Journal of Physical Science and Innovation
ISSN: 2277-0119 **Volume 10, No. 3, 2018**

NUMERICAL SIMULATIONS ON THE EFFECT OF RECYCLE AND TIME DELAYON THE CUBIC AUTOCATALYTIC REACTION MODEL

Yakubu, A. A.[1], Yatim, M. Y.[2]

[1]Department of Mathematical Sciences, Ibrahim Badamasi Babangida University, Lapai, Nigeria;

[2]School of Mathematical Sciences, UniversitiSains Malaysia, P.O.Box 11800, Penang, Malaysia

email: aaishaty@ibbu.edu.ng

ABSTRACT

The effect of recycle and time delay on the cubic autocatalytic reaction model with linear decay in the absence of an autocatalyst in a continuous stirred tank reactor (CSTR) is studied. The model comprises a system of nonlinear ordinary differential equation which describes the autocatalytic behavior of two chemicals (a reactant and an autocatalyst) flowing into the CSTR. When the system is affected by recycle r(using different values of r) without time delay T, the concentration of the reactant decomposes until it reaches equilibrium while the concentration of the autocatalyst oscillates in an unstable pattern, but with increase in time τ. However, when the system is affected by both recycle and time dalay, the concentrations oscillations is quite small and unstable for the autocatalyst.

Keywords: *Continuous stirred tank reactor (CSTR),Nonlinear ODE, Recycle and Time delay*

INTRODUCTION

During the early stages of cubic autocatalator research in an isothermal and non-isothermal CSTR (Abasaeed (2000); Gray & Scott, 1984;Gray & Scott, 1985; Kanse *et al.,* (2012);Kay & Tomlin, 1989;King

et al., 2003;Mann (2009); Nauman (2008); Uppal & Poore, 1974), the effect of recycle and delay on the stability of the reactor and reactants were neglected. Badola *et al.* (1991) analyzed the bursting solution for cubic autocatalysis in a CSTR with recycle and time delay. The solutions to the delay differential equations were obtained using semi implicit RungeKutta method. Incorporating a variable-step size algorithm and a cubic spline interpolation routine was built into the main algorithm. The analysis showed that in the absence of recycle, the system has three steady states. They also carried out the investigation in order to show the existence of bursting solutions in certain regions of the parameter space. However, they only considered the case when the system is feed with both reactant and autocatalyst and bifurcation analysis was exempted.

The effect of delay on the stability of the non-isothermal CSTR sustaining first-order reaction was investigated byBalasubramanian *et al.* (2005). They observed that the system changes the dynamic instability characteristics as a result of the delay. Gangadhar & Balasubramanian (2010)studied the numerical bifurcation analysis of delayed recycle stream in a CSTR using DDE-BIFTOOL in Matlab. A first-order irreversible elementary reaction was considered. They found that the system exhibits delay dependent stability under non-isothermal operation of the CSTR..

Ariffin and Balasubramanian (2013) carried out a research on the dynamic behavior of the cubic autocatalytic reaction with time delay using the DDE23 in Matlab. They compared the results of Badola *et al.* (1991) and Balasubramanian *et al.* (2005) and also included bifurcation analysis in their studies. They observed that in the absence

of delay, the system is dynamically unstable for the parameters considered. However, the system changes the dynamic instability characteristics to stable as a result of delay. Their analysis was only restricted to the presence of both reactant and autocatalyst as studied by Badola *et al.* (1991).

In this paper, the setup of a CSTR having a recycle stream is been considered. The mass balance equation of the model will be derived, thereafter, the dynamics of the model is studied. The effect of the recycle and time delay on the model will be studied in the absence of an autocatalyst. Numerical simulations are carried out to observe the concentration behavior of the chemicals.

The Model Formation

In this section, the reaction model with recycle and delay parameters is developed. For this setup, the exit stream of the reactor is sent through the separation system and the unconverted reactant is sent to the CSTR via the recycle stream which will lead to a time delay in the reaction process. Fig 1 represents the schematic diagram of a CSTR with a recycle stream to help understand better the movements of the chemicals in and out of the tank.

From the law of conservation of mass, the mass balance equation for reactant A and autocatalyst B is generated. This is given by

Mass accumulation = mass input – mass output $\pm$ rate of reaction.

