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Modeling and simulation of the packed-bed reactor for anaerobic treatment process of the refinery effluents

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A B S T R A C T

In this study, the modeling and simulation of a packed bed reactor for treating refinery effluent using anaerobic processes were conducted. MATLAB computer programming language was employed, specifically utilizing the ordinary differential equations (ODEs) 45 model. The simulation employed the fourth-order Runge-Kutta algorithm (RK4) to investigate the impact of reactor length on the rate of contaminant treatment, focusing on mitigation. The results obtained from the simulation indicated that an increase in biomass concentration led to a decrease in the effluent's concentration (sludge concentration). This decrease in effluent concentration correlated with an increase in biomass concentration, which refers to the concentration of bacteria or the bacteria population within the reactor. The findings of this research hold significant utility in various aspects. Firstly, they can be applied for monitoring purposes, providing valuable insights into the ongoing treatment process. Additionally, the simulation allows for the prediction of treatment efficiency under different conditions, enabling researchers and operators to optimize the process. Furthermore, the ability to model the rate of effluent degradation based on microbe concentration offers valuable information for designing and operating similar anaerobic treatment systems effectively. Overall, this research contributes to the understanding and advancement of anaerobic treatment processes in packed bed reactors, providing a valuable tool for engineers and scientists working in the field of wastewater treatment and bioremediation.

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Capsule Summary: A modeling and simulating a packed bed reactor to treat refinery effluent using anaerobic processes was investigated. The findings are valuable for monitoring, predicting, and optimizing the contaminants removal rate based on microbe concentration, offering insights into efficient wastewater treatment.

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INTRODUCTION

Mathematical modeling is an important tool for rapid and reliable chemical reactor development and design. The models are built up from basic studies of the reaction mechanism and kinetics, the transfer processes, and the interactions within the system (Tchobanoglous et al., 2003; Jakobsen, 2009; Nathanson et al., 2022; Levenpiel, 2001). Mathematical modeling plays an important role in the development of a chemical reactor. It helps in understanding the experimentally observed processes by

testing their reactor models on well-established software, the equations are written in terms of mathematical objects that correspond directly to physical quantities if the objects change as part of the phenomenon, they are generally called variables while if they are fixed, they are generally called parameters (Abbas et al., 2017).

A model is a description of a system using mathematical concepts and language. Mathematical modeling refers to the process of creating a mathematical model (Pollution Prevention Case Stusies, 2021; Appels et al., 2008). Mathematical modeling (numerical modeling) of reactors is a powerful tool for understanding, designing, and predicting processes and process equipment in the chemical industry, including the conservation of momentum, energy, and material. Chemical reactions, composition, fluid movement, and temperature distribution in three dimensions and time may all be described using numerical computer modeling (Boe, 2006; Coulson and Richardson, 1991; Green and Perry, 1997; Almed, 2012).

A chemical reactor is an enclosed volume in which a chemical reaction takes place (Aida, et al., 2015; Altina, 2018; Anderson et al., 2000; Pereira et al., 2008) In chemical engineering, it is often considered to be a process vessel used to carry out a chemical reaction. Packed-bed reactors are tubular reactors loaded with solid catalyst particles that are used when it is intended to operate the reactor continuously but without back mixing of re232actants and products. Material flows through the reactor as a plug; they are also called plug flow reactors (PFR). Plug flow reactors are tubular reactors consisting of a hollow pipe or tube through which reactants flow. Furthermore, in the ideal reactor the compositions, and possibly the temperature and pressure also change between inlet and outlet of the reactor in the longitudinal direction. In the elementary treatment of tubular reactors, longitudinal dispersion, i.e., mixing by diffusion and other processes in the direction of flow, is also neglected. The advantage of using a packed bed reactor is the higher conversion per weight of catalyst than other catalytic reactors. The conversion is based on the amount of the solid catalyst rather than the volume of the reactor (Balanche et al., 1999; Zhigiang et al., 2010; Gondar et al., 2000; Sponza and Ulukon, 2005)

