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NUMERICAL INVESTIGATION OF THE EFFECTS OF TEMPERATURE AND BIOMASS DENSITY ON THE PRODUCTS EVOLUTION FROM WOOD PYROLYSIS

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Abstract: Interest in wood and other biomass as a source of renewable energy has been on the rise as it will help reduce the current reliance on fossil fuels. The aim of this study was to utilize Python 3 programming language in computing the numerical solutions to the differential equations using Euler's method for evaluating the effects of biomass density and system temperature on product evolution and yields during pyrolysis. It was observed that the rate of biomass degradation and product evolution is more rapid at higher temperatures. The final concentration of char decreased as the instantaneous temperature increased. At higher temperatures, gaseous products evolve at a higher rate and exist at a higher proportion in equilibrium. It was also observed that biomass density does not have a significant effect on the rate of the biomass degradation and the nature of the product evolution but biomass with higher density gives more char yield than those with lower densities.

Keywords: biomass pyrolysis; numerical solution; python; density

INTRODUCTION

Interest in biomass as a source of renewable energy has been on the rise as it will help reduce the current reliance on fossil fuels. Also the negative environmental impact of fossil fuels use will consequently be ameliorated. Biomass is identified as natural high-molecular organic substances of lignocellulosic structure (Fu, Hu, Xiang, et al., 2009). Even the largest coal consuming country in the world; China, is now turning towards greener energy sources (Fu et al., 2010). The fraction of the biomass energy consumed in developing countries is between 40% to 50% since these countries have large areas for agriculture (Gani & Naruse, 2007). Biomass from agricultural residues is recognized as one of the most promising sources of renewable energy because of their availability, cheap price and abundance (Fu, Hu, Sun, et al., 2009).

The products of the pyrolysis process are oil/tar, synthesis gas and char. Biomass consists of mainly three components; hemicellulose, cellulose and lignin (Qu, Guo, Shen, Xiao, & Zhao, 2011). They possess very different thermal behaviours (Wang, Zhou, Liang, Song, & Zhang, 2015). The pyrolysis products may be considered to be from the overall conversion of the main components hence, the possibility of predicting the pyrolysis product distribution according to the component proportion in a biomass. Simplifying reaction sequences and overall reaction kinetics for biomass pyrolysis has been proposed and studied over the years (Prakash & Karunanithi, 2008). For numerous biomass samples, kinetics and reaction sequence has been exhaustively examined (Gavin, Stuart, & Emilio, 2016). Pious O. Okekunle and Adeoye (2016) undertook a generic numerical modelling for biomass aimed at studying thermo-physical property effects on product yield. The use of python for kinetic modelling of wood pyrolysis degradation and product evolution is unreported in open literature.

This study aims on taking a step further by utilizing a numerical modelling technique (Euler's method) and Python 3 programming language (on Python v2.7 software) to elucidate the effect of temperature and wood density on the pyrolysis products evolution. It is modelling cum property-effect studies. The approach will encompass the generation of differential governing equations to describe the wood pyrolysis process and these includes solid mass conservation equations, mass conservation equations for gas and tar, energy equation and total pressure equation. Furthermore, Python 3 programming language will be used in computing the numerical solutions to the differential equations using an appropriate computational technique (Euler's method). Graphical plots will be developed and analysed to show the effects of biomass density and system temperature on product evolution and yields during pyrolysis.

METHODOLOGY

— Pyrolysis Mechanism and Kinetics

Pyrolysis is mathematically described through a system of coupled equations. The basic equations are those of chemical kinetics, heat transfer and mass transfer. The pyrolysis mechanism adopted for this research was developed by Chan (1983) and shown in Figure 1. In this mechanism, biomass decomposes via three competing reactions into gas, charcoal and tar. The secondary reaction takes place in the gas/vapour-phase within the pores of the charcoal. Consecutively the tar is converted by two secondary reactions into secondary gases and charcoal. The rate of the reaction is proportional with the concentration of the tar vapours.

