References
REFERENCES

CHAPTER-I


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LIST OF PUBLICATIONS BASED ON THE THESIS


LIST OF CONFERENCES/SEMINARS/WORKSHOPS

PRESENTED AND ATTENDED

1. Participated in one day seminar on Reproductive Health organized by the Population Education Resource Centre of Centre for Adult, Continuing Education and Extension & College Development Council, Alagappa University, Karaikudi and State Resource Centre for Non formal Education, Chennai on 18th August 2006 at Alagappa University.

2. Participated one day First Aid Training Programme for YRC volunteers of Alagappa University on 11th April 2007 at the University Auditorium.

3. Participated in two days national seminar on Educating Children with Learning Difficulties organized by the Special Education Centre/ Disability Unit, Alagappa University, Karaikdi on 11th and 12th April 2008 in Alagappa University, Karaikudi.


6. Participated in five days training programme on “Diagnosing and addressing learning problems of children at secondary level in Tamilnadu” organized by Regional Institute of Education (NCERT) at Mysore during from 25th February to 1st March 2013.

7. Presented the paper “Mathematical modelling of a biofilm; The Adomian decomposition method” in the DST & CSIR sponsored national conference on Advances and Applications in Mathematical Modelling, organized by the Department of Mathematics, The Madura College (Autonomous), Madurai during 15th and 16th April 2013.
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Reprints of publications
Analytical Solution of the Concentration in a Packed-bed Immobilized Enzyme Reactor using Homotopy Perturbation Method

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Abstract

A mathematical model of packed-bed immobilized enzyme (IME) reactor is presented. The model is based on system of reaction-diffusion equations containing a non-linear term related to Michaelis-Menten kinetics of the enzymatic reaction. A simple and closed approximate analytical expression of the steady-state concentrations and effectiveness factor in a Packed-bed immobilized enzyme reactor are derived for all values of the reaction diffusion parameters. In this paper, He’s Homotopy perturbation method is implemented to give approximated and analytical expression of concentration of substrate and effectiveness factor for all values of the parameters.

Keywords: Mathematical model; Steady-state; Homotopy perturbation method; Packed-bed reactor; immobilized enzyme; Michaelis-Menten kinetic.

Introduction

In many cases, for immobilized enzyme reactors, it is not possible to use the plug-flow model due to can not suppress potentially disturbing effects such as mass transfer limitations, axial dispersion and bypassing. Therefore, any realistic analysis of the packed-bed enzymatic reactor should include some fundamental aspects of the process such as liquid-phase (external) and the solid-phase (internal) mass transfer, intrinsic kinetic parameters, and reactor hydrodynamics. These physical considerations determine a mathematical model representing reactor behavior as a function of operational conditions [1, 2]. Packed-beds are commonly employed for solid–fluid contacting in heterogeneous catalysis for several reasons: (i) it facilitates the contact and subsequent separation between reactant and catalyst; (ii) it allows
reuse of the enzyme without the need for a prior separation; (iii) a continuous mode of operation can be used easily.

Immobilization of enzymes on suitable support materials has resulted in their extended use in batch and continuous bioreactors. For immobilized enzymes, however, there are several factors which affect the observed kinetics that could be significantly different from the intrinsic kinetics of the free enzyme. These factors include interparticle and intraparticle diffusion limitations, steric and conformation effects, the partitioning of substrate between the support and bulk of the solution, conformation and spatial effects due to the immobilization mechanism which may cause disfiguration of the enzyme and micro-environmental effects due to the interactions of the support on the enzyme-substrate reaction resulting in a change in the enzymatic reaction mechanism.

Lilly et al. [3] proposed a method to characterize packed-bed immobilized enzyme (IME) reactors, in which the exit concentration of substrate consumed is linearly plotted against the logarithm of the exit unconverted fraction of substrate and the apparent Michaelis constant. On the other hand, Peter et al. [4] found that such a plot, made by using experimental data in the packed-bed immobilized \( \beta \)-galactosidase reactor, was deviated from linearity. Although several attempts [5, 6] were made to theoretically interpret the experimental results, no decisive conclusion has been derived because the models introduced were not sufficient. Shiraishi previously derived expressions for the apparent kinetic parameters of IME reactions [7]. Shiraishi studied the design equation for a packed-bed immobilized enzyme reactor is expressed in terms of apparent kinetic parameters and the relationship between the exit concentration of substrate consumed and the logarithm of the exit unconverted fraction of substrate [8].

However, to the best of author’s knowledge, no general analytical results of substrate concentration and effectiveness factor for all values of dimensionless parameters \( \alpha \) and \( \gamma_E \) have been published. The purpose of this communication is to derive approximate analytical expressions for the steady-state concentrations for all values of \( \alpha \) and \( \gamma_E \) using Homotopy Perturbation method.

**Mathematical formulation of the problem**

The boundary value problems which have to be solved in this case can be written in the following forms [8]:

\[
\frac{D_e}{x^{G-1}} \frac{d}{dx} \left( x^{G-1} \frac{dS}{dx} \right) = \frac{V_m S}{K_m + S}
\]

(1)

with the boundary conditions:

\[
\frac{dS}{dx} = 0 \text{ when } x = 0
\]

(2)

\[
D_e \frac{dS}{dx} = k_L (S_b - S) \text{ when } x = R
\]

(3)
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The effectiveness factor $E_f$ can be calculated as

$$E_f = \frac{G(K_m + S_b)}{RV_mS_b} \left( D_e \frac{dS}{dx} \right)_{x=R} \tag{4}$$

We introduce the following set of dimensionless variables:

$$U = \frac{S}{S_b}, \quad X = \frac{x}{R}, \quad \gamma_E = \frac{V_mR^2}{De k_m}, \quad \alpha = \frac{S_b}{k_m}, \quad m = \ldots \tag{5}$$

The governing non-linear reaction/diffusion Eqs. (1-3) are expressed in the following non-dimensional form as:

$$\frac{d^2U}{dX^2} + \frac{G - 1}{X} \frac{dU}{dX} = \frac{\gamma_E U}{1 + \alpha U} \tag{6}$$

with the boundary conditions:

$$X = 0, \quad \frac{dU}{dX} = 0 \tag{7}$$

$$X = 1, \quad \frac{dU}{dX} = m(1 - U) \tag{8}$$

The effectiveness factor is given by

$$E_f = \frac{(1 + \alpha) \left[ \frac{dU}{dX} \right]_{X=1}}{\gamma_E} \tag{9}$$

Analytical solution of steady state concentration using HPM

Recently, many authors have applied the HPM to various problems and demonstrated the efficiency of the HPM for handling non-linear structures and solving various physics and engineering problems [9-12]. This method is a combination in topology and classic perturbation techniques. Ji Huan He used the HPM to solve the Lighthill equation [13], the Duffing equation [14] and the Blasius equation [15]. The idea has been used to solve non-linear boundary value problems, integral equations and many other problems [16-17]. The HPM is unique in its applicability, accuracy and efficiency. The HPM uses the imbedding parameter $p$ as a small parameter and only a few iterations are needed to search for an asymptotic solution. Using this method (see Appendix B and C), we can obtain the following solution to Eqs. (6) - (8). For the case of slab ($G = 1$), the concentration of the substrate becomes
The effectiveness factor is given by

\[
U(X) = 1 + \frac{\gamma_E E^2}{2} \left( \frac{\gamma_E m + 2 \gamma_E}{2m} \right) + \frac{\gamma_E \left( \frac{\alpha}{m} + \frac{1}{6m} + \frac{\alpha}{2} + \frac{1}{24} - \frac{\alpha X^2}{12} - \frac{X^4}{24} \right)}{2m + \frac{1}{4} + \frac{1}{m^2} + \frac{1}{2m} - \frac{X^2}{2m}}
\]

(10)

The effectiveness factor is given by

\[
Ef = \frac{(1 + \alpha)}{\gamma_E} \left[ \gamma_E - \gamma_E \left( \frac{1}{6} + \alpha \right) - \gamma_E \left( \frac{1}{m} + \frac{1}{2} \right) \right]
\]

(11)

For the case of rod \((G = 2)\), the concentration of the substrate becomes

\[
U(X) = 1 + \frac{\gamma_E^2}{24m^2} \left[ m^2 X^4 - 12mX^2 - 6m^2 X^2 + 20m + 24 + 5m^2 \right] + \frac{\gamma_E}{m} \left[ 2\alpha + \alpha m - \alpha mX^2 \right]
\]

(12)

The effectiveness factor is given by

\[
Ef = \frac{(1 + \alpha)}{\gamma_E} \left[ \frac{\gamma_E^2}{24m^2} \left( -8m^2 - 24m \right) - 2\gamma_E \alpha \right]
\]

(13)

Results and Discussion

Figs. 1(a)-(b) to 2(a)-(b) represent the normalized steady-state concentration of substrate \(U(X)\) for different values of dimensionless parameters \(\alpha\) and \(\gamma_E\). From this figure 1, it is evident that for the case of slab, the values of the concentration of substrate is constant when \(X = 0.1\) and then increases slowly. From this figure 2, it is obvious that the values of the concentration of substrate decreases when \(X \geq 0.1\). Also, from the figures 1(a)-2(b), it is known that, the concentration of substrate increases when dimensionless parameter \(\alpha\) and \(\gamma_E\) are increases for \(m = 0.01, 1\). The effectiveness factor \(Ef\) for various values of \(\gamma_E\) and \(\alpha\) is plotted in Figs. 3 and 4. From these figures, it is obvious that, the values of the effectiveness factor slowly increases when \(\gamma_E\) and \(\alpha\) is increases.

