DYNAMIC MODEL OF UNPRETREATED PLANTAIN TRUNK BIOMASS HYDROLYSIS FOR BUTANOL PRODUCTION

PATIENCE O. EVANS[1] & EVANS C. EGWIM[2]
[1]Department of Mathematics, Federal Polytechnic Bida, Niger State, Nigeria.
[2]Department of Biochemistry, Federal University of Technology Minna, Niger State, Nigeria.
E-mail: e.egwim@futminna.edu.ngg, patevansjj@gmail.com
Phone: +234-706-553-0033

Abstract
Lignocellulose biomass promises to be a cheap source of Butanol. The kinetic model for the hydrolysis of Unpretreated Plantain Trunk Biomass (UPTB) for the production of Butanol was examined. The process from biomass to glucose and to Butanol was subjected to mathematical modeling using an initial value of UPTB as 1000mg/ml. The optimum yield of glucose from UPTB is 450mg/ml while that for Butanol was 974ppm. The results showed that glucose depletion followed an exponential pattern with R-Squared values of 0.8643 for unpretreated biomass while that of Butanol yield follows a second order polynomial with R-Squared of 0.9775. The work concludes that Butanol yield increases with increase in the time of reaction.

Keywords: Dynamics, Models, Initial Value, Optimum, Biomass, Butanol, Polynomial.

Introduction
Production of butanol by the anaerobic fermentation is one of the oldest industrial methods for obtaining this important industrial solvent. It is of particular interest due to the role it can play as one the future biofuels. Biobutanol is a next-generation liquid biofuel with properties similar to those of gasoline. There is a widespread effort to commercialize biobutanol production from agricultural residues, such as corn stover, which do not compete with human and animal foods It is expected that production biobutanol can reduce consumption of oil and natural gas by the automobile industry and reduce emissions of harmful gases into the atmosphere (Nawa, *et al*., 2016)

According to Olaoye and Kolawole (2013), logistic model can be used to illustrate the kinetics of biomass conversion with respect to time while the modified Gomperta model can be used to test the kinetics of ethanol production at a steady temperature. Literature supports that the utilization of mathematical model will contribute to a better understanding of effects of various factors, affecting production of ethanol (Evans *et al*., 2021).

Farah *et al*. (2011), used computer simulation of four different kinetic models which are: Monod, Contois, Modified Monod and Teisser to investigate *S. cerevisiae* growth kinetics and ethanol productivity. It was observed that Teisser model gave marginally better fit than other models tested as it obtained the highest correlation coefficient of 0.96299, Gábor. (2017). According to Alfa *et al*. (2012), biogas produced from boiled *Cymbopogon citratus* (Lemon Grass) is a potential cost-effective alternative energy source in Nigeria.

Sheetal and Patil (2014) reviewed some literature and observed that kinetic models describing the behavior of microbiological systems are very useful tool. Kinetics of biomass production with respect to time could be illustrated by logistic models. They concluded that, utilization of mathematical model would contribute to a better understanding of effects of various factors affecting the production processes. In other words, models enable us to understand, design and control the fermentation process better and could also be used for further process development, (Saa and Nielsen, 2017).

The present work is therefore designed to use consecutive reaction mathematical model to study the kinetics of the hydrolysis of plantain biomass to glucose and the fermentation of glucose to butanol using *Costridium acetobutylicum*.

Methodology

In the production of butanol from plantain trunk biomass, we consider a pattern of a consecutive reaction where the product of one reaction becomes the reactant for the other reactions.

Model of Conversion of Plantain Trunk Biomass to Ethanol without Pretreatment

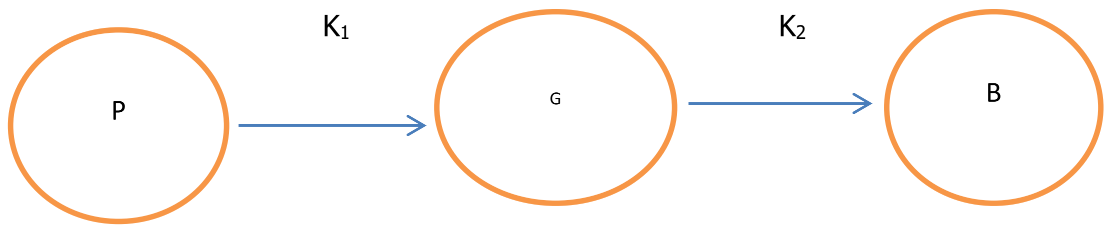

Figure 1: Model of Conversion of Plantain Trunk Biomass to Ethanol without Pretreatment.

