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NUMERICAL MODELING OF RESIDUAL WOODY BIOMASS TORREFACTION

Jesús David Rhenals-Julio
Juan Pablo Arteaga Ramos
Carlos Manuel Romero Luna
Ivonete Avila

UNESP – São Paulo State University, Institute of Sciences and Engineering of Itapeva, Rua Geraldo Alckmin, 519, 18409-010, Itapeva-SP, Brazil.
rhenals.julio@unesp.br; juan.arteaga@unesp.br; carlos.romero-luna@unesp.br; ivonete.avila@unesp.br.

Abstract. *In the global context, biomass has been gaining relevance as a renewable energy source, this is due to its high availability in some regions and its direct relationship with sustainable development, however, the direct application of biomass as fuel in combustion and gasification systems faces great challenges due to some properties of biomass, However, these drawbacks can be addressed by means of the torrefaction process, which increases the energy density of biomass by concentrating the fixed carbon present and also reduces the compatibility with water by thermally degrading the hemicellulose. In this work, a model of dry, non-oxidative torrefaction of pine forest residues was developed in order to identify the most appropriate temperature and residence time parameters for this process, using a two-stage species transport model with Arrhenius kinetics coupled to a heat transfer model in cylinders, The model was solved using a finite difference scheme, analyzing the temperature distribution over time and the impact of temperature and residence time on biomass composition, mass yield, heating value and energy yield. The results show that the highest heating value was 21 MJ/kg and was reached at a temperature of 525 K, however, the highest energy yield was obtained at 500 K, since at this temperature the mass loss was lower. It was also found that, for particle diameters of 10 mm, after 35 min, the temperature distribution is approximately constant. On the other hand, it was observed that, at a temperature of 500 K, the formation biomass composition is dominated by natural biomass and the intermediate solid, while the fraction of carbon present is very small. As for the composition of volatiles, it was found that light volatiles were emitted in higher amount than secondary volatiles. Finally, the results of the calorific value obtained in the model were compared with experimental results from the literature, finding that the percentage of error calculated was in the range of 1-5%, so it is concluded that the two-phase model with Arrhenius kinetics and one-dimensional heat transfer provides reliable results in terms of heating value.*

Keywords: *Torrefaction, modeling, biomass,*

1. INTRODUCTION

In the global energy context, biomass has been gaining importance as an energy source, due to its high availability in some regions and its renewable nature. For the utilization of biomass energy, various conversion processes have been proposed, which can be classified into thermochemical and biochemical (Tamminen et al., 2016). Biomass utilization has major disadvantages due to its physicochemical characteristics, such as, low lignin content, heterogeneity in particle size, low energy and mass density (Gómez-Vásquez et al., 2021).

Torrefaction is a thermochemical conversion process that eliminates some of the disadvantages of using biomass in its natural state for energy generation. It consists of heating the biomass to temperatures between 200 °C and 300 °C for a certain time, in an inert atmosphere, thus obtaining a torrified product with properties similar to coal, which would be a viable alternative to partially or totally replace this fuel in combustion or gasification processes. , 2021; González Martínez et al., 2022).

Experimental studies show that the relevant parameters in the torrefaction process are temperature, residence time, heating rate, biomass composition and particle size (Bates & Ghoniem, 2012; Medic et al., 2010). Torrified biomass contains 70% to 90% of the mass of the original feedstock while 10% to 30% is released in as gaseous species, which are usually exploited to generate the heat needed in the process by combustion, provided that their water content and

CO2 /CO ratio are low (Bergman et al., 2005; van der Stelt, 2011). However, many authors point out the importance of recovering some components found in volatile species, either because they can be used as input for production or other valuable compounds or because they present harmful effects on the environment (Alonso et al., 2016; Detcheberry et al., 2016).

Torrefaction modeling is essential for the investigation of reaction mechanisms, reactor design and scale-up, optimization and large-scale application of biomass treatment systems by torrefaction (Feng et al., 2022). Simulation of the torrefaction process involves the coupling of fluid dynamic equations with chemical reaction kinetics equations and the use of numerical techniques for the joint solution of these equations. Although experimental investigations are still necessary for the study of roasting, the development of simulation models of this process is important to know more details of the phenomenology and to reduce the number of experiments necessary to study the influence of the variables.

