RESEARCH ARTICLE

MODELLING AND SIMULATION OF PYROLYSIS OF CASSAVA PEEL IN A FIXED BED REACTOR

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ABSTRACT

Modeling of a fixed bed reactor for pyrolysis of cassava peels for the production of bio oil , bio char and bio gas has been studied. Model equations were developed using mass, energy and momentum balance equations coupled with rate equations, deduced from primary and secondary reaction mechanism. Simulation of the model equations was carried out at pyrolysis temperatures of 300^oC, 400^oC, 500^oC and 600^oC, adopting kinetic values in literatures, using the finite element method in COMSOL multiphysics programming environment. The results obtained showed decrease in char yield from 44.7% to 18.6% with increase in temperature, whilst bio gas increases from 16.7% to 54.4% as temperature increase from 300^oC to 600^oC. A maximum yield of bio oil was observed at 300^oC which was comparable to results in literature. The simulation predicts the pyrolysis behavior of agricultural waste in a fixed bed reactor which will be useful for design and optimization purposes.

INTRODUCTION

Developing a model to approximate real life process is important in Chemical Engineering for design purposes. Usually, models are developed from fundamental mathematical principles to more complex formulas. Simulation of models becomes necessary in order to solve such complex formulas easily to understand the parameters needed and validate such parameters with experimental values. Modeling and simulation of biomass pyrolysis process have been carried out by some researchers in order to understand the process parameters, thermochemical conversion to products (J. D. Murillo *et al*. 2017) and design of the reactor (N. Kazakova *et al*. 2015) used for the process. Biomass pyrolysis is a solid-gas reaction and the process is represented by global kinetic models which accounts for the decomposition of biomass to primary products such as bio gas, bio oil and bio char (Hashimoto *et al*. 2011).Such models are investigated to provide data for modeling and simulation of the pyrolysis process (M. Van de Velden. 2008,A. Tabal *et al*.2021) and the reactor (P. Lamarche *et al*. 2013). A. Grana *et al*. (2010) studied on the detailed kinetics of fixed bed gasifiers and proposed a two-stage reaction mechanism for the pyrolysis of biomass. Most of the kinetic parameters have been fitted in experimental data to validate the models developed. However, (K. Hashimoto *et al*. 2011) observed that the model developed from the experimental data of one biomass material may not be applied to other biomass materials. This might be due to the variability of different biomass materials. The effect of temperature and biomass particle size has also been considered in modeling biomass pyrolysis process. Z. Luo *et al*. (2005) conducted and developed a model of wood flash pyrolysis in fluidized bed reactor. The model predicted the effect of reaction temperature on the pyrolysis products. They observed that a moderate dense bed temperature of 500 C, and lower suspension bed temperature were more suitable for optimizing bio-oil production, because decomposition takes place at such temperatures with less effect of secondary cracking of oil.K. Papadikisa *et al*. (2009) modeled and simulated biomass pyrolysis processand established that particle sizes did not significantly affect the product yield but the heat transfer inside the particle affected the product yield. Di Blasi (2004) modeled wood gasification process in a fixed bed reactor and included heat and mass transfer in the decomposition process. Researchers have also carried out modeling and simulation of biomass pyrolysis processes using computer softwares. J. Ward *et al*. (2013) developed a computational model of pyrolysis process with different biomass materials and simulationusing Aspen plus software to analyze the performance of the process. It was established that biomass with high cellulose and low moisture contents are suitable materials for bio oil production.