Industrial wastewater or effluent is water which has been used for industrial purposes and has been mixed with solids either suspended or dissolved (Idongesit et al., 2018). It is a byproduct of the production of commercial items. Water is necessary for practically every step of production across a wide range of industries, including the manufacture of food, drinks, clothing, and paper and chemical goods (Dezotti et al., 2017; Cakir and Stenstrom, 1999; Lweandowski and Defilippi, 2002). Water used in manufacturing operations can pick up a variety of impurities, which must be removed using water treatment techniques before discharge from the industrial manufacturing plant to fulfill regulatory standards. Suspended solids (TSS), fats-oils-grease (FOG), pH, bacteria, selenium, heavy metals, and other controlled chemicals and compounds are examples of components that may require treatment (Dagde et al., 2011; Seghezzo et al., 1998; Lee et al., 2015; Schroder et al., 1997; Ma et al., 2014). Sludge is largely water with some solid particles extracted from liquid sewage. Primary sludge is made up of particles that settle during primary treatment in primary clarifiers. Secondary sludge is sludge that has been separated in secondary clarifiers and is utilized in secondary treatment bioreactors or procedures that use inorganic oxidizing agents. To protect our ecosystems and human health, industrial effluents must be treated before it is released back into the environment. Treatment of refinery effluents has the potential to save energy by producing biogas from wastewater through anaerobic digestion, resulting in a source of cost-effective renewable energy that contributes to sustainability and water reuse by reclaiming high-quality effluent and lowering plant operating costs.

In this project, the Monod kinetic model and Edward–Haldane kinetic model are to be used with materials balances for biomass and the sludge to develop mathematical models for the anaerobic process of treatment of sludge in plug-flow reactor. These mathematical models used with MATLAB software results in defined values and variation of the various parameters. A knowledge of these values and their variation enhances optimum operation for maximal performance of the anaerobic reactor (Metcalf and Eddy, 2003; Shanshan et al., 2016; Syed et al., 2016).

Growing industrial set-ups have increased the release of pollutants, affecting the entire ecosystem. Wastewater from industrial processes, if released directly into the environment before proper treatment, is a source of pollution. It results in large pollution of rivers and other water bodies, consequently endangering living species including any surrounding population dependent on these water sources. (Vivek et al., 2014; Suruki and Yamaya, 2005). Efficient removal strategies of these toxic pollutants before releasing them into various water bodies are therefore highly necessary for a healthy environment.

Various types of technologies and strategies are being developed and employed for contamination removal from wastewater released from several industries. Some contaminants can be treated using anaerobic biological processes. This project will be used to predict or study the behavior of anaerobic system using a packed bed reactor and how it is used for the treatment of the effluent. The aim of the study is to develop a mathematical model of a packed bed reactor for anaerobic sludge treatment of refinery effluents.

MATERIAL AND METHODS

The materials used for this project are; journals, technical papers and textbooks, laptop, MATLAB Online Basics, industrial plant data, literature data of the kinetics of reaction in the operating conditions of process. According

to Sampson (2016), sludge wastewater was obtained from a typical petrochemical company in Port Harcourt, Nigeria. Methanogenic bacteria were isolated from the intestine of a cow and Oxoid AnaeroGen TM AN 0035A gas park was used to create Anaerobic condition in the reactor.

Methods

Modeling is a systematic mathematical approach that aids to formulate, simplify, and analyze behaviors and patterns in problems that arise in real life. Additionally, the use of mathematical models enables the investigation of hypotheses and hypothetical scenarios that are often inaccessible to research, as well as parameter ranges that may be difficult to obtain experimentally or computationally (Rahumpour et al., 2011). Aspen HYSYS can be used to describe the operation of the process by designing and simulating the process reactor in other to validate the mathematical models developed from principles of conservation of mass and energy. Here in the modeling of the packed bed reactor, we are concerned in determining mathematical equations that can be used to predict the growth of microorganism and the depletion of substrate in the reactor. These equations can simply be referred to as models.

Mathematical model development

A mathematical model of the reactor was developed to describe the operation of anaerobic digestion of sludge (substrate) by methanogenic bacteria (biomass) in a packed bed reactor (Scheme 1). The model was developed from first principles by applying the principles of conservation of mass. The analysis of the energy balance was neglected due to the nature of anaerobic systems.