Different authors have studied the modeling of the roasting process, using different approaches for this, (Prins et al., 2006) developed a model for the prediction of mass loss during roasting, considering a two-step degradation process from experimental results of isothermal thermogravimetry. Subsequently (Bates & Ghoniem, 2012) developed a semi-empirical torrefaction model with prediction of volatiles composition adjusted with experimental data, also predicting the variations of solids composition by mass balance, for this they used an Arrhenius kinetic model, also considering that the process occurred in two phases.

For their part (Sarvaramini et al., 2013) investigated the release of volatiles as a function of time for cellulose, xylan and lignin torrefaction reactions measured by a thermogravimetric method using a distributed activation energy model and a three-parameter log-normal distribution function.

2. MATERIALS AND METHODS

2.1 Characteristics of the process

The biomass torrefaction process was modeled, considering the effects of heat transfer. The particles were modeled as cylinders, with the properties of pine wood. It was considered that the biomass entered the rector at room temperature and came in contact with the carrier gas entering the reactor at the torrefaction temperature, so that the heat transfer between the particle and the gas was considered by pure convection. The convective heat transfer coefficient was calculated with Churchill and Bernstein's semi-empirical model, (Bejan & Kraus, 2003) as shown in equation (1).

$$\frac{hD}{k} = 0.3 + \frac{0.62\,\mathrm{Re}^{1/2}\,\mathrm{Pr}^{1/3}}{\left[1+(0.4/\mathrm{Pr})^{2/3}\right]^{1/4}}\left[1+\left(\frac{\mathrm{Re}}{282000}\right)^{5/8}\right]^{4/5} \qquad (1)$$

The Figure 1 shows the diagram of the simulated process.

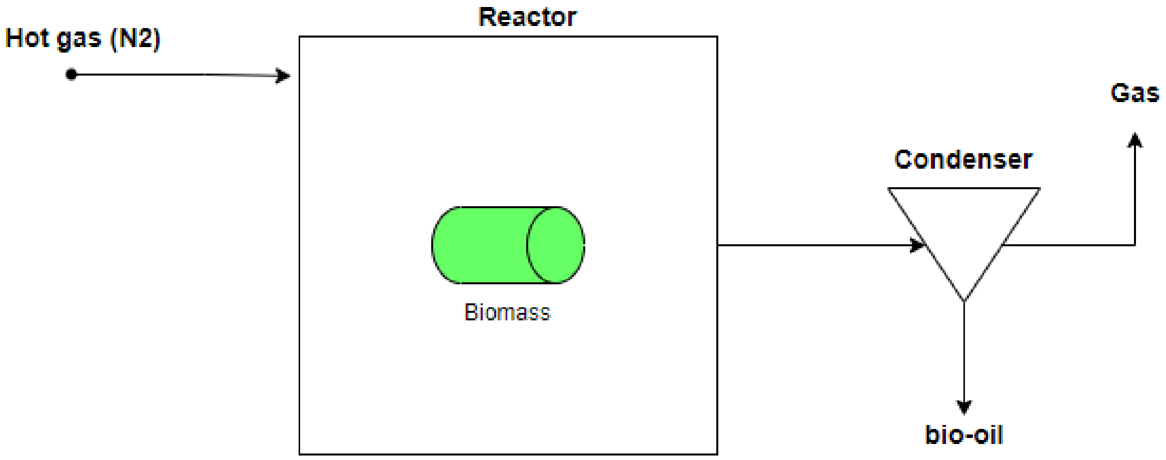

Figure 1. Diagram of the torrefaction process

The torrefaction process was simulated considering four gas inlet temperatures, 475, 500, 525 and 550 K.

2.2 Modeling torrefaction biomass

The following considerations were taken into account when modeling the torrefaction process:

- The gas enters the reactor at roasting temperature.

- The reactions occur according to the multiple surface model (intrinsic kinetics in the porous medium are disregarded).
- Chemical reactions were modeled with the first-order Arrhenius equation.
- Biomass particles were modeled as cylinders.
- Heat transfer was considered one-dimensional.

Torrefaction was modeled as a two-stage process as proposed by Bates & Ghoniem, (2012), in the first stage primary volatiles (V1) are emitted and an intermediate solid (B) is generated while in the second stage secondary volatiles (V2) are emitted and biochar is obtained at the end of the process (C). As shown in Figure 2.