Figs. 5(a)-(b) to 6(a)-(b) represent the normalized steady-state concentration of substrate \(U(X)\) for different values of dimensionless parameters \(\alpha\) and \(\gamma_E\) for the case of rod \(G = 2\). From these figures, it is inferred that, the dimensionless concentration \(U(X)\) for all values of \(m\) and \(\gamma_E\). The effectiveness factor increases quite rapidly as dimensionless reaction diffusion parameters \(\gamma_E\) and \(\alpha\) are increases, approaching to high values, which corresponds to internal diffusion controlled processes. Moreover, it is also well known that, a constant value of dimensionless
parameters $\gamma_E$ and $\alpha$, the effectiveness factor increases with increasing value of $\gamma_E$ and $\alpha$. The effectiveness factor $Ef$ for various values of $\gamma_E$ and $\alpha$ is plotted in Figs. 7 and 8. From these figures, it is apparent that, the value of the effectiveness factor is very small when $\gamma_E$ and $\alpha$ is less than 0.5. When $\gamma_E$ and $\alpha$ are greater than 1, the effectiveness factor is increases.

**Figure 1(a-b):** Normalised concentration profile $U(X)$ as a function of dimensionless parameter $X$. The concentrations were computed using Eq. (10) for various values of the reaction/diffusion parameter $\alpha$ and for the fixed value of $m = 0.01, \gamma_E = 0.1$.

**Figure 2(a-b):** Normalised concentration profile $U(X)$ as a function of dimensionless parameter $X$. The concentrations were computed using Eq. (10) for various values of the reaction/diffusion parameter $\gamma_E$ and for the fixed value of $m = 1, \alpha = 5$. 
Figure 3: Dimensionless effectiveness factor $Ef$ versus $\alpha$ for various values of $\gamma_E$ for the fixed value of $m = 0.01$.

Figure 4: Dimensionless effectiveness factor $Ef$ versus reaction diffusion parameter $\gamma_E$ for various values of $\alpha$ for the fixed value of $m = 1$. 
Figure 5(a-b): Normalised concentration profile $U(X)$ as a function of dimensionless parameter $X$. The concentrations were computed using Eq. (12) for various values of the reaction/diffusion parameter $\alpha$ and for the fixed value of $m = 0.01, \gamma_E = 0.1$.

Figure 6(a-b): Normalised concentration profile $U(X)$ as a function of dimensionless parameter $X$. The concentrations were computed using Eq. (12) for various values of the reaction/diffusion parameter $\gamma_E$ and for the fixed value of $m = 1, \alpha = 5$. 
Figure 7: Dimensionless effectiveness factor $Ef$ versus $\alpha$ for various values of $\gamma_E$ for the fixed value of $m = 0.01$.

Figure 8: Dimensionless effectiveness factor $Ef$ versus reaction diffusion parameter $\gamma_E$ for various values of $\alpha$ for the fixed value of $m = 1$. 
Conclusions
The time independent non-linear reaction-diffusion equation has been formulated and solved analytically. Analytical expressions for the concentration and effectiveness factor are derived by using the HPM. The primary result of this work is simple approximate calculations of concentration and effectiveness factor for all values of dimensionless parameters $\alpha$ and $\gamma_k$. The HPM is an extremely simple method and it is also a promising method to solve other non-linear equations. This method can be easily extended to find the solution of all other non-linear equations.

References

Appendix A

In this appendix we outline the basic idea of Homotopy Perturbation method. This method has eliminated the limitations of the traditional perturbation methods. On the other hand it can take full advantage of the traditional perturbation techniques, so there has been a considerable deal of research in applying homotopy technique for solving various strongly nonlinear equations. To explain this method, let us consider the following function

\[ A(u) - f(r) = 0, \quad r \in \Omega \]  
(A1)

with the boundary conditions of

\[ B(u, \frac{\partial u}{\partial n}) = 0, \quad r \in \Gamma \]  
(A2)

where \( A, B, f(r) \) and \( \Gamma \) denote a general differential operator, a boundary operator, a known analytical function and the boundary of the domain \( \Omega \), respectively. Generally speaking, the operator \( A \) can be divided into a linear part \( L \) and a nonlinear part \( N \). Eq. (A1) can therefore, be written as

\[ L(u) + N(u) - f(r) = 0 \]  
(A3)

By the Homotopy technique, we construct a Homotopy \( H(r, p) : \Omega \times [0,1] \to R \) which satisfies

\[ H(v, p) = (1 - p)[L(v) - L(u_0)] + p[A(v) - f(r)] = 0, \]  
\[ p \in [0,1], \ r \in \Omega \]  
(A4)

or

\[ H(v, p) = L(v) - L(u_0) + pL(u_0) + p[N(v) - f(r)] = 0, \]  
(A5)

where \( p \in [0,1] \) is an embedding parameter, and \( u_0 \) is an initial approximation of Eq. (A1), which satisfies the boundary conditions. Obviously, from Eqs. (A4) and (A5), we will have

\[ H(v, 0) = L(v) - L(u_0) = 0 \]  
(A6)

\[ H(v, 1) = A(v) - f(r) = 0. \]  
(A7)

When \( p = 0 \) Eq. (A4) or Eq. (A5) become a linear equation; when \( p = 1 \) it
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become a non-linear equation. So the changing process of \(p\) from zero to unity is just that of \(L(\nu) - L(t_0) = 0\) to \(A(\nu) - f(r) = 0\). We can first use the embedding parameter \(p\) as a “small parameter”, and assume that the solutions of Eqs. (A4) and (A5) can be written as a power series in \(p\)

\[v = v_0 + pv_1 + p^2v_2 + .....\]  

(A8)

Setting \(p = 1\) results in the approximate solution of Eq. (A1):

\[u = \lim_{p \to 1} v = v_0 + v_1 + v_2 + .....\]  

(A9)

The combination of the perturbation method and the Homotopy method is called the HPM.

Appendix B

Solution of the equation (6) for \(G=1\) using Homotopy perturbation method. In this appendix, we indicate how Eq. (10) in this paper is derived. Furthermore, a Homotopy was constructed to determine the solution of Eq. (6) for \(G=1\)

\[(1-p) \left[ \frac{d^2U}{dx^2} \right] + p \left[ \frac{d^2U}{dx^2} + \alpha \frac{d^2U}{dx^2} - \gamma E U \right] = 0\]  

(B1)

The initial approximation is as follows:

\[X=0, \frac{dU}{dx} = 0\]  

(B2)

\[X=1, \frac{dU}{dx} = m(1-U)\]  

(B3)

\[X=0, \frac{dU_i}{dx} = 0\]  

(B4)

\[X=1, \frac{dU_i}{dx} = m(1-U), \forall \ i = 1, 2, \ldots\]  

(B5)

The approximate solutions of (B1) is

\[U = U_0 + pU_1 + p^2U_2 + p^3U_3 + \ldots\]  

(B6)

Substituting Eq. (B6) and into Eq. (B1) and comparing the coefficients of like powers of \(p\)

\[p^0: \frac{d^2U_0}{dx^2} = 0\]  

(B7)

\[p^1: \frac{d^2U_1}{dx^2} + \alpha U_0 \frac{d^2U_0}{dx^2} - \gamma E U_0 = 0\]  

(B8)
Solving the equations (B7) to (B9), and using the boundary conditions (B2) and (B3), we can find the following results

\[ U_0(X) = 1 \]  
\[ U_1(X) = \frac{\gamma_E X^2}{2} - \frac{(\gamma_E m + 2 \gamma_E)}{2m} \]  
\[ U_2(X) = \gamma_E \left[ \frac{\alpha}{m} + \frac{1}{6m} + \frac{\alpha}{2} + \frac{1}{24} - \frac{X^2}{2} + \frac{X^4}{24} \right] + \frac{\gamma_E^2}{2m} \left[ \frac{1}{4} + \frac{1}{m^2} + \frac{1}{2m} - \frac{X^2}{2m} - \frac{X^2}{4} \right] \]

According to the HPM, we can conclude that

\[ U(X) = \lim_{p \to 1} U(X) = U_0 + U_1 + U_2 \]

Using Eqs. (B10), (B11) and (B12) in Eq. (B13), we obtain the final result as described in Eq. (10).

