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MODELLING THE PYROLYSIS AND COMBUSTION OF WOOD

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Abstract: This paper examines the chemical kinetics of cellulosic material with fixed and varying temperatures. The combustion kinetics of wood together with Arrhenius equation is used in derivation of the model. The governing nonlinear ordinary differential equations with initial conditions are solved numerically. The results obtained are presented graphically for the purpose of showing the pyrolysis and combustion of wood and impact of wood burning for both fixed and varying temperatures. It is observed that charcoal and gases yields are the end products formed during the processes. However it is observed that gases are highly produced at varying temperatures. However for both fixed and varying temperatures, the decomposition reaction of wood (cellulose) in the system leads to the separation of the components of wood giving charcoal and gases as end products, but the gases are highly produced at moderate temperatures.

Keywords: Pyrolysis, combustion, decomposition, activation energy ratio.

2000 AMS Subject Classification: 47H17; 47H05; 47H09

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1. Introduction

Studies related to combustion kinetics of wood have aimed at understanding the mechanisms and rates of wood combustion for modelling heating in buildings, designing wood stoves, furnaces and boilers. The resulted models have been utilized to examine the effect of wood size, moisture content and temperatures on the rates of pyrolysis and formation of tar, volatiles and char (Bryden *et al*, 2002) Combustion of wood is a particular complex series of chemical reactions and processes. Naturally we understand that a piece of wood will burn when subjected to sufficient heat. Drying will begin by evaporation of water and the resulting water vapour escape through the porous fuel. Pyrolysis is the process that enables combustion to occur when wood reaches a sufficiently high temperature. Chemical reactions then cause the solid material to decompose into a combination of gases (volatile and non-volatile), tar and char and the left over solids made of carbon. When the released volatile gases encounter oxygen, the resulting oxidation can lead to flaming combustion (Riensche and Lewis, 2009). Most people in the world live in the rural areas where they use wood fuel for their cooking using stoves. It is assumed that large quantities of carbon dioxide are produced from these stoves; but due to the increased population growth and repeat fragmentation of the village forests, the wood fuel is probably unsustainable. Rather, it leads to increased collection of fuel wood from the village forests and consequent deforestation and hence desertification (Miaha *et al*, 2008). The fast pyrolysis of natural polysaccharides as industrial process was investigated and found that the pyrolysis of cellulosic materials show promise as a means for the production of useful chemicals in industries (Radlein *et al*, 1991). The studies on the analysis of different kinetic models in the dynamic pyrolysis of cellulose revealed that simultaneous fitting of various curves in dynamic conditions of different heating rates is a technique for calculating kinetic parameters which minimizes the apparent compensation between pre-exponential factor and activation energy (Conesa *et al*, 1994).

Radlein *et al.*, (1991), studied the fast pyrolysis of natural polysaccharides as industrial process and found that pyrolysis of cellulosic materials show a promise of a means for the production of useful chemicals in industries. Conesa *et al.*, (1994), studied the analysis of different kinetic models in the dynamic pyrolysis of cellulose and found that simultaneous fitting of various curves in dynamic conditions of different heating rates is a technique for calculating kinetic parameters which minimize the apparent compensation between pre-exponential factor and activation energy.

In this paper it is intended to formulate and analyze a mathematical model of the pyrolysis and combustion of wood and determine the effects of variation of the related parameters at both fixed and varying temperatures.

2. Model formulation

Under the influence of heat, cellulose produces easily levoglucosan that decomposes into polymers. These three components disintegrate further to C, CO, CO_2, H_2O and combustible volatiles and finally react with oxygen to form glowing ignition and flaming combustion respectively figure 1**.** Note that the pyrolysis is usually the first chemical reaction that occurs in the burning of wood and other organic substances.

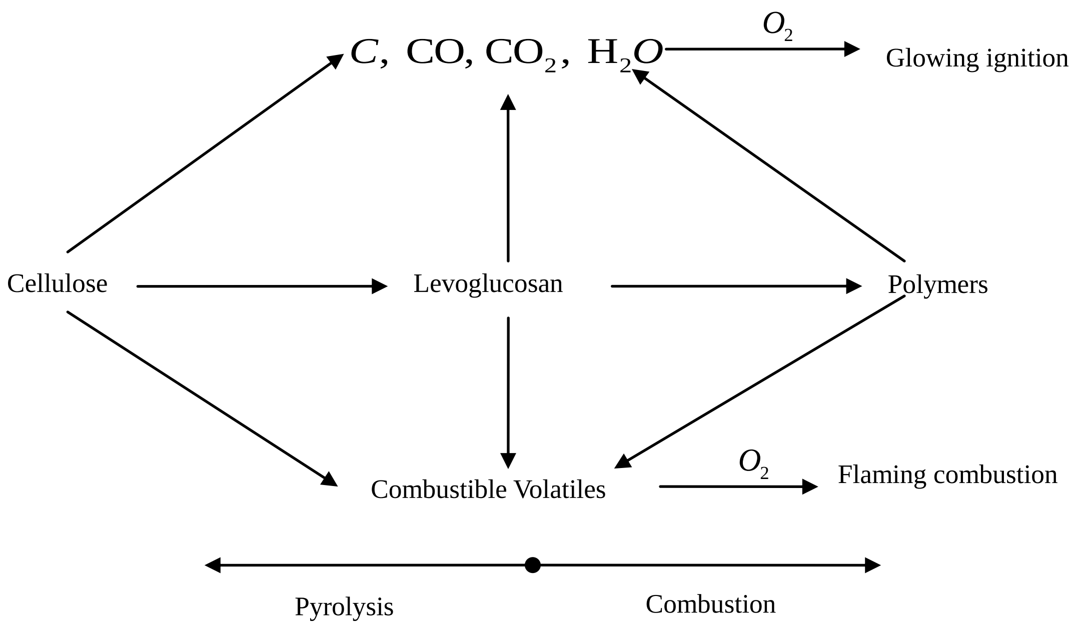

Figure 1: Schematic diagram for the pyrolysis and combustion of wood

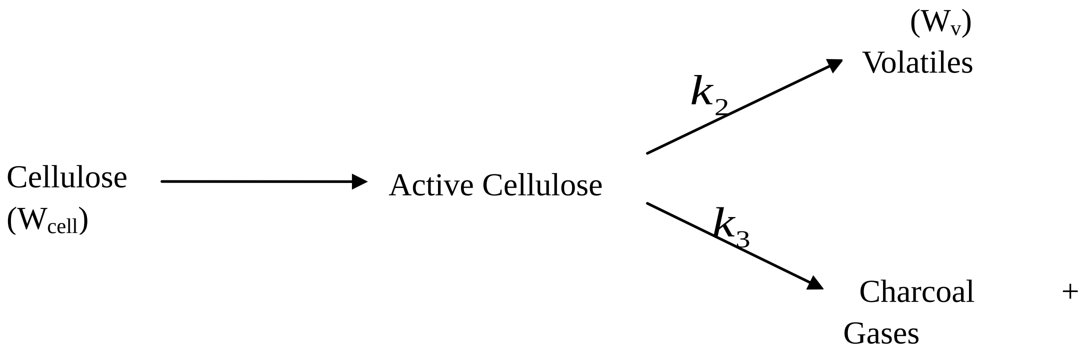

Figure 2: Combustion kinetics of wood

If we let

W_{cell} =mass of wood before decomposition,

W_A =mass fraction present of active cellulose at time τ,

W_v =mass fraction of volatiles,

W_c =mass fraction of charcoal,

W_g =mass fraction of gases,

T =absolute temperature,

T_0 = the initial temperature,

τ is the time,

$k_{i(i=1,2,3)}$ are the rate constants,

$\delta_{i(i=1,2)}$ = the coefficients of deposition.