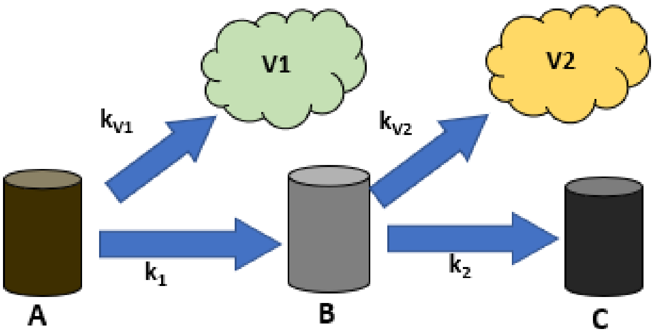

Figure 2. Torrefaction kinetic model

The kinetics of each stage of the process were represented by means of the first-order Arrhenius equation, according to the following equation (2)

$$k_i = A_i \exp\left(\frac{E_i}{RT}\right) \quad (2)$$

The Table 1 shows kinetics parameters of de Arrhenius equation.

Table 1. Kinetics parameters (Bates & Ghoniem, 2012)

Kinetics	**A (s^{-1})**	**E ($J\ mol^{-1}$)**
k_1	$2{,}48\times10^{4}$	75976
k_{V1}	$3{,}23\times10^{7}$	114214
k_2	$1{,}10\times10^{10}$	151711
k_{V2}	$1{,}59\times10^{10}$	151711

2.3 estimation of biomass properties

In the proposed model it is necessary to estimate the conductivity, specific heat and density of each solid phase present in the system, since these properties are necessary in the calculations of mass conservation and heat transfer. For specific heat and thermal conductivity, the temperature-dependent equations for biomass in its natural state and biochar according to Koufopanos et al (1991) were adopted (see equations 3-6).

$$C_{P,A} = 1112 + 4.58\cdot\left(T - 273.15\right) \quad (3)$$

$$k_A = 0.13 + \left(3\cdot10^{-4}\right)\cdot\left(T - 273.15\right) \quad (4)$$

$$C_{P,C} = 1003.2 + 2.09\left(T - 273.15\right) \quad (5)$$

$$k_C = 0.8 + \left(1\cdot10^{-4}\right)\cdot\left(T - 273.15\right) \quad (6)$$

The intermediate solid phase is difficult to evaluate experimentally, so it is proposed to estimate its properties by averaging the property value for biomass and biochar.

$$C_{P,B} = \frac{C_{P,A} + C_{P,C}}{2} \quad (7)$$

$$k_B = \frac{k_A + k_C}{2} \quad (8)$$

Finally, to simplify the solution of the heat transfer model, an effective value for the conductivity and specific heat was estimated to represent these properties for all the solid phases present, as shown in equations 9 and 10.

$$C_{P,eff} = \sum_i x_i \cdot C_{P,i} \quad (9)$$

$$k_{eff} = \sum_i x_i \cdot k_i \quad (10)$$

2.4 Solution of modeling equations

The developed model consists of simultaneously solving the heat transfer equations with the species conservation equations. The solution of these equations was calculated by the finite difference method with a scheme centered in space and advanced in time. Equation 11 gives the temperature distribution in the biomass particle as a function of radial distance from the center of the geometry and time.

$$\frac{1}{r} \cdot \frac{\partial}{\partial r}\left(r \cdot k \cdot \frac{\partial T}{\partial r} \right) = \rho \cdot c \cdot \frac{\partial T}{\partial t} \quad (11)$$

Equations 12 through 16 represent the conservation of all species present in the system as a function of temperature and time.

$$\frac{dm_A}{dt} = -\left(k_1 + k_{V1}\right) \cdot m_A \quad (12)$$

$$\frac{dm_B}{dt} = k_1 \cdot m_A - \left(k_2 + k_{V2}\right) \cdot m_B \quad (13)$$

$$\frac{dm_C}{dt} = k_2 \cdot m_B \quad (14)$$

$$\frac{dm_{V1}}{dt} = k_{V1} \cdot m_A \quad (15)$$

$$\frac{dm_{V2}}{dt} = k_{V2} \cdot m_B \quad (16)$$

The above equations must be solved in a coupled manner under the following initial and boundary conditions.

$$-k \frac{\partial T\left(r_0, t\right)}{\partial r} = h \cdot \left[T_\infty - T\left(0, t\right) \right] \quad (17)$$

$$T\left(r, 0\right) = 300\ K \quad (18)$$

$$m_A\left(0\right) = \rho \cdot V \quad (19)$$

$$m_B\left(0\right) = m_C\left(0\right) = m_{V1}\left(0\right) = m_{V2}\left(0\right) = 0 \quad (20)$$

Finally, as output variables we considered the higher heating value of the biomass (HHVBT), calculated using equation 21, the mass yield of the process (YBT) calculated with equation 22 and the energy yield of the process (ER) estimated with equation 23.