Model assumption

The following assumptions were made in the development of the model equations.

i. Readily biodegradable substrate, which serves as source of carbon and energy, are present and accessible to the methanogenic bacteria.
ii. The components in the reactor moves in a plug flow manner because of the relatively flat velocity profile due to the packing. This means the concentration varies along the length of the reactor bed.
iii. The reactor operates at steady state.
iv. Pressure drop effects along the reactor were neglected.
v. There is no mixing along axial direction.
vi. Perfect mixing and the composition of the reacting mixture is uniform along the radial direction.
vii. Constant density.
viii. There is no radial variation in concentrations, temperatures and velocities.
ix. Constant inlet velocity which is equal to the axial velocity.

Material balance

The material balance on the reactors was developed based on the principle of conservation of mass. According to the principle of conservation of mass.

$$\begin{pmatrix}\text{Rate of accumulation}\\ \text{of component i}\\ \text{within the reactor}\end{pmatrix}=\begin{pmatrix}\text{Rate of input}\\ \text{of component}\\ \text{i into the reactor}\end{pmatrix}-\begin{pmatrix}\text{Rate of output}\\ \text{of component}\\ \text{i from the reactor}\end{pmatrix}\pm\begin{pmatrix}\text{Rate of generation or}\\ \text{deplection of species i}\\ \text{by chemical reactor}\end{pmatrix}$$

In the case of this study, the terms in Eq. 1 can be defined as, rate of accumulation = microbial growth, Rate of generation or depletion due to chemical reaction = Microbial biodegradability of wastewater (substrate). The general form of the steady state materials balance for the substrate and biomass is shown below.

$$\begin{pmatrix}\text{Rate of accumulation}\\ \text{of component i}\\ \text{or microbial growth in}\\ \text{the reactor}\end{pmatrix}=\begin{pmatrix}\text{Rate of input}\\ \text{of component}\\ \text{i into the reactor}\end{pmatrix}-\begin{pmatrix}\text{Rate of output}\\ \text{of component}\\ \text{i from the reactor}\end{pmatrix}\pm\begin{pmatrix}\text{Microbial biodegradability}\\ \text{of wastewater}\\ \text{in the reactor}\end{pmatrix}$$

Rate of Accumulation of component

$$\text{i} = \frac{\partial C_i}{\partial t}dV = Adz\frac{\partial C_i}{\partial t} = Adz(C_{i1,t+\Delta t} - C_{i1,t}) \quad (1)$$

At steady state in a PFR, rate of accumulation = 0. Rate of input of component i = F_i, Rate of output of component i = $F_i + dF_i$, Rate of depletion of component i = $(-r_i)dV = (-r_i)Adz$, substituting terms into Eq. 1 gives:

$$0 = F_i - (F_i + dF_i) + (-r_i)dV \quad (2)$$

$$F_i - F_i - dF_i + (-r_i)dV = 0$$

$$-dFi = (-r_i)dV \quad (3)$$

But $F_i = v_0 C_i$ and $dV = Adz$

$$-d(v_0 C_i) = (-r_i)Adz$$

$$-v_0 dC_i = (-r_i)Adz = \frac{dC_i}{dz} = -\frac{A}{v_0}(-r_i) \quad (4)$$

Equation (4) is the mathematical model in terms of concentration of species i. Where, dC_i is the differential change in the concentration of species i, mol/m^3, dV is the differential volume, m^3, C_i is the concentration of species i, mol/m^3, dC_i is the differential change in the concentration of species i, mol/m^3, F_i is the molar flow rate, i, mol/s, $\frac{dC_i}{dz}$ is the change in concentration. dz is the differential thickness of the fluid plug, m, the index i refers to the species I $(-r_i)$ is the rate of reaction term, mol/$m^3 s$, A is the transverse cross-sectional area of the tubular reactor, m^2, v_0 is the volumetric flow rate of the input, m^3/s.

The model equation (3.4) can also be express in terms mole fraction.

Recall: $y_i = \frac{C_i}{C}$ (5)

$C_i = Cy_i$ (6)

$dC_i = Cdy_i$ (7)

Where, y_i is the mole fraction of species i and C is the total concentration. Substituting Eq. 7 into equation (4) gives

$\frac{Cdy_i}{dz} = -\frac{A}{V_o}(-r_i)$ (8)

Rearranging equation

$\frac{dy_i}{dz} = -\frac{A}{V_o C}(-r_i)$ (9)

But, $v_o C = F_i$ (10)

$F_i = V_o C$ (11)

Substitute the equations

$\frac{dy_i}{dz} = -\frac{A}{F_i}(-r_i)$ (12)

Where, F_i is the molar flowrate of reacting species. Equation (12) represents the mathematical model for the packed bed reactor in terms of mole fraction.