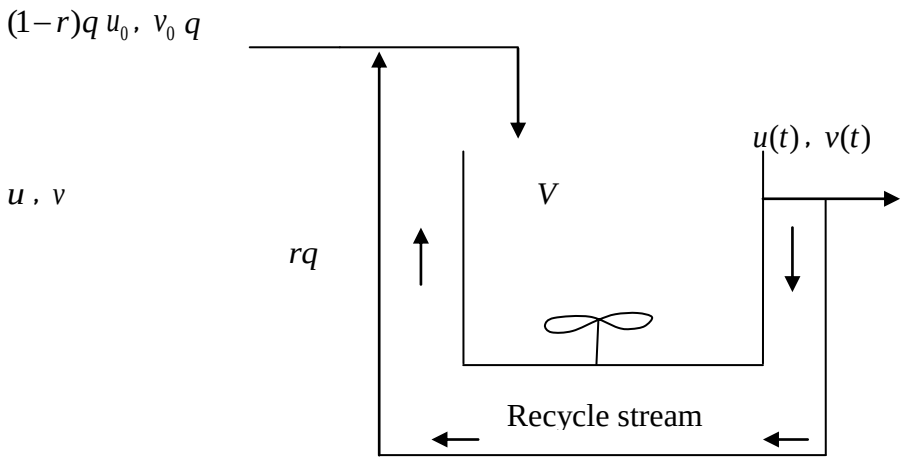


Fig1 *The CSTR with recycle stream*

Mathematically this can be expressed as

$$V\frac{du}{dt} = (1-r)qu_0 + rqu(t-T) - qu - Vk_1uv^2, \tag{1}$$

$$V\frac{dv}{dt} = (1-r)qv_0 + rqv(t-T) - qv + V(k_1uv^2 - k_2v). \tag{2}$$

The molar concentration of reactant A and autocatalyst B are governed by the delay differential equations (1) and (2), where q is the volumetric flow rate (m^3s^{-1}), T is the time delay and r is the recycle ratio. Also from Fig1, the term rq represents the flow rate of the recycle stream, while $(1-r)q$ represents the flow rate of the external input feed.

Dividing (1) and (2) by V, gives

$$\frac{du}{dt} = \frac{q}{V}(1-r)u_0 + \frac{q}{V}ru(t-T) - \frac{q}{V}u - k_1uv^2, \tag{3}$$

$$\frac{dv}{dt} = \frac{q}{V}(1-r)v_0 + \frac{q}{V}rv(t-T) - \frac{q}{V}v + k_1uv^2 - k_2v. \tag{4}$$

From Badola et al., (1991), who studied the bursting solutions for the cubic autocatalysis in the presences of an aotucatalyst. They noted that

in the absence of a recycle stream, $r=0$, while when $r=1$, it represents no input from the external feed, therefore, $(1-r)q=0$, hence complete recycling. Also from initial stages while $t<T$, (when no contribution from the recycle stream exists due to delay time) the external input is assumed to operate at a higher flow rate which decreases itself by an amount equal to rq when $t=T$. They also related in a simple fashion the solution behavior of the system in the absence of recycle $(r=0)$, with that of the CSTR operating with recycle $(0<r<1)$ but without delay $(T=0)$, by utilizing $x[t-0]=x$ and $y[t-0]=y$. Thus, (3) becomes

$$\frac{du}{dt}=\frac{q}{V}ru(t-T)-\frac{q}{V}u-k_1uv^2. \tag{5}$$

Non-Dimensional

In this section the non-dimensional variables are defined in the form of

$$x=\frac{u_0-u}{u_0},\ y=\frac{v}{u_0},\ y_0=\frac{v_0}{u_0},\ \tau=k_1u_0^2t,\ \alpha=\frac{k_2}{k_1u_0^2},\ \gamma=\frac{q}{Vk_1u_0^2} \tag{6}$$

From (6), $u=u_0(1-x)$, but $\frac{du}{dt}=u_0\frac{dx}{dt}$ and also $v=yu_0$.

