SIMULATING THE DYAMICS OF AN ISOTHERMAL BATCH REACTOR

Effong, E. E., Kalu, E.I., Ikezue, E.N. and Nwanekezie, M. N.
Department of Chemical Engineering, Chukwuemeka Odumegwu Ojukwu University, Uli, Anambra State.

ABSTRACT

The results of the simulation of a reversible batch reactor using Ordinary Differential Equation Solver (ODE45) is presented. It employs the Clasical Runge – Kutta (4.4) method to integrate the equations. Hypothetical values of the rate constants K_1, K_2, K_3 and K_4 were employed in the analysis. K_1 value was unaltered at $1s^{-1}$, while K_2 varied from 0.5, 0.75, $1.0s^{-1}$, K_3 and K_4 values were fixed at 0.2, 0.5, $0.75s^{-1}$. Results of the concentration profile shows that component A falls from 1.0 mol/dm^{-3} to 0.04mol/dm^{-3}, component B from 0 to 0.53mol/dm^{-3} then drops, to 0.18mol/dm^{-3}, and component C rises from 0.0 to a maximum value of 0.70mol/dm^{-3}.

Keywords: Simulation, Modeling, Reversible, Batch, Reactor.

1.0 INTRODUCTION

The focus of a model builder is how to achieve maximum yield of the desired product in a reasonable time frame. Chemical Kinetics is concerned with the velocity or time rate of reaction and the mechanisms of the reaction. The rate constant determines how quantitative the yield of the reaction is. Therefore efforts aimed at optimizing the rate would enhance yield maximally. Computer aided mathematical application is a growing trend used in modeling and simulation of reaction kinetics to achieve such a desired optimum yield (Ullan and Wolkenhauer, 2011). In many chemical processes of transformation of reactants into products, only the disappearance of the reactants and appearance of the final products may be observed (Sharma and Pathania, 2006). But for batch reactions occurring in steps, intermediate products may be formed which may not be detected because they are promptly used up in the subsequent step to yield the main product. The rate of reaction generally decreases with time but the coefficient of determination (rate constant) remains unchanged throughout the reaction. The rate depends on the active concentration of the reactants and is greatly influenced by temperature among other factors such as the nature and concentration of the reacting species (Higham, 2007).

Khamforosh (2011) presented a fuzzy logic (FL) which were used to model the performance of a batch reactor system and, hence, the conversion profile at varying operating conditions.

Hakeem *et al*. (2010) outlined a mathematical model capable of determining suitable operating conditions to produce TiO_2 nanoparticles with specified average diameter.

Da Cunha *et al*. (2011) presented a growth of Bacillus thuringiensis var. israelensis, a bioinsecticide producer,

Prokopová *et al*. (2013) outlined the analysis, mathematical modelling and simulation of reactors which are used in the chemical and tanning technology.

Schilling *et al*. (1999). Showed how an empirical model was applied to describe the growth related formation of scleroglucan in batchwise cultivation of *Sclerotium rolfsii*.

Rolando *et al*. (2010) presented a mathematical model for limonene epoxidation over PW-Amberlite in a batch reactor and used for reactor simulation and optimization.

Salmi *et al*. (2000) outlined dynamic modelling principles for typical catalytic three-phase reactors, batch autoclaves and fixed (trickle) beds.

2.0 MODEL DEVELOPMENT

The reaction steps were

$$A \underset{k_3}{\overset{k_1}{\rightleftharpoons}} B \underset{k_4}{\overset{K_2}{\rightleftharpoons}} C$$