Kinetic model

The Monods kinetic model is given by Coulson and Richardson (1991) as:

$\mu = \frac{\mu_m S}{K_s + S}$ (13)

Where, μ is the specific growth rate. K_s , the Monods constant and S the feed or sludge concentration. Let C_s be the instantaneous concentration of the substrate (sludge). Hence the Monods equation becomes:

$\mu = \frac{\mu_m C_s}{K_m + C_s}$ (14)

Where, K_m is the Monods constant, μ_m is a constant. From Eq. 14, the rate of change in concentration of the biomass $\frac{dC_B}{dt}$ and the rate of change in concentration of sludge (substrate) $\frac{dC_s}{dt}$ can be expressed in terms of microbial growth of the biomass as:

$\frac{dC_B}{dt} = \mu C_B = \frac{\mu_m C_B C_S}{K_m + C_S}$ (15)

$\frac{dC_S}{dt} = -\frac{1}{\gamma}\mu C_B = -\frac{\mu_m C_B C_S}{\gamma(K_m + C_S)}$ (16)

The negative sign in equation (16) depicts microbial biodegradation of the industrial wastewater and γ is known as the yield coefficient.

Coulson & Richardson (1991) gives g a modification of the Monods equation taking into consideration the consumption of cellular material to produce maintenance energy:

$\mu = \frac{\mu_m C_s}{K_m + C_s} - K_d$ (17)

Where, the constant K_d is referred to as endogenous respiration coefficient or specific maintenance rate.

Component balance of the species in the feed mass balance for the biomass (B)

From Levenspiel (2001) for a general reaction.

$r_A V = kVC_A$ (18)

Microbial biodegradability

$r_B V = \mu V C_B$ (19)

Hence, $r_B = \mu C_B$ (20)

Where, C_B is the instantaneous concentration of bacteria culture; V is the volume of the anaerobic reactor; □ is the specific growth rate; r is the rate of microbial biodegradation. Substituting equation (19) into the model equation (4); we have Eq. 21 and putting equation (17) into equation (21) gives Eq. 22.

$\frac{dC_B}{dz} = -\frac{A}{v_0}\mu C_B$ (21)

$\frac{dC_B}{dz} = -\frac{A}{v_0}\frac{\mu_m C_B C_S}{K_m + C_S} - K_d C_B$ (22)

Equation (22) is the model for the rate of change of the concentration of the biomass along the differential length of the tubular reactor, i.e., the rate of microbial growth.

Mass balance for the industrial wastewater (S)

From equation (16), rewriting equation (20) for the rate of the substrate (sludge) gives Eq. 23 and substituting equation (23) into the model equation (4) gives Eq. 24. Putting equation (17) into equation (24) gives Eq. 25.

$r_S = -\frac{1}{\gamma}\mu C_S$ (23)

$\frac{dC_S}{dz} = \frac{1}{\gamma}\frac{A}{v_0}\mu C_B$ (24)

$\frac{dC_S}{dz} = \frac{1}{\gamma}\frac{A}{v_0}\frac{\mu_m C_B C_S}{K_m + C_S}$ (25)

Equation (25) is the model for the rate of change of the concentration of the substrate (sludge) along the differential length of the tubular reactor, i.e., the rate of microbial biodegradation of the sludge wastewater.

Biomass yield (X)

The yield of the methanogenic bacteria can be calculated by subtraction the initial biomass concentration (C_{B0}) from the final biomass concentration (C_B). Thus, the instantaneous biomass yield can be calculated along the reactor length by taking the difference between subsequent biomass concentrations.

$$X = C_B - C_{B0} \quad (26)$$

Yield coefficient (Y)

This is the ratio of the actual yield of biomass to the amount of substrate consumed in the process. It represents how the substrate is efficiently converted by the microorganisms to products (microbial growth efficiency).

$$Y = \frac{Biomass\ produced,\ X}{Substrate\ consumed,\ S} = \frac{C_B - C_{B0}}{C_{S0} - C_S} \quad (27)$$

Where: C_B is the final biomass concentration, C_{B0} is the initial biomass concentration, C_S is the final substrate concentration and C_{S0} is the initial substrate concentration.