The dynamic model for the production of Butanol from pretreated plantain trunk biomass was formulated and Excel software was used to plot the graphs

The ODEs that describe the rate of change of each reactant with time is written as

$$\frac{dP(t)}{dt} = -K_1P(t) \quad (1)$$

$$\frac{dG(t)}{dt} = K_1P(t) - K_2G(t) \quad (2)$$

$$\frac{dB(t)}{dt} = K_2G(t) \quad (3)$$

were,

P = Unpretreated Plantain trunk biomass concentration

G = Glucose concentration

B = Buthanol concentration

We consider an initial value problem in which we consider initial time t=0, for the above reaction,

$$[P] = [P_0], [G] = 0, [B] = 0$$

$$P_0 = [P] + [G] + [B] \quad (4)$$

Integrating equation (1),

$$\int \frac{dP}{dt} = \int -k_1P \quad (5)$$

Applying separation of variable,

$$\int \frac{dP}{P} = -k_1 \int dt \tag{6}$$

Integrating from P_0 to P and 0 to t,

$$\int_{P_0}^{P} \frac{dP}{P} = -k_1 \int_0^t dt \tag{7}$$

$$\ln P - \ln P_0 = -k_1 t \tag{8}$$

$$[P] = Pe^{-k_1 t} \tag{9}$$

Substituting equation 9, into equation 2, we obtain,

$$\frac{dG}{dt} = k_1 P_0 e^{-k_1 t} - k_2[G] \tag{10}$$

Adding $k_2[G]$to both sides of (10), we obtain,

$$\frac{dG}{dt} + k_2[G] = k_1 P_0 e^{-k_1 t} \tag{11}$$

Using integrating factor method,

$$G.IF = e^{\int f(x)dx} = e^{\int f(x)dx}.y(x)dx + C$$

$$e^{\int k_2 dt}.[G] = e^{\int k_2 dt}.k_1[P_0]e^{-k_1 t} + C \tag{12}$$

We obtain,

$$e^{k_2 t}[G] = \frac{k_1 P}{k_2 - k_1} e^{(k_2 - k_1)t} + C \tag{13}$$

At t=0, $[G] = [G_0]$

$$e^{k_2(0)}[G_0] = \frac{k_1 P_0}{k_2 - k_1} e^{(k_2 - k_1)0} + C \tag{14}$$

We obtain the constant c as,

$$C = G_0 - \frac{k_1 P_0}{k_2 - k_1} \tag{15}$$

Substitute the value of constant C, into equation13, we have,

$$e^{k_2 t}[G] = \frac{k_1 P_0}{k_2 - k_1} e^{(k_2 - k_1)t} + G_0 - \frac{k_1 P_0}{k_2 - k_1} \tag{16}$$

Diving both sides by $e^{k_2 t}$

$$[G] = \frac{k_1 P_0}{k_2 - k_1} e^{(-k_1)t} + G_0 e^{-k_2 t} - \frac{k_1 P_0}{k_2 - k_1} e^{-k_2 t} \tag{17}$$

Let $G_0 = 0$, we have,

$$[G] = \frac{k_1 P_0}{k_2 - k_1}\left(e^{-k_1 t} - e^{-k_2 t}\right) \tag{18}$$

From equation 4,

$$[B] = P_0 - [P] - [G] \tag{19}$$

hence,

$$[B] = P_0 - P_0 e^{-k_1 t} - \frac{k_1 P_0}{k_2 - k_1}\left(e^{-k_1 t} - e^{-k_2 t}\right) \tag{20}$$

Simplifying equation 20, we obtain,

$$[B] = P_0\left(1 + \frac{k_1 e^{-k_2 t} - k_2 e^{-k_1 t}}{k_2 - k_1}\right) \qquad (21)$$

Equation (9), (18) and (21) was solved using maple to determine the concentration of the biomass, glucose yield and ethanol produced.

Result and Discussion

The result generated from the maple simulation at $k \ = 1.5 and\, k_2 = 0.8$ has its initial values as:

Considering the process from Plantain trunk biomass to Glucose

$$P(t) = 1000\, e^{-\frac{3}{2}t} \qquad (22)$$

$$G(t) = -1000\, e^{-\frac{3}{2}t} + 1000 \qquad (23)$$

Table 1: A Table of Glucose Yield with Time from Plantain Trunk Biomassat constant pH, Temperature and Enzyme concentration.