A: $\frac{dC_A}{dt} = K_1C_A + K_3C_B$ **(1)**

B: $\frac{dC_B}{dt} = K_1C_A + K_4C_c - (K_2 + K_3)C_B$ **(2)**

C: $\frac{dC_c}{dt} = K_2C_B - K_4C_C$ **(3)**

Numerical Solution

$$y_{i+1} = y_i + \frac{h}{6}\{k_1 + 2k_2 + 2k_3 + k_4\} \quad \textbf{(4)}$$

where

$$k_1 = f(\chi_i, y_i) \quad \textbf{(5)}$$

$$k_2 = f\left(\chi_i + \frac{h}{z}, y_i + \frac{1}{2}k_1\right) \quad \textbf{(6)}$$

$$k_3 = f\left(\chi_i + \frac{h}{z}, y_i + \frac{1}{2}k_2\right) \quad \textbf{(7)}$$

$$k_4 = f(\chi_i + h, y_i + k_3) \quad \textbf{(8)}$$

Equations 1,2,3 were combined to obtain the lumped parameter model as

$$\frac{d^2c_A}{dt^2} + a_1\frac{dc_A}{dt} + a_2c_A = a_3 \quad \textbf{(9)}$$

Where $a_1 = K_1 + K_2 + K_3 + K_4$ **(10)**

$$a_2 = K_1K_2 + K_3K_4 + K_1K_4 \quad \textbf{(11)}$$

$$a_3 = K_1K_4C_{A0} \quad \textbf{(12)}$$

C_{A0} = 1 mole,

$\frac{dC_A(0)}{dt}$ = - 1

Equation 9 was solved using Classical Runge – Kutta (4.4) method to obtain the solutions leading to fig. 1,2,3, and 4

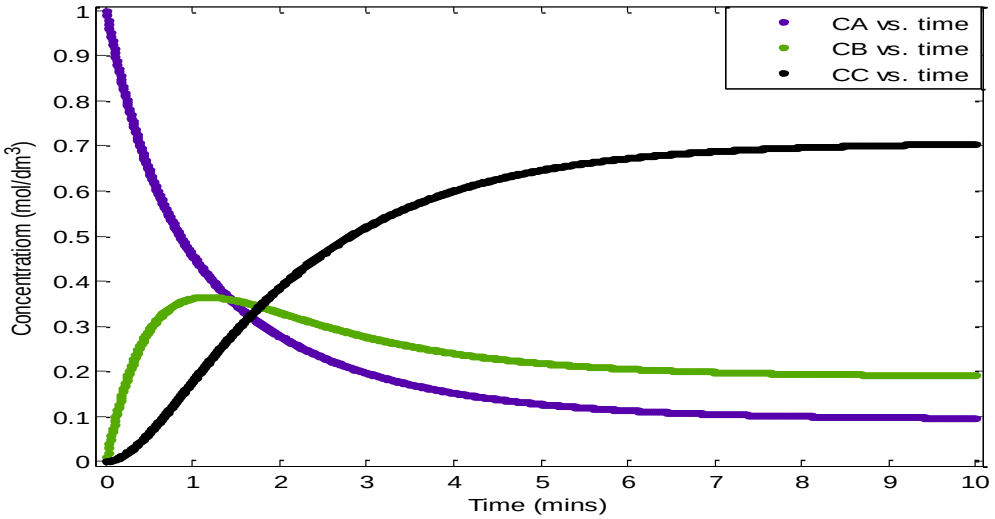

Fig. 1: Concentration profile for $K_1 = 1$, $k_2 = 0.75$, $k_3 = 0.5$, $k_4 = 0.2$ and $C_{A0} = 1$, $C_{B0} = 0$, $C_{C0} = 0$.