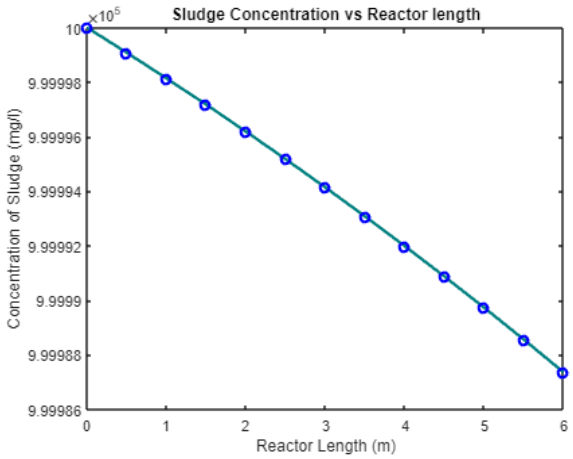


Fig. 1: Sludge substrate concentration versus reactor length

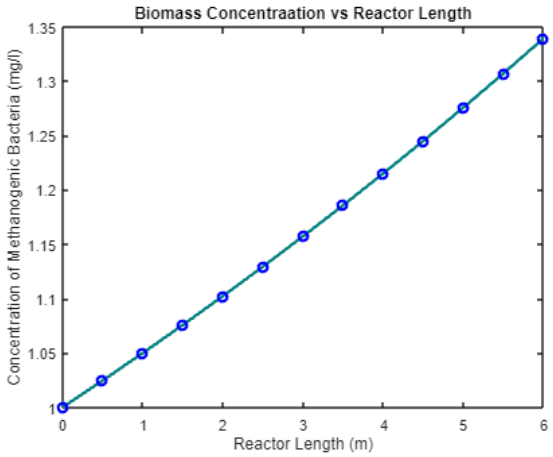
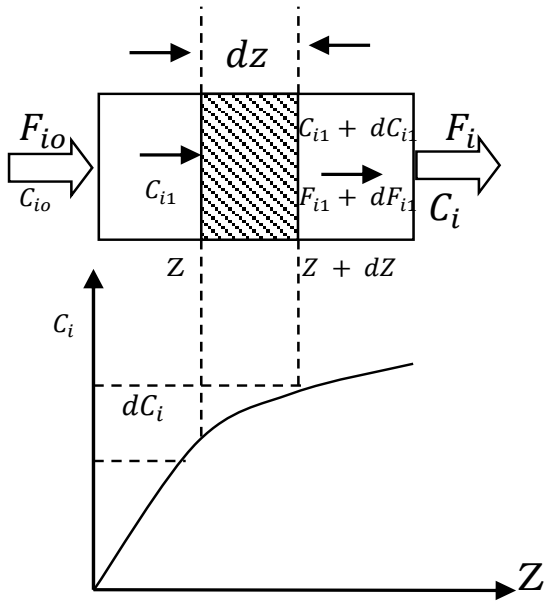