**Appendix C**

Solution of the equation (6) for \( G = 2 \) using Homotopy perturbation method. In this appendix, we indicate how Eq. (12) in this paper is derived. Furthermore, a Homotopy was constructed to determine the solution of Eq. (6) for \( G = 2 \)

\[ (1 - p) \left[ \frac{d^2 U}{dX^2} \right] + p \left[ \frac{d^2 U}{dX^2} + \frac{1}{X} \frac{dU}{dX} + \alpha U \frac{d^2 U}{dX^2} + \frac{\alpha U}{X} \frac{dU}{dX} - \gamma_E U \right] = 0 \]

and the initial approximations are as follows:

\[ X = 0, \quad \frac{dU}{dX} = 0 \]  
\[ X = 0, \quad \frac{dU_i}{dX} = 0 \]  
\[ X = 1, \quad \frac{dU_i}{dX} = m(1 - U) \]  
\[ X = 1, \quad \frac{dU_i}{dX} = m(1 - U) \quad \forall \quad i = 1, 2, \ldots \]
The approximate solutions of (C1) is
\[ U = U_0 + pU_1 + p^2U_2 + p^3U_3 + \ldots \] (C6)

Substituting Eq. (C6) and into Eq. (C1) and comparing the coefficients of like powers of \( p \)
\[ p^0: \quad \frac{d^2U_0}{dX^2} = 0 \] (C7)
\[ p^1: \quad \frac{d^2U_1}{dX^2} + \frac{1}{X} \frac{dU_0}{dX} + \alpha U_0 \frac{d^2U_0}{dX^2} + \frac{\alpha U_0}{X} \frac{dU_0}{dX} - \gamma E U_0 = 0 \] (C8)
\[ p^2: \quad \frac{d^2U_2}{dX^2} + \frac{1}{X} \frac{dU_1}{dX} + \alpha U_0 \frac{d^2U_1}{dX^2} + \alpha U_1 \frac{d^2U_0}{dX^2} + \frac{\alpha U_0}{X} \frac{dU_1}{dX} + \frac{\alpha U_1}{X} \frac{dU_0}{dX} - \gamma E U_1 = 0 \] (C9)

Solving the equations (C7) to (C9), and using the boundary conditions (C2) and (C3), we can find the following results
\[ U_0(X) = 1 \] (C10)
\[ U_1(X) = \frac{\gamma E X^2}{2} - \frac{\gamma E}{m} \frac{X^2}{2} \] (C11)
\[ U_2(X) = \frac{\gamma E^2 X^4}{24} - \frac{\gamma E^2 X^2}{2m} \frac{X^2}{4} - \alpha \gamma E X^2 \frac{\gamma E X^2}{2m} \frac{X^2}{2m} + \frac{\gamma E^2}{m} \frac{X^2}{m} + 2 \alpha \gamma E + \gamma E \frac{X^2}{6m} - \frac{\gamma E}{24} \]
\[ + \frac{\gamma E}{2m} + \frac{\gamma E}{4} + \alpha \gamma E + \frac{\gamma E}{2} \] (C12)

According to the HPM, we can conclude that
\[ U(X) = \lim_{p \to 1} U(X) = U_0 + U_1 + U_2 \] (C13)

Using Eqs. (C10), (C11) and (C12) in Eq. (C13), we obtain the final result as described in Eq. (12).
Modelling of Immobilized Glucoamylase Kinetics by Flow Calorimetry

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A mathematical modeling of immobilized glucoamylase kinetics by flow calorimetry is discussed. The model is based on non-stationary diffusion equation containing a non-linear term related to kinetics of the enzymatic reaction. This paper presents the complex numerical methods (The modified Adomian decomposition method) to solve the non-linear differential equations that describe the diffusion coupled with a non-linear reaction terms. Approximate analytical expressions for substrate concentration have been derived for all values of enzyme reactions parameters.

Keywords: Flow calorimetry; Immobilized glucoamylase; Kinetic measurement; intrinsic kinetics; The modified Adomian decomposition method, Boundary value problems.

1. INTRODUCTION

Since the 1990s [1-7] there has been an important transition in the development of immobilized enzymes. Approaches used for the design of immobilized enzymes have become increasingly more rational; this is reflected in the use of more integrated and sophisticated immobilization techniques to solve problems that cannot be easily solved by previously developed single immobilization approaches. In this phase, the major focus of enzyme immobilization was on the development of robust enzymes that are not only active but also stable and selective in organic solvents. Although in the period from the 1970s to the 1980s it was recognized that many enzymes are active and stable in organic solvents under appropriate conditions, the enzymes used are usually less active or stable in organic solvents than in conventional aqueous media [8]. For this reason development of more robust
immobilized enzymes which can work under hostile conditions, especially in non-aqueous media came to the forefront of many research interests in this period [9-11]. Immobilization of enzymes on suitable support materials has resulted in their extended use in batch and continuous bioreactors. For immobilised enzymes, however, there are several factors which affect the observed kinetics that could be significantly different from the intrinsic kinetics of the free enzyme.

Immobilized biocatalysts (IMB) – enzymes are still in the interest of people working in different branches. They constitute principal parts of devices of very variable scale and application starting from microgram amounts of IMB in special analytical devices up to industrial reactors with IMB loading of hundreds of kilograms. This is valid in the stage of IMB screening and design, as for the specification of operational conditions in which they should be used. Therefore, there is always the need coming with a new IMB to find sufficiently accurate, simple and fast experimental technique of investigation of their kinetic properties.

Vladimir Stefuca et.al [12] described the principles and applications of flow calorimetry (FC) in the investigation of the IMB properties. The FC can be used practically for every enzyme-substrate system, under the condition that a sufficient reaction heat is produced and the substrate is in soluble form [13]. Wide applications of glucoamylase in starch industry research focused in the improvement of the enzyme properties by methods of enzyme screening, molecular biology and enzyme engineering. Research in this area can be facilitated by developing suitable methods for the investigation of kinetic properties of immobilized glucoamylase.

Vladimir Stefuca et.al [12] simplified this task by reducing the experiment to the initial rate measurement in combination with the FC avoiding the requirement of a more complicated chemical analysis. For the purpose of the methodology development, the enzyme was immobilized in controlled-pore glass (CPG) particles and a well defined substrate – maltodextrin (MDX) - was used. However, to the best of author’s knowledge, the steady state analytical expression of immobilized glucoamylase and effectiveness factor have not been derived. In this paper, we have obtained the analytical expression of immobilized glucoamylase and effectiveness factor for all values of parameters for steady state condition using the modified Adomian decomposition method.

2. MATHEMATICAL FORMULATION OF THE NON-LINEAR DIFFUSION PROBLEM

We assume that the glucoamylase was immobilized in porous particles. The experimental set-up used for the measurements is depicted in Fig. 1. The main part of the system is a thermostatic cell with the immobilished enzyme column. The column is operated as a small packed bed reactor. Since biocatalyst particle is spherical shape, the material balance reaction diffusion equation is given by [12]

\[
D_e \left( \frac{d^2 c_s}{dr^2} + \frac{2}{r} \frac{dc_s}{dr} \right) - v_r = 0
\]

(1)

with boundary conditions:
\[
\frac{dc_s}{dr} = 0 \text{ at } r = 0, \tag{2a}
\]
\[
c_s = c_{sb} \text{ at } r = R, \tag{2b}
\]

where \( r \) is the particle radial coordinate, \( R \) the particle radius and \( D_e \) the substrate (MDX) effective diffusion coefficient, \( c_s \) is the substrate concentration and \( c_{sb} \) is the bulk substrate concentration.