Substituting the values of u and v into (5), and dividing through by u_0, the equation becomes

$$\frac{dx}{dt}=\frac{q}{V}rx(t-T)-\frac{q}{V}x+k_1u_0^2y^2(1-x).$$

Using chain rule that is $\frac{dx}{d\tau}=\frac{dx}{dt}\times\frac{dt}{d\tau}$, and from (6), $t=\frac{\tau}{k_1u_0^2}$, as such, $\frac{dt}{d\tau}=\frac{1}{k_1u_0^2}$, thus,

$$\frac{dx}{d\tau}=\left(\frac{q}{V}rx(\tau-T)-\frac{q}{V}x+(1-x)k_1u_0^2y^2\right)\frac{1}{k_1u_0^2},$$

$$\frac{dx}{d\tau}=\frac{q}{Vk_1u_0^2}rx(\tau-T)-\frac{q}{Vk_1u_0^2}x+(1-x)y^2.$$

But $\gamma = \frac{q}{Vk_1u_0^2}$, therefore

$$\frac{dx}{d\tau} = \gamma rx(\tau - T) - \gamma x + (1-x)y^2. \quad (7)$$

From (6), we have that $v = u_0 y$, therefore $\frac{dv}{dt} = u_0 \frac{dy}{dt}$, substituting the value for v into (4) and also substituting the non-dimesionless variables gives

$$\frac{dy}{d\tau} = \gamma(1-r)y_0 + \gamma ry(\tau - T) - \gamma y + (1-x)y^2 - \alpha y. \quad (8)$$

Equations (7) and (8) are the governing ODE when there is time delay which is the same as used by Badola *et al.*, (1991). While in the absence of time delay equation (7) and (8) becomes

$$\frac{dx}{d\tau} = \gamma rx - \gamma x + (1-x)y^2, \quad (9)$$

$$\frac{dy}{d\tau} = \gamma(1-r)y_0 + \gamma ry - \gamma y + (1-x)y^2 - \alpha y. \quad (10)$$

NumericalSimulations

The numerical simulation of the cubic autocatalytic reaction with the effect of recycle and time delay is considered in this section. The simulations will be carried for the case where there is absence of an autocatalyst. The simulations will be studied for different values of recyle and time delay. It is of importance to know what happens to model in the absence of an autocatalyst as this has been one of the shortcomings of previous research.

The effect of recycle and time delay in the absence of autocatalyst

In this section, the dynamic behavior of the effect of recycle and time delayon the cubic autocatalytic reaction will be studied with and

without the presence of time delay respectively. The simulation will also be performed using different values for the recycle r. Some of the values used are as considered by Ariffin and Balasubramanian (2013), were they studied the dynamics of recycle and time delay in the presence of an autocatalyst. The simulation analysis is shown in Fig2 without time delay for the concentration of the reactant x and autocatalyst y.