Fig. 2: Biomass concentration versus reactor length



Scheme 1: Hypothetical representation of packed bed reactor

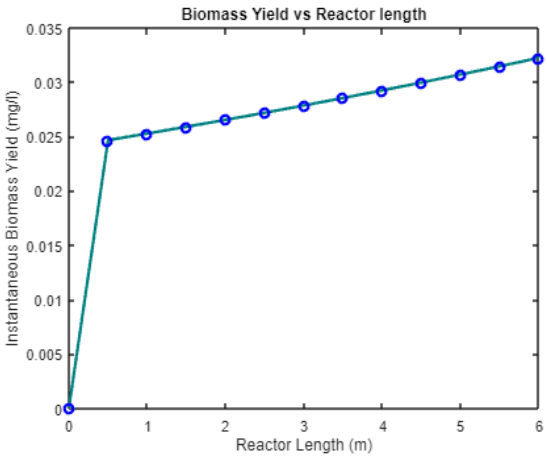


Fig. 3: Biomass yield versus reactor length

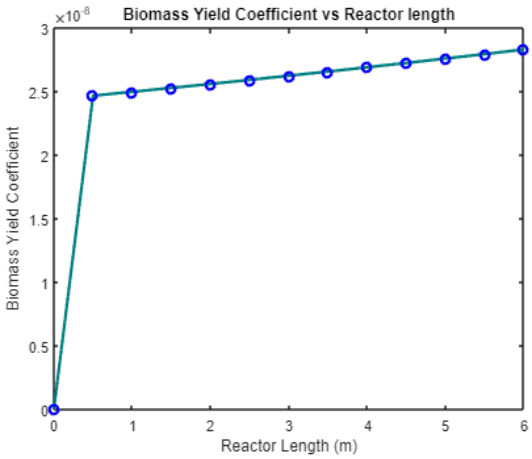


Fig. 4: Biomass yield coefficient versus reactor length

Solution techniques

The developed model equations will be solved using MATLAB Online Basics from Mathworks by employing the fourth order Runge Kutta algorithm in solving the resultant system of ordinary differential equations (ODEs).

Initial conditions

The biomass (methanogenic bacteria) acts on the substrate (wastewater) to produce biogas, consisting of methane, carbon dioxide, with very small amounts of water vapor and traces of other contaminant gases. The data and initial condition of the feed at the inlet is summarized in Table 1.

Runge-Kutta Algorithm

The fourth-order Runge-Kutta (RK4) algorithm for solving a system of ordinary differential equations is adopted for the solution. The RK4 method provides the approximate value of y (C_i in our case) for a given point x (dz). The algorithm is used to numerically compute simultaneous functions in which there are multiple variables to be determine. The global error of the fourth-order Runge-Kutta algorithm is O(h4). The algorithm used for solving the model as shown below.

% Considering the simultaneous ODEs as: $C_A, C_B, C_C, C_D, .., C_N$

Input: $C_{A0}, C_{B0}, C_{C0}, C_{D0}, \dots, C_{N0}$

Step $= h$; *numberofsteps* $= N$

Output: $C_{i(N+1)}$ *to the solution* $C_{I(Zn+1)}$ *at* $Z_{N+1} = Z_o + (N+1)h$

for $n = 0, 1, \dots, N-1$

% Firstvector: Increment based on the slope at the beginning of the interval

$k_{11} = hf_o(Z_o, C_{A(0)})$

$k_{12} = hf_o(Z_o, C_{B(0)})$

$k_{13} = hf_o(Z_o, C_{C(0)})$

$k_{14} = hf_o(Z_o, C_{D(0)})$

% Secondvector: Increment based on the slope at the midpoint of the interval

$k_{21} = hf_o(Z_o + {}^1/_2\, h, C_{A(0)} + {}^1/_2\, k_{11}, C_{B(0)} + {}^1/_2\, k_{12} \dots)$

$k_{22} = hf_o(Z_o + {}^1/_2\, h, C_{A(0)} + {}^1/_2\, k_{11}, C_{B(0)} + {}^1/_2\, k_{12} \dots)$

$k_{23} = hf_o(Z_o + {}^1/_2\, h, C_{A(0)} + {}^1/_2\, k_{11}, C_{B(0)} + {}^1/_2\, k_{12} \dots)$

$k_{24} = hf_o(Z_o + {}^1/_2\, h, C_{A(0)} + {}^1/_2\, k_{11}, C_{B(0)} + {}^1/_2\, k_{12} \dots)$

% Thirdvector: Increment based on the slope at the midpoint of the interval

$k_{31} = hf_o(Z_o + {}^1/_2\, h, C_{A(0)} + {}^1/_2\, k_{21}, C_{B(0)} + {}^1/_2\, k_{22} \dots)$

$k_{32} = hf_o(Z_o + {}^1/_2\, h, C_{A(0)} + {}^1/_2\, k_{21}, C_{B(0)} + {}^1/_2\, k_{22} \dots)$

$k_{33} = hf_o(Z_o + {}^1/_2\, h, C_{A(0)} + {}^1/_2\, k_{21}, C_{B(0)} + {}^1/_2\, k_{22} \dots)$