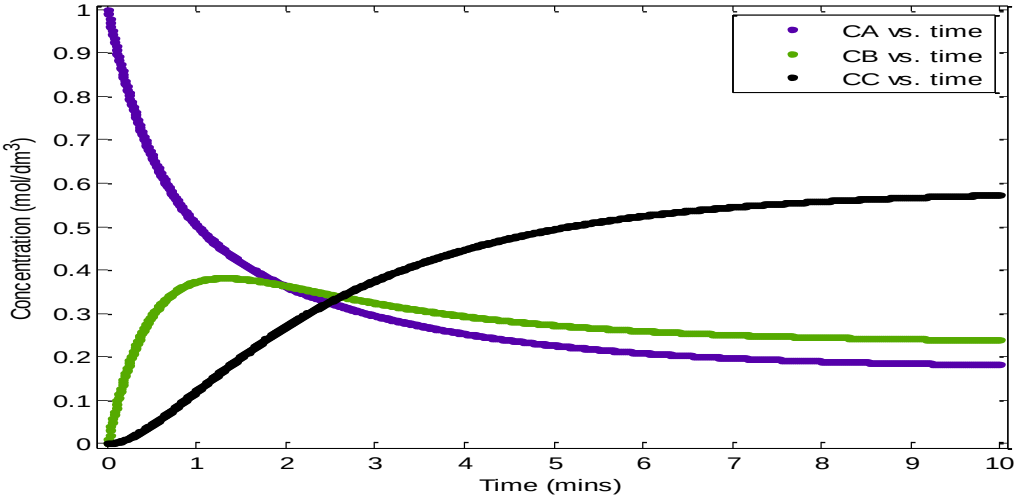

Fig. 2: Concentration profile for $K_1 = 1$, $k_2 = 0.5$, $k_3 = 0.75$, $k_4 = 0.2$ and $C_{A0} = 1$, $C_{B0} = 0$, $C_{C0} = 0$

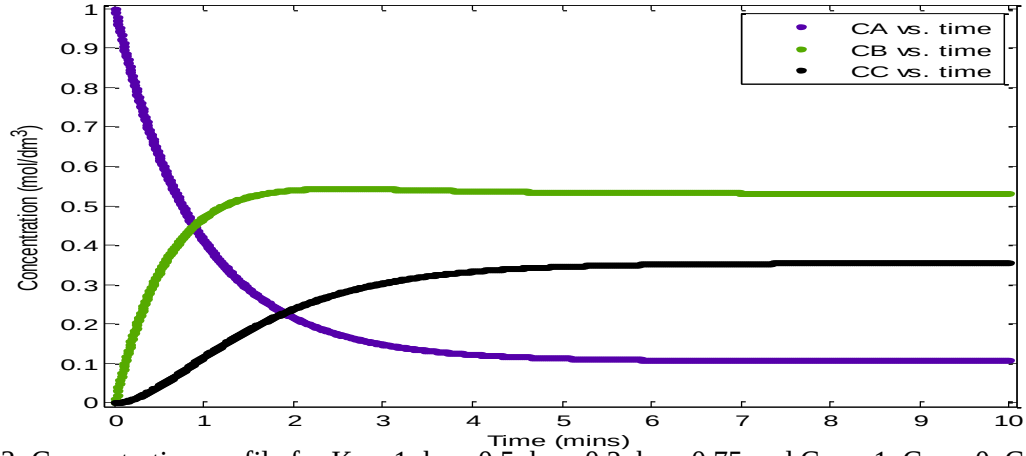

Fig. 3: Concentration profile for $K_1 = 1$, $k_2 = 0.5$, $k_3 = 0.2$, $k_4 = 0.75$ and $C_{A0} = 1$, $C_{B0} = 0$, $C_{C0} = 0$.