Then the model equations obtained from combustion kinetics of wood can be written as:

$$\frac{dW_{cell}}{d\tau} = -k_1 W_{cell},$$
$$\frac{dW_A}{d\tau} = k_1 W_{cell} - (k_2 + k_3) W_A,$$
$$\frac{dW_c}{d\tau} = \delta_1 k_3 W_A \tag{1}$$
$$\frac{dW_g}{d\tau} = \delta_2 k_3 W_A,$$
$$\frac{dT}{d\tau} = k_1 W_{cell},$$

with initial conditions that

$$T(0) = T_0 \ , \ W_{cell}(0) = W_0, \ W_A(0) = 0, \ W_c(0) = 0, \ W_g(0) = 0$$

We introduce the dimensionless variables into the equations (1) as

$$x = \frac{W_{cell}}{W_0}, \ y = \frac{W_A}{W_0}, \ z = \frac{W_c}{W_0}, \ m = \frac{W_g}{W_0}, \ \theta = \frac{E_1(T - T_0)}{RT_0^2},$$

$$\lambda_1 = k_{10} t_a e^{-\frac{E_1}{RT_0}}, \ \lambda_2 = k_{20} t_a e^{-\frac{E_2}{RT_0}}, \ \lambda_3 = k_{30} t_a e^{-\frac{E_3}{RT_0}}$$

$$r_2 = \frac{E_2}{E_1}, \ r_3 = \frac{E_3}{E_1}, \ \varepsilon = \frac{RT_0}{E_1}, \ \lambda_0 = \frac{E_1 \lambda_1 W_0}{RT_0^2}, \ t = \frac{\tau}{t_a},$$

and

$k_i = k_{i0} e^{-\frac{E_i}{RT}}, \ i = 1, 2, 3$ is the Arrhenius reaction rate.

We therefore obtain the dimensionless governing equations as:

$$\frac{dx}{dt} = -\lambda_1 x e^{\frac{\theta}{(1+\varepsilon\theta)}},$$

$$\frac{dy}{dt} = \lambda_1 x e^{\frac{\theta}{(1+\varepsilon\theta)}} - y\left(\lambda_2 e^{\frac{r_2\theta}{(1+\varepsilon\theta)}} + \lambda_3 e^{\frac{r_3\theta}{(1+\varepsilon\theta)}}\right),$$

$$\frac{dz}{dt}=\delta_1\lambda_3 y e^{\frac{r_3\theta}{(1+\varepsilon\theta)}}, \tag{2}$$

$$\frac{dm}{dt}=\delta_2\lambda_3 y e^{\frac{r_3\theta}{(1+\varepsilon\theta)}},$$

$$\frac{d\theta}{dt}=x\lambda_0 e^{\frac{\theta}{(1+\varepsilon\theta)}}.$$

with the initial conditions

$\theta(0)=0$, $x(0)=1$, $y(0)=0$, $z(0)=0$, $m(0)=0$.

In the system (2), $r_{i(i=2,3)}$ are the ratios of activation energies, $\lambda_{i(i=0,1,2,3)}$ are the conductivities of wood, θ is the temperature of wood, t is time, t_a is the ambient time, ε is the activation energy parameter, R is the universal gas constant, $E_{i(i=1,2,3)}$ are the activation energies, and x, y, z, m are the mass fractions for cellulose, active cellulose, charcoal and gases respectively.

2.1 Pyrolysis and combustion of wood

Case (a) Model with Fixed temperature (say $\theta=\theta_a$): We substitute $\theta=\theta_a$ to the dimensionless model system (2) to get

$$\begin{aligned}\frac{dx}{dt}&=-\lambda_1 Ax,\\ \frac{dy}{dt}&=\lambda_1 Ax-y\left(\lambda_2 B+\lambda_3 C\right),\\ \frac{dz}{dt}&=\delta_1\lambda_3 Cy,\\ \frac{dm}{dt}&=\delta_2\lambda_3 Cy,.\end{aligned} \tag{3}$$

where

$$A=e^{\frac{\theta_a}{(1+\varepsilon\theta_a)}},\quad B=e^{\frac{r_2\theta_a}{(1+\varepsilon\theta_a)}},\quad C=e^{\frac{r_3\theta_a}{(1+\varepsilon\theta_a)}}$$

with the initial conditions,

$x(0)=1$, $y(0)=0$, $z(0)=0$, $m(0)=0$.

Case (b): Model with variable temperature i.e. large activation energy (say $\varepsilon = 0$). We substitute $\varepsilon = 0$ into the dimensionless model equations (2), the new model equations become:

$$
\begin{aligned}
&\frac{dx}{dt} = -\lambda_1 x e^{\theta},\\
&\frac{dy}{dt} = \lambda_1 x e^{\theta} - y\left(\lambda_2 e^{r_2\theta} + \lambda_3 e^{r_3\theta}\right),\\
&\frac{dz}{dt} = \delta_1 \lambda_3 y e^{r_3\theta},\\
&\frac{dm}{dt} = \delta_2 \lambda_3 y e^{r3\theta},\\
&\frac{d\theta}{dt} = x\lambda_0 e^{\theta},
\end{aligned}
\tag{4}
$$

with the initial conditions $\theta(0) = 0, x(0) = 1, y(0) = z(0) = m(0) = 0.$

3 Results and discussion

Models (3) and (4) are first order initial value problems. The two dimensionless non linear systems together with their initial conditions are solved numerically using ode45 Runge-Kutta approach to determine the proportional material formed. Graphical results for both cases are presented and discussed with respect to various embedded parameters in the systems.

To analyse the simulation to the combustion kinetics in the model system, we again assign numerical values to the parameters encountered in the problem. At the initial stage (i.e. $t = 0$), the temperature of the wood is (cellulose) assumed to be equal to that of the ambient and there has been no production of any of the components involved in the decaying of the cellulose. However at $t > 0$, the decomposition reaction in the system progressed lead to separation of the components involved in the pyrolysis and combustion processes. Here it is assumed that the temperature of wood is not fixed, but it is very high (i.e. high activation energy) and vary with time. Figures 3(a) and 3(b) below demonstrate the effects of various thermo-physical parameters on the wood (cellulose) for constant and varying temperatures respectively for estimated parameter values.

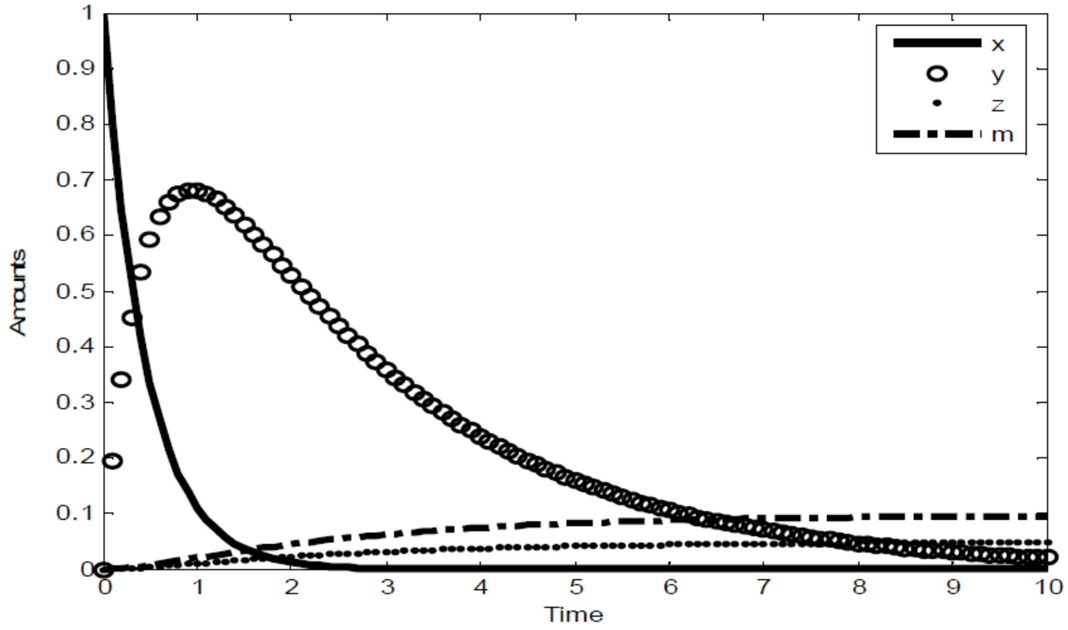

Figure 3(a): The pyrolysis and combustion of wood for $\delta_1 = 0.1, \delta_2 = 0.2$, $\lambda_1 = 0.3$, $\lambda_2 = 0.2$, $\lambda_3 = 0.2$. for a fixed temperature

