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Modelling the Biokinetics of Urease Sorption in the Fluidized Bed Reactor

Ukpaka, Chukwuemeka Peter[1] --- Igwe, Felix[2]

[1]Department of Chemical/Petrochemical Engineering

[2]Department of Biochemistry Rivers State University of Science and Technology Nkpolu, Port Harcourt, Nigeria

(Corresponding Author)

ABSTRACT

The model equation for the sorption of urease in a fluidized bed reactor was developed taking into consideration gradient and temperature gradient across the bed height. The ordinary differential equation obtained was simulated using MATLAB (7.9.0 4D) and it was observed that concentration gradient changes across the bed. Urease Test determine the ability of microorganisms to degrade urea by means of the enzyme urease. The equation for the modelling of the Biokinetics of urease sorption using fluidized bed reactor was used to study the effects of both the concentration and temperature of the urease in the bed of reactor height. The obtained differential equation was simulated using MATLAB (7.9.0 4D) and it was observed that the concentration of urease and temperature changes across the bed. Finally, the results obtained reveals the usefulness of MATLAB – 7.9.0 4D computer programme language for monitor, predicting and simulation of biokinetics model for urease sorption in a fluidized bed reactor.

Keywords: Urease, Biokinetics, Matlab – 7.9.0 4D, Modelling, Fluidized bed reactor.

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1. INTRODUCTION

The research demonstrate the usefulness of urease test to determine the ability of microorganisms to degrade urea by means of the enzyme urease. Research conducted on urease reveals that the prediction of the mode of occurrence of urease in terms of bacteria, several species of yeast and a number of higher plants was presented by Choi & Ray, [1].

Investigation carried out revealed that urease belong to the super family of amidorhydrolases and phosphotriesterases. It is an enzyme that catalyzes the hydrolysis of urea into carbon dioxide ammonia. The reaction occurs as follows:

$(NH_2)_2CO + H_2O \rightarrow CO_2 + 2NH_3$

The biochemical reaction stated above revealed that the urease catalyses the hydrolysis of urea to produce ammonia carbamate. Most especial urease are found in numerous bacteria, fungi, algae, plants, and some invertebrates as well as in soils, as a soil enzyme. One mechanism for the catalyses of the reaction involving urease was proposed by Ukpaka, [5, 6]; Ukpaka, [3, 9]. Urea or carbimide (from the Greek word means Oupia) is an organic compound with the chemical formula $CO(NH_2)_2$. The molecule has two – NH_2 groups joined by a Carbonyl (C=O) functional group. Urea serves an important role in the metabolism of nitrogen containing compound by animals and it's the main nitrogen containing substance in the urine of mammals. It is odourless, colourless solid, highly soluble in water and practically non-toxic. Urea is widely used in fertilizers as a source of nitrogen and an important material in the chemical industry [8, 2].

Fluidized bed reactor technology has been invented so many years ago. And its commercial use has been growing since the last decade; little is still know about the behaviour regarding to temperature, concentration, production and urease adsorption characteristics in the reactor [12, 13]. [1, 7, 4, 10, 11]. Various research has be conducted on the inhibitions of urease as well as extensively studied because of their potential uses like: Therapy against bacterial urease (eg: Helicobacter pylori) that induced human pathogenic states, such as, urinary stone formation, peptic ulcer, pyelonephritis and hepatic coma., to protect soil from pH elevation and loss of nitrogen after use of urea fertilizer by controlling hydrolysis of urea in soil, and as analytical technique for determining substances acting as enzyme inhibitor. Urease inhibitors can be broadly classified into two categories: substrate structural analogs (hydroxyurea and hydroxamic acid) and Inhibitors that affect the mechanism of reaction (phosphodiamidates). By chemical structure, urease inhibitors can be divided into four major groups. The first group is formed by theolic compounds, since theolate anions react directly with the metallocenter of urease. The second group is of hydroxamic acid and its derivatives. Inhibitors of this group compete with urea for binding with the urease active site. The third group is the most effective inhibitors, which include substituted phosphorodiamidatesInvestigation conducted on enzyme immobilized membrane in static conditions were grouped into two distinctive processes that affect the overall rate of adsorption, which involves the molecules diffusion from the bulk solution to an area close to the membrane surface then transfer from this nearby position to the adsorbed state [1]. The adsorption process is said to be diffusion controlled if the porosity allows the diffusion of the substance through the bed packed region. In this case, Langmuir isotherm is used to interpret adsorption at the solid-liquid interface. According to the model, there is a thin layer with a thickness of a few molecular diameters only, immediately adjacent to the surface [12, 13, 15, 16, 3, 11, 14]. The reaction-controlled adsorption occurs within this layer and the rate of adsorption on the membrane surface is described by the following equation.