**Figure 1.** Experimental calorimetric recirculation system.

For substrate inhibition model the reaction rate, \( v_r \) is given by

\[
v_r = \frac{V_m c_s}{K_m + c_s + \frac{c_{sb}^2}{K_i}} \tag{3}
\]

where \( V_m, K_m \) and \( K_i \) are kinetic parameters. The steady state effectiveness factor is [12]

\[
v = \frac{3(1 - \varepsilon)D_e}{R\varepsilon} \left[ \frac{dc_s}{dr} \right]_{r=R} \tag{4}
\]

where \( \varepsilon \) is void fraction of IMB bed. The system governs the substrate concentration \( c_s \) when there is no competitive inhibition in the reaction. The non-linear equation is made dimensionless by defining the following parameters

\[
u = \frac{c_s}{c_{sb}}, \quad X = \frac{r}{R}, \quad k = \frac{V_m R^2}{K_m D_e}, \quad \alpha = \frac{c_{sb}}{K_m}, \quad \beta = \frac{c_{sb}^2}{K_i K_m} \tag{5}
\]
where $u(X)$ represents dimensionless concentration, $X$ is dimensionless distance. $k, \alpha$ and $\beta$ are dimensionless parameters. The equation (1) reduces to the following dimensionless form

$$\frac{d^2 u}{dX^2} + \frac{2}{X} \frac{du}{dX} - \frac{ku}{1+au + \beta u^2} = 0$$

(6)

The boundary conditions reduce to

$$\frac{du}{dX} = 0 \text{ at } X = 0$$

(7a)

$$u = 1 \text{ at } X = 1$$

(7b)

The dimensionless effective factor ($\eta$) is given by [1]

$$\eta = \frac{R^2 \Delta \nu}{3(1 - \varepsilon)C_0} \left( \frac{du}{dX} \right)_{X=1}$$

(8)

3. ANALYTICAL SOLUTION OF BOUNDARY VALUE PROBLEM USING THE MODIFIED ADOMIAN DECOMPOSITION METHOD (MADM)

The modified adomian decomposition method is an extremely simple method to solve the nonlinear differential equations. In the recent years, much attention is devoted to the application of the adomian decomposition method to the solution of various scientific models [14]. The MADM yields, without linearization, perturbation, transformation or discretisation, an analytical solution in terms of a rapidly convergent infinite power series with easily computable terms.

The decomposition method is simple and easy to use and produces reliable results with some iteration used. The results show that the rate of convergence of modified Adomian decomposition method is higher than standard Adomian decomposition method [15-19]. Furthermore, the obtained result is of high accuracy. Using this modified Adomain decomposition method (see Appendix A), the solution of the boundary value problem (Eqs. 6 - 7) is

$$u(X) = 1 - M + \frac{7NM}{60} + \left( \frac{6M - NM}{6} \right) X^2 + \frac{NM}{20} X^4$$

(9)

where $M = \frac{k}{6(1 + \alpha + \beta)}$ and $N = \frac{k(1 - \beta)}{(1 + \alpha + \beta)^2}$ for $k \leq 1$

(10)

The above expression is valid when $k$ is small ($k \leq 1$) and all possible values of parameters $\alpha$ and $\beta$. The experimental range of the numerical values of the dimensionless parameters are $k = 0.001$
to 1000, $\alpha = 0.001$ to 0.1 and $\beta = 0.001$ to 0.1. When $k$ is large ($k > 1$), the substrate concentration becomes

$$u(X) = \frac{\sinh(\sqrt{k}X)}{X \sinh(\sqrt{k})} \text{ for } k > 1$$

The effective factor using eqns. (9) and (11) becomes

$$\eta = \frac{2M(15 - N)}{15} \text{ for } k \leq 1$$

$$= \sqrt{k} (\coth \sqrt{k}) - 1 \text{ for } k > 1$$

4. NUMERICAL SIMULATION

Figure 2. Dimensionless substrate concentration $u(X)$. The concentrations were computed using Equation (11) for various values of $\alpha$ and $\beta$ and for a fixed value of $k = 1$.

An analytical solution for non-linear reaction diffusion equation in immobilized glucoamylase kinetics solved using the modified Adomian decomposition method. To show the efficiency of the present method, our problem is compared with the numerical solution (MATLAB program). We have used the function pdex1 in MATLAB software, to solve the initial-boundary value problems numerically.

The default parameters employed in Vladimir Stefuca et.al [1] and in this study are given in Table. 1. The numerical solution is compared with our analytical results in Figs 3-6 and Tables 2-4. The relative difference between the analytical dimensionless substrate concentration $u$ and numerical reference results does not exceed 0.22% for all values of the parameters. Upon comparison, it gives a
satisfactory agreement for all values of the dimensionless parameters $k$, $\alpha$ and $\beta$. The MATLAB program is also given in Appendix (C).

**Table 1.** Numerical values of the parameters used in this work. The fixed values of the dimensionless parameters are $c_{sb} = 100$ g/l, $K_m = 0.15$ gdm$^{-3}$ to 0.96 gdm$^{-3}$, $K_i = 470$ gdm$^{-3}$s$^{-1}$ to 1910gdm$^{-3}$s$^{-1}$, $V_m = 3.8$ gdm$^{-3}$s$^{-1}$ to 4.2 gdm$^{-3}$s$^{-1}$ and $D_e=9.4\times10^{-9}$dm$^2$s$^{-1}$. These are dimensionless parameters used in Vladimir Stefuca et al.[1]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Numerical values of parameter used in Vladimir Stefuca et al[1]</th>
<th>Numerical values of parameters used in this work</th>
</tr>
</thead>
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<tr>
<td>$\alpha = \frac{c_{sb}}{K_m}$</td>
<td>$10^{-6}$ to $10^{-4}$</td>
<td>(a) 0.01 (b) 0.01 (c) 0.05, 0.1</td>
</tr>
<tr>
<td>$\beta = \frac{c_{sb}^2}{K_i K_m}$</td>
<td>$10^{-8}$ to $10^{-6}$</td>
<td>(a) 0.001, 0.001, 0.001, 0.001, 0.001, 0.001</td>
</tr>
<tr>
<td>$X = \frac{r}{R}$</td>
<td>0 to 1</td>
<td>(a) 0 to 1 (b) 0 to 1 (c) 0 to 1</td>
</tr>
<tr>
<td>$k = \frac{V_m R^2}{K_m D_e}$</td>
<td>to $1000$</td>
<td>(a) 0.001, 0.001, 0.001, 0.001, 0.001, 0.001, 0.001, 0.001</td>
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</tbody>
</table>

Figure 3. Dimensionless substrate concentration $u$. The concentrations were computed using Eq. (11) for various values of the reaction/diffusion parameter $k$ and for a fixed small value of dimensionless diffusion co-efficients $\alpha = 0.001$ and $\beta = 0.001$. The key to the graph: ‘—’ represent Eq.11 for $k \leq 1$ and Eq.13 for $k > 1$ and ‘+++’ represents the simulation result.
Figure 4. Dimensionless substrate concentration $u$. The concentrations were computed using Eq. (11) for various values of the reaction/diffusion parameter $k$ and for a fixed small value of dimensionless diffusion co-efficients $\alpha = 0.01$ and $\beta = 0.01$. The key to the graph: ‘___’ represent Eq.11 for $k \leq 1$ and Eq.13 for $k > 1$ and ‘+++’ represents the simulation result.

Figure 5. Dimensionless substrate concentration $u$. The concentrations were computed using Eq. (11) for various values of the reaction/diffusion parameter $k$ and for a fixed small value of dimensionless diffusion co-efficients $\alpha = 0.05$ and $\beta = 0.05$. The key to the graph: ‘___’ represent Eq.11 for $k \leq 1$ and Eq.13 for $k > 1$ and ‘+++’ represents the simulation result.
Figure 6. Dimensionless substrate concentration $u$. The concentrations were computed using Eq. (11) for various values of the reaction/diffusion parameter $k$ and for a fixed small value of dimensionless diffusion co-efficients $\alpha = 0.1$ and $\beta = 0.1$. The key to the graph: ‘__’ represent Eq.11 for $k \leq 1$ and Eq.13 for $k > 1$ and ‘+++’ represents the simulation result.

Upon comparison, it gives a satisfactory agreement for all values of the dimensionless parameters $k, \alpha$ and $\beta$. The MATLAB program is also given in Appendix (C).
Table 3. Comparison of dimensionless concentration of analytical and numerical of $u$ for various small values of $k$ when $\alpha = 0.1, \beta = 0.1$

<table>
<thead>
<tr>
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Table 4. Comparison of dimensionless concentration of analytical and numerical of $u$ for various large values of $k$ when $\alpha = 0, \beta = 0$

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<th>Error %</th>
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5. DISCUSSION

5.1 Concentration profile

The kinetics response of calorimetric recirculation systems depends on the concentrations of glucoamylase. The concentrations of glucoamylase depends on the following three factors $k, \alpha$ and $\beta$. Thiele modulus, $k$ represents the ratio of the characteristic time of the enzymatic reaction to that of substrate diffusion. The variation in the Thiele modulus $k$ can be achieved by varying either the radius of the particle or kinetic parameters. The Thiele modulus is indicative of the competition between the diffusion and reaction in the calorimetry. When $k$ is small, the kinetics dominates and the uptake of glucoamylase in the enzyme matrix is kinetically controlled. Under these conditions, the glucoamylase concentration profile across the membrane is essentially uniform. When $k$ is large, diffusion limitations are the principal resistance.