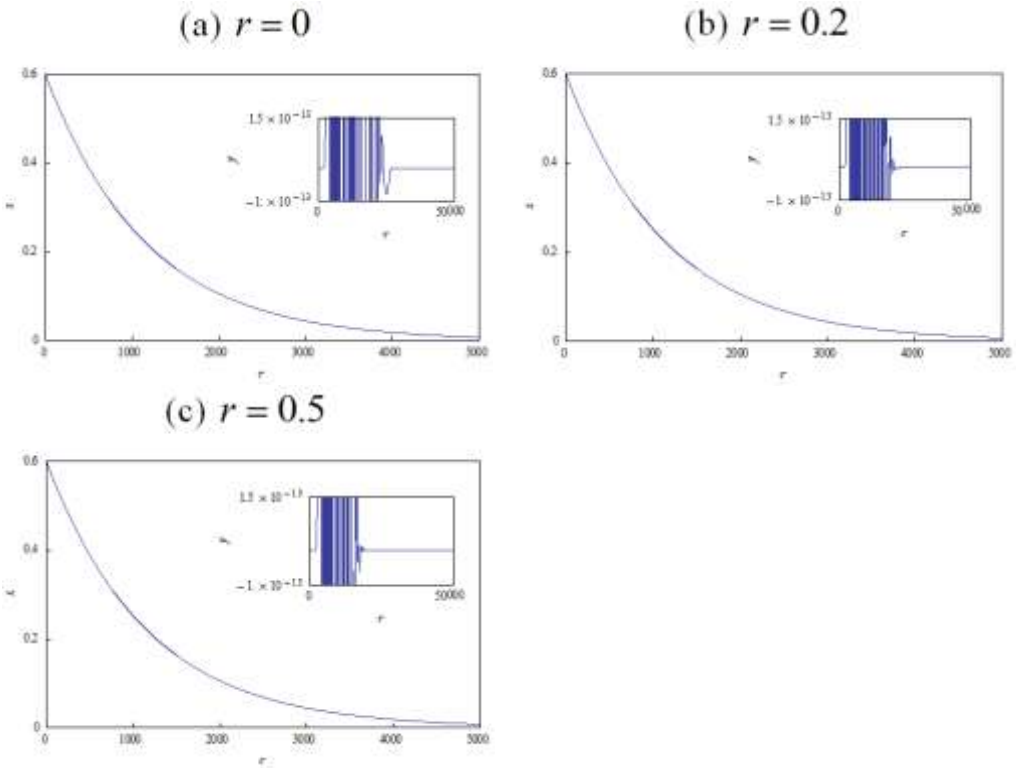
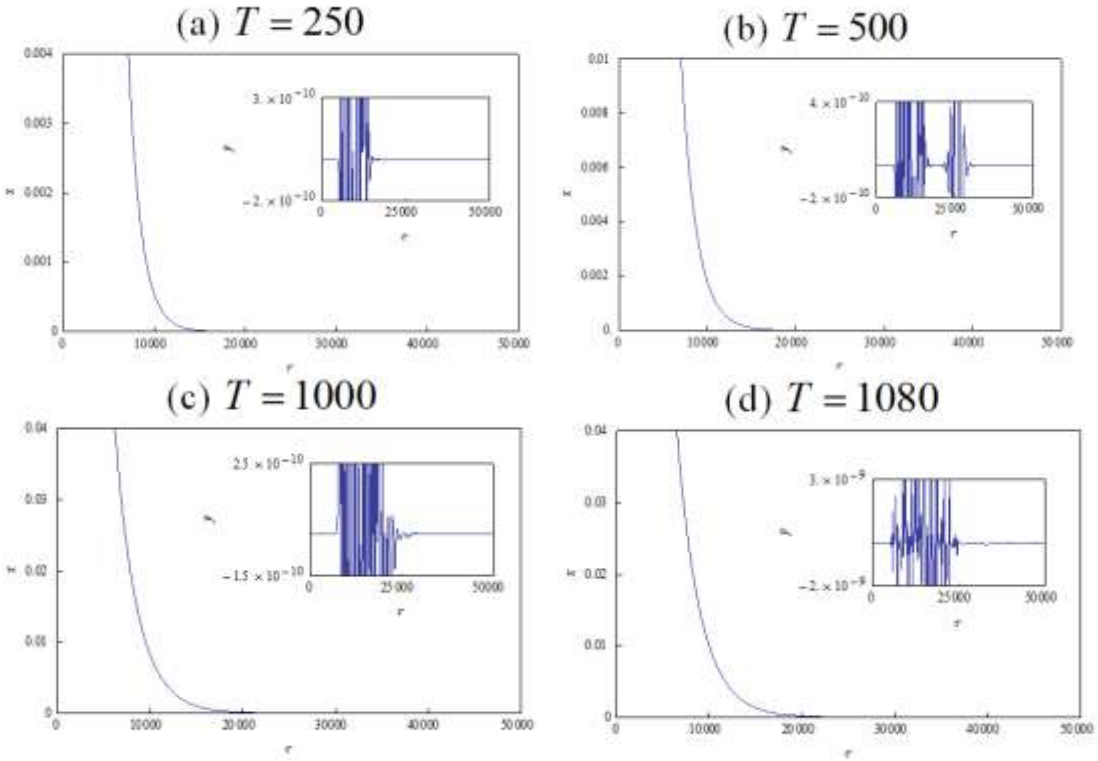


Fig2 *Behavior of the reactant* x *and autocatalyst* y *in the absence of delay,* $T = 0$ *for (a)* $r = 0$, *(b)* $r = 0.2$ *and (c)* $r = 0.5$, *in the absence of an autocatalyst*

From the simulation analysis carried out, it is observed that the concentration of the reactant decomposes until it reaches an equilibrium state. While the concentration of the autocatalyst oscillates in an unstable pattern, but with increase in time τ, the reaction

becomes stable as it heads towards an equilibrium state. Though the concentration values in the absence of the autocatalyst is so small but if not acknowledged, could have an effect on the end product.

The next simulation shows the dynamics of the system in the presence of time delay $(T > 0)$. The dynamics will be observed in two states one of which the recycle parameter is fixed and the time delay is varied, while the other has a fixed value for the time delay and the recycle parameter is varied. Fig3 illustrates the concentration behavior of the autocatalyst with different values of time delay for a fixed value of recycle parameter $(r = 0.5)$.