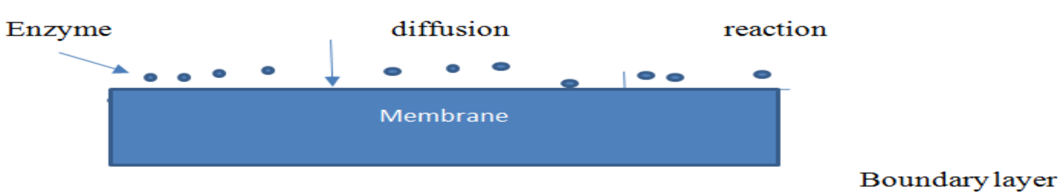

Figure-1. The concepts of enzyme adsorption process

Source: Choi & Ray, [1]

The aim of the research work is to develop mathematical model that can monitor and predict the temperature build up upon increase in microbial concertation in a fluidized bed reactor as well as the rate of sorption of the urease in the bed reactor height influence in the process, using mathematical concepts known as matlab computer programming language as presented in the paper.

2. MATERIALS AND METHODS

2.1. Model Development

In order to develop mathematical model for the monitoring and predicting the characteristics of the biokinetics of fluidized bed reactor for urease adsorption, the following assumptions were considered as stated below.

2.2. Assumptions

1. Particle are assumed to be spherical in shape and homogeneous in size, and the biofilm is homogeneous with respect to thickness, porosity, composition, and density.
2. Growth kinetics follow a substrate inhibition model
3. Concentration gradients are significant only in the direction perpendicular to the support surface; thus a one dimensional model is considered.
4. Contribution of suspended microorganisms in substrate biodegradation is not neglected.

2.3. The Model

The conservation law of mass concept was applied on resolving the mathematical problem in this case, as shown in equation (1) below.

The modeling performance for a fluidized bed reactor is derived from material balance equation.

$$\begin{bmatrix} Rate\ of\ inflow \\ of\ crude\ oil\ into\ the \\ reactor \end{bmatrix} - \begin{bmatrix} Rate\ of\ outflow \\ of\ crude\ oil\ out \\ of\ the\ reactor \end{bmatrix} + \begin{bmatrix} Rate\ of \\ generation/consumption \\ within\ the\ reactor \end{bmatrix} = \begin{bmatrix} Rate\ of\ accumulation \\ within\ the\ reactor \end{bmatrix}$$

(1)

The mathematical expression for parameters defined in equation (1) is given as:

Accumulation of substrate in the bed = $\frac{\mu d\mathrm{Cur}}{dz}$, Inflow of substrate =$K_i C_{ur(in)}$, Outflow of substrate = -$k_i C_{ur\ (out)}$

For the general mass balance equation can be expressed as, thus:

Accumulation of the substrate in the bed = inflow of substrate – outflow of substrate (2)

Substituting the mathematical tools defined above into equation (2), we have

$$\frac{\mu d\mathrm{Cur}}{dz} = K_i\, C_{ur(in)} - K_i\, C_{ur(out)} \quad (3)$$

$$\frac{\mu dCur}{dz} = \frac{ki}{b}\left(C_{ur(in)} - C_{ur(out)}\right) \quad (4)$$

Dividing through equation (4) by μ, we have

$$\frac{dCur}{dz} = \frac{ki}{\mu}(C_{ur(in)} - C_{ur(out)}) \quad (5)$$

Where, K_i is the mass transfer coefficient, µ is the flow rate of urease, c_{ur} is the concentration of urease, and z is the bed height, (distance)

