

Pyrolysis of large biomass particles: model validation and application to Coffee Husks valorization

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Abstract

Coffee husk is a valuable source of energy in Ethiopia. Pyrolysis of thermally thick biomass particles plays a crucial role across several industrial applications. Despite its significance, the enthalpy changes associated with volatile species release and residual biochar formation during the process are often overlooked. Predictive models for the pyrolysis of large particles and designing a new generation of pyrolyzers are crucial, particularly for industrial-scale applications. Thus, this work introduces a comprehensive one-dimensional (1D) model, BioSMOKE1D, to capture the intricacies of pyrolysis in thick biomass particles and aid in designing optimized pyrolyzers. The model integrates a solid-phase kinetic mechanism, transport limitations, and secondary gas-phase tar-cracking reactions. The BioSMOKE1D has been thoroughly validated and exhibits impressive predictive accuracy by replicating various experiments on large biomass particles. The model successfully reproduces temperature measurements, mass loss profiles, and speciation data at lower temperature measurements. However, incorporating gas-phase mechanisms and secondary tar-cracking reactions has achieved better accuracy at higher temperatures (above 650 °C). Unfortunately, to the authors' knowledge, no experimental data is available for the pyrolysis of large coffee husk particles. Therefore, several parametric analyses are performed to determine the effect of model parameters on the pyrolysis yields for pelletized coffee husks. The findings indicate that biomass particle size, temperature, and initial moisture content significantly affect conversion time, energy consumption, pyrolysis product yields, and species distributions. Larger biomass particle sizes correspond to slower conversion rates and increased energy consumption. This modeling tool holds promises for optimizing the utilization of coffee husks as a renewable energy source, mitigating agricultural waste, and boosting economic growth. Furthermore, the insights from this study provide valuable inputs for optimizing pyrolysis processes in industrial-scale applications of these resources.

1. Introduction

The global energy supply is primarily derived from fossil fuels, leading to significant increases in atmospheric CO₂ and its concomitant effects [1]. A shift to cleaner, more sustainable resources is essential to tackle the challenges [2]. Biomass is a versatile energy resource that can be converted into various fuels including biofuels, with feedstocks ranging from agricultural and forest residues to municipal solid waste (MSW)[3]. Pyrolysis is a precursor to various thermochemical processes that convert low-energy-density biomass into high-energy-density biofuels in oxygen-depleted atmospheres [4]. However, it is not widely considered commercially successful due to complex feedstock chemistry, product instability, poor fuel

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properties, and heterogeneity in product composition [5]. The process occurs at temperatures ranging from 300 to 600°C, producing solid char, liquid tar, and permanent gases [6]. The temperature and species distribution inside the particle are significantly affected by particle properties such as moisture content, biomass compositions, porosity, and operating conditions like temperature, particle size, and geometry [7]. Indeed, understanding the coupled effects is critical to improving the process and producing the desired products. Figure 1 depicts a cross-section of a typical centimeter-size biomass particle undergoing decomposition and the involved heating-related phenomena. In this regard the general objective of this work is to validate the 1D model and investigate the pyrolysis characteristics of large biomass particle application to coffee husks volarization.

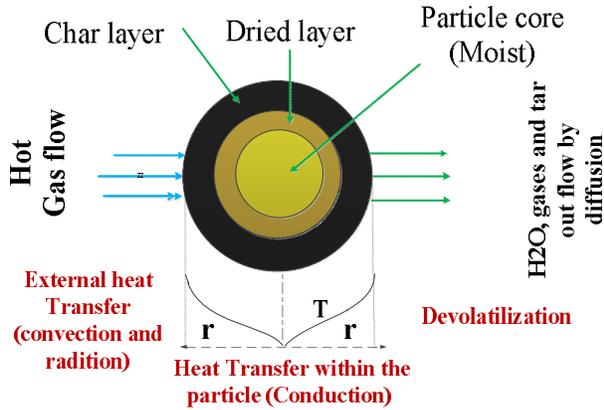


Figure.1 : Cross-section of a centimeter size biomass particle undergoing decomposition (Adapted with permission from [8])

2. Modelling framework

In this section, both the pyrolysis mechanism and the computational modeling framework are discussed.

A. Kinetics mechanism of biomass pyrolysis

The detailed multistep pyrolysis mechanism discussed in this section is based on the one originally proposed by [9] and the one modified in the later stage by Debiagi et al. [10], which contains 32 reactions with 58 species (29 volatiles species and 29 solid species).

B. Computational framework

The large biomass particle is modeled as a continuous system to solve heat and mass transport within the particle, where heat transfer takes place through conduction and convection [11]. To solve the transient 1D system, a C++ numerical solver based on the OpenSMOKE++ [12], framework is employed. The particle is discretized in a finite volume approach in isochoric shells, which exchange heat and mass by convection and diffusion phenomena.