Eq. 9 and Eq. 11 represent the analytical expressions for the dimensionless concentration of glucoamylase $u(X)$. Eq. 9 is valid for $k \leq 1$ and Eq. 11 is valid for $k > 1$. Fig. 2 presents the dimensionless substrate concentration $u(X)$. The concentrations were computed using Eq. 9 for various
values of $\alpha$ and $\beta$ and for a fixed value of $k = 1$. From Fig. 2, it is inferred that the concentration increases when the values of $\alpha$ and $\beta$ increases. In Figs. 3-6, simulation and analytical results are compared. From these figures, it is inferred that the value of the concentration $u$ increases when $k$ decreases but there is no significant difference in the concentration. When $k \leq 1$, the concentration is uniform.

5.2 Effectiveness factor

![Figure 7(a)](image1)

Figure 7(a). Dimensionless effectiveness factor $\eta$. The dimensionless effectiveness factor were computed using Eq. (14) for various values of dimensionless diffusion co-efficients $\alpha$ and $\beta$.

![Figure 7(b)](image2)

Figure 7(b). Dimensionless effectiveness factor $\eta$. The dimensionless effectiveness factor were computed using Eq. (15) for large values of dimensionless parameter $k$. 
Eqs.12 and 13 represent the analytical expressions for the dimensionless effectiveness factor $\eta$. The normalized effectiveness factor $\eta$ versus $k$ plotted in Fig. 7(a). This figure illustrates the effectiveness factor $\eta$ for $k \leq 1$ and all practical values of $\alpha$ and $\beta$. In this figure, the effectiveness factor increases when the parameters $\alpha$ and $\beta$ decreases. But there is no significant difference in the effectiveness factor for all practical values of the parameters $\alpha$ and $\beta$. Fig 7(b) illustrates the effectiveness factor $\eta$ versus $k$ for various values of $\alpha$ for $k > 1$. In this figure the effectiveness factor increases when the value of $k$ increases. From these figures (7(a) and 7(b)), we conclude that the value of $\eta$ increases when the reaction diffusion parameter $k$ increases.

6. CONCLUSIONS

We have presented a theoretical model of immobilized glucoamylase kinetics by flow calorimetry. An approximate analytical expression of substrate concentration and effectiveness factor for all possible values of the kinetic parameters are derived using the Adomian decomposition method [15-17]. The accuracy of the approximate analytical solutions of non-linear differential equations has been verified by comparison with numerical solutions. The theoretical results is very much useful to determine the reaction rate and intrinsic kinetic parameters of immobilized glucomylase.

ACKNOWLEDGEMENTS

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References

Appendix A: Basic concepts of the modified Adomian decomposition method

Consider the non-linear differential equation in the form

\[ y^{(n)} + \frac{2n}{x} y' + \frac{n(n-1)}{x^2} y = g(x) - F(x, y) \quad n \geq 0 \quad (A.1) \]

with initial condition

\[ y(0) = A, \quad y'(0) = B \]

where \( F(x, y) \) is a real function, \( g(x) \) is the given function and \( A \) and \( B \) are constants. We propose the new differential operator, as below

\[ L = x^{-n} \frac{d^2}{dx^2} (x^n y) \quad (A.2) \]

So, the problem (A.1) can be written as,

\[ L y = g(x) - F(x, y) \quad (A.3) \]

The inverse operator \( L^{-1} \) is therefore considered a two-fold integral operator, as below.

\[ L^{-1}() = x^{-n} \int_0^x \int_0^x x^n () \, dx \, dx \quad (A.4) \]

Applying \( L^{-1} \) on both sides of Eq. (A.1), we find

\[ A + Bx + L^{-1} g(x) - L^{-1} F(x, y) = L^{-1} \left( y^{(n)} + \frac{2n}{x} y' + \frac{n(n-1)}{x^2} y \right) \]

\[ = x^{-n} \int_0^x \int_0^x x^n \left( y^{(n)} + \frac{2n}{x} y' + \frac{n(n-1)}{x^2} y \right) \, dx \, dx \quad (A.5) \]

\[ = x^{-n} \int_0^x (x^n y' + nx^{n-1} y) \, dx \]

\[ = y(x) - y(0) \]

The Adomian decomposition method introduce the solution \( y(x) \) and the nonlinear function \( F(x, y) \) by infinity series.
\[ y(x) = \sum_{n=0}^{\infty} y_n(x) \]  
(A.6)

and

\[ F(x, y) = \sum_{n=0}^{\infty} A_n \]  
(A.7)

where the components \( y_n(x) \) of the solution \( y(x) \) will be determined recurrently and the Adomian polynomials coefficients \( A_n \) of \( F(x, y) \) are evaluated using the formula

\[
A_n(x) = \frac{1}{n!} \frac{d^n}{dx^n} \left[ N \left( \sum_{n=0}^{\infty} \left( \frac{d}{dx} y_n \right) \right) \right]_{x=0}
\]  
(A.8)

By substituting Eq. (A.7) and Eq. (A.8) into Eq. (A.6),

\[
\sum_{n=0}^{\infty} y_n(x) = A + Bx + L^{-1}g(x) - L^{-1} \sum_{n=0}^{\infty} A_n
\]  
(A.9)

Using modified Adomian decomposition method, the components \( y_n(x) \) can be determined as

\[
y_0(x) = A + Bx + L^{-1}g(x) \\
y_{n+1}(x) = -L^{-1}(A_n), n \geq 0
\]  
(A.10)

which gives

\[
y_0(x) = A + Bx + L^{-1}g(x) \\
y_1(x) = -L^{-1}(A_0) \\
y_2(x) = -L^{-1}(A_1) \\
y_3(x) = -L^{-1}(A_2) \\
\vdots
\]  
(A.11)

From Eq. (A.9) and Eq. (A.11), we can determine the components \( y_n(x) \), and hence the series solution of \( y(x) \) in Eq. (A.6) can be immediately obtained.

**Appendix B: Solution of non-linear Eq. (6) by using modified Adomian decomposition method**

In this appendix, we derive the general solution of nonlinear Eq. (6) by using Adomian decomposition method. We write the Eq. (6) in the operator form,

\[ L(u(X)) = kN[u(X)] \]  
(B.1)

where
\[ L = X^{-1} \frac{\partial^2}{\partial X^2} X \text{ and } N[u(X)] = \frac{u}{1 + \alpha u + \beta u^2} \]  

(B.2)

Applying the inverse operator \( L^{-1} \) on both sides of Eq. (B.1) yields

\[ u(X) = A X + B + k L^{-1} N[u(X)] \]  

(B.3)

where \( A \) and \( B \) are the constants of integration. We let,

\[ u(X) = \sum_{n=0}^{\infty} u_n(X) \]  

(B.4)

\[ N[u(X)] = \left( \frac{u}{1 + \alpha u + \beta u^2} \right) = \sum_{n=0}^{\infty} A_n \]  

(B.5)

In view of Eqs. (B.4) and (B.5), Eq. (B.3) gives

\[ \sum_{n=0}^{\infty} u_n(X) = A X + B + k L^{-1} \sum_{n=0}^{\infty} A_n \]  

(B.6)

We identify the zeroth component as

\[ u_0(X) = A X + B \]  

(B.7)

and the remaining components as the recurrence relation

\[ u_{n+1}(X) = k L^{-1} A_n \quad n \geq 0 \]  

(B.8)

where \( A_n \) are the Adomian polynomials of \( u_0, u_1, u_2, \ldots, u_n \). We can find the first few \( A_n \) as follows:

\[ A_0 = N(u_0) = \frac{k}{1 + \alpha + \beta} \]  

(B.9)

\[ A_1 = \frac{d}{d\lambda} \left[ N(u_0 + \lambda u_1) \right] = \frac{k(1 - \beta)u_1}{(1 + \alpha + \beta)^2} \]  

(B.10)

The remaining polynomials can be generated easily, and so,

\[ u_0(X) = 1 \]  

(B.11)

\[ u_1(X) = \frac{k}{6(1 + \alpha + \beta)} (X^2 - 1) \]  

(B.12)
\[ u_2(X) = 1 + \frac{7k^2(1-\beta)}{360(1+\alpha+\beta)^3} - \frac{k^2(1-\beta)}{36(1+\alpha+\beta)^3}X^2 + \frac{k^2(1-\beta)}{120(1+\alpha+\beta)^3}X^4 \quad (B.13) \]

Adding (B.11) to (B.13) we get Eq. (9) in the text.

**Appendix C: The Matlab program to find the numerical solution of Equation 6**

```matlab
function pdex4
m = 2;
x = linspace(0,1);
t = linspace(0,1000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u = sol(:,:,1);
figure
plot(x,u(end,:))
title('u(x,t)')

% --------------------------------------------------------------
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = 1.*DuDx;
r=1;
a=0.01;
b=0.1;
F = -(r*u)/((1+(u*a)+(b*u^2)));
s=F;
% --------------------------------------------------------------
function u0 = pdex4ic(x);
u0 = [1];
% --------------------------------------------------------------
function [pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
pl = 0;
ql = 1;
pr = ur-1;
qr = 0;
```

**Appendix D: Nomenclature**

- \(r\) particle radial coordinate
- \(R\) particle radius
- \(D_e\) substrate (MDX) effective diffusion coefficient \(t (=9.4 \times 10^{-9} \text{ dm}^2\text{s}^{-1})\)
- \(v_r\) reaction rate
- \(V_m, K_m,\) and \(K_i\) are kinetic parameters
- \(u(X)\) dimensionless concentration
- \(X\) dimensionless distance
- \(c_s\) substrate concentration
\( \nu \) effective factor
\( c_{sb} \) bulk substrate concentration
\( \eta \) dimensionless effective factor
\( \varepsilon \) void fraction of IMB bed
\( N, M \) dimensionless constants.