2.4. The Energy Balance

The energy balance equation can be expressed as stated in equation (1), thus

The energy concept for a fluidized bed reactor is derived from energy balance equation as stated in equation (6).

$$\begin{bmatrix} Rate\ of\ inflow \\ of\ energy\ into\ the \\ reactor \end{bmatrix} - \begin{bmatrix} Rate\ of\ outflow \\ of\ energy\ out \\ of\ the\ reactor \end{bmatrix} + \begin{bmatrix} Rate\ of energy \\ generation/consumption \\ within\ the\ reactor \end{bmatrix} = \begin{bmatrix} Rate\ of\ accumulation \\ of\ energy\ within\ the\ reactor \end{bmatrix}$$

(6)

The mathematical expression for the energy balance in terms of the enzyme is defined as: Inflow of enzyme into the bed = $H_{mT(i),}$ Outflow of enzyme from the bed =H_{mTout}

Therefore, the general energy balance becomes;

$$C_{ur}\, C\frac{\mu dT}{dz} = HmT_i – HmT_{i\ out} \quad (7)$$

$$C_{ur}\, C\frac{\mu dT}{dz} = Hm\ (T_i – T_{out}) \quad (8)$$

$$\frac{dT}{dz} = \frac{Hm\ (Ti – Tout)}{Cur.C.\mu} \quad (9)$$

2.5. Computational Procedures

The following computational parameters were choose to simulate the rate of sorption of urease in a fluidize bed reactor, such as flow rate u (kg/hr), initial concentration of urease (g/m^3), initial and final temperature Tin and Tout (^oc), enthalpy of system H_m, equilibrium constant k_i, and all parameters used in the simulation are presented in Tables as stated in the paper in area of the results and discussion.

3. RESULTS AND DISCUSSION

The rate of sorption of urease in the fluidized bed reactor was monitored, predicted and simulated using the data stated in the various tables and the application of parameters into the developed mathematical as well as the application of MATLAB computer programme language yielded the results presented in the figures presented in this paper.

Table-1. The functional parameters used in the simulation of the rate of sorption of urease in a fluidized bed reactor.

PARAMETERS	UNITS	VALUE
u	Kg/hr	122,2
K_i		1.32×10^{-3}
C_{ur}	g/m^3	600
μ_{ur}		700
Hm	J	37.620
T_{in}	K	660
T_{out}	K	300
$C_{ur(in)}$	g/m^3	0.00046
C_{mr}	g/m^3	50

Source: Choi & Ray, [1]

Using the values of the functional parameters stated in table 1 and inputting the values into the mathematical expression obtained and the application of the matlab computer programming language yielded to the graph presented in Figure 2 below.