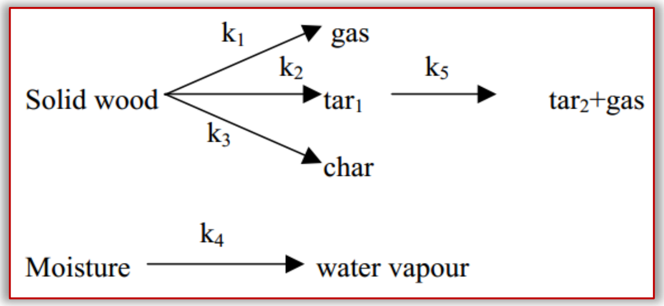


Figure 1. Pyrolysis mechanism by Chan (1983)

For each of the reactions in figure 1, the kinetic constants are presented in table 1. The constants are for the Arrhenius equation given as equation 1

$$k_i = A_i \exp\left(-\frac{E_i}{RT}\right) \quad (1)$$

The values of the pre-exponential factor and activation energy are shown in Figure 1.

Table 1. Kinetic Constants used by Chan (1983)

	Reaction	A_i (sec^{-1})	E_i (kJ/mol)
1	Wood → Gas	1.3×10^8	140
2	Wood → $(Tar)_1$	2×10^8	133
3	Wood → Char	1.08×10^7	121
4	Moisture → Water Vapour	5.13×10^6	87.9
5	$(Tar)_1$→ $(Tar)_2$ +Gas	1.48×10^6	144

— Development of Governing Equations

The governing equations used to describe the processes that occurred during pyrolysis of biomass consist of the solid mass conservation equations, mass conservation equations for gas and tar, energy equation and total pressure equation.

» Solid Mass Conservation Equation

Mass balance equation for each of the reaction yielding char, tar and gas

$$\frac{\partial \rho_{sw}}{\partial t} = -(K_1 + K_2 + K_3)\rho_{sw} \quad (2)$$

Char mass balance

$$\frac{\partial \rho_c}{\partial t} = K_3\, \rho_{sw} \quad (3)$$

» Mass Conservation Equations for Gas, Tar, Water Vapour and Moisture

Mass equations for the inert gas used (Nitrogen) Using two-dimensional cylindrical coordinate system from the equation of continuity

$$N_2\text{:} \quad \frac{\partial(\varepsilon\rho_{N_2})}{\partial t} + \frac{\partial(\rho_{N_2}U)}{\partial z} + \frac{1}{r}\frac{\partial(r\rho_{N_2}V)}{\partial r} = S_{N_2} \quad (4)$$

NB: θ direction is zero.

The source term, $S_{N_2} = 0$

$$N_2\text{:} \quad \frac{\partial(\varepsilon\rho_{N_2})}{\partial t} + \frac{\partial(\rho_{N_2}U)}{\partial z} + \frac{1}{r}\frac{\partial(r\rho_{N_2}V)}{\partial r} = 0 \quad (5)$$

Mass equation for the gas produced

$$\text{gas:} \quad \frac{\partial(\varepsilon\rho_g)}{\partial t} + \frac{\partial(\rho_g U)}{\partial z} + \frac{1}{r}\frac{\partial(r\rho_g V)}{\partial r} = S_g \quad (6)$$

where $S_g = K_1\rho_{sw} + \varepsilon K_5 \rho_{t_1}$

Mass equation for the water vapour produced water vapour:

$$\frac{\partial(\varepsilon\rho_w)}{\partial t} + \frac{\partial(\rho_w U)}{\partial z} + \frac{1}{r}\frac{\partial(r\rho_w V)}{\partial r} = S_w \quad 7)$$

where $S_w = K_4\rho_m$

Mass equation for the tar_1 and tar_2 produced tar_1:

$$\frac{\partial(\varepsilon\rho_{t_1})}{\partial t} + \frac{\partial(\rho_{t_1}U)}{\partial z} + \frac{1}{r}\frac{\partial(r\rho_{t_1}V)}{\partial r} = S_{t_1} \quad (8)$$

where $S_{t_1} = K_2\rho_{sw} - \varepsilon K_5 \rho_{t_1}$

$$tar_2\text{:} \quad \frac{\partial(\varepsilon\rho_{t_2})}{\partial t} + \frac{\partial(\rho_{t_2}U)}{\partial z} + \frac{1}{r}\frac{\partial(r\rho_{t_2}V)}{\partial r} = S_{t_2} \quad (9)$$