TIME (DAYS)	P (MG/ML)	G (MG/ML)
0	1000	0
1	223.1301601	776.8698399
2	49.78706837	950.2129316
3	11.10899654	988.8910035
4	2.478752177	997.5212478
5	0.55308437	999.4469156
6	0.123409804	999.8765902
7	0.027536449	999.9724636
8	0.006144212	999.9938558
9	0.001370959	999.998629
10	0.000305902	999.9996941

Considering the process from Glucose to Butanol

$$G(t) = 800\, e^{-\frac{4}{5}t} \qquad (24)$$

$$B(t) = -800\, e^{-\frac{4}{5}t} + 801 \qquad (25)$$

Considering the process from Unpretreated Plantain trunk biomass to Glucose and to butanol

$$P(t)=1000e^{-\frac{3}{2}t} \tag{26}$$

$$G(t)=-\frac{1500}{7}e^{-\frac{3}{2}t}+\frac{1500}{7}e^{-\frac{4}{5}t} \tag{27}$$

$$B(t)=\frac{8000}{7}e^{-\frac{3}{2}t}-\frac{1500}{7}e^{-\frac{4}{5}t}+1000 \tag{28}$$

Figure 2 shows the dynamics of UPTB and glucose yield.

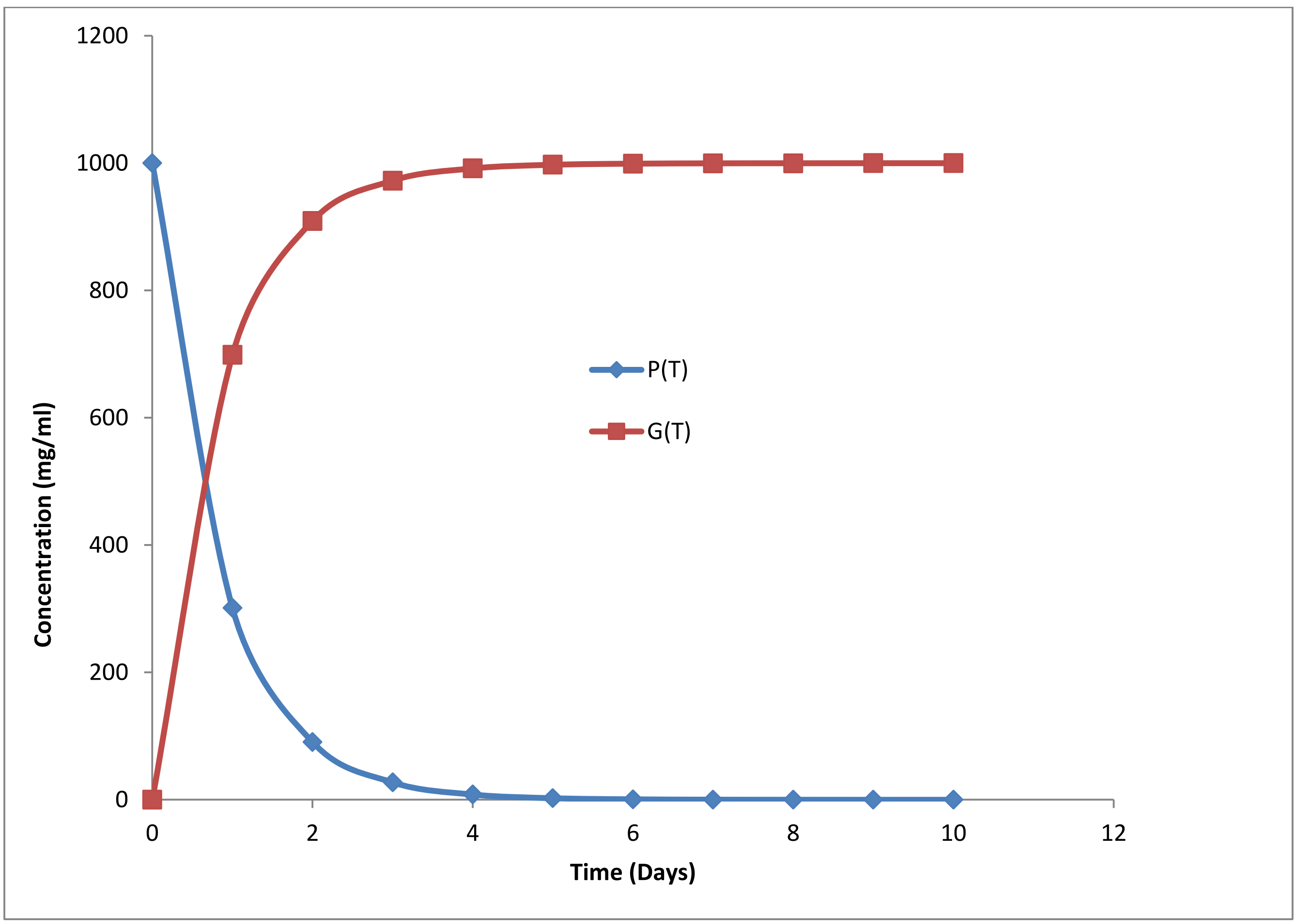

Figure 2: A Plot of the Rate of Change of Plantain Trunk Biomass and Glucose with Time.

The Plantain trunk biomass decreases at the rate of $\alpha = 1.5$ from the initial value of 1000g/l to 0.0003059mg/ml at day 10. The result shows that as the UPTB decreases the glucose increases. This agrees with the work of Olaoye and Kolawole (2013), who showed that Logistic model can be used to illustrate the kinetics of biomass conversion with time.

The plot of Glucose depletion and Butanol yield is given in Figure 3.