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Theoretical Analysis of Mass Transfer with Chemical Reaction Using Absorption of Carbon Dioxide into Phenyl Glycidyl Ether Solution

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ABSTRACT

Theoretical analysis corresponding to the diffusion and reaction kinetics in a chemical reaction between carbon dioxide and phenyl glycidyl ether solution is presented. Analytical expressions pertaining to the concentration of carbon dioxide (CO₂), phenyl glycidyl ether solution (PGE) and flux are obtained in terms of reaction rate constants. In this paper, a powerful analytical method, called the Adomian decomposition method (ADM) is used to obtain approximate analytical solutions for nonlinear differential equations. Furthermore, in this work the numerical simulation of the problem is also reported using Scilab/Matlab program. An agreement between analytical and numerical results is noted.

Keywords: Carbon Dioxide; Phenyl Glycidyl Ether Solution; Nonlinear Differential Equations; Adomian Decomposition Method; Boundary Value Problems

1. Introduction

Carbon dioxide is generally a useful gas that is made up of a carbon atom and two oxygen atoms. It is very important in plant photosynthesis, manufacturing carbonated soft drinks, powering pneumatic systems in robots, used in fire extinguisher, removing caffeine from coffee, etc., Carbon dioxide has the potential to provide a vast and cheap source of carbon. Turning it into useful products would also reduce its environmental impact as a greenhouse gas. Scientists have shown that ionic liquids are selective catalysts for converting carbon dioxide into synthetic intermediates called cyclic carbonates, but it is difficult to separate and recycle the liquid catalyst.

Recently, the chemical fixation of carbon dioxide has become an important research topic [1], because of the danger posed by global warming, and conversion of carbon dioxide into valuable substances is an extremely attractive solution. The reaction with oxiranes leading to five-membered cyclic carbonate (oxirane-reaction) is well-known among many examples [2,3]. These carbonates can be used as aprotic polar solvent and sources for polymer synthesis [4]. In the oxirane-reaction, high pressure (5 - 50 atm) of CO₂ has been thought to be necessary [2]. The oxirane—reactions under atmospheric pressure have been reported [4].

Many organic and inorganic compounds including ammines, phosphines, quaternary ammonium salts, and alkali metal salts are known to catalyze the oxirane-reaction [3]. The kinetics of the reaction between CO₂ and phenyl glycidyl ether (PGE) have been studied using catalyst THA-CP-MS41, The reaction rate constants were obtained using the measured absorption rate of and analyzed with the mass transfer mechanism associated with the chemical reactions.

Park et al. [5] investigated the chemical absorption of carbon dioxide and phenyl glycidyl ether solution containing the catalyst THA-CP-MS41 in a heterogeneous system. To our knowledge no analytical solutions of this model have been reported. The purpose of this communication is to derive simple approximate analytical expression for the steady-state concentrations of CO₂, PGE and flux using the Adomian decomposition method.

2. Mathematical Formulation of the Problem and Analysis

Figure 1 shows the schematic representation of the stirred-cell absorber [5]. The overall reaction between CO₂ and phenyl glycidyl ether (PGE) to form the 5—membered cyclic carbonate is as follows:

\[ \text{CO}_2 + \text{RCH(O)} = \text{CO}_2 + \text{RCH(O)} \rightarrow \text{RCO}_2 \text{HO} \tag{1} \]
Figure 1. Shows the schematic representation of the stirred-cell absorber [5]. A, B, C: Valve; D: Absorber; E: Impeller; F: Liquid bottle; G: Funnel; H: Soap film meter; I: Gas chromatography.

where $R$ is a functional group of $-\text{CH}_2\text{-O-CH}_3$. The overall reaction of Equation (1) consists of two consecutive steps: 1) a reversible reaction between PGE (B) and THA-CP-MSplex (C$_1$); 2) an reversible reaction between O$_2$ (A) to form QX and five-membered cyclic carbonate (C):

$$B + QX \leftrightarrow C_1 \quad (2)$$

$$A + C_1 \rightarrow C + QX \quad (3)$$

At steady state condition, the consecutive chemical reaction rate of CO$_2$ to form C$_1$ is given as follows:

$$r_{A,cons} = \frac{C_a S_t}{k_1 + \frac{1}{k_1 K_i C_A} + \frac{C_A}{k_3 C_A}} \quad (4)$$

where, $S_t$ is the surface area of catalyst, $C_A$ and $C_B$ are the concentration of CO$_2$ and PGE respectively. $K_i$ is the reaction equilibrium constant, $k_1$ is the forward reaction rate constant in Equation (2) and $k_3$ is the forward reaction rate constant in Equation (3). The mass balances of CO$_2$ and PGE, using film theory accompanied by the consecutive chemical reactions are given as follows [5]:

$$D_A \frac{d^2 C_A}{dz^2} = \frac{C_a S_t}{k_1 + \frac{1}{k_1 K_i C_A} + \frac{C_A}{k_3 C_A}} \quad (5)$$

$$D_B \frac{d^2 C_B}{dz^2} = \frac{C_a S_t}{k_1 + \frac{1}{k_1 K_i C_A} + \frac{C_A}{k_3 C_A}} \quad (6)$$

where $D_A$ and $D_B$ are the diffusivity of CO$_2$ and PGE respectively and $z$ is the distance. The boundary conditions are:

$$C_A = C_{AI}, \frac{dC_A}{dz} = 0 \quad \text{at} \quad z = 0 \quad (7)$$

$$C_A = C_{Al}, \frac{dC_A}{dz} = C_{Bo} \quad \text{at} \quad z = z_L$$

Equations (5), (6) and the boundary conditions (7) can be normalized by employing the following parameters:

$$a = \frac{C_a}{C_{AI}}, \quad b = \frac{C_B}{C_{Bo}}$$

$$\alpha_1 = \frac{z^2 S_t C_a K_i k_3}{D_A}, \quad \alpha_2 = \frac{z^2 S_t C_a K_i k_3}{D_B}$$

$$\beta_1 = \frac{C_a K_i k_3}{k_1}, \quad \beta_2 = \frac{C_a K_i k_3}{k_1}$$

where, $a$ is the concentration of CO$_2$, $b$ is the concentration of PGE, $\alpha_1, \alpha_2, \beta_1, \beta_2$ normalized parameters and $x$ is the dimensionless distance. Now the two nonlinear reaction/diffusion Equations (5), (6) in normalized form becomes as follows:

$$\frac{d^2 a}{dx^2} = \frac{\alpha_1 ab}{1 + \beta_1 a + \beta_2 b} \quad (8)$$

$$\frac{d^2 b}{dx^2} = \frac{\alpha_1 ab}{1 + \beta_1 a + \beta_2 b} \quad (9)$$

The above Equations (8), (9) are the system of nonlinear differential equations. While no general method of solving these nonlinear problems has been proposed, several rigorous procedure such as Adomian decomposition method [6-10], Homotopy perturbation method [11-15] and Homotopy analysis method [16-21] etc., have been analyzed. Here, Adomian decomposition method is used to solve these nonlinear differential equations. The boundary conditions becomes,

$$a = 1, \quad \frac{db}{dx} = 0 \quad \text{at} \quad x = 0 \quad (10)$$

$$a = k, \quad b = 1 \quad \text{at} \quad x = 1$$

where, $k = \frac{C_a}{C_{AI}}$. The enhancement factor of CO$_2$ defined as the ratio of the flux of CO$_2$ with chemical reaction to that without chemical reaction is as follows,

$$\beta = \left[ \frac{da}{dx} \right]_{x=0} \quad (11)$$

3. Analytical Solutions of Concentrations of CO$_2$ and PGE under Steady-State Condition Using the Adomian Decomposition Method