where $S_{t_2} = \varepsilon K_5 \rho_{t_1}$

Mass equation for the moisture produced moisture:

$$\frac{\partial(\varepsilon\rho_m)}{\partial t} + \frac{\partial(\rho_m U)}{\partial z} + \frac{1}{r}\frac{\partial(r\rho_m V)}{\partial r} = S_m \quad (10)$$

where $S_m = -K_4\rho_m$

Intra-particle tar and gas transport velocity Using Darcy's Law

$$U = \frac{-B}{\mu}\left(\frac{\partial \rho}{\partial z}\right) \quad (11)$$

$$V = \frac{-B}{\mu}\left(\frac{\partial \rho}{\partial r}\right) \quad (12)$$

where μ is the viscosity, ε is the porosity

$$\varepsilon = 1 - \frac{\rho_{sw,sum}}{\rho_{sw,o}}\left(1 - \varepsilon_{sw,0}\right) \quad (13)$$

where $\varepsilon_{sw,0}$ = initial porosity of wood, $\rho_{sw,sum}$ = sum of wood density and $\rho_{sw,o}$ = initial wood density. The permeability B of the wood biomass:

$$B = (1 - \eta)\, B_{sw} + \eta B_c \quad (14)$$

where η = degree of pyrolysis

$$\eta = 1 - \frac{\rho_{sw} + \rho_c}{\rho_{sw,o}} \quad (15)$$

— Solution Procedure

The numerical methods listed above are to be programmed to create simple and efficient python codes that output the numerical solutions at the required degree of accuracy, arrays (vectors and matrices) are created and manipulated using 'Numpy' and the plotting functions of 'matplotlib' are used to present the results graphically. The necessary tools and libraries needed to carry out the analysis effectively were Python 3 programming language (on Python v2.7 software), SciPy (mathematical solvers), NumPy (n-dimensional array package), Matplotlib (comprehensive plotting), Pandas (data structures and analysis), iPython (interactive console) and Spyder (a Python IDE similar to Matlab).

RESULTS AND DISCUSSION

— Effect of Temperature

Considering the quantity of data generated from the numerical study, it is very important to carefully present the characteristic features of the concentration profiles of various species resulting from the pyrolysis process.