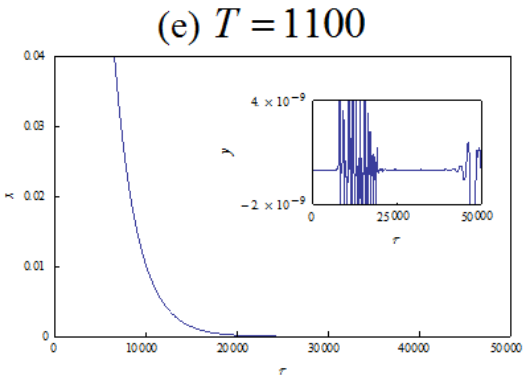


Fig3 *Behavior of the reactant* x *and autocatalyst* y *with a fixed value of recycle parameter* $r = 0.5$ *for (a)* $T = 250$, *(b)* $T = 500$, *(c)* $T = 1000$, *(d)* $T = 1080$ *and (e)* $T = 1100$, *in the absence of an autocatalyst*

In the absence of the autocatalyst, Fig 3 reveals that the amplitude in the concentrations oscillation is quite small and unstable for the autocatalyst. Though, with increase in the time delay, the frequency reduces and gradually there is a relaxation in the amplitude. However, it is also observed that the pattern of oscillation when $T = 250$ to $T = 500$ is different from when $T = 1000$ to $T = 1080$, and at $T = 1100$ the oscillation assumes its previous form.

Subsequently, the next analysis displays the behavior of the autocatalyst with variation in the recycle parameter at a fixed value of time delay $(T = 1080)$. This value is considered because its oscillatory pattern is different from others. Thus, we want to see if a change in values of the recycle parameter will have an effect on this behavior. Fig 4 displays the the behavior in the concentration of the autocatalyst with varied recycle parameter at a fixed value of time delay.