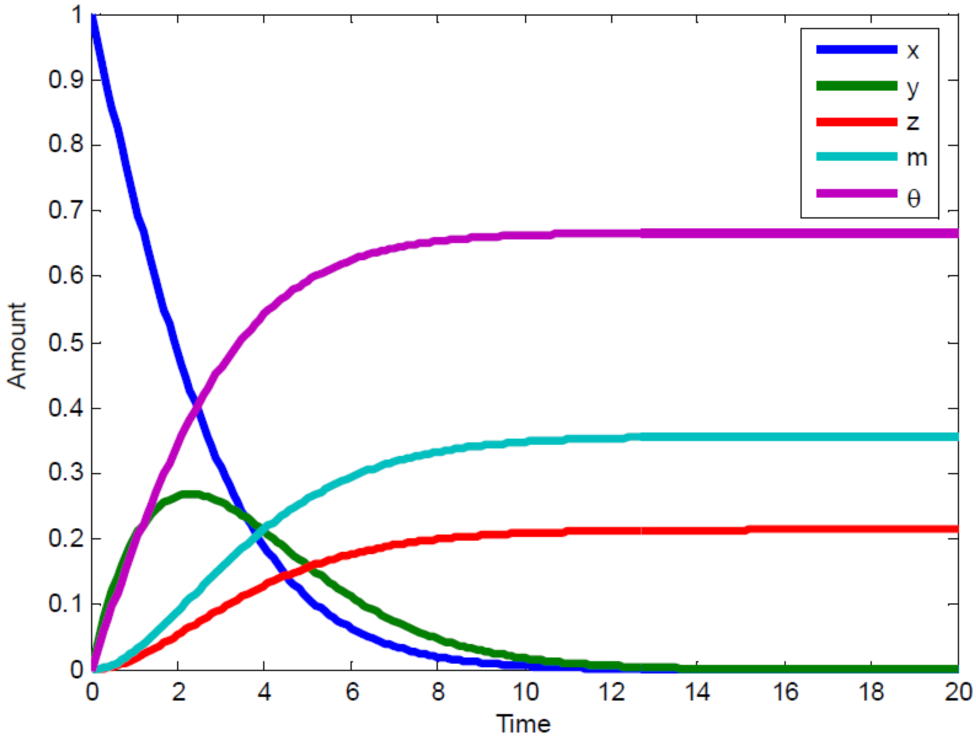

Figure 3(b): The pyrolysis and combustion of wood for $\delta_1 = 0.3$, $\delta_2 = 0.5$, $\lambda_0 = 0.2$, $\lambda_1 = 0.3$, $\lambda_2 = 0.2$, $\lambda_3 = 0.5$, $r_2 = 0.02$, $r_3 = 0.002$ for varying temperatures

It is noted that as the time advances, the amount of cellulose decreases, approaching zero with an accumulation of active cellulose until it attains its steady state. Later on, the active cellulose is disintegrated to two components, charcoal and gases, but the gases are abundantly produced than charcoal specifically at varying temperature (figure 3(b)). This situation enhances greenhouse effect in the atmosphere, whereas the global average surface temperature known as global warming increases.

3.1 Effect of conductivity on wood burning

Figures 4(a) and 4(b) below illustrate the decay of cellulose with two different thermal conductivities (i.e. $\lambda_1 = 0.3$ and $\lambda_1 = 0.5$) both for fixed temperature and varying temperatures respectively.

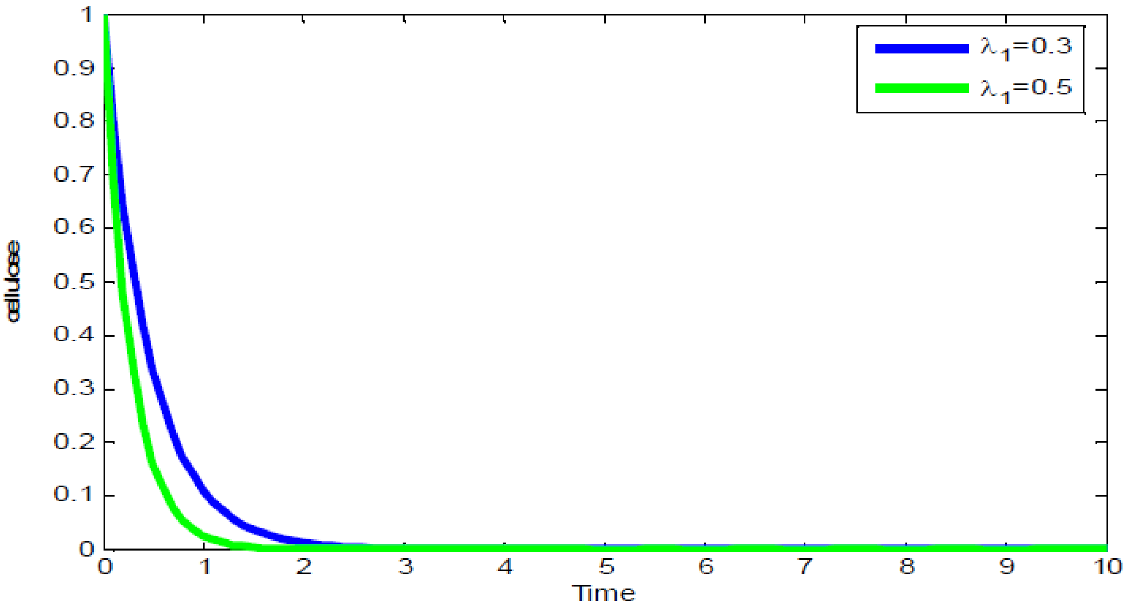

Figure 4(a): Variation of conductivities on cellulose for $\lambda_1 = 0.3$ and $\lambda_1 = 0.5$ at a fixed temperature

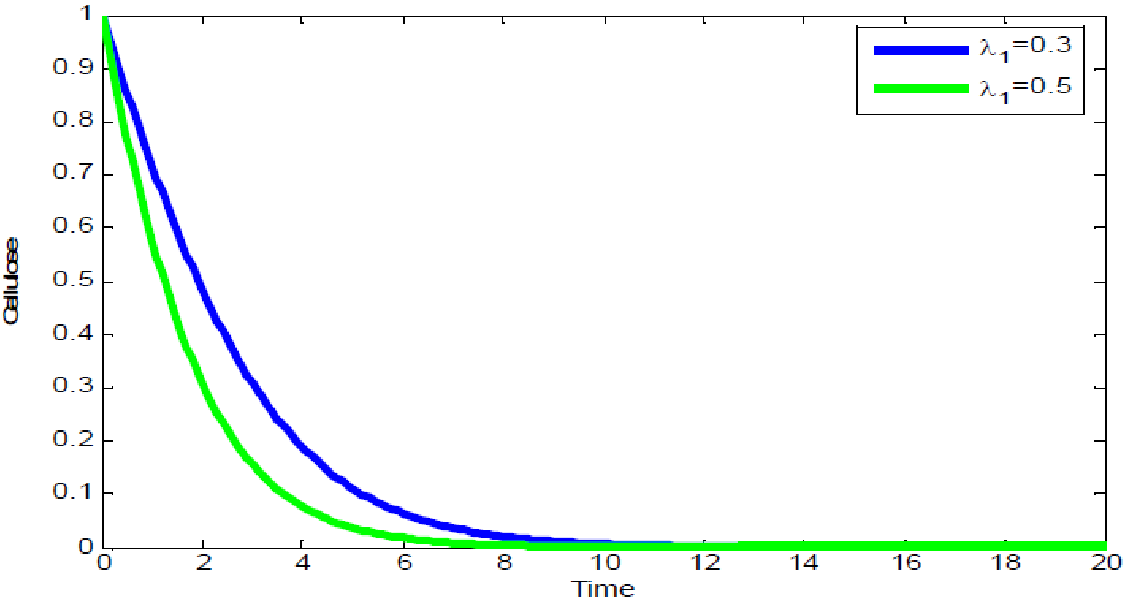

Figure 4(b): Variation of conductivities on cellulose for $\lambda_1 = 0.3$ and $\lambda_1 = 0.5$ at varying temperatures

In both cases, it is seen that whenever conductivity is increased the rate of decay increases i.e. conductivity is proportional to the rate of decay of cellulose.

Figures 5(a) and 5(b) below show the deposition of active cellulose with different values of thermal conductivities (i.e $\lambda_3 = 0.3$ and $\lambda_3 = 0.5$) both for fixed temperature and varying temperatures respectively . The green line represents the deposition rate of active cellulose with conductivity of 0.5 units and blue one indicates the deposition rate of active cellulose with conductivity of 0.3 units.

