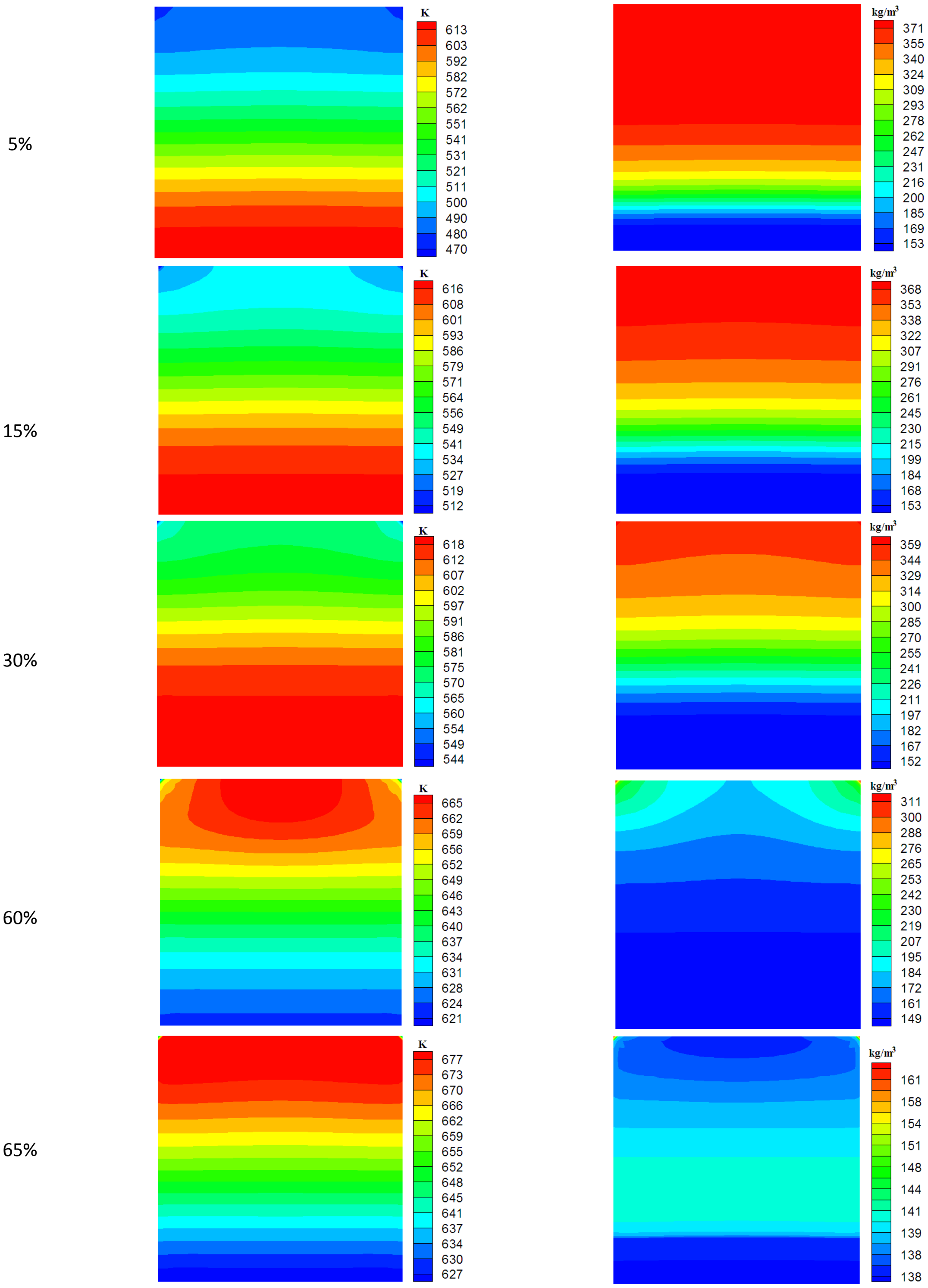


Fig. 3 Temperature (left) and the density (right) profile for wood conversions