The following mass and energy balances are introduced describing the evolution of the mass of solid species k in shell i , $m_{k,i}^S$, gas species k in shell i , $m_{k,i}^G$, and the temperature of shell i , T_i

$$\frac{dm_{k,i}^S}{dt} = \dot{\Omega}_{k,i}^S V_i^S \quad (1)$$

$$\frac{dm_{k,i}^G}{dt} = \dot{\Omega}_{k,i}^S V_i^S + \dot{\Omega}_{k,i}^G V_i^G + \left[J_{k,i-\frac{1}{2}}^m S_{i-\frac{1}{2}} - J_{k,i+\frac{1}{2}}^m S_{i+\frac{1}{2}} \right] \quad (2)$$

$$\frac{dT_i}{dt} \left(\sum_{k=1}^{N_s^G} c_{p,k,i}^G m_{k,i}^G + \sum_{k=1}^{N_s^S} c_{p,k,i}^S m_{k,i}^S \right) = \left[J_{i-\frac{1}{2}}^T S_{i-\frac{1}{2}} - J_{i+\frac{1}{2}}^T S_{i+\frac{1}{2}} \right] + \left(\sum_{k=1}^{N_s^G} h_{k,i}^G \frac{dm_{k,i}^G}{dt} + \sum_{k=1}^{N_s^S} h_{k,i}^S \frac{dm_{k,i}^S}{dt} \right) \quad (3)$$

The fluxes are evaluated considering mass diffusion, Darcy fluxes, and heat transfer by conduction and mass fluxes as:

$$J_{k,i}^m = -\Gamma_{k,i}^I \rho_i^I \frac{d\omega_{k,i}^G}{dr} - \rho_i^G \omega_{k,i}^G \frac{1}{\mu_i^I Da} \frac{dP_i}{dr} \quad (4)$$

$$J_i^T = -\lambda_i^I \frac{dT_i}{dr} - \sum_{k=1}^{N_s^G} h_{k,i}^G J_{k,i}^m \quad (5)$$

3. Result and discussion

The simulation results and experimental data at various operating temperatures, particle sizes, and wood species are compared in this section to evaluate the proposed methodology for the pyrolysis of large biomass particles.

Figure 2 shows the comparison of model predictions and experimental temperature profiles at the center ($r = 0$) and middle ($R = r/2$) for poplar wood particles at three different reactor temperatures [13]. The results show that two distinct thermal events, endothermic and exothermic reactions, occur at the particle center, and the BioSMOKE1D model predictions correctly describe these thermal phenomena.

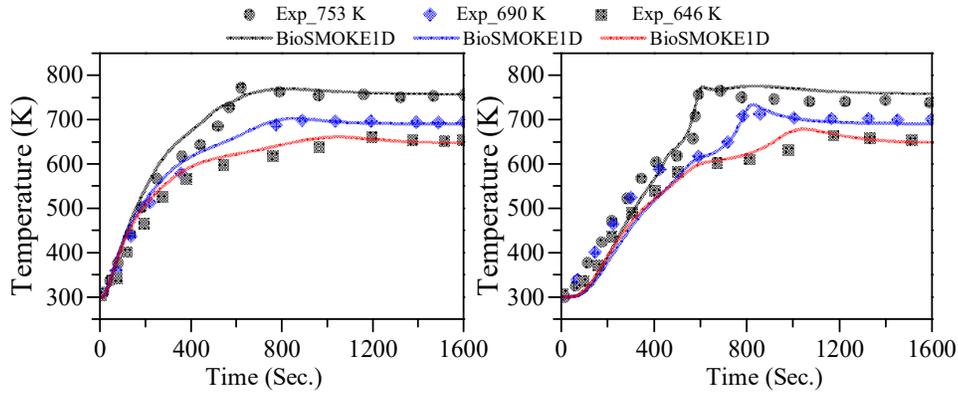


Figure 2: Temperature profile at two different positions middle ($r= R/2$) (left panel) and center ($r= 0$) (right panel) for 38.1 mm diameter of poplar wood spheres pyrolyzed at three different temperatures HT-753 K (black), MT-690 K (blue) & LT- 646 K (red), comparison between experimental [13] (symbol) and BioSMOKE1D (solid lines).

Table 1 exhibit quantitative comparison of the present model and experimental data at the three different temperatures shown in Figure 2. The errors were determined to quantify the model's

accuracy. In all cases, the average percentage error and standard deviation for the experimental data are lower in the prediction of the current models.

Table 1 : Comparison of model prediction results with those experimental measurements for different temperature ranges at the center ($r=0$) and half ($r = R/2$) of a spherical particle of 3.81 cm.

	Center ($r=0$) Temperature [K]			$r= R/2$ Temperature [K]		
	LT- 646	MT- 690	HT-753	LT- 646	MT- 690	HT-753
Relative Error (E_{pe})(%)	3.37	5.31	2.63	7.15	6.38	8.57
Standard deviation (SD)	0.04	0.07	0.06	0.09	0.10	0.13

Figure 3 shows the predicted global mass yields compared with measurements for two different particle sizes with diameters of 19.05 mm (cylindrical) [13] and 38.1 mm (spherical) [13], respectively. Overall, the model predictions and experimental data show similar patterns. The difference between the experimental yields could be attributed to secondary tar reactions occurring in the biomass particle. The other possible justification for the uncertainties could also result from cracking occurring in the reactor, but the authors did not report information on the residence times involved during experimental measurement.