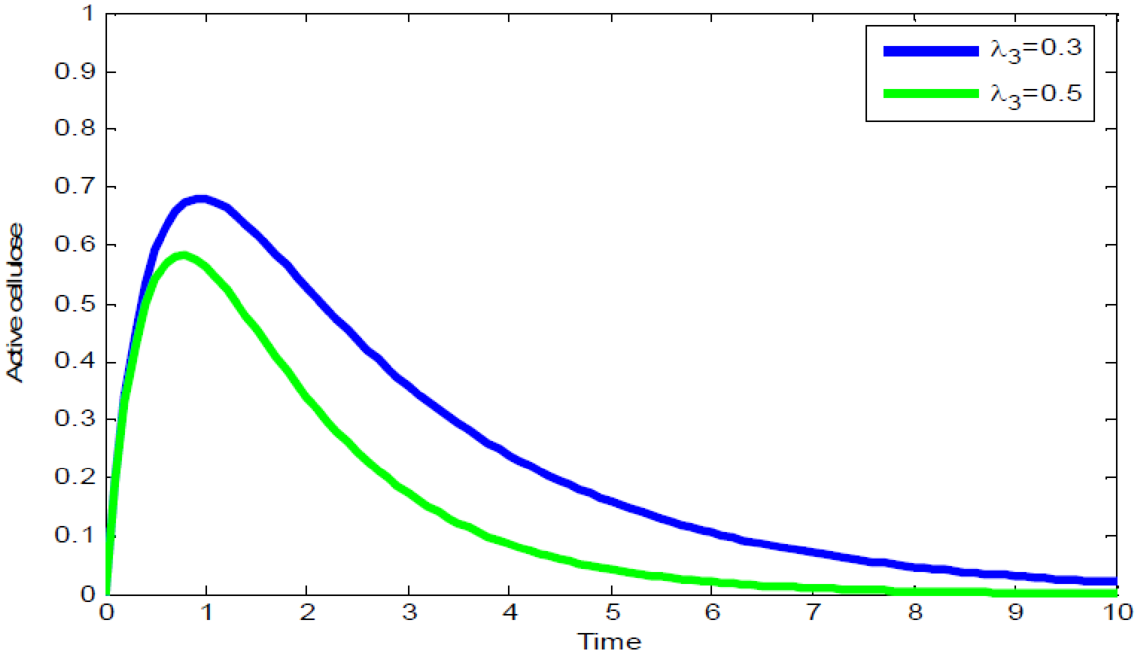

Figure 5(a): Variation of thermal conductivities on active cellulose for $\lambda_3 = 0.3$ and $\lambda_3 = 0.5$ for fixed temperature.

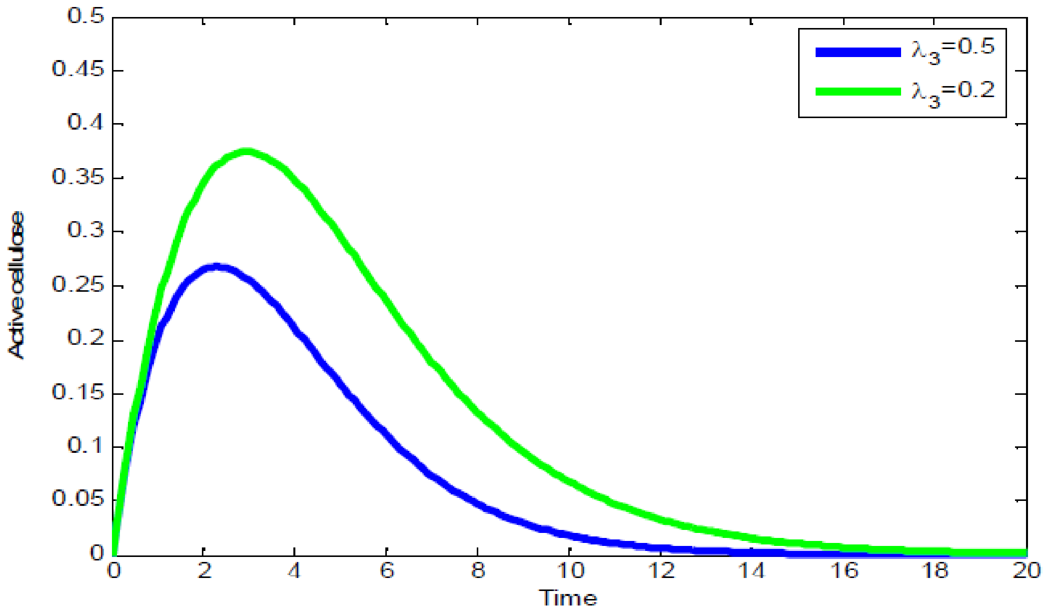

Figure 5(b): Variation of thermal conductivities on active cellulose for $\lambda_3 = 0.2$ and $\lambda_3 = 0.5$ for varying temperatures.

It is noted that there are considerable changes of different conductivities with the amount of active cellulose accumulated, but the amount is lowered at high activation energy than that of the moderate temperature

Figures 6(a) and 6(b) illustrate the charcoal and gases yield with two thermal conductivities (i.e. $\lambda_3 = 0.2$ and $\lambda_3 = 0.5$) for a fixed temperature.

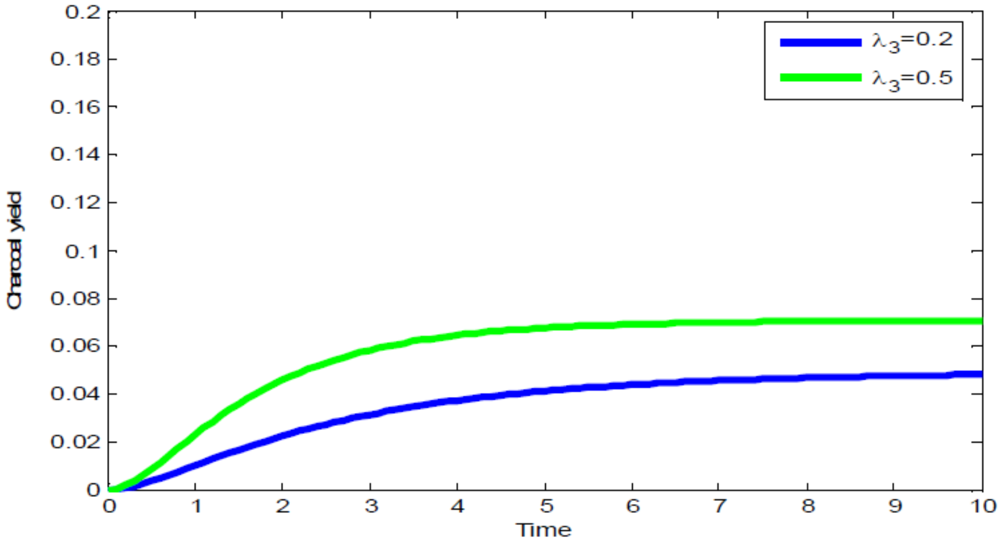

Figure 6(a): Variation of thermal conductivities on charcoal for $\lambda_3 = 0.2$, and $\lambda_3 = 0.5$

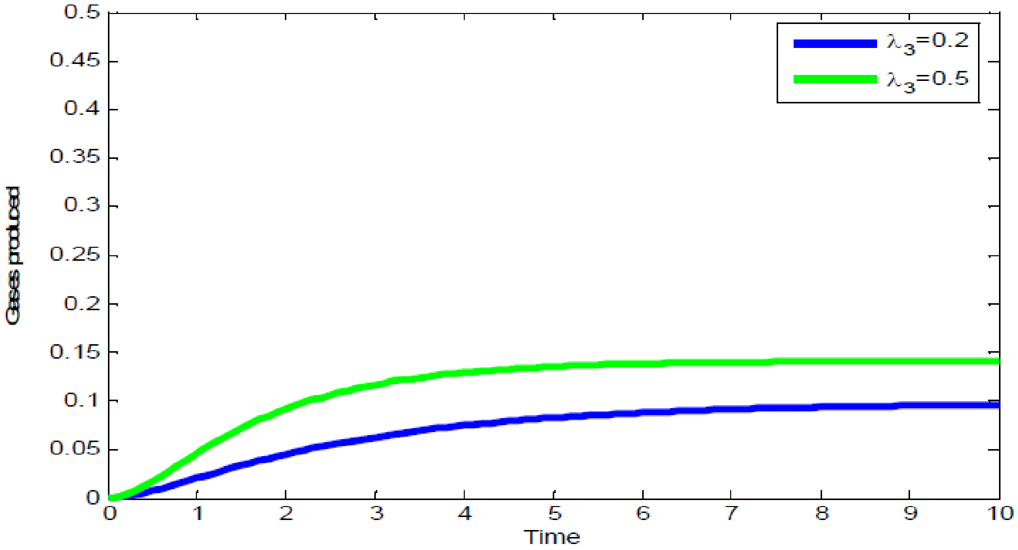

Figure 6(b): Variation of conductivities on gases for $\lambda_3 = 0.2$ an $\lambda_3 = 0.5$

It is seen that the production of gases and charcoal are proportional to the thermal conductivities of wood, but the gases are produced in large quantities.