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I. M. Idriss *et al*. (2017) also carried modeling and simulation of beech wood using Aspen plus and predicted the effect of pyrolysis temperature and wood particle size on the composition of liquid and gaseous products.B. Alexandre*et al*. (2015) investigated on modeling and simulation of fixed-bed pyrolysis of debark residue using COMSOL 5.0 software to determine the effect of the physical parameters of fuel on pyrolysis product yields and tar cracking. Though some researchers have modeled and simulated biomass pyrolysis processes with different biomass materials, little information is available in literature on modeling and simulation of cassava pyrolysis except for O. L. Ki *et al*, (2013) who investigated the modeling and simulation of pyrolysis of cassava peel in a fixed bed reactor using MATLAB software.Therefore this study will model and simulate the pyrolysis of cassava peels using COMSOL software and predict product yield which will be useful for design and optimization purposes

MATERIALS AND METHODS

The material used for the investigation was cassava peels and the composition of the material is shown in Table 1. The development of the process model and simulation was carried out using COMSOL 5.4. The two-stage reaction system is a fixed bed reactor with a diameter of 0.15m and a total height of 0.15 m. This reactor consists of 0.5 m packed bed. The experiment was conducted at pyrolysis temperatures of 300°C, 400°C, 500°C, and 600°C

Table 1. Proximate and Ultimate Analysis of Cassava peel (Farrow et al. 2018)

Proximate analysis		Ultimate analysis	
Parameter	Value (%)	Parameter	Value (%)
Moisture (ar)	7.0	C (db)	42.4
Volatile matter (daf)	76.6	H (db)	6.0
Fixed carbon (daf)	20.5	N (db)	1.1
Ash (db)	2.9		

Modeling

Model Assumptions

The following assumptions were adopted (Di Blasi, 2004, Ki *et al*. 2013)

- Biomass particle is spherical.
- Heat transfer inside the biomass particle is only conduction.
- Temperature gradient inside the biomass particle is a function of the radius position with surface temperatures less or equal to the temperature in the system
- Density, specific heat capacity, and thermal conductivity are constant.

The pyrolysis model built in the simulation environment is presented in Figure 1.
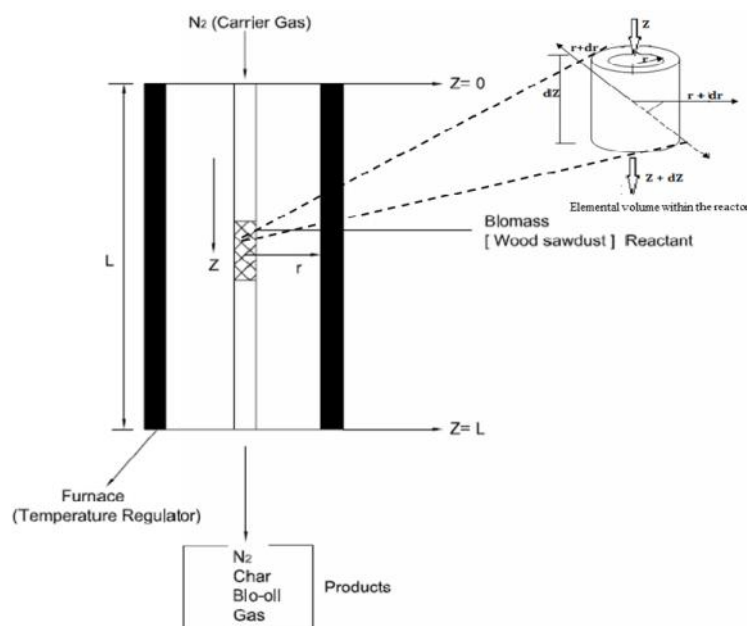