$k_{34} = hf_o(Z_o + {}^1/_2\, h, C_{A(0)} + {}^1/_2\, k_{21}, C_{B(0)} + {}^1/_2\, k_{22} \dots)$

% Fourthvector: Increment based on the slope at the end of the interval

$k_{41} = hf_o(Z_o + h, C_{A(0)} + k_{31}, C_{B(0)} + k_{32} \dots)$

$k_{42} = hf_o(Z_o + h, C_{A(0)} + k_{31}, C_{B(0)} + k_{32} \dots)$

$k_{43} = hf_o(Z_o + h, C_{A(0)} + k_{31}, C_{B(0)} + k_{32} \dots)$

$k_{44} = hf_o(Z_o + h, C_{A(0)} + k_{31}, C_{B(0)} + k_{32} \dots)$

% Vector of dependent variables

$$\Delta C_A = \frac{1}{6}(k_{11} + 2k_{12} + 2k_{13} + k_{14})$$

$$\Delta C_B = \frac{1}{6}(k_{21} + 2k_{22} + 2k_{23} + k_{24})$$

$$\Delta C_C = \frac{1}{6}(k_{31} + 2k_{32} + 2k_{33} + k_{34})$$

$$\Delta C_D = \frac{1}{6}(k_{41} + 2k_{42} + 2k_{43} + k_{44})$$

Output: Z_{N+1}; $C_{A(N+1)}$; $C_{B(N+1)}$; $C_{C(N+1)}$; $C_{D(N+1)}$

end stop, In general, $C_{i(n+1)} = C_{i(n)} + \Delta C_i$

where: $i = A, B, C$ *and* D

RESULTS AND DISCUSSION

Model simulation results

This chapter discusses the results from the simulation and solution of the mathematical model equations developed for the anaerobic process of sludge treatment in a packed bed reactor and the process kinetics. MATLAB Online Basics from Mathworks which provides access to MATLAB and Simulink from any standard web browser with internet access was used for the simulation of the developed model equations. The 4th order Runge-Kutta algorithm was used in solving the models which were in the form of ordinary differential equations (ODEs) to compute the concentrations of the biomass (methanogenic bacteria culture) and the substrate in the sludge wastewater.

The biomass yield coefficient and the instantaneous yield as the reaction progress along the length of the reactor was also computed. Initial conditions are shown in Table 1 and Table 2 demonstrate the result from the MATLAB program. The rate of change in concentration of the substrate (sludge) across the reactor length was automatically approximated and truncated by the MATLAB program. See in Figures 1, 2, 3 and 4 for a graphical representation of the results. For an anerobic sludge treatment process in plug flow reactor, the following model equations were developed (Eqs. 27-28).

$$\frac{dC_B}{dz} = \frac{A}{v_0}\frac{\mu_m C_B C_S}{K_m + C_S} - K_d C_B \quad (27)$$

$$\frac{dC_S}{dz} = -\frac{1}{\gamma}\frac{A}{v_0}\frac{\mu_m C_B C_S}{K_m + C_S} \quad (28)$$

The results of the anaerobic digestion process for sludge wastewater treatment predicted by the plug flow reactor

Table 1: Parameters and initial conditions (Sampson et al., 201)

Parameters	Values
CB0	1.0 g/L
µm	0.037/h
VSS	9.6 mg
BCOD	600 mg
γ	0.016
Km	0.02 kmol/m3
Kd	0.025/d
D	0.18/h
CS0	1000000 mg/L

models developed with respect to the reactor length is shown in Figures 1, 2, 3 and 4. Figures 1 and 2 show the variation of the concentration of the sludge substrate and the biomass (methanogenic bacteria culture) respectively across the reactor length. From Figure 1, the concentration of the substrate decreased across the reactor length which was predicted by the negative sign in the model equation (16) showing microbial biodegradation of the sludge. The concentration of the biomass increased along the reactor length as shown in Figure 2. Yield is an important variable in chemical reactor modeling and it was also computed and the result shown in Figures 3 and 4 obtained from the Matlab output.