Figures 7(a) and 7(b) illustrate the charcoal and gases yield with two thermal conductivities (i.e. $\lambda_3 = 0.2$ and $\lambda_3 = 0.5$) for varying temperatures.

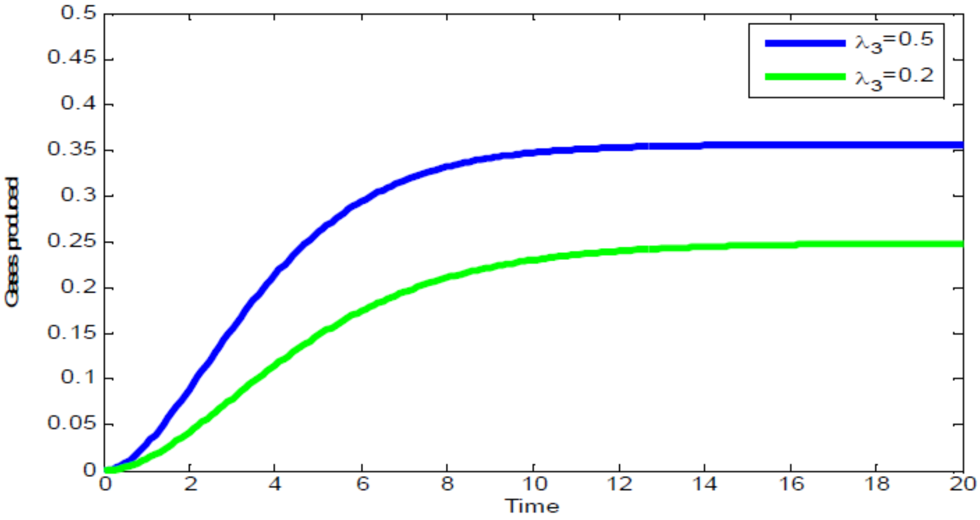

Figure 7(a): Variation of conductivities on gases for $\lambda_3 = 0.2$ and $\lambda_3 = 0.5$

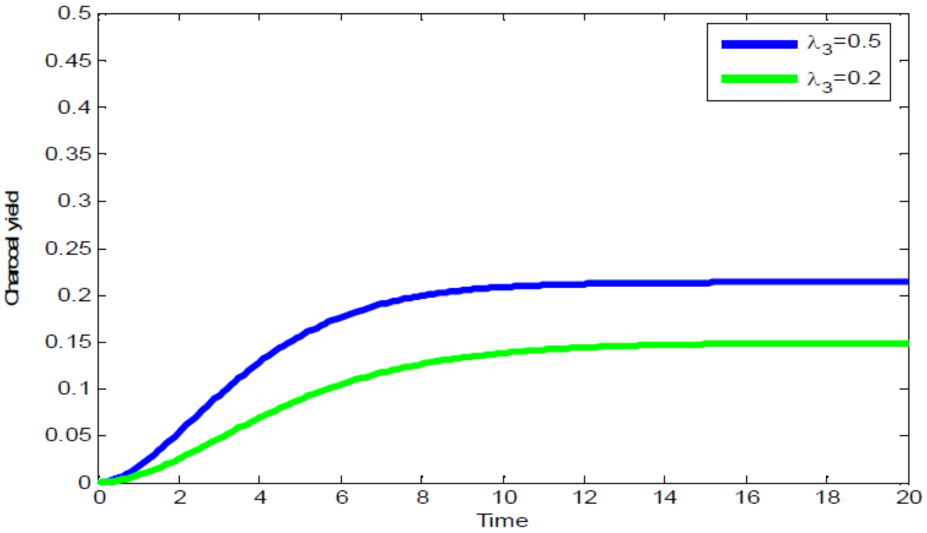

Figure 7(b): Variation of thermal conductivities on active cellulose for $\lambda_3 = 0.5$ and $\lambda_3 = 0\,.$

It is clear that the production of gases and charcoal are proportional to the thermal conductivities of wood, but the gases are produced in large quantities

Figure 8 below illustrate how temperature varies with two different thermal conductivities of cellulose (woods) with the same activation energy i.e. $\lambda_0 = 0.2$ and $\lambda_0 = 0.3$.

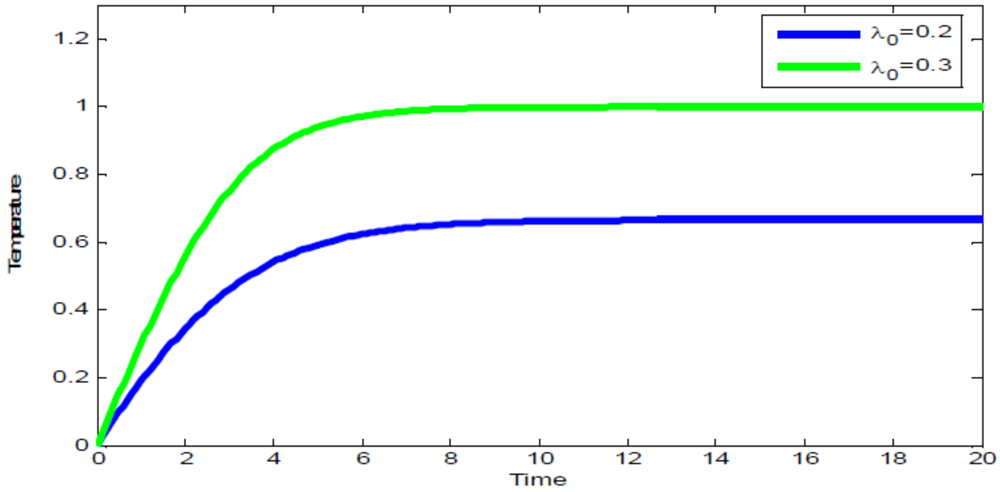

Figure 8: The effect of conductivities on temperature for $\lambda_0 = 0.2$ and $\lambda_0 = 0.3$

It can be observed from the graph that, at the same activation energy, the higher the thermal conductivity the higher the temperature.

3.2 Effect of the coefficient of deposition on wood burning

Gases and charcoal production are also affected by deposition coefficients of wood. In this section we show the effect of coefficient of deposition δ on combustion of wood while maintaining the other model parameters constant. Figures 9(a) and 9(b); illustrate the behaviour of charcoal and gases formation with different deposition coefficients for a fixed temperature.

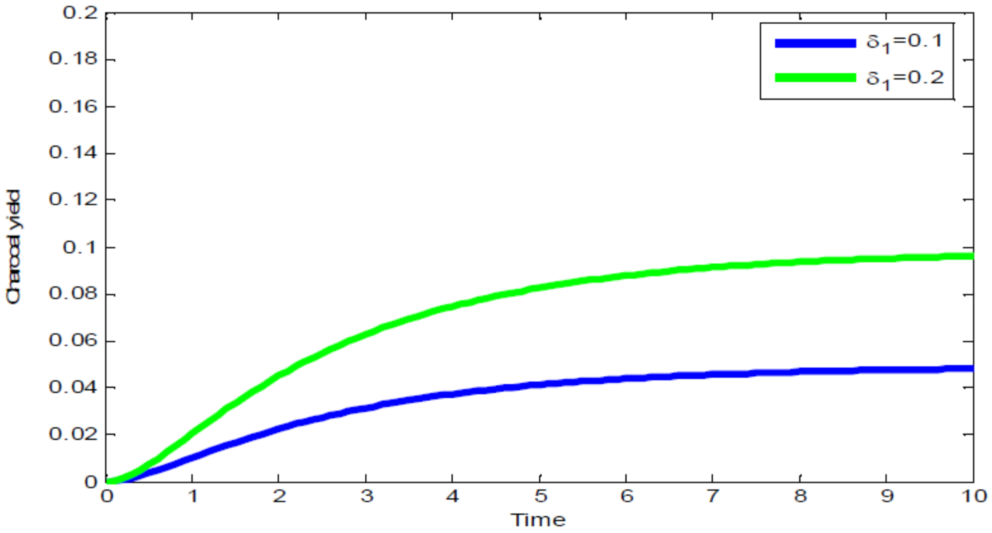

Figure 9(a): Variation of deposition coefficients on charcoal for $\delta_1 = 0.1$ and $\delta_2 = 0.2$ for a fixed temperature