Figure 1. Fixed bed Reactor for Biomass Pyrolysis

Kinetic modeling: Figure 2 represents the conversion of cassava into the primary products and further conversion of the primary products into secondary products. The reaction kinetic equations, values of reaction rate constants and other parameters used in this work were adopted from O.L. Ki *et al*. (2013) and are presented in equations 1-5
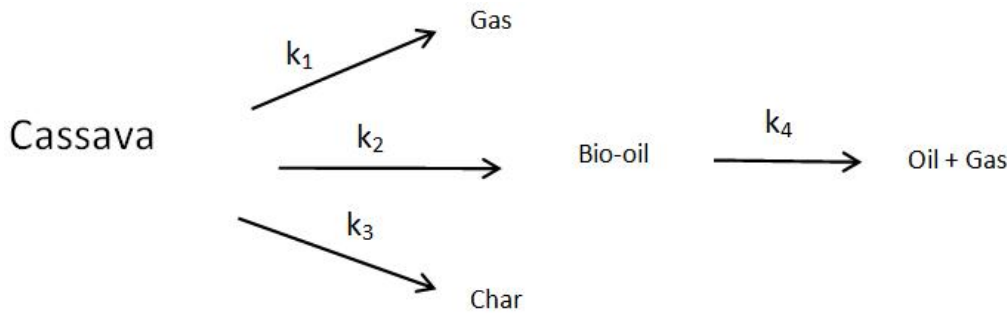

Figure 2. Pyrolysis of Cassava into primary and secondary products(M. Van de Velden et al. (2008)

$$\frac{dY_B}{d} = -(k_1 + k_2 + k_3).Y_B = -k.Y_B \tag{1}$$

$$\frac{dY_{G1}}{d} = k_1.Y_B \tag{2}$$

$$\frac{dY_{O1}}{d} = k_2.Y_B \tag{3}$$

$$\frac{dY_C}{d} = k_3.Y_B \tag{4}$$

$$\frac{dY_{O2}}{d} = \frac{dY_{G2}}{d} = k_4.Y_{G1} \tag{5}$$

Where Y is the mass fraction and the subscripted notations $B, C, G1, O1, G2,$ and $O2$ refer to biomass, char, primary gases, primary liquid, secondary gases, and secondary liquid, respectively. The kinetic equations and the calculated rate constants in equations 6-10 were taken from Van de Velden *et al*. (2008) since the reaction proposed is similar

$$k = 28057.18 \exp\left(-\frac{8\quad.7}{RT_S}\right) \tag{6}$$

$$k_1 = 14300 \exp\left(-\frac{1}{RT_S}\right) \tag{7}$$

$$k_2 = 21332.77 \exp\left(-\frac{8\quad.1}{RT_S}\right) \tag{8}$$

$$k_3 = 6431.74 \exp\left(-\frac{8\quad.7}{RT_S}\right) \tag{9}$$

$$k_4 = 7900 \exp\left(-\frac{8}{RT_S}\right) \tag{10}$$

Model Equations for the Pyrolysis reaction

Initial and Boundary Conditions: The model in this work was developed from the general mass balance, component balance and energy balance equations in equation (11-13)

$$\varepsilon\frac{\partial c_j}{\partial} = -\varepsilon u_z \frac{\partial c_j}{\partial} + \varepsilon D_{j,z}\frac{\partial^2 c_j}{\partial z^2} + \sum_{i\in r} \quad \alpha_{i,j}r_i^* \tag{11}$$

Where $\alpha_{i,j}$ is the stoichiometry of reaction *i* for component j and r_i^* is the rate of reaction *i*. Eq. (1) can be expressed in terms of mass fraction x_j thus;

$$\varepsilon\frac{\partial x_j}{\partial} = -\varepsilon u_z \frac{\partial x_j}{\partial} + \rho D_{j,z}\frac{\partial^2 x_j}{\partial z^2} + \sum_{i\in r} \quad \alpha_{i,j}r_i^* \tag{12}$$

where $D_{j,z}$ and are the axial and radial diffusivity respectively. The total mass fraction expected at the exit of the reactor should be equal to 1 i.e. $\sum_j x_j = 1$. The yield can be estimated thus;

$$\rho_f C_p \; \varepsilon \frac{\partial T_b}{\partial} = -\varepsilon \rho_f u_z C_p \; \frac{\partial T_b}{\partial} + \lambda \frac{\partial^2 T_b}{\partial z^2} + \Delta H_i \alpha_{i,j} w_i^* + Q \tag{13}$$