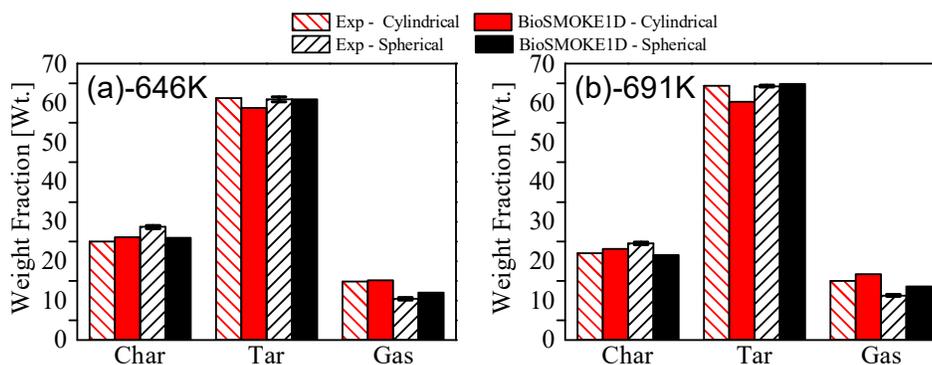


Figure 3 : Experimental measurements of gas, tar, and solid yields as fractions of initial dry poplar wood with different particle sizes and two different geometries with (Cylindrical $D = 19.05$ mm, $L = 40$ mm) and (Spherical 38.1 mm), as compared to model predictions at 646 & 691 K [13].

On the other aspect, during thermal degradation of different biomass particle sizes, there is noticeable variation in the pyrolysis reaction time and energy required to decompose the particles. During thermal decomposition, the energy requirement increases substantially with particle size due to the greater heat transfer limitations and transport phenomena associated with larger particles and extended reaction times. The simulation results clearly demonstrate that energy demand rises significantly as particle size increases. This is primarily attributed to the reduced rates of mass and heat transfer in larger particles, which have a lower surface area-to-volume ratio. Smaller particles, despite their higher surface area, decompose more readily and require significantly less energy. Figure 4 (a) shows the heat flow in (W) and Figure 4 (b) shows the thermal decomposition curve as a function of particle size.

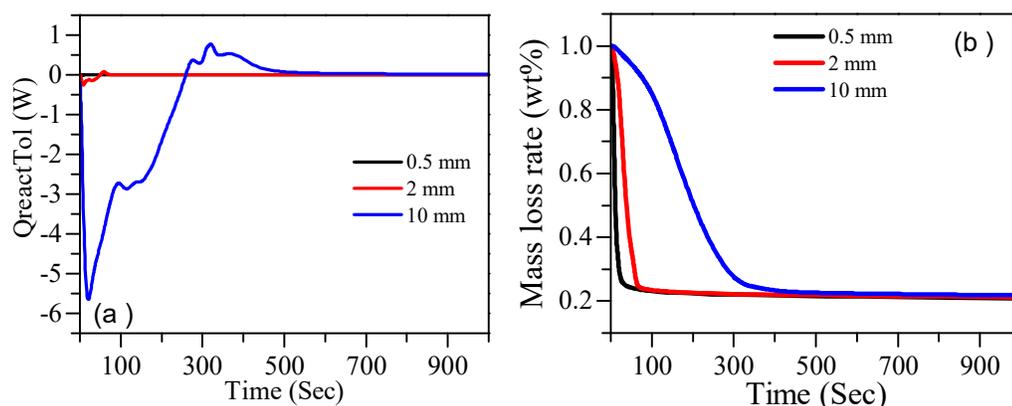


Figure 4 : Comparison of Energy required (endothermic) and thermal decomposition characteristics of large and smaller particles.

4. Conclusion

For the pyrolysis of large biomass particles, the results also revealed that intraparticle temperatures determine the characteristics of pyrolysis reactions. It also shows that the CRECK-S-B kinetic model of biomass pyrolysis, coupled with a simple 1D model for large particles, reasonably replicates the overshooting of the center temperature of large particles, while also rationally predicting the effect of temperature on the degree of pyrolysis for different biomass particles. The comparison of experimental and model results has also provided insights into the mechanisms and kinetics of biomass pyrolysis, highlighting the importance of parameters such as particle size, geometry, and biomass composition in determining pyrolysis characteristics and pyrolysis product distributions of large biomass particles. Particle size also significantly affects energy consumption and reaction time. The results also provide a means of optimizing the use of large biomass particles for industrial applications with the pellet size of coffee husk for biofuel production, but further research is necessary to determine the techno-economic viability of this feedstock for commercial applications.

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