In this paper, the Adomian decomposition method (see Appendix A) is used to solve nonlinear differential equations. The ADM [6-10] yields, without linearization, per-
turbation or transformation, an analytical solution in terms of a rapidly convergent infinite power series with easily computable terms. The basic principle of this method is described in Appendix A and detailed derivation of dimensionless concentration of CO₂ and PGE, from the nonlinear Equations (8) and (9) are described in Appendix B. Using this method (refer Appendix B), we obtain the analytical expression corresponding to the concentrations of CO₂ and PGE as follows:

\[
a(x) = (k-1)x + 1 + \frac{\alpha_x}{2\beta_1}(x-1) - \frac{\alpha_1(1+\beta_1)}{\beta_1^2(k-1)^2} \left( \log(1+\beta_1 + \beta_1((k-1)x+1))-\log(1+\beta_1 + \beta_1k)-1 \right) \\
(1+\beta_1 + \beta_1((k-1)x+1))(1+\beta_2 + \beta_1k) \left( \log(1+\beta_2 + \beta_1k)-1 \right)
\]

\[
b(x) = 1 + \frac{\alpha_2}{2\beta_1}(x^2-1) - \frac{\alpha_1(1+\beta_1)}{\beta_1^2(k-1)^2} \left( \log(1+\beta_1 + \beta_1((k-1)x+1))-\log(1+\beta_2 + \beta_1k)-1 \right) \\
(1+\beta_1 + \beta_1((k-1)x+1))(1+\beta_2 + \beta_1k) \left( \log(1+\beta_2 + \beta_1k)-1 \right)
\]

From Equation (11), we obtain the flux as

\[
b = 1 - k - \frac{\alpha_1(1+\beta_1)}{\beta_1^2(k-1)^2} \left( \log(1+\beta_2 + \beta_1k)-1 \right)
\]

4. Numerical Simulation

The function pde2 in Scilab/Matlab software which is a function of solving the initial-boundary value problems for the two reaction/diffusion equations is used to solve Equations (8) and (9). The normalized concentrations of CO₂ and PGE are compared with simulation results in Figures 1 and 2. A satisfactory agreement is noted. The Scilab/Matlab program is also given in Appendix C. In Table 1, the simulation results compared with ADM results, the maximum error is 0.64%.

5. Results and Discussion

Equations (12) and (13) represent the new closed and simple approximate analytical expressions of the normalized concentrations of CO₂ and PGE for all values of parameters \(\alpha_1, \alpha_2, \beta_1, \beta_2, \) and \(k\). The current response is given in Equation (14). The concentration profiles of CO₂ and PGE are shown in Figures 2 and 3. The concentration of CO₂ increases when the normalized parameter \(k\) increases (refer Figure 2(a)). The concentration of CO₂ decreases when the parameters \(\beta_1\) and \(\beta_2\) decreases (refer Figures 2(b) and (c)). In Figure 3, the concentration of PGE increases when the normalized parameter \(\alpha_2\) or surface area of catalyst increases and diffusivity of PGE decreases. Equation (14) represents the normalized flux. The value of flux increases as the parameters \(\beta_1\) and \(\beta_2\) or reaction equilibrium constant increases (refer Figures 4(a) and (b)). In Figure 4(c), the value of flux decreases as the parameters \(\alpha_1\) or or surface area of catalyst increases and diffusivity of CO₂ decreases.

6. Conclusions

This paper presents a theoretical treatment of carbon dioxide and phenyl glycidyl ether solution in chemical reaction. Also, we have discussed the mathematical models of CO₂ absorption into the PGE solution. We have solved the nonlinear differential equations both analytically and numerically. The approximate analytical expressions for
Figure 2. Normalized concentration of CO$_2$ for various values of parameters is plotted using Equation (12). (a) $\alpha_1 = 0.1$, $\beta_1 = 0.5$, $\beta_2 = 0.7$; (b) $k = 0.1$, $\alpha_1 = 1$, $\beta_2 = 0.001$; (c) $k = 0.1$, $\alpha_1 = 3$, $\beta_1 = 1$. The key to the graph (stacked line) represents Equation (12) and (dotted line) represents the numerical simulation.

Figure 3. Normalized concentration of PGE for various values of parameters is plotted using Equation (13). The key to the graph (stacked line) represents the Equation (13) and (dotted line) represents the numerical simulation.
the steady state concentrations of CO₂ and PGE for all values of parameters using the Adomian decomposition method. These theoretical results are useful to evaluate the overall reaction rate constant and enhancement factor of CO₂. A satisfactory agreement with the numerical result is noted.

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REFERENCES


Appendix A

Basic Concept of the Adomian Decomposition Method (ADM)

Adomian decomposition method [22-27] depends on decomposing the nonlinear differential equation

$$F(x, y(x)) = 0$$ (A.1)

into the two components

$$L(y(x)) + N(y(x)) = 0$$ (A.2)

where \(L\) and \(N\) are the linear and the nonlinear parts of \(F\) respectively. The operator \(L\) is assumed to be an invertible operator. Solving for \(L(y(\chi))\) leads to

$$L(y(x)) = -N(y(x))$$ (A.3)

Applying the inverse operator \(L^{-1}\) on both sides of Equation (A.3) yields

$$L^{-1}y(x) = N^{-1}y(x)$$ (A.4)

where

$$L^{-1} = \frac{d^2}{dx^2}, \quad N^{-1} = \frac{\alpha_{ab}}{1 + a\beta_1 + b\beta_2}$$ (B.1)

Applying the inverse operator \(L^{-1}\) on both sides of Equation (B.1) and (B.2) yields

$$a(x) = Ax + B + L^{-1}N[a(x)]$$ (B.4)

$$b(x) = Ax + B + L^{-1}N[b(x)]$$ (B.5)

Applying the inverse operator \(L^{-1}\) on both sides of Equation (A.3) yields

$$y(x) = \varphi(x) - L^{-1}\left[\sum_{n=0}^{\infty} A_n(x) \right]$$ (A.5)

where

$$\sum_{n=0}^{\infty} y_n(x) = y(x), \quad A_n(x) = \frac{1}{n!} \left[ \frac{d^n}{dx^n} N\left(\sum_{j=0}^{\infty} \chi^j y_j(x) \right) \right]_{\chi = 0}$$ (A.6)

and

$$\sum_{n=0}^{\infty} A_n(x) = N(y(x)) \quad n \geq 0$$

Then equating the terms in the linear system of Equation (A.5) gives the recurrent relation

$$y_n = \varphi(x), \quad y_{n+1} = -L^{-1}(A_n) \quad n \geq 0$$ (A.7)

However, in practice all the terms of series in Equation (A.5) cannot be determined, and the solution is approximated by the truncated series \(\sum_{n=0}^{\infty} y_n(x)\).

Appendix B

Analytical Expression of Concentrations of CO\(_2\) and PGE Using the Adomian Decomposition Method

To solve Equations (8) and (9) using the Adomian decomposition method, we write the Equations (8) and (9) in the operator form,

$$L[a(x)] = N[a(x)]$$ (B.1)

$$L[b(x)] = N[b(x)]$$ (B.2)

where

$$L = \frac{d^2}{dx^2}, \quad N[a(x)] = \frac{\alpha_{ab}}{1 + a\beta_1 + b\beta_2}$$ (B.3)

According to the ADM, the solution \(a(x)\) and \(b(x)\) can be elegantly computed by using the recurrence relation

$$a_n(x) = Ax + B, \quad a_{n+1}(x) = L^{-1}N[a(x)] = L^{-1}A_n(x)$$ (B.6)

$$b_n(x) = Ax + B, \quad b_{n+1}(x) = L^{-1}N[b(x)] = L^{-1}B_n(x)$$ (B.7)

where \(A_n\) and \(B_n\) are the Adomian polynomials of \(a\) and \(b\) respectively. We can find the first few Adomian polynomial coefficients \(A_n\) and \(B_n\) using Equation (A.6) as follows:

$$A_n(x) = N(a_n) = \frac{\alpha_{ab} b_n}{1 + a\beta_1 + b\beta_2}$$ (B.8)

$$B_n(x) = N(b_n) = \frac{\alpha_{ab} b_n}{1 + a\beta_1 + b\beta_2}$$ (B.9)

The remaining polynomials \(A_n(x)\) and \(B_n(x)\) can be generated easily, using Equation (A.6). Applying the following boundary conditions

$$a_0(0) = 1, \quad a_1(0) = k$$

and

$$a_i(0) = 0, \quad a_i(1) = 0$$ (B.10)

for \(i \geq 1\)

$$b_0(0) = 0, \quad b_1(0) = 1$$

and

$$b_i(0) = 0, \quad b_i(1) = 0$$ (B.11)

for \(i \geq 1\)

From Equations (B.6) and (B.7) using the above conditions we obtain the following results:

$$a_n(x) = (k - 1)x + 1$$ (B.12)
Adding Equations (B.12) and (B.13), (B.14) and (B.15), we get the concentration of CO$_2$ and PGE (Equations (12) and (13)) in the text.