Where T_b is the temperature of the bulk fluid, λ is the thermal conductivity, ε is the porosity, C_p is the heat capacity of the fluid, i for component j and r_i^* is the rate of reaction i. The related initial and boundary conditions are presented in equations 14-19. Initial conditions: At $t = 0\ s$

$$Y_g = 0, Y_c = 0, Y_G = 0, Y_B = 0, T_g = 303k, T_s = 303k, \tag{14}$$

Boundary conditions:

Side wall and axis: $\left.\frac{\partial T_g}{\partial}\right|_{r=0} = \left.\frac{\partial T_s}{\partial}\right|_{r=0} = \left.\frac{\partial Y_i}{\partial}\right|_{r=0} = \left.\frac{\partial Y_i}{\partial}\right|_{r=R} = 0 \tag{15}$

$$\lambda_{g,e} \; \left.\frac{\partial T_g}{\partial}\right|_{r=R} = h_w(T_f \; - T_g) + \sigma \varepsilon_r(T^4_f \; - T^4_g) \tag{16}$$

$$\lambda_{s,e} \; \left.\frac{\partial T_s}{\partial}\right|_{r-R} = h_w(T_f \; - T_s) + \sigma \varepsilon_r(T^4_f \; - T^4_s) \tag{17}$$

Bottom face:

Case of a fixed bed: $z = 0$

$$T_g = T_{i_1}, T_s = T_{i_1}, \quad u_g = u_{i_1} \tag{18}$$

Top face:

$$\left.\frac{\partial T_s}{\partial}\right|_{z-H} = \left.\frac{\partial T_g}{\partial}\right|_{z-H} = \left.\frac{\partial Y_i}{\partial}\right|_{z-H} = 0 \tag{19}$$

h = 5.69+ 0.0098T_s , Cp = 1449J kg^{-1} K^{-1}, k= 0.156W m^{-1} K^{-1}, ρ_b = 289kg m^{-3}, v = 0.226, and D = 2.8834×10^{-7} m^2.s^{-1} (Ki *et al.* (2013)

Fluid Phase: The general equations for the oil and gas component balance in the reaction remain the same, due to the nature of diffusivity or convective flow of their molecules as presented in equations 20 (a-d) while the energy balance is presented in equation 21.

$$V \cdots_g \frac{|Y_{G1}}{|t} \Gamma V \cdots_g u_g \frac{|Y_{G1}}{|x} Z Diff \cdots_g \frac{|^2 Y_{G1}}{|x^2} X w_{G1} \; X k_1 Y_B \cdots_s \tag{20a}$$

$$V \cdots_g \frac{|Y_{G2}}{|t} \Gamma V \cdots_g u_g \frac{|Y_{G2}}{|x} Z Diff \cdots_g \frac{|^2 Y_{G2}}{|x^2} X w_{G2} \; X k_4 Y_{O1} \cdots_s \tag{20b}$$

$$V \cdots_g \frac{|Y_{O1}}{|t} \Gamma V \cdots_g u_g \frac{|Y_{O1}}{|x} Z Diff \cdots_g \frac{|^2 Y_{O1}}{|x^2} X w_{O1} \; X k_2 Y_B \cdots_s \tag{20c}$$

$$V \cdots_g \frac{|Y_{O2}}{|t} \Gamma V \cdots_g u_g \frac{|Y_{O2}}{|x} Z Diff \cdots_g \frac{|^2 Y_{O2}}{|x^2} X w_{O2} \; X k_4 Y_{O1} \cdots_s \tag{20d}$$

Energy balance:

$$V \cdots_g C_{Pg} \frac{|T_g}{|t} \Gamma \cdots_g u_g C_{Pg} \frac{|T_g}{|x} Z \}_g \frac{|^2 T_g}{|x^2} X h_{gs} S(T_s \; Z T_g) \Gamma \quad_i \cdots_s w_i \zeta H_i \Gamma Q_{rad} \tag{21}$$

Solid Phase: The char component balance simplified in equation 22a since char is solid with negligible diffusion and the energy balance is presented in equation 22b.