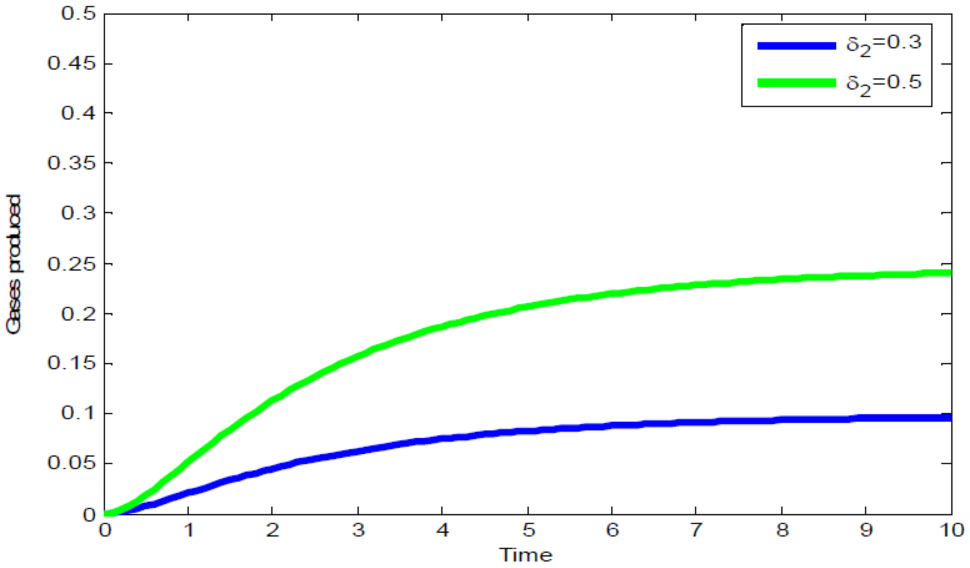

Figure 9(b): Variation of deposition coefficients on gases for $\delta_2 = 0.3$ and $\delta_2 = 0.5$ for a fixed temperature

Figures 10(a) and 10(b); illustrate the behaviour of charcoal and gases formation with different deposition coefficients for varying temperatures.

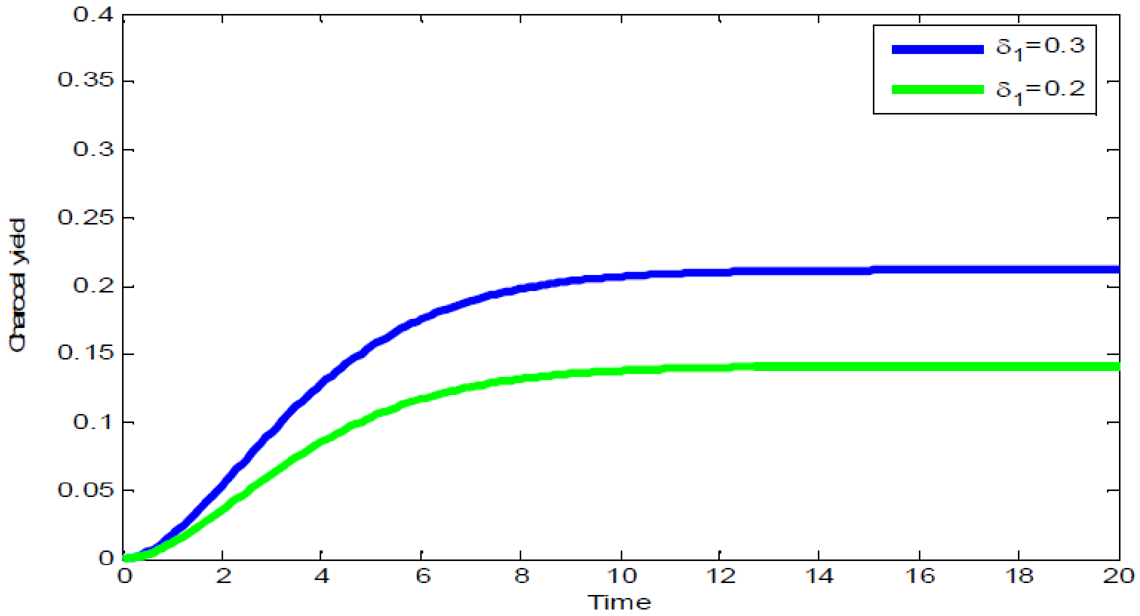

Figure 10(a): Variation of deposition coefficients on charcoal for $\delta_1 = 0.2$ and $\delta_2 = 0.3$ for varying temperatures.

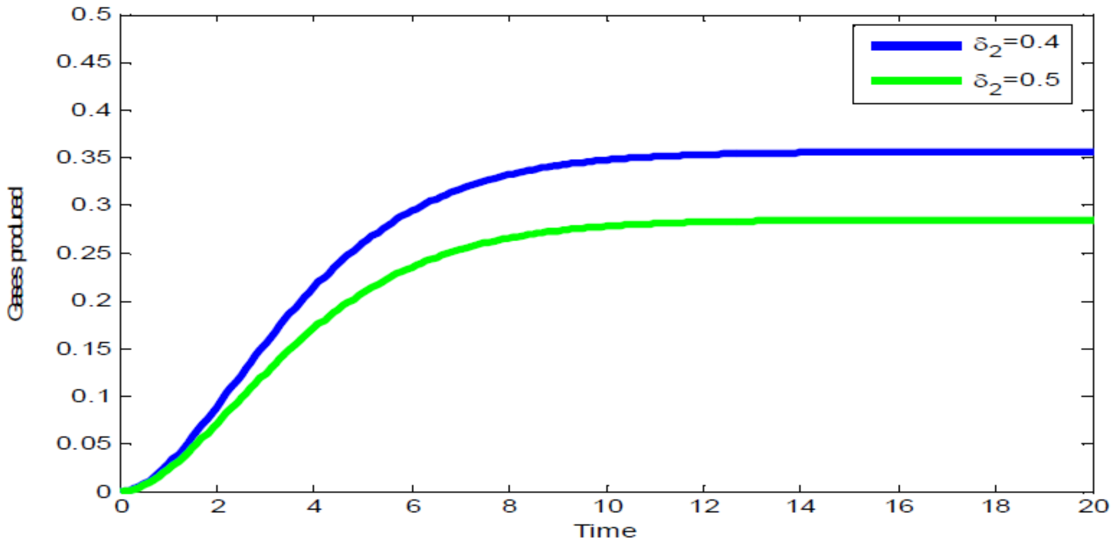

Figure 10(b): Variation of deposition coefficients on gases for $\delta_1 = 0.4$ and $\delta_2 = 0.5$ for varying temperatures.

It is observed that in both cases, as the coefficient of deposition increases, the gases and charcoal formation for the fixed and varying temperatures also increase until the limiting values are attained. High proportions of charcoal and gases production are seen at high activation energy compared to the case of fixed temperature for the same parameter values.

3.3 Effects of activation energy ratios on wood burning

Figures 11 and 12 represent the rate of increase of active cellulose with different ratios of activation energies,

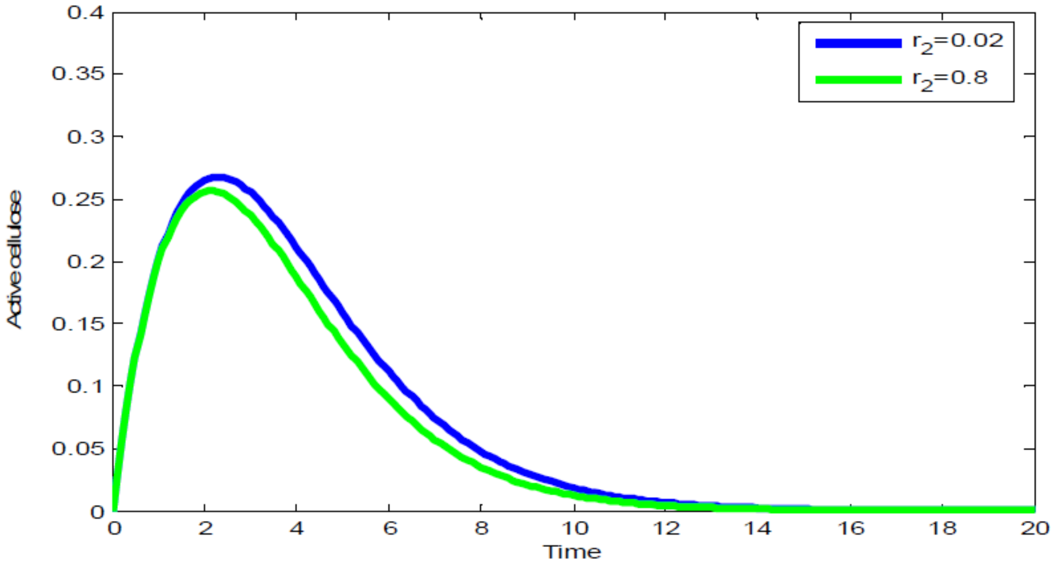

Figure 11: Variation of ratios of activation energies on active cellulose for $r_2 = 0.02$ and $r_2 = 0.8$