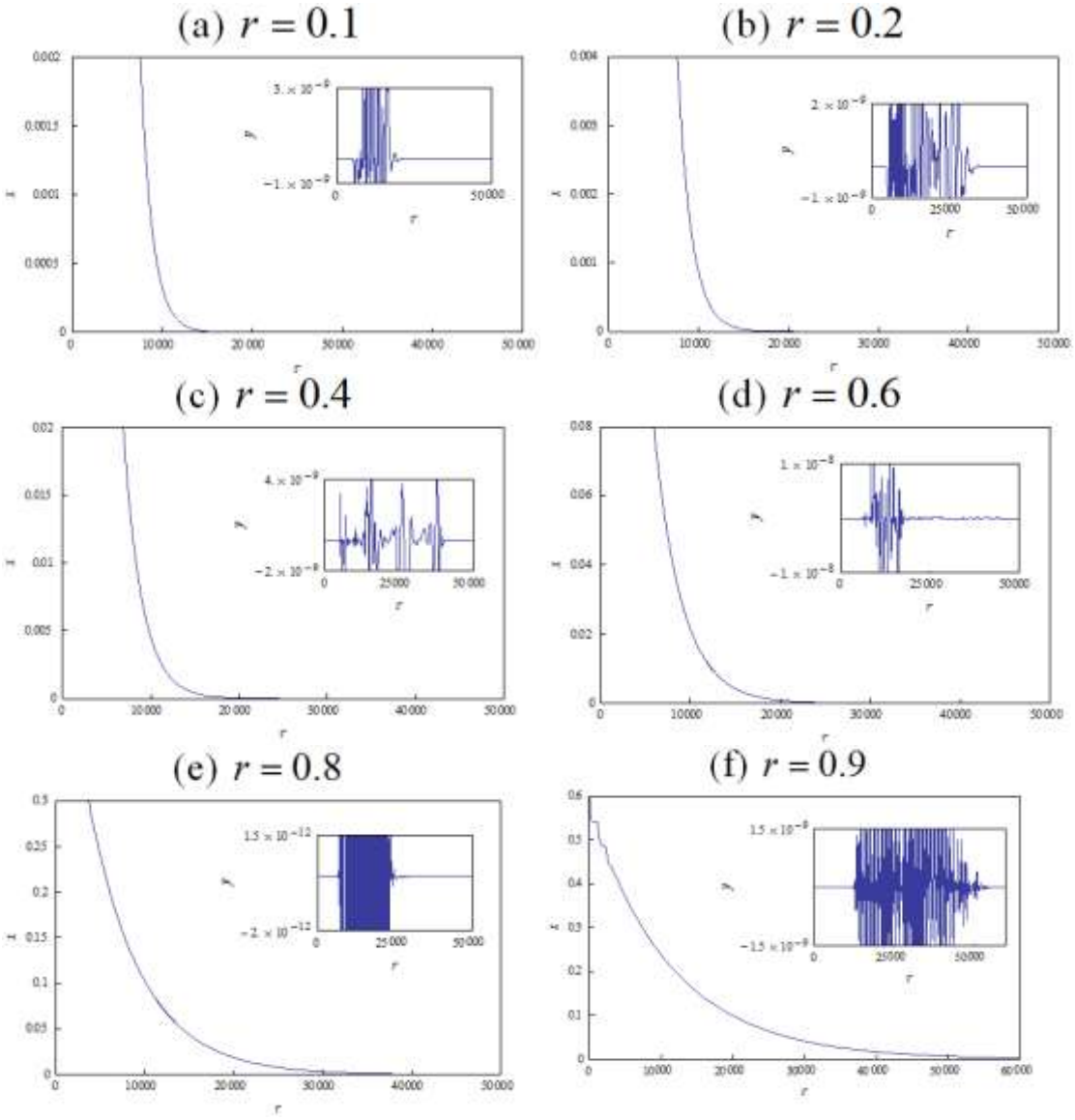


Fig4 *Behavior of the reactant* x *and autocatalyst* y *with a fixed value of time delay* $T = 1080$ *for (a)* $r = 0.1$, *(b)* $r = 0.2$, *(c)* $r = 0.4$, *(d)* $r = 0.6$, *(e)* $r = 0.8$ *and (f)* $r = 0.9$, *in the absence of an autocatalyst*

Fig 4 reveals that at $r = 0.4$, there is a relaxation state in the frequency of the oscillation which exhibits an unstable pattern. The oscillation however, disappears as the reaction heads towards completion. The

Figure also reveals that even with an increase in the recycle parameter, the oscillations will always head towards an equilibrium state.

CONCLUSION

At the end of this paper,the numerical simulation of the model was carried out in the case where there is an absence of autocatalyst. Different values of recycle r and time delay T were analyzed and the result of the observations were translated. The reactant x is always decomposing for all cases in the absence of the autocatalyst, while the autocatalyst y oscillates before reaching an equilibrium state.

REFERENCE

Abasaeed, A. (2000). Bifurcation and chaos for a mutating autocatalator in a CSTR. *Bioprocess Engineering,***22,** 337-346.

Ariffin, K. J. & Balasubramanian, P. (2013). Dynamic Behavior of Cubic Autocatalytic Reactions with Time Delay. *Proceedings of the 6th International Conference on Process Systems Engineering* (PSE ASIA), 27.

Badola, P., Rajani, P., Kumar, V. R. & Kulkarni, B. (1991). Bursting solutions for cubic autocatalysis in a continuous stirred tank reactor with recycle and time delay. *The Journal of Physical Chemistry,***95,** 2939-2941

Balasubramanian, P., Pushpavanam, S., Kienle, A. & Balaraman, K. (2005). Delay effect in a coupled reactor-separator system sustaining non isothermal reaction. *Industrial & Engineering Chemistry Research,***44,** 3619-3625.

Gray, B. F. & Scott, S. K. (1985). Multistability and sustained oscillations in isothermal, open systems. Cubic autocatalysis and the influence of competitive reactions. *Journal of the Chemical Society, Faraday Transactions 1: Physical Chemistry in Condensed Phases,***81,** 1563-1567.

Gray, P. & Scott, S. (1984). Autocatalytic reactions in the isothermal, continuous stirred tank reactor: Oscillations and instabilities in the system A+ 2B⟶ 3B; B⟶ C. *Chemical Engineering Science,***39,** 1087-1097.

Kanse, N. G., Dhanke, P. B. & Thombare, A. (2012). Modeling and Simulation Study of the CSTR for Complex Reaction by Using Polymath. *Research Journal of Chemical Sciences,***2,** 79-85.

Kay, S., Scott, S. & Tomlin, A. (1989). Quadratic autocatalysis in a non-isothermal CSTR. *Chemical engineering science,***44,** 1129-1137.

King, A. C., Billingham, J. & Otto, S. R. (2003). *Differential Equations: Linear, Nonlinear, Ordinary, Partial.* USA: Cambridge University Press.

Mann, U. (2009). *Principles of chemical reactor analysis and design: new tools for industrial chemical reactor operations*. New York: John Wiley & Sons.

Reference to this paper should be made as follows: Yakubu, A. A., Yatim, M. Y. (2018), Numerical Simulations on the Effect of Recycle and Time Delayon the Cubic Autocatalytic Reaction Model. J. of Physical Science and Innovation, Vol. 10, No. 3, Pp. 1-12