$$\cdots_s \frac{|Y_c}{|t} \Gamma V \cdots_s u_s \frac{|Y_c}{|x} Z Diff \cdots_s \frac{|^2 Y_c}{|x^2} X w_c \; X k_3 Y_B \cdots_s \tag{22a}$$

Char energy balance:

$$V \cdots_s C_{Ps} \frac{|T_s}{|t} \Gamma \cdots_s u_s C_{Ps} \frac{|T_s}{|x} Z \}_s \frac{|^2 T_s}{|x^2} X h_{gs} S(T_s \; Z T_g) \Gamma \quad_i \cdots_s w_i \zeta H_i \Gamma \cdots_s w_{char} \zeta H_{char} \tag{22b}$$

Where,

$$SX\frac{6(1Zv)}{d_P}$$ (23)

Momentum balance

$$u_z \; XZ\frac{k}{\sim_g}(\frac{|P}{|z}ZP_g\,g)$$ (24)

RESULTS AND DISCUSSION

Product yield: The results of the products obtained from the simulation are presented in Figures 3-5. In Figure 3, it was observed that char yield decreased with increase in temperature from 300°C to 600°C. This might be due to enhanced decomposition of the biomass and secondary thermal decomposition of char (A. Pattiya, 2011). The maximum bio oil yield of 30.89% was obtained at 300°C in Figure 4. The decomposition of hemicellulose and cellulose takes place at temperature between 200-350°C (Y. K. Park *et al.*2012). These components are responsible for the evolution of volatile matters which comprises of condensable and non-condensable gaseous substances. The condensable vapour forms the liquid (bio oil) while the non-condensable vapour form the bio gas. The maximum bio oil yield at 300°C might be due to enhanced production of condensable volatile matters due to high content of cellulose (J. Ward *et al.* 2013) which decomposed at that temperature. However, the decreased in bio oil yield from 30.89 to 22.14% as temperature increased from 300°C to 400°C might be as a result of primary cracking of bio oil. From 400°C to 500°C, an increase in bio yield was observed from 22.14% to 27.6% probably due to more gasification reactions of the char to form more condensable, which in turn forms bio oil. A further decrease in bio oil yield was also observed from 27.6% to 25.8% as temperature increases from 500°C to 600°C likely due to secondary cracking of bio oil to gaseous matter. The gaseous products increased with increasing temperature from 300°C to 600°C as presented in Figure 5. The possible reason for the continuous increase in the yield of gaseous product might be due to secondary cracking of bio oil and char gasification reactions (A. Pattiya, 2011).The simulated results are presented in Table 4, which followed a similar trend in literature (O. L.Ki *et al.* 2013)
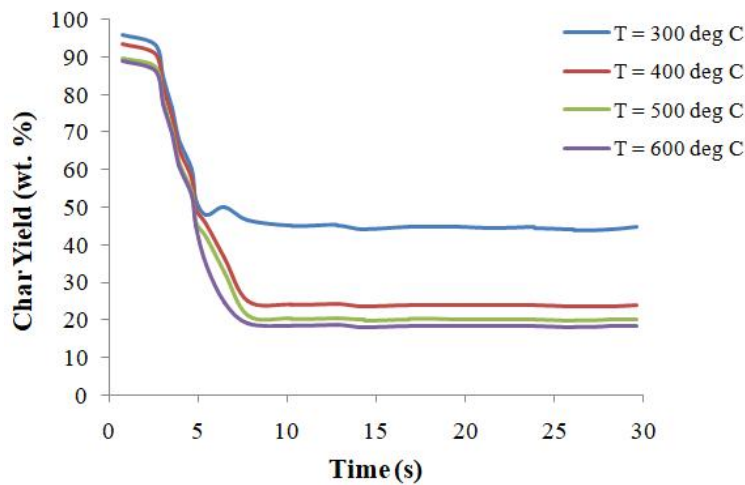