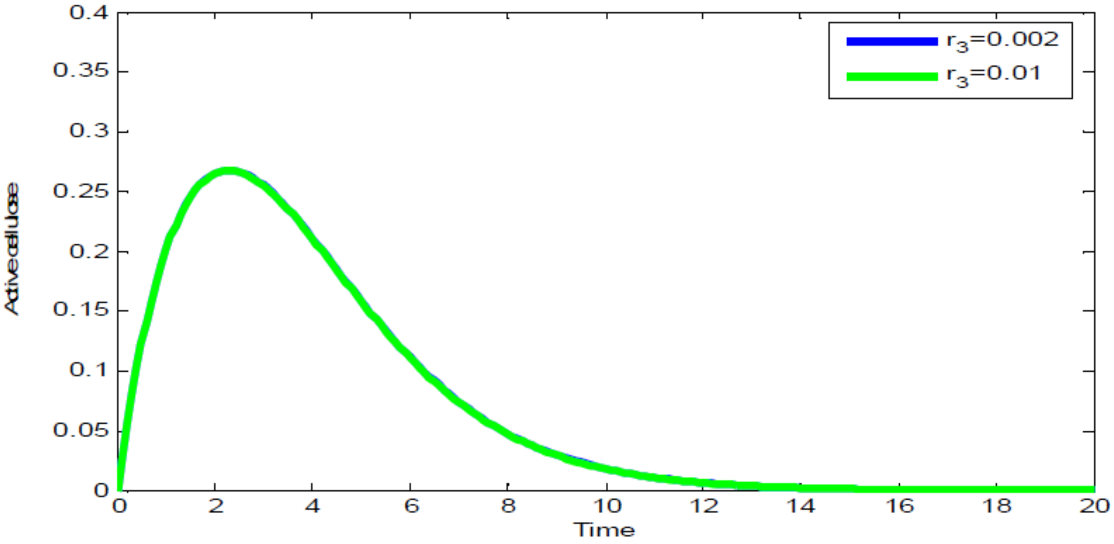

Figure 12: Variation of ratios of activation energies on active cellulose for $r_3 = 0.002$ and $r_3 = 0.01$

It can be seen from the figure 11 that there is a slight change on the rate of accretion of active cellulose but there is no significant change of active cellulose as seen in figure 12.

Figures 13 and 14 represent charcoal and gases yields respectively with no significance change when the ratios of activation energies are varied.

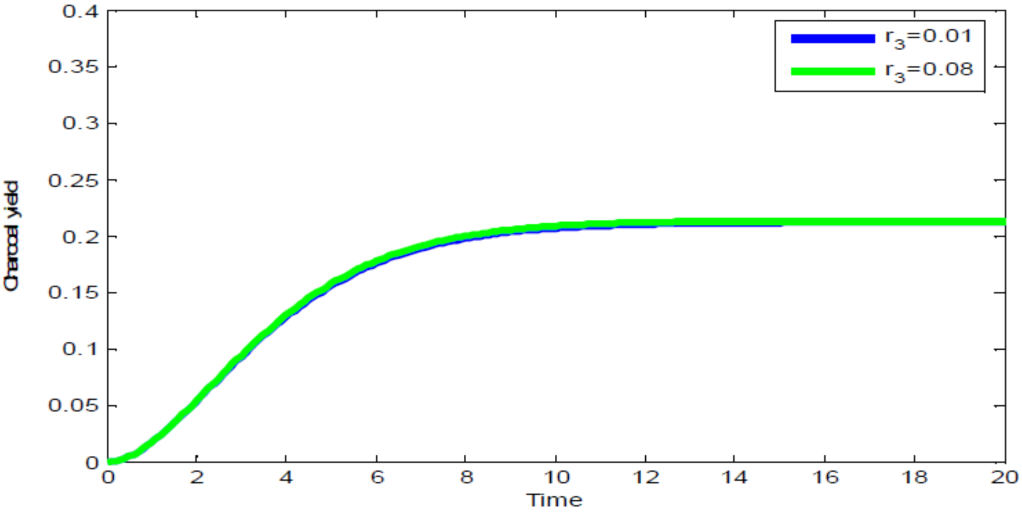

Figure 13: Variation of ratios of activation energies on charcoal yield for $r_3 = 0.01$ and $r_3 = 0.08$

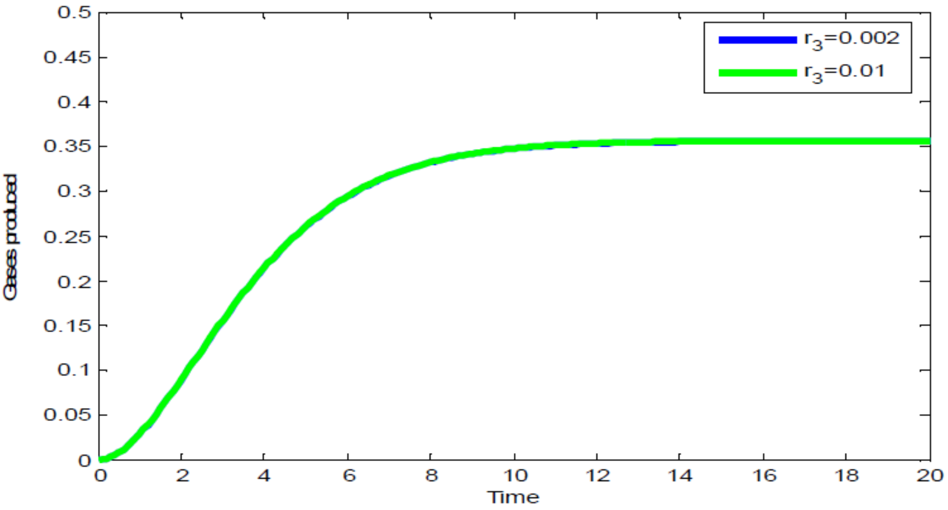

Figure 14: **V**ariation of ratios of activation energies on gases for $r_3 = 0.002$ and $r_3 = 0.01$

It is seen that there is no significance change for the yields if the ratios of activation energy for both cases are varied.

3.4 Relationships among the variables for the large activation model (model (4))

In the pyrolysis process, the cellulose disintegrate to give active cellulose as intermediate product before it undergo decomposition to give charcoal and gases which are the end products. Gases are usually highly produced as seen in figures 23 and 24 below.