$$HHV_{BT} = x_A \cdot HHV_A + x_B \cdot HHV_B + x_C \cdot HHV_C \quad (21)$$

$$Y_{BT} = \frac{\left(m_A\right)_{final} + \left(m_B\right)_{final} + \left(m_C\right)_{final}}{\left(m_A\right)_{initial}} \quad (22)$$

$$ER = \frac{m_{BT} HHV_{BT}}{m_A HHV_A} \quad (23)$$

3. RESULTS AND DISCUSSION

3.1 Impact of temperature on heating value and energy efficiency

The results of the heating value of the torrified biomass are presented in Figure 3, where it is observed that the temperature of 525 K allows obtaining the highest values in the heating value. For lower temperature values, the calorific value is lower, due to the excessive volatile material present, with low calorific value. While for values higher than 525 K, thermal degradation of species with great contribution to the heating value occurs.

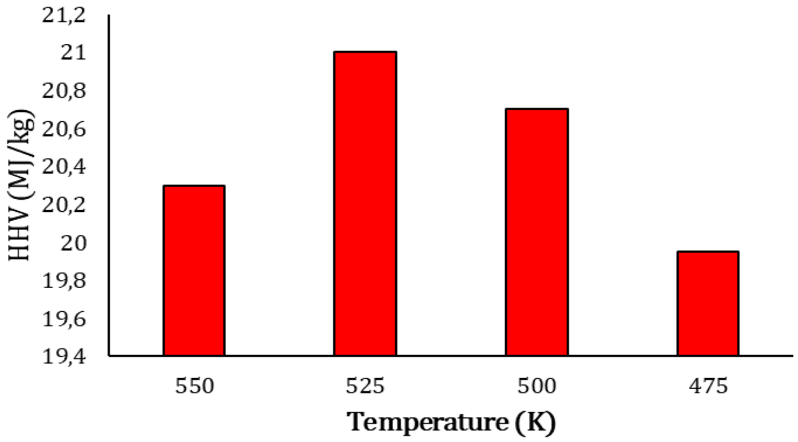

Figure 3. Impact of temperature on heating value

Regarding the impact of temperature on energy yield, it was found that the optimum temperature was 500 K, because the mass yield starts to drop very quickly for higher temperature values (see Figure **4**).

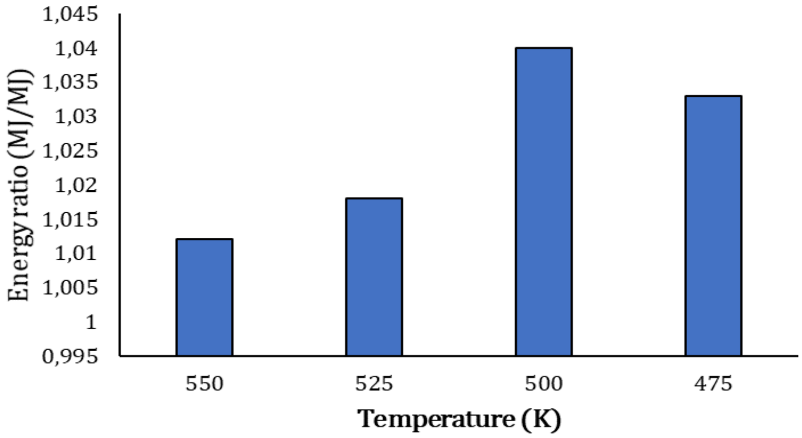

Figure 4. Impact of temperature on energy efficiency

3.2 Particle temperature distribution

The results of the temperature distribution in the biomass particle are presented in Figure 5. Where the temperature at the center (blue line) is compared with the temperature at the surface (red line) showing that after 20 min of heating the temperature of the particle at all points is approximately the same.