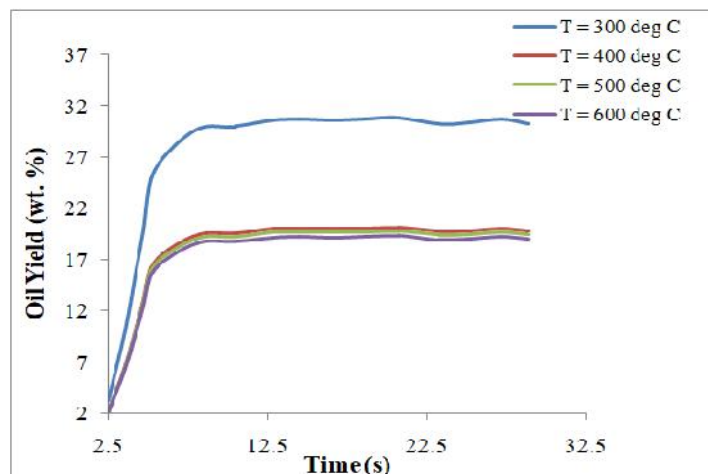**Figure 3. Char yield verse time at different pyrolysis temperature**

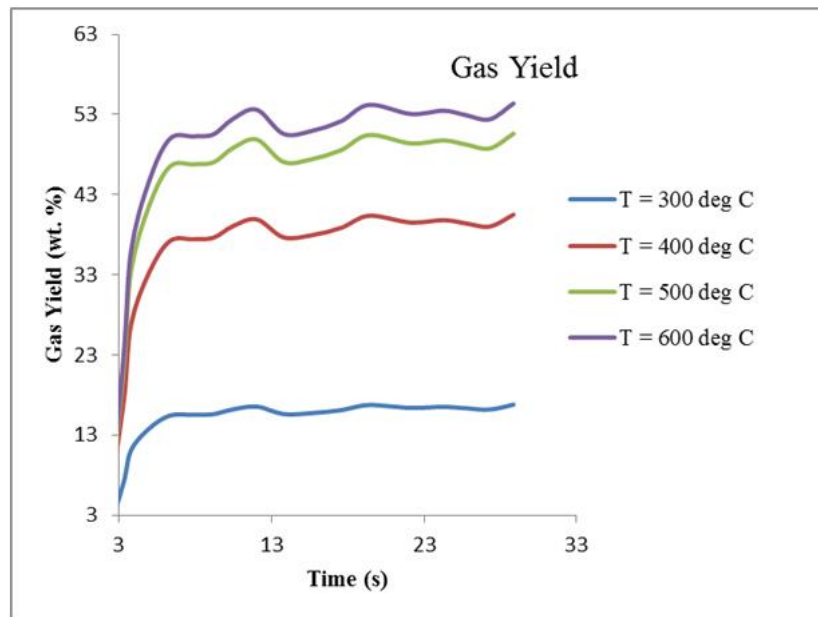**Figure 4 .Oil yield verses time at different pyrolysis temperature**

Figure 5. Gas yield vs time at different pyrolysis temperature

Table 5. Verification of product yield with literature values

T(^{o}C)	This work			Ki et al.(2013)		
	Char (wt %)	Bio oil (wt%	Gas (wt%)	Char (wt %)	Bio oil (wt%	Gas (wt%)
300	44.7	30.89	16.72	-	-	-
400	23.6	22.14	40.4	41.3	34.6	24.1
500	20.2	27.6	50.6	27.6	47.5	24.6
600	18.6	25.8	54.41	22.9	43.4	33.7

Conclusion

In this study, model equations were developed in a fixed bed reactor for the pyrolysis of cassava peels to produce bio oil. The model equations were simulated using COMSOL 5.4 software. The percentage of bio oil (30.89%) from simulation shows that cassava peel waste is a source of bio oil, which could be used for the production of bio oil. The maximum yield at 300°C indicates that bio oil could be produced favorably at this temperature, which will be useful for design purposes.

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