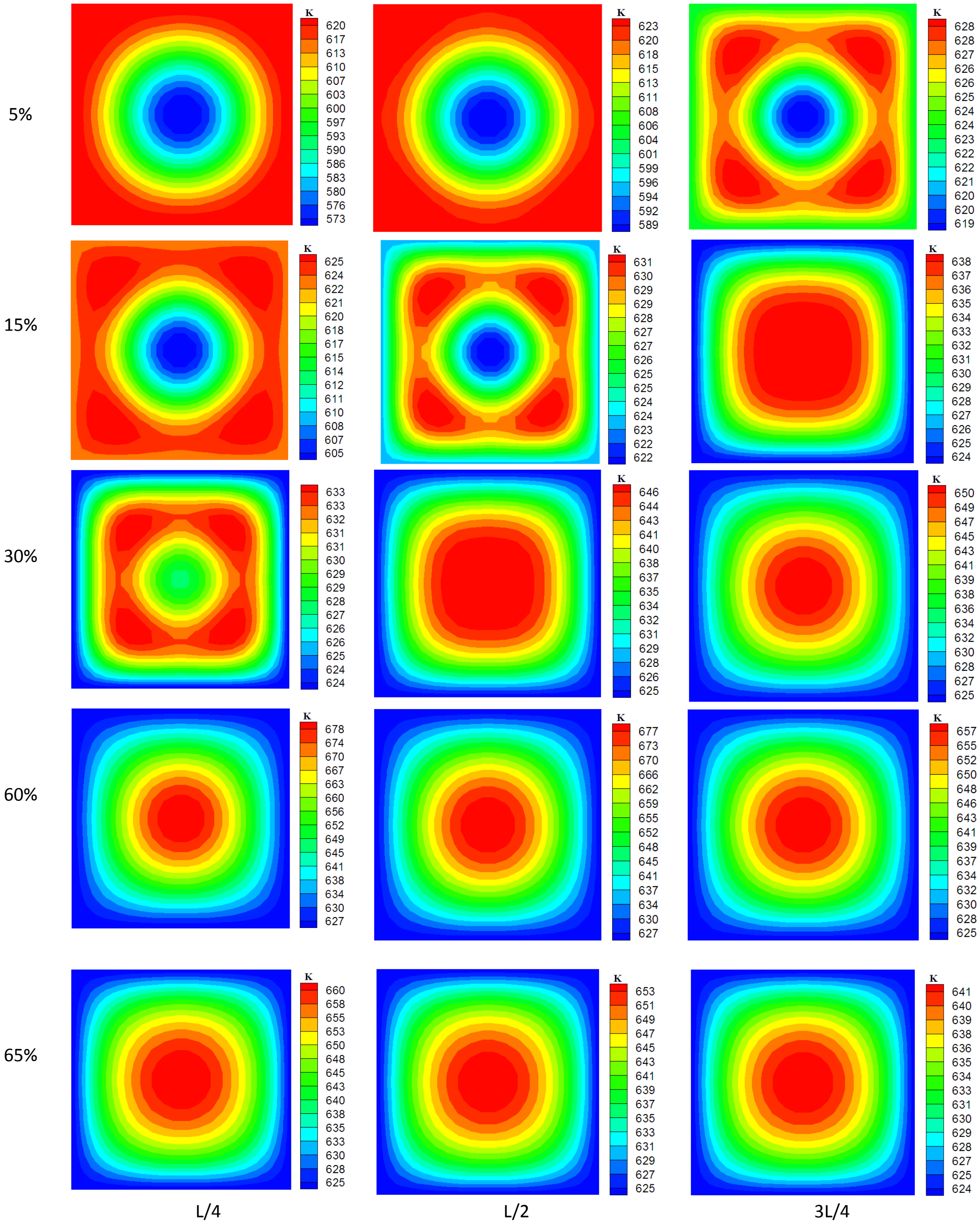


Fig. 4 Temperature profile in the xy plane at z = L / 4, L / 2 and 3L / 4

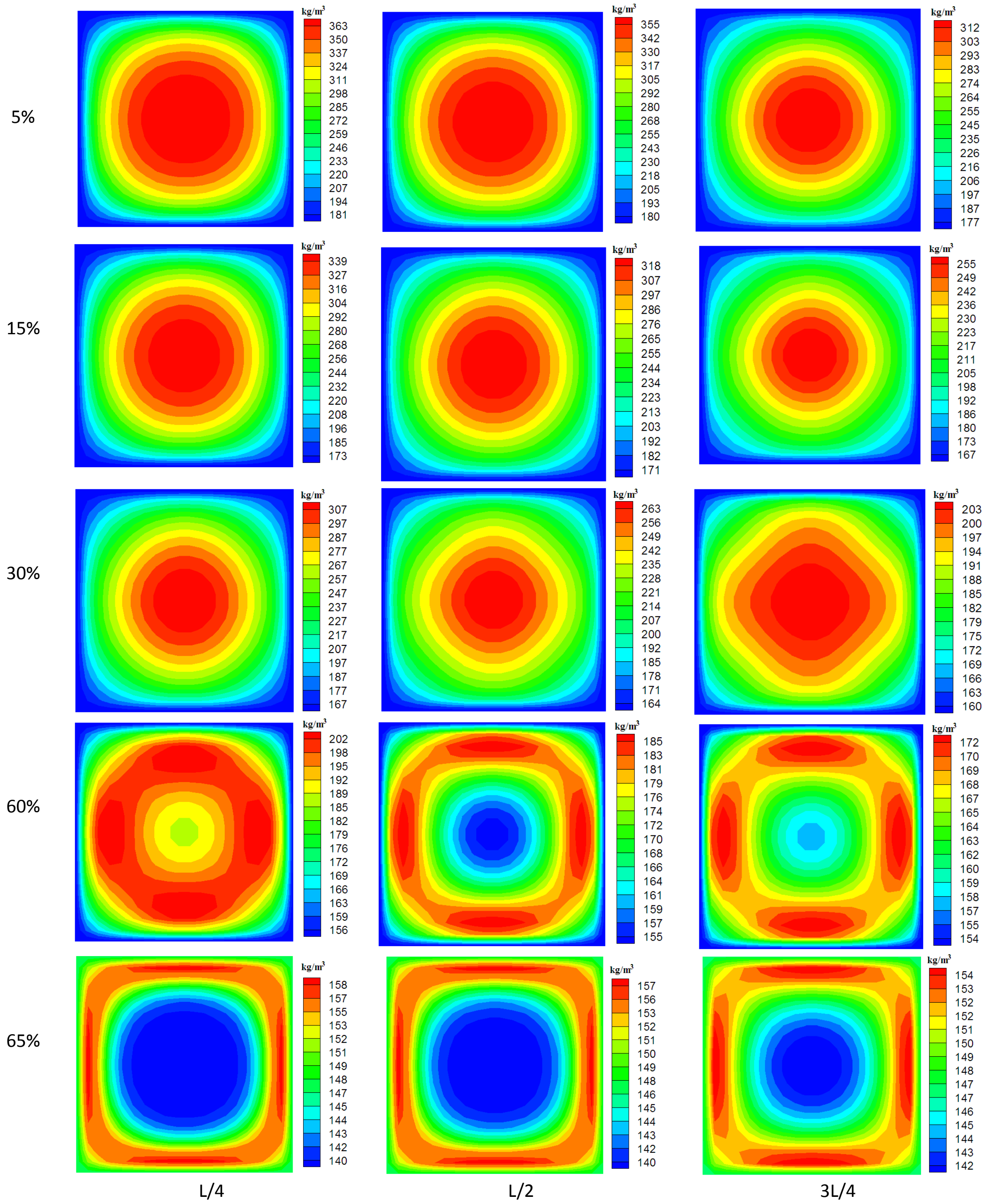