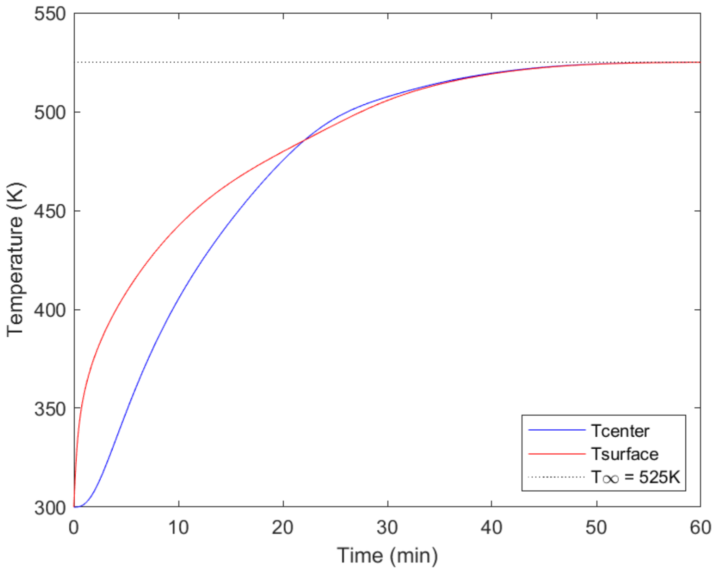

Figure 5. Particle temperature distribution

3.3 Chemical species as a function of time

Figure 6 presents the results of the concentration of chemical species as a function of residence time (in solid lines the concentration in the center and in dotted lines the concentration at the surface), finding that the highest degradations presented correspond to the first stage of the process, where intermediate solids and primary volatiles are generated. While the amount of biochar generated is very little, these results are consistent with those presented by Bates & Ghoniem (2014).

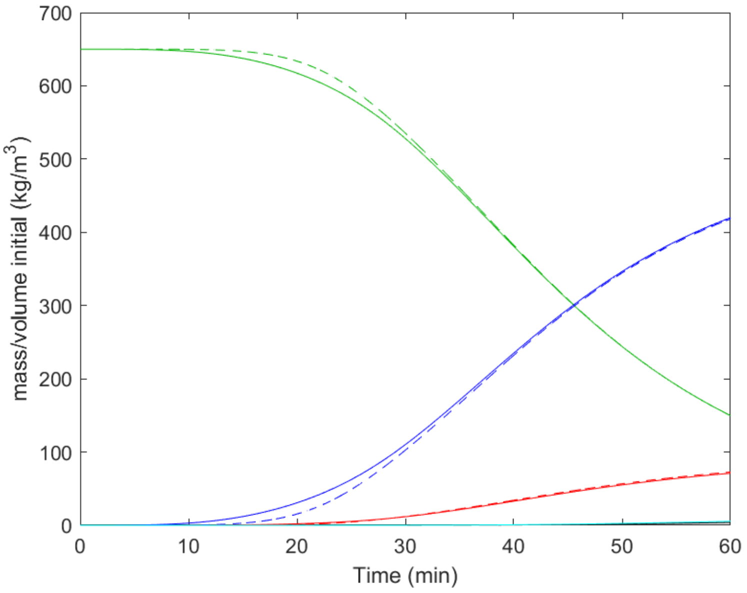

Figure 6. Concentration of chemical species

3.4 Impact of residence time on mass yield, calorific value and energy yield.

The results of the residence time on the mass yield of the process are shown in **Figure 7**, where residence times of more than 30 minutes generate an excessive degradation of the material present in the reactor.

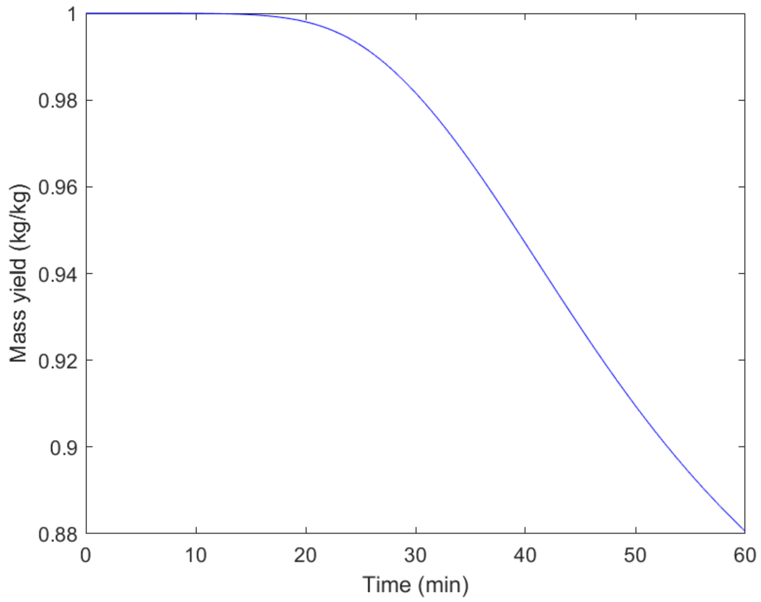

Figure 7. Mass yield vs time

Figure **8** presents the impact of residence time on the calorific value, where it is observed that longer residence times produce higher heating values.