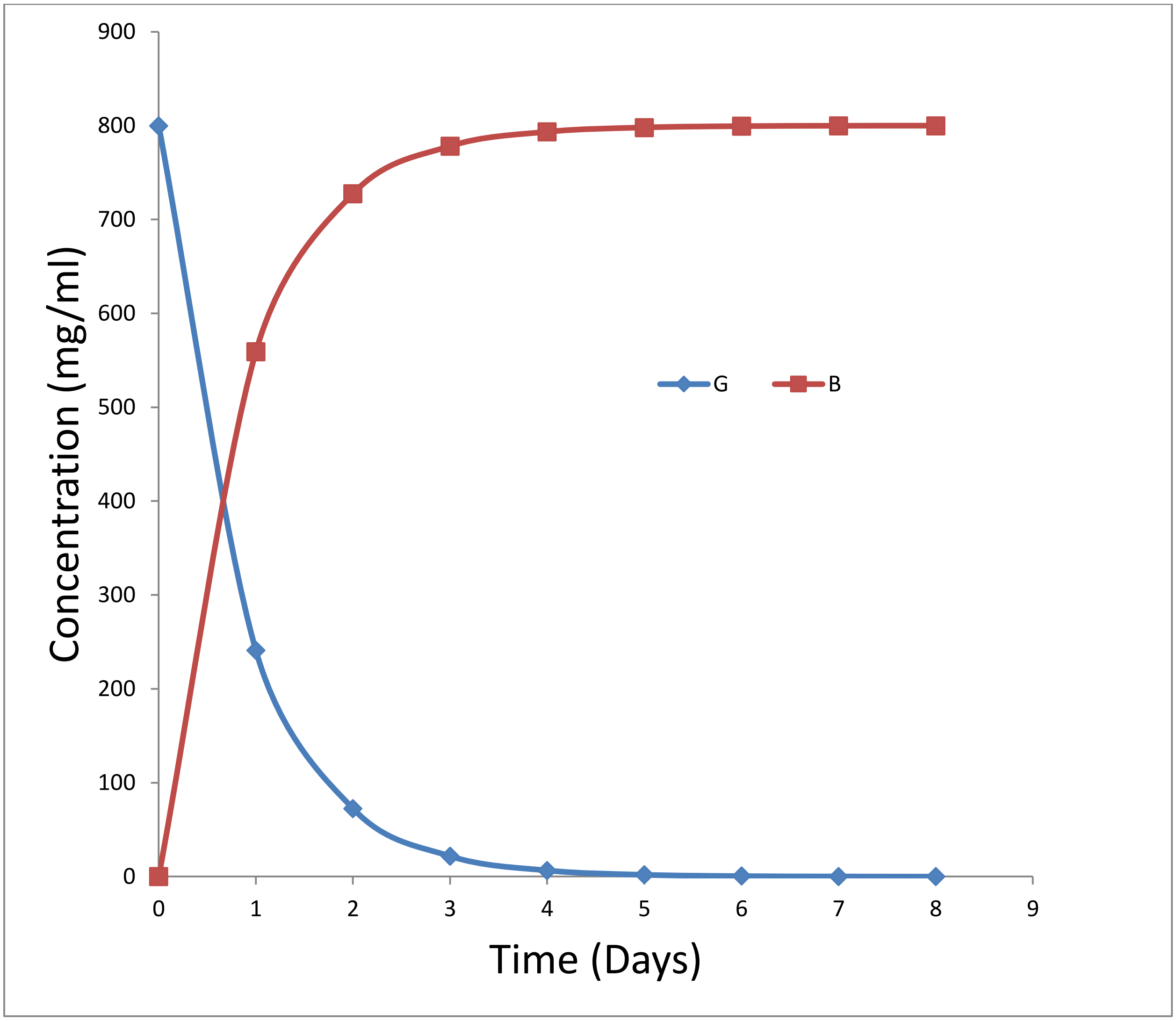

Figure 3: A Plot of the Rate of Change of Glucose Concentration and Butanol Yield with Time

In Figure 3, as the glucose yield decreases the Butanol also increases due to the utilization of the available glucose for the butanol production. This agrees with the work of Olaoye and Kolawole (2013), who showed that the modified Gomperta model can be used to test the kinetics of ethanol production at steady temperature.

The graph for the kinetics of butanol produced from UPTB is given in Figure 4.