Fig. 5 Density profile in the xy plane at z = L / 4, L / 2 and 3L / 4

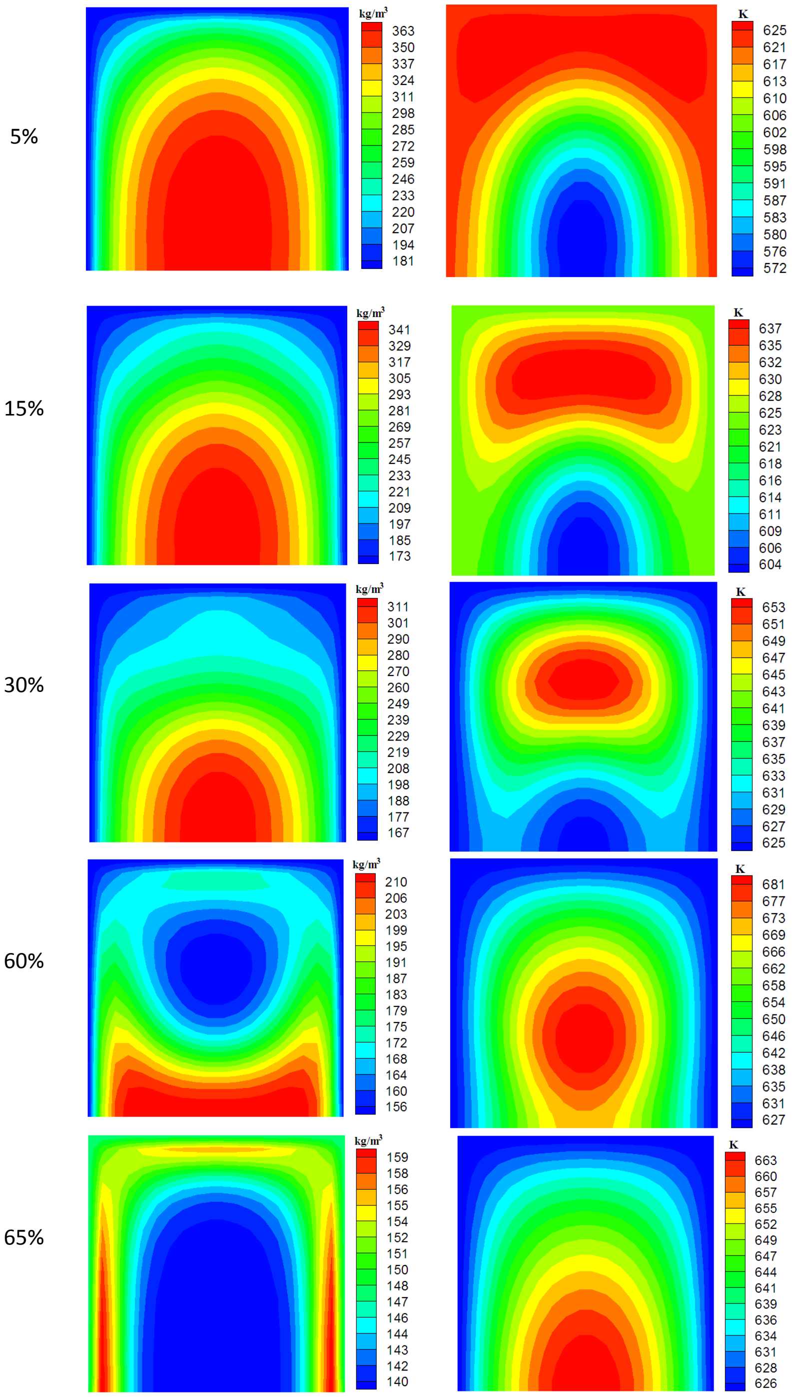


Fig. 6 Temperature and the density profile in the zx plane at y = H / 2

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