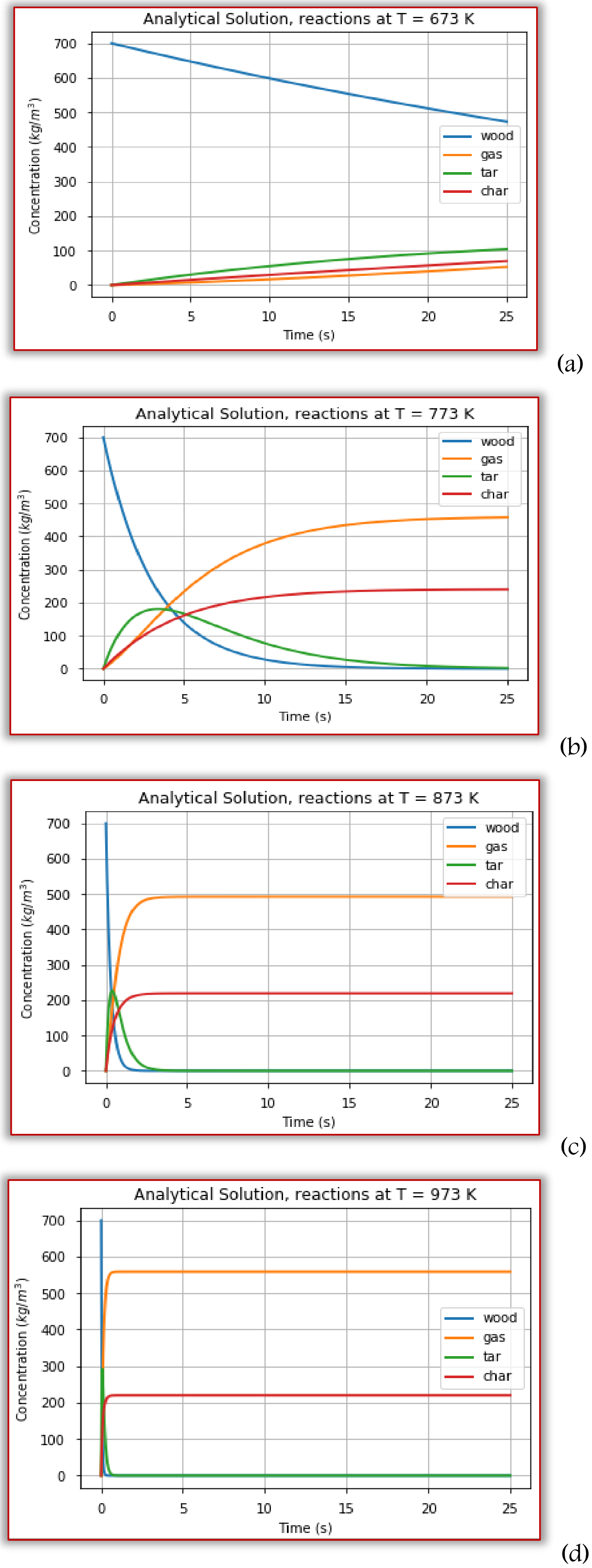


Figure 2(a-d). Biomass and product species concentration profiles with time sample density of 700kg/m³ and temperature of (a) 673 K (b) 773 K (c) 873 K (d) 973 K

Figures 2 shows the species concentration profiles for wood pyrolysis process. As shown in the figures, the initial temperature being high enough to initiate the process leads to the almost immediate decomposition of biomass.

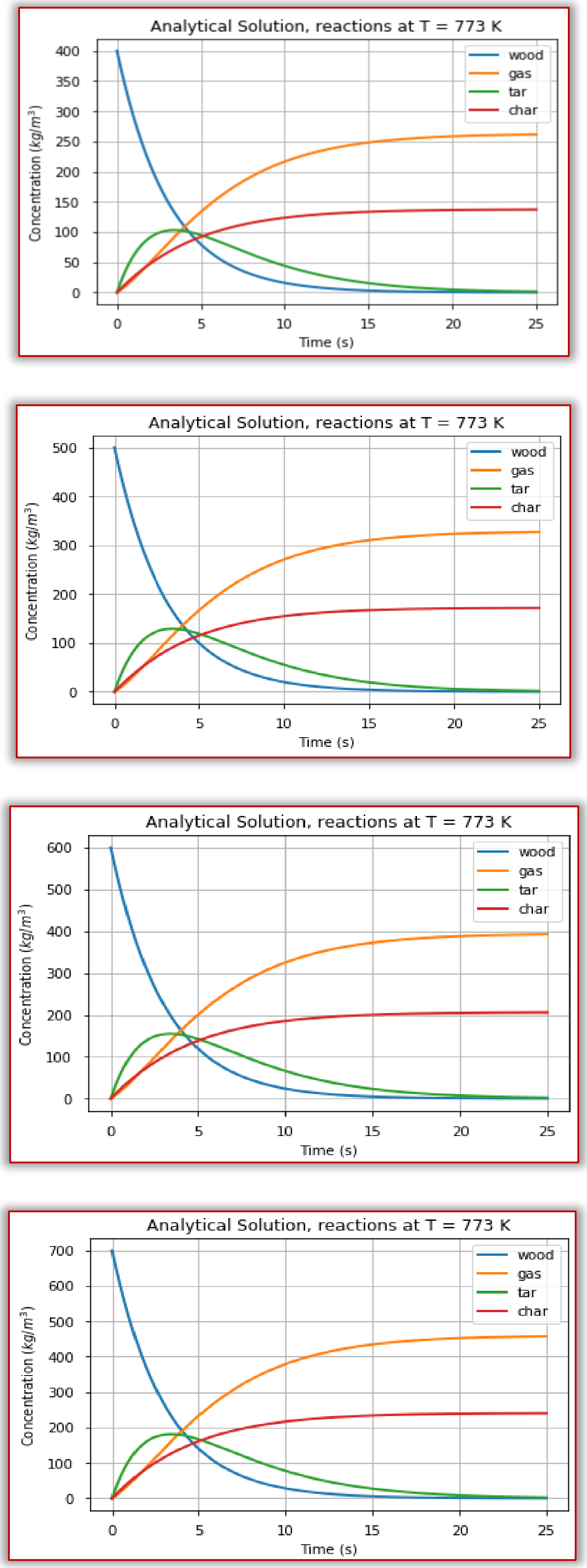
Figure 2a, 2b, 2c and 2d shows product evolution and biomass concentration loss at an instantaneous temperature of 673K, 773K, 873K and 973K respectively. This biomass decomposition reaction resulted in the formation of gas, tar and intermediate solid. As the temperature increased, the tar and intermediate solid formed further participated in some secondary reactions, characterized by decrease in the concentration of the two species, resulting in the production of more gas and char. The process was terminated when biomass concentration had become so low that no significant decomposition reaction took place any more.