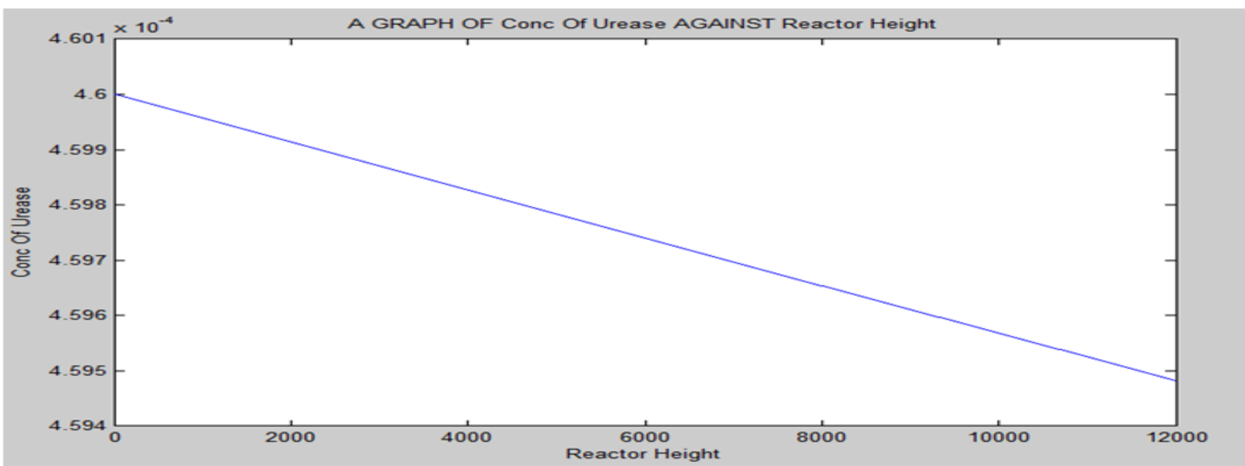

Fig-2. The graph of urease concentration against the bed height

Source: simulated by the researchers

The result presented in Figure 2 illustrates decrease in urease concentration with increase in bed reactor height. The variation in urease concentration can be attributed to the variation in the bed reactor height in the fluidized system as well as the influence of the functional parameters used in simulating the process. The various outputs obtained shows that increase in the Reactor length (bed height) revealed that the concentration of urease decreases as the urease enters the fluidized bed reactor; it is absorbed by the microorganism and therefore leading to a decrease in the concentration. At the bottom of the bed or the fluidized bed reactor, the concentration of urease is more adsorbed than at the top of the reactor. From the graph obtained from the simulated data, it shows that temperature increases across the bed length during the adsorption of the urea in the fluidized bed reactor.

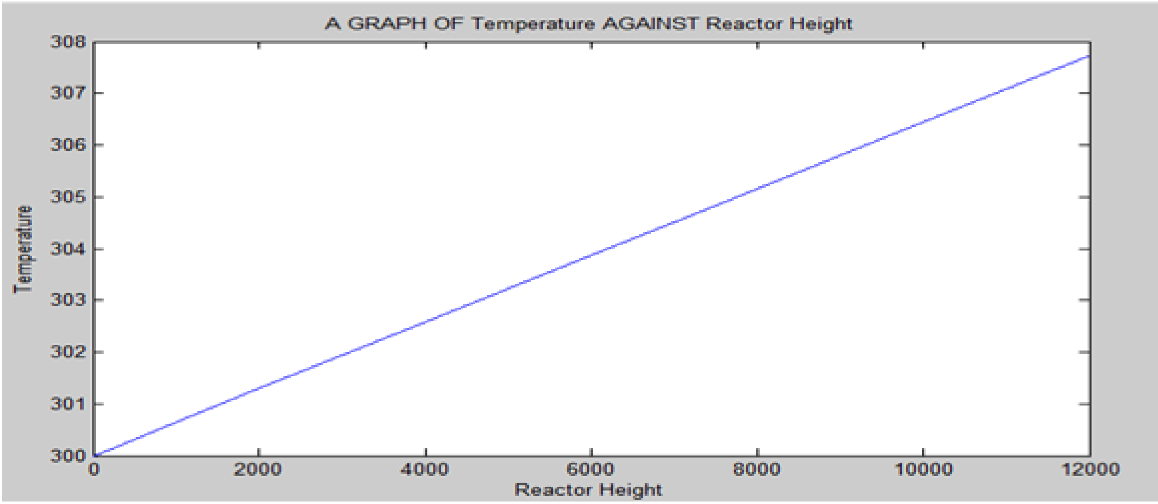

Fig-3. The graph of the temperature gradient against the bed height

Source: simulated by the researchers

The Figure 3 illustrates the bioenergy of the urease in the fluidized bed reactor upon the influence of bed reactor height. The result obtained reveals that increase in the bed reactor height resulted to increase in urease temperature build up in the fluidized bed reactor, the concept is acceptable only the functional parameters and coefficient does not influence the microbial activity in the fluidized bed reactor.

4. CONCLUSION

The simulation of the fluidized bed bioreactor by inputting some functional parameters revealed the significance of the matlab computer programming in monitoring and predicting the characteristics of the biomass build in a fluidized bed bioreactor upon the rate of sorption of the substrate by the urease within the bed packed height. In this research work, the model equation for the adsorption of urease in the fluidized bed reactor was developed considering the length of the bed as the material moves along the bed, concentration and temperature changes across the bed height. It is recommended experimental approach should conducted to ascertain effectively prediction on the profile of the changes in the biomass concentration, temperature build up as well the rate of adsorption of substrate (urea).

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