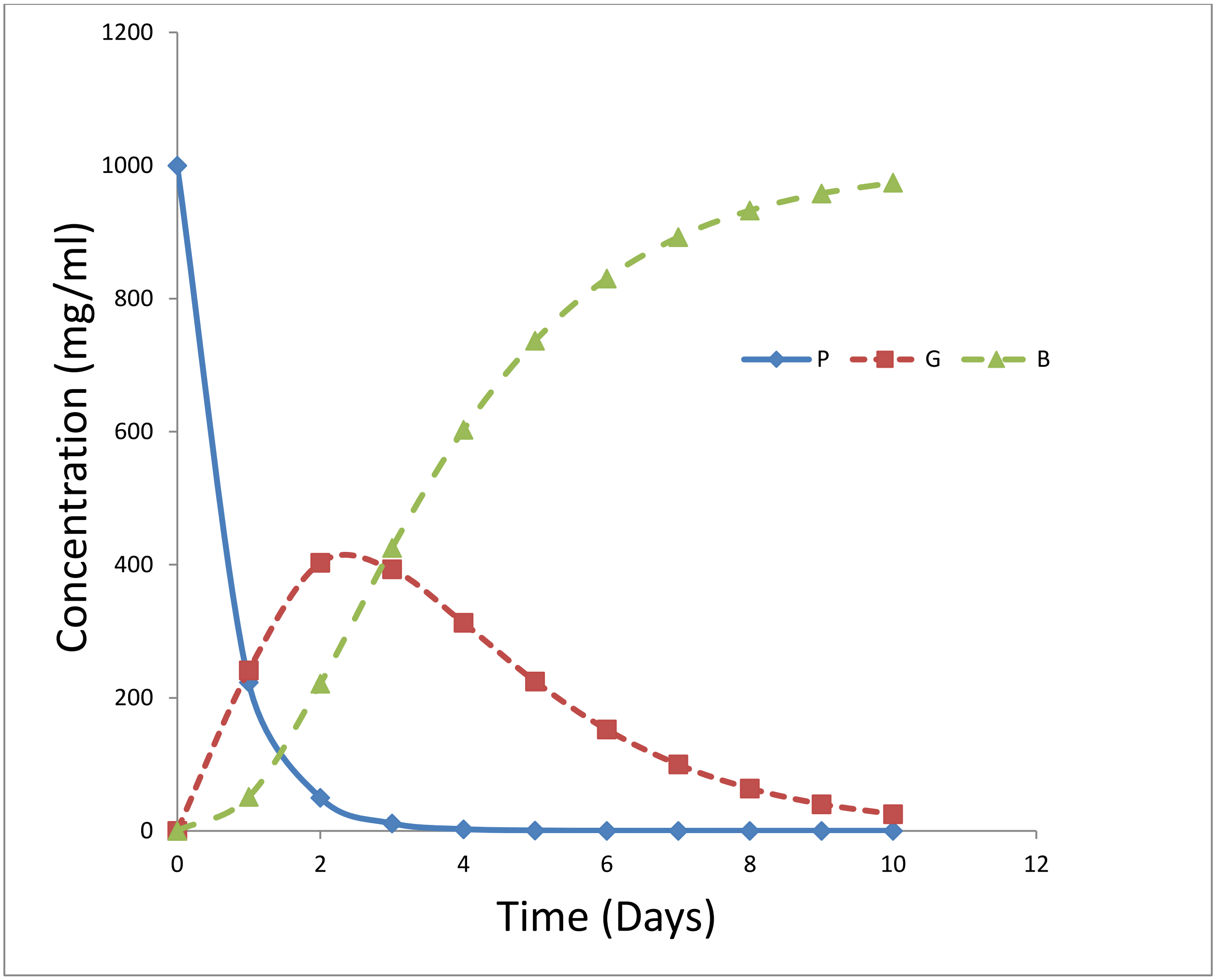

Figure 4: A Plot of the Rate of Change of Unpretreated Plantain Trunk Biomass, Glucose Yield and Butanol Produced with Time

The rate of change of butanol with time is inversely proportional to that of biomass. As the glucose yield increases the butanol also increases to an optimum value at day 2 when it starts decreasing due to the utilization of the available glucose for the butanol production, this agrees with our previous findings that hydrolysis increases glucose and ethanol yield (Evans *et al.,* 2021).

The results in Figures 2, 3, and 4 agrees with real life situation, the graphs are well fitted this indicates that the prediction can be trusted for application in real life and that the model is realistic which can be used for industrial purposes.

Conclusion

In conclusion the dynamic models obtained were used to determine glucose yield and butanol production. The rate of production of glucose from the biomass is 1.5 and of butanol from glucose is 0.8. The glucose yield is inversely proportional to the biomass consumption and the butanol yield is inversely proportional to the glucose.

The optimum glucose yield from unpretreated PTB was 450mg/ml while that for Butanol is 974ppm. The results showed that glucose depletion followed an exponential pattern with R^2 values of 0.8643 for unpretreated biomass while that of Butanol yield follows a second order polynomial with R^2 of 0.9775. The work also concludes that at day 2 almost all the biomass was consumed in the process.

References

Alfa, M., Okuofu, C. A., Adie, D. B., Dahunsi, S. O., Oranusi, U. S., & Idowu, S. A. (2012). Evaluation of biogas potentials of *Cymbopogon citratus* as alternative energy in Nigeria. *International Journal of Green Chemistry and Bioprocess,* 2(4), 34-38.