It can be observed that the rate of biomass degradation and product evolution is more rapid at higher temperatures. This was due to the fact that as the instantaneous temperature increased, the rate of chemical reaction was accelerated, resulting in a speedy completion of the pyrolysis process. Furthermore, within the 25 seconds consideration time, concentration equilibrium was not achieved for 673K instantaneous temperature. The equilibrium was almost immediately achieved at the higher end of the temperature considered. At higher temperatures, gaseous products evolve at a higher rate and exist at a higher proportion in equilibrium. Other process modelling techniques (thermodynamic approach) have made similar observations albeit for banana residues (Ighalo & Adeniyi, 2019) and rice husk (Adeniyi, Odetoye, Titiloye, & Ighalo, 2019).

The summation of the final concentration of initial biomass, tar, gas, intermediate solid and char is always the same. This is based on the conservation of mass concept to physical system. It can be observed from Figure 2 that the final concentration of char decreased as the instantaneous temperature increased. This is attributable to the fact that increase in instantaneous temperature favours the yield of fluid phase (tar and gas) products during primary pyrolysis (Adeniyi et al., 2019) and also facilitated secondary reactions. The decrease in the final concentration of the intermediate solid with increasing instantaneous temperature is also attributable to this reason. The final concentration of gas appeared to be inconsistent as instantaneous temperature increased because secondary reactions, which led to more gas yield, depend on both residence time and temperature, and the extent of these reactions is based on a trade-off between the two factors.

— Effect of Biomass Density

Figures 3 show the effect of biomass density on the pyrolysis product evolution.



(a)

(b)

(c)

(d)

Figure 3(a-d). Biomass and product species concentration profiles with time at 773 K and sample density of (a) 400 kg/m³ (b) 500 kg/m³ (c) 600 kg/m³ (d) 700 kg/m³

It is observed that biomass density does not have a significant effect on the rate of the biomass degradation and the nature of the product evolution. Although the profiles were similar for all samples considered, the peaks and the final values of the product species concentration profiles, the extent of secondary reactions and the time required for the completion of the pyrolysis process were different for different biomass densities. Wood with higher density gives more char yield than those with lower densities. This is in agreement with the observation of Pious O Okekunle, Akogun, Alagbe, and Osinuga (2015) for hard and soft wood pyrolysis.

CONCLUSION

In this study, Python 3 programming language was successfully used in computing the numerical solutions to the differential equations using Euler's method for evaluating the effects of biomass density and system temperature on product evolution and yields during pyrolysis. It was observed that the rate of biomass degradation and product evolution is more rapid at higher temperatures. This was due to the fact that as the instantaneous temperature increased, the rate of chemical reaction was accelerated, resulting in a speedy completion of the pyrolysis process. The final concentration of char decreased as the instantaneous temperature increased. At higher temperatures, gaseous products evolve at a higher rate and exist at a higher proportion in equilibrium. It was also observed that biomass density does not have a significant effect on the rate of the biomass degradation and the nature of the product evolution. Wood with higher density gives more char yield than those with lower densities.

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