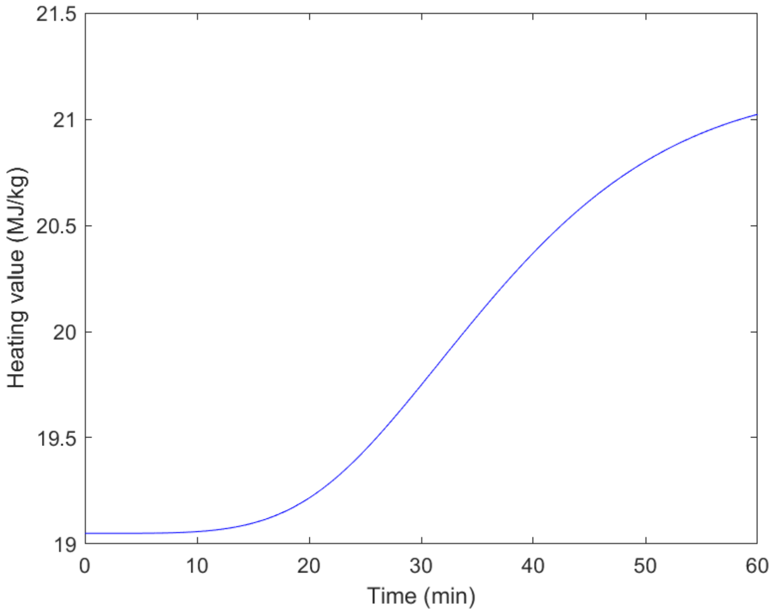

Figure 8. High heating value vs time

Figure 9 shows the energy yield of the process as a function of residence time, where it is observed that the highest yields are reached for times close to 30 minutes, this is due to the fact that before this time the gain of calorific value of the biomass is low, while for higher times large mass losses are generated.

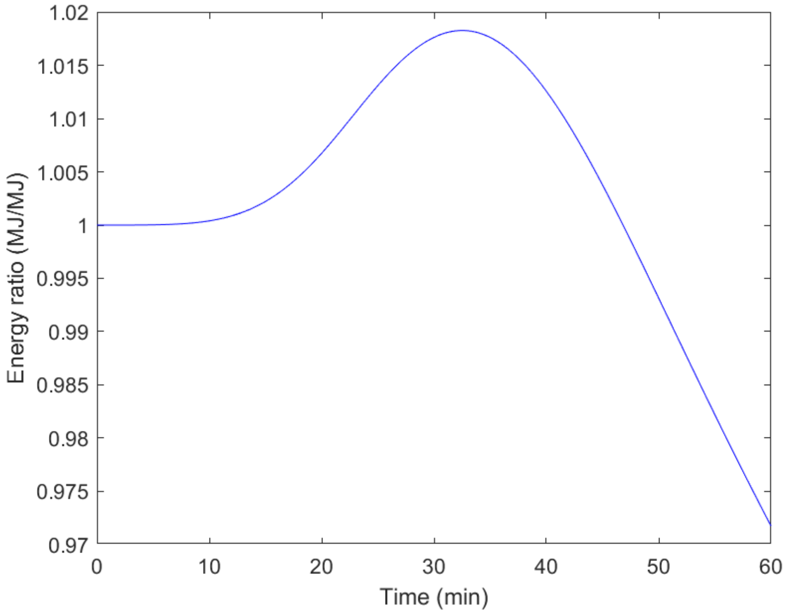

Figure 9. Energy ratio vs time

3.5 Validation of the model

The results of the comparison of the model results with experimental results from the literature are presented in Table **2**, where it can be seen that the percentages of errors presented are less than 5%, which indicates that the proposed model gives good precision in the estimations of the calorific value.

Table 2. Comparison of heating value with other studies

HHV (MJ/kg)	**Reference**	**%Error**
20.84	(Roman poundso & Conte, 2021)	0.8%
21.9	(Khalsa et al., 2016)	4.11%
22.04	(Gucho et al., 2015)	4.72%

4. CONCLUSIONS

The multi-surface model with global kinetics and one-dimensional heat transfer seems to be adequate to simulate biomass torrefaction. Of the temperatures evaluated, the best alternative for pine torrefaction is 525 K. The developed model showed a low error percentage compared to the heating value presented in the literature.

5. ACKNOWLEDGEMENTS

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