Evans, P. O., Jiya, M., Nyor, N., & Yisa, J. (2021). Mathematical modeling of enzyme hydrolysis and fermentation of banana trunk biomass for optimum ethanol production. A paper presented at the International Conference on Contemporary Developments in Mathematical Sciences (ICCDMS) In Honour Of Prof. K. R. Adeboye Book of Proceedings, 368-381.

Farah, A., Ahmad, T. J., Mohd, H. K., & Maizirwan, M. (2011). Study of growth kinetic and modeling of ethanol production by *Saccharomyces cerevisae*. *African Journal of Biotechnology,* 16(81), 18842-18846.

Gábor, L. (2017). Analytical solutions for the rate equations of irreversible two-step consecutive processes with mixed second order later steps. *Journal of Mathematical Chemistry,* 55(3), 832-848.

Nawa, R. B., Lauren, S., Ajay, S., Thaddeus, C. E., Katrina, C., & Ann, C. (2016). Acetone-butanol-ethanol fermentation of corn stover: current production methods, economic viability and commercial use. *FEMS Microbiology Journal*, 363, fnw033.

Olaoye, O. S., & Kolawole, O. S. (2013). Modeling of the kinetics of Ethanol fermentation from Glucose biomass in batch culture with a non – structural model. *International Journal of Engineering Research and Application*, 3(4), 562 – 565.

Saa, P. A., & Nielsen, L. K. (2017) Formulation, construction and analysis of kinetic models of metabolism: A review of modelling frameworks. *Biotechnology Advancement*, (8), 981-1003. doi: 10.1016/j.biotechadv.2017.09.005. Epub 2017 Sep 13.

Sheetal, B. G., & Patil, I. D. (2014) Economic study of fermentation kinetics for production of ethanol from damaged sorghum and corn grains: A Critical Review. *Pratibha: International Journal of Science, Spiritual, Business and Technology* (IJSSBT), 2(2), 32-37.