Figure 1 shows the plot of the relationship of concentration of the sludge and the effect of reactor length in anaerobic sludge treatment using methanogenic bacteria culture as the biomass. Indeed, the result obtained reveals decrease in the concentration of the sludge (substrate) with increase in the length of the plug-flow reactor. The result clearly shows the role played by the concentration of the biomass in terms of methanogenic bacteria as well as revealing that the concentration of the sludge decreases with increase in reactor length as well as increase in microbial activities. The downward slope (negative slope) clearly validates the negative sign in the model equation (16) which shows microbial biodegradation of the sludge by the methanogenic bacteria.

Figure 2 shows the plot of the relationship of the concentration of biomass and the reactor length in anaerobic sludge treatment process using methanogenic bacteria culture as the biomass. It is clearly shown from the result that the concentration of the biomass increases with increase in the reactor length in a plug-flow reactor which resulted in a straight line with positive slope passing through the origin. The result revealed that, as the reaction progress across the length of the reactor, there is microbial growth as the methanogenic bacteria feed on the substrate. This means that there is formation of new cells in the biomass which leads to increased microbial activities.

Figure 3 shows the relationship between the biomass yield and the effect of reactor length. This is the instantaneous biomass yield at any given point along the reactor length of a plug-flow reactor. The result obtained reveals that at the start of the reaction, there was a steep

Table 2: Results from MATLAB program

Reactor length (m)	Concentration of biomass (Methanogenic bacteria) (mg/L)	Substrate concentration in sludge (mg/L)	Biomass yield (mg/L)	Yield coefficient
0	1	1000000	0	0
0.5	1.0246	1.0000e+06	0.0246	2.4646e-08
1.0	1.0499	1.0000e+06	0.0253	2.4950e-08
1.5	1.0758	1.0000e+06	0.0259	2.5259e-08
2.0	1.1023	1.0000e+06	0.0265	2.5572e-08
2.5	1.1295	1.0000e+06	0.0272	2.5891e-08
3.0	1.1573	9.9999e+05	0.0278	2.6216e-08
3.5	1.1858	9.9999e+05	0.0285	2.6545e-08
4.0	1.2150	9.9999e+05	0.0292	2.6880e-08
4.5	1.2450	9.9999e+05	0.0299	2.7221e-08
5.0	1.2757	9.9999e+05	0.0307	2.7567e-08
5.5	1.3071	9.9999e+05	0.0314	2.7920e-08
6.0	1.3393	9.9999e+05	0.0322	2.8278e-08

rise in the value of the biomass produced (yield) from 0 mg/L at length, x = 0 to 0.0246 mg/L at length, x = 0.5 m. Afterwards, the biomass yield increased linearly throughout the course of the reaction with increase in the reaction length. Figure 4 shows the relationship between the biomass yield coefficient and the effect of reactor length. This is the ratio of the amount of biomass produced to the substrate consumed as the reaction progress across the reactor length of a plug-flow reactor. The result obtained reveals that initially, the yield coefficient, Y = 0 when reactor length, x = 0 after which there was a steep rise in the value of the yield coefficient when the process started from 0 mg/L to 0.0246 mg/L, while the substrate is being consumed simultaneously. Afterwards, the biomass yield coefficient increased linearly throughout the course of the reaction with increase in the reaction length.

CONCLUSIONS

This work entails the modeling of detailed mathematical models and MATLAB computer program that simulates the anaerobic operation of a packed bed reactor for treatment of sludge wastewater. The kinetics of the process was obtained from literature and incorporated into the models to ensure proper behavior and description of the process when simulated. The results obtained from the developed mathematical models showed that rate of change in concentration of the biomass (methanogenic bacteria culture) and the rate of change in concentration of the substrate in the wastewater sludge for the anaerobic plug-flow reactor follow a linear model as proved by the results and straight-line graphs obtained from the MATLAB program. The yield followed a similar pattern. The research demonstrates the following conclusions;

i. The modelling and simulation of packed-bed reactor for anaerobic treatment is influenced by the bed height and the flow rate characteristics of the effluent.
ii. The research also demonstrates that the initial concentration of the effluent is a major factor on the effectiveness of the anaerobic process of contaminant mitigation using a packed-bed reactor.
iii. The MATLAB computer software used for the simulation of the biomass concentration, substrate concentration repeats to reactor length revealed increase in both biomass (microbial growth) and increase in substrate utilization.

DECLARATION OF COMPETING INTEREST

The authors declare no competing financial interest.

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