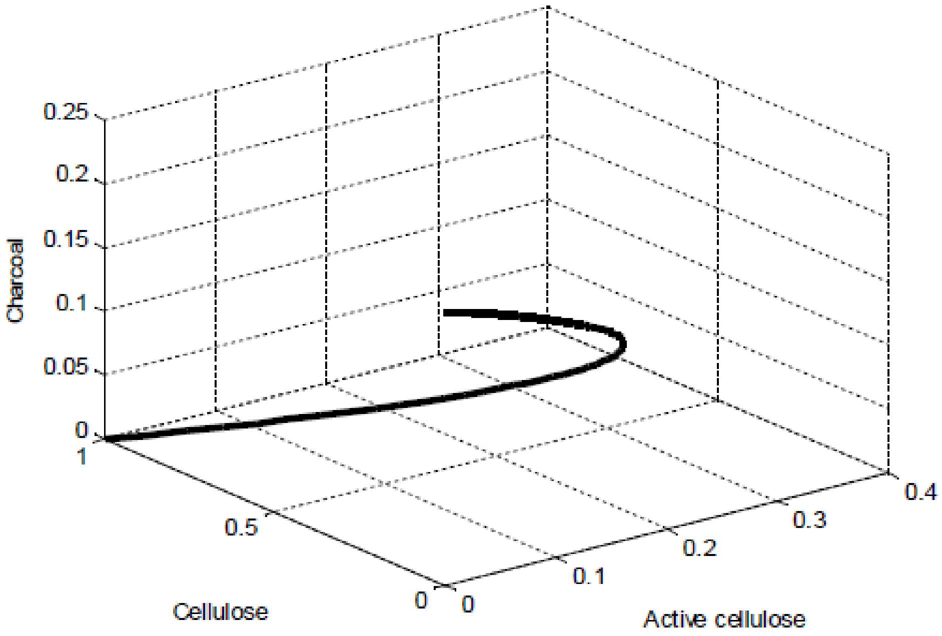

Figure 23: Variation of cellulose, active cellulose and charcoal

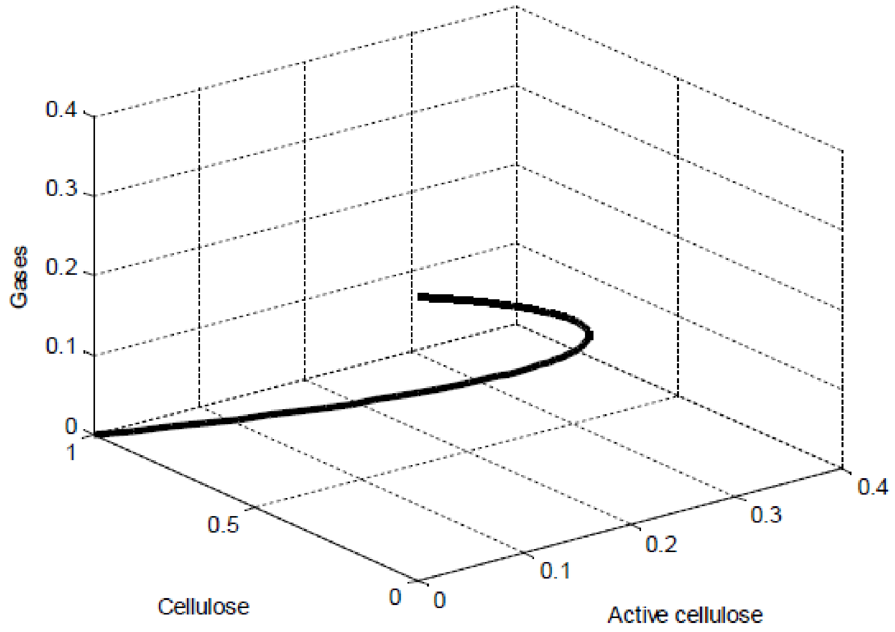

Figure 24: Variation of cellulose, active cellulose and gases yield

Figure 25 below shows the variation of cellulose, active cellulose with temperature.

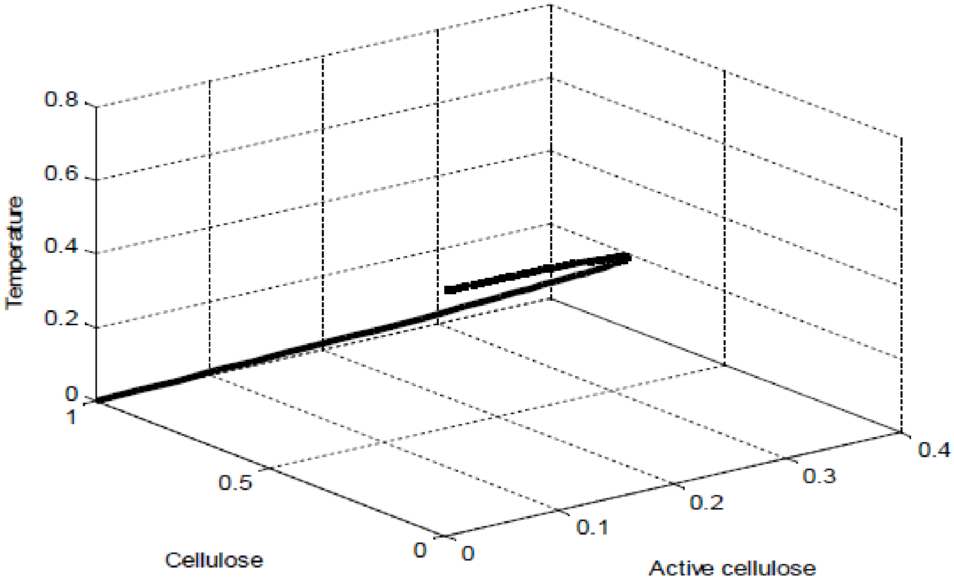

Figure 25: Variation of cellulose, active cellulose and temperature

It is noted that there is accretion of active cellulose as the cellulose start to disintegrate until it attains its steady state value and then decreases with the temperature rise.

Figure 26 shows the variation of active cellulose, charcoal and gases

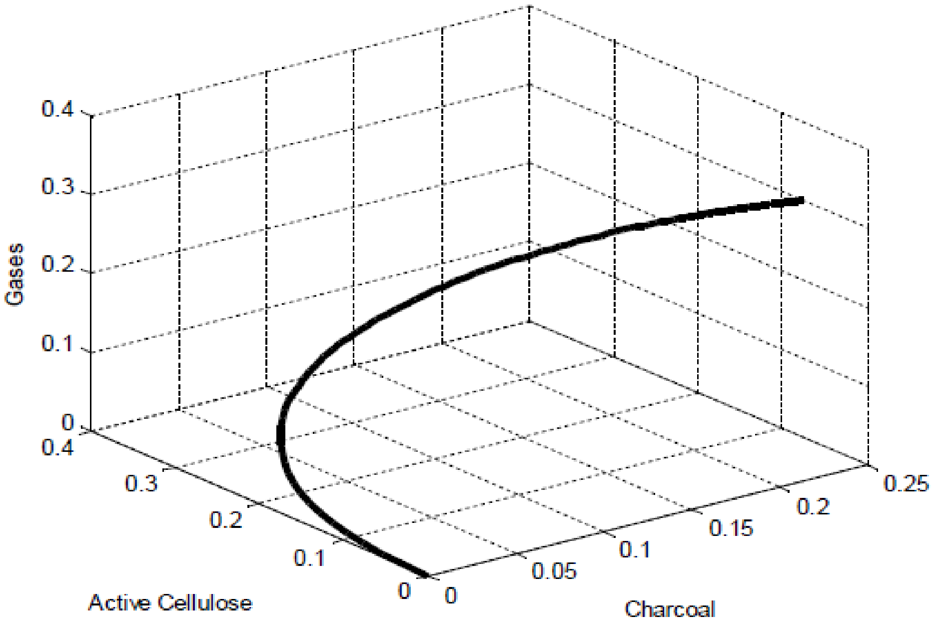

Figure 26: Variation of active cellulose, charcoal and gases

It can be seen that the decomposition of active cellulose increase until it attains its activated point, then it starts to decrease to produce gases and charcoal

4.0 Conclusions

In this paper, the pyrolysis and combustion of wood (cellulose) with respect to wood (cellulose) decomposition was investigated both for fixed and varying temperatures respectively. The governing nonlinear differential equations with initial conditions were solved numerically using Runge-Kutta method.

The computational results show that for fixed temperatures, the decomposition reaction of wood (cellulose) lead to separation of the components of wood through pyrolysis process to yield active cellulose, charcoal and gases. During the decomposition, as the time progresses, the amount of cellulose decrease and approach zero while active cellulose accumulates until it attains its steady state value and then it decreases in the same manner as the cellulose, thereafter decompose to charcoal and gases. It is shown that the thermal conductivity and coefficient of deposition play a key role in the decomposition and accretion processes. Therefore using wood with high thermal conductivity and coefficient of deposition amounts in the yield of large amount of charcoal and gases. Also it is revealed that gases are abundantly produced than charcoal and this enhances greenhouse effect in the atmosphere. and thus increasing global warming.

The effects of various parameters on the wood (cellulose) at high activation energy $(\varepsilon = 0)$ were demonstrated and the results were almost the same but at moderate temperature more gases are released. Also it was shown that the ratios of activation energy parameter values have no significant effect on wood burning.

REFERENCES

[1] K.M. Bryden ,K.W. Ragland,C.J. Rutland, Modelling Thermally Thick Pyrolysis of Wood, Biomass and Bioenergy, 22(2002), 41-53.

[2] R.M. Riensche, R.R. Lewis, Modelling and Rendering Physically-Based Wood Combustion, In proceedings (conf/isvc/RienscheL09), Springer, 5875(2009), 896-905.

[3] M.D. Miaha, A.H. Rashid, M.Y. Shin M. Y, Wood fuel use in the traditional cooking stoves in the rural floodplain areas of Bangladesh: A socio environmental perspective, Institute of Forestry and Environmental Sciences, University of Chittagong, Bangladesh article info Article history, 2008.

[4] D. Radlein, J. Piskorz, D.S. Scott, Fast pyrolysis of natural polysaccharides as a potential Industrial process, Journal of Analytical and Applied Pyrolysis, Elsevier, Volume: 19, Issue: 19(1991), 41-63.

[5] J.A. Conesa, J.A. Caballero, A. Marcilla, R. Font R., Analysis of different kinetic models in the dynamic pyrolysis of cellulose**,** J. Anal. Appl. Pyrol., 30(1994), 101-120.