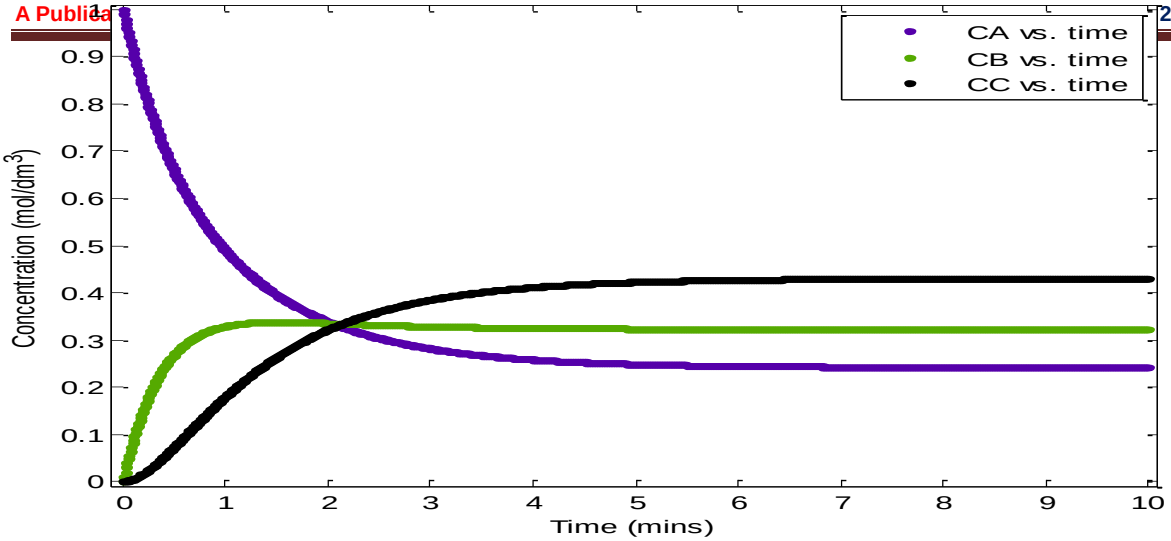

Fig. 4: Concentration profile for $K_1 = 1$, $k_2 = 1$, $k_3 = 0.75$, $k_4 = 0.75$ and $C_{A0} = 1$, $C_{B0} = 0$, $C_{C0} = 0$

3.0 DISCUSSION OF THE RESULTS

Figure 1, 2, 3, 4 shows the plot of concentrations of A, B, and C with various variations in the hypothetical values of the rate constants,K_1, K_2, K_3 and K_4.

In comparison of Figure 2 to interchange with Figure 4.1.1 of K2 and K3 values in relation shows that the concentration of A drops from 1.0 to 0.18 in Figure 2, while the drop in figure 4.1.1 is approximately 0.1, Specie B rises from 0.0 to 0.38 in Figure 2 while about 0.37 in Figure 1 .However this concentration values tends to drop to different values (0.24 in Figure 2 and 0.24 in Figure 1),Component C increase in both Figures from 0.0 to 0.58 in Figure 2 and 0.70 in Figure 1,This shows that the reduction in the interchange value of K2 and K3 with K1 held constant at 1.0 and the lowest value in K4,results in increase in component c and a decrease in the concentration of component b, correspondingly an increase in the value of K3 and a decrease in K4 results in higher concentration of a, with an increase in the concentration of c.

Figure 2 and 3 in comparison with the interchange of K3 and K4 values in relation shows that the concentration of A drops from 1.0 to 0.18 in Figure 2,while the drop in Figure 3 is about 0.10.Species B rises from 0.0 to about 0.38 in Figure 2 and about 0.52 in Figure 4.1.6, so therefore the concentration values tends to drop to different values (0.24 in Figure 2 and 0.52 in Figure 4.1.6),Component C increases in both Figures from 0.0 to 0.58 in Figure 2 and 0.36 in Figure 3. This shows that the reduction in the interchange value of K3 and K4 with K1 held constant at 1.0 and 0.50 K2, which results in a decrease in component C and an increase in the concentration of component b, responds to a decrease in the value of K3 and an increase in K4, results in high concentration of A, and a decrease in the concentration of C and B.

CONCLUSION

Simulation of kinetic models using Matlab functions solver, ODE45 programme proved to be a reliable tool for obtaining dependable results of industrial chemical processes. The results obtained in this study showed that maximum yield of the product C (0.70mol/dm^3) was obtained when the coefficient of determinant K_1 of the reaction was 3.5 x 10^{-1}.this maximum result was achieved within an optimized time frame of 4- 10 minutes under constant temperature.

RECOMMENDATION

It is recommended that this work be extended using alternative concentration and rate constants.

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