### Appendix C

Scilab/Matlab program for the numerical solution of the system of nonlinear Equations (8) and (9)

```matlab
function pdex4
m = 0;
x = linspace(0,1);
t=linspace(0,100000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
```

```matlab
function pdex4pde(x,t,u,DuDx)
c = [1; 1];
f = [1; 1] .* DuDx;
```

```matlab
function pdex4bc(xl,u0)
pl = [ul(1)-1;0];
ql = [0; 1];
pr = [ur(1)-0.1; ur(2)-1];
qr = [0; 0];
```

### Nomenclature

**Symbols**
- C: Concentration of CO$_2$ (M)
- C: Concentration of PGE (M)
- D: Diffusivity of CO$_2$ (m$^2$/s)
- D: Diffusivity of PGE (m$^2$/s)
- K: Reaction equilibrium constant (1/M)
- rA,cons: Reaction rate of CO$_2$ in consecutive model (M/s)
- S: Surface area of catalyst (m$^2$)
- z: Distance (m)
- zL: Film thickness (m)
- a: Normalized concentration of CO$_2$ (Dimensionless)
- b: Normalized concentration of PGE (Dimensionless)
- $\alpha$, $\alpha$, $\beta$, $\beta$, $k$: Normalized parameters (Dimensionless)
- $\beta$: Flux of CO$_2$ (Dimensionless)

**Subscripts**
- A: CO$_2$
- B: PGE
- L: Bulk solution
- o: Feed or solvent
Mathematical modelling of a biofilm: The Adomian decomposition method

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ABSTRACT

A mathematical modelling by a biofilm under steady state conditions is discussed. The nonlinear differential Equations in biofilm reaction is solved using the Adomian decomposition method. Approximate analytical expressions for substrate concentration have been derived for all values of parameters \( \delta \) and \( S_L \). These analytical results are compared with the available numerical results and are found to be in good agreement.

Keywords: Mathematical Modeling; Simulation; Adomian Decomposition Method; Initial Boundary Value Problems

1. INTRODUCTION

Microorganisms biofilms adhere to the interfaces between gas and liquid phases, liquid and solid phases, or two liquid phases [1]. Their activity can have an adverse effect, e.g., biofilms damage materials [2], and water purification technology [3]. The situation is largely similar to the case of heterogeneous reaction in a porous layer [4,5]; however, for the biofilm kinetics, there are a number of specific features. The dependence of the biochemical reaction rate on a substrate concentration is described by a saturating curve and can not be characterized by a power function [3,6]. Dueck et al. [7-9] described the mathematical modeling of evaluation of biofilm with allowance for its erosion. Recently, Minkov et al. [10] obtained the analytical expression for the substrate flux into the biofilm for a square law of microbial death rate with steady-state conditions has been reported. The purpose of this communication is to derive approximate analytical expressions for the steady-state concentration of substrate and flux into the biofilm using the Adomian decomposition method for all values of biofilm thickness and substrate concentration outside the biofilm.

2. MATHEMATICAL FORMULATION OF THE PROBLEM

It is assumed that the substrate consumption is described by the Michaelis-Menten kinetics. The Equation of which are derived on the basis of the theory of enzymatic reactions [3,5] on the particle surface of biofilm [10] is of the following form:

\[
D_f \frac{d^2 S_f}{dz^2} = q \frac{S_f}{K + S_f} X_f
\]

(1)

The boundary conditions are

\[
\begin{align*}
& z = 0, \quad \frac{dS_f}{dz} = 0 \\
& z = L_f, \quad S_f = S_i
\end{align*}
\]

(2)

(3)

The biomass balance [10].

\[
Y_f \frac{S_f}{K + S_f} X_f = bX_f^2
\]

(4)

From Eq.4, the concentration of active biomass can be expressed through the substrate concentration. Now the Eq.1 can be written in the form

\[
D_f \frac{d^2 S_f}{dz^2} = q^2 Y \left( \frac{S_f}{K + S_f} \right)^2
\]

(5)

where \( S_i \) is the substrate concentration in the biofilm, \( K \) is the Michaelis-Menten constant, \( z \) is the co-ordinate, \( L_f \) is the biofilm thickness, \( D_f \) is the diffusion coefficient.
within the biofilm, \( b \) is the Microbial death constant, \( q \) is the substrate consumption rate constant, \( S_1 \) is the substrate concentration outside the biofilm and \( Y \) is the biomass yield per unit amount of substrate consumed respectively. The non-linear ODE (Eq.5) is made dimensionless by defining the following parameters:

\[
S = \frac{S_f}{K}, x = \frac{z}{L_f}, \delta = \frac{Y q L_f}{bKD_f}, S_e = \frac{S_e}{K}
\]

(6)

The above Eq.5 reduces to the following dimensionless form:

\[
\frac{d^2 S}{dx^2} = \delta \left( \frac{S}{1+S} \right)^2
\]

(7)

\[
x = 0, \quad \frac{dS}{dx} = 0
\]

(8)

\[
x = 1, \quad S = S_e
\]

(9)

The dimensionless concentration flux into the biofilm is given by

\[
\psi(x) = \frac{1}{\sqrt{\delta}} \frac{dS}{dx}
\]

(10)

### 3. SOLUTION OF BOUNDARY VALUE PROBLEM BY THE ADOMIAN DECOMPOSITION METHOD

The Adomian’s decomposition method has been successfully applied to linear and nonlinear problems. One of its advantages is that it provides a rapid convergent series solution. However, in this method, some modifications are proposed by several authors [11-15]. By applying the Adomian’s decomposition method, a new iterative method to compute nonlinear Equations are developed. The Adomian decomposition method is an extremely simple method [11-15] to solve the non-linear differential Equations. First iteration is enough. Furthermore, the obtained result is of high accuracy. Using this Adomian decomposition method (see Appendix A and B), the solution of Eq.7 becomes:

\[
S(x) = S_e + \frac{\delta \left( \frac{S_e}{1+S_e} \right)^2}{2} (x^2 - 1)
+ \frac{\delta^2 S_e}{(1+S_e)^3} \left( \frac{x^3}{12} - \frac{x^2}{6} + \frac{5}{12} \right) + \frac{\delta^2 S_e^2}{4(1+S_e)^3} \left( \frac{x^6}{30} - \frac{x^4}{6} + \frac{x^2}{2} \right)
- \frac{\delta^2 S_e^3}{(1+S_e)^3} \left( \frac{x^9}{30} - \frac{x^6}{6} + \frac{x^3}{2} \right) + \frac{2\delta^2 S_e^2}{(1+S_e)^3} \left( \frac{x^6}{360} - \frac{x^4}{24} + \frac{5x^2}{24} \right)
+ \frac{3\delta^2 S_e^3}{4(1+S_e)^3} \left( \frac{x^9}{30} - \frac{x^6}{6} + \frac{x^3}{2} \right) - \frac{2\delta^2 S_e^2}{(1+S_e)^3} \left( \frac{x^6}{360} - \frac{x^4}{24} + \frac{5x^2}{24} \right)
+ \frac{3\delta^2 S_e^3}{360(1+S_e)^3} (-155 + 66S_e)
\]

(11)

The solution of concentration flux into the biofilm is obtained as

\[
\psi = \frac{1}{\sqrt{\delta}} \delta \left( \frac{S_e}{1+S_e} \right)^2 - \frac{2}{15} \frac{\delta^2 S_e^3}{(1+S_e)^6} + \frac{8}{15} \frac{\delta^2 S_e^3}{(1+S_e)^6} + \frac{8}{15} \frac{\delta^2 S_e^3}{(1+S_e)^6}
\]

(12)

### 4. NUMERICAL SIMULATION

The non-linear differentials Eq.7 is also solved by numerical methods. The function bvp4c in Matlab software which is a function of solving two-point boundary value problems (BVPs) for ordinary differential equations is used to solve this equation. The Matlab program is also given in Appendix C. Its numerical solution is compared with Adomian decomposition method in Tables 1 and 2 and Figures 1-3 for various value of parameters.

### 5. RESULTS AND DISCUSSION

An approximate analytical expression of concentrations \( S \) is given in the Eq.11. The concentration \( S(x) \) is plotted in Figures 1-3 for various values of \( \delta \) and \( S_e \). From these figures, it is evident that the value of concentration gradually increases as the dimensionless biofilm thickness \( \delta \) decreases. Figures 4 to 5 represent the concentration \( S(x) \) for various values of \( S_e \). From these figures it is observed that, the value of the concentration increases when \( S_e \) increases. When \( \delta \leq 1 \), the

---

**Figure 1.** Normalized concentration profile \( S(x) \) as a function of dimensionless distance \( x \). The concentrations were computed using Eq.11 for various values of the \( \delta \) when \( S_e = 0.05 \), (—) denotes Eq.11 and (…) denotes the numerical simulation.
**Table 1.** Comparison of normalized steady-state concentration $S(x)$ with simulation results for various values of $x$ and for some fixed values of $S_L = 0.5$.

<table>
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<th>Simulation</th>
<th>Error %</th>
<th>$S(x)$ (when $\delta = 1$)</th>
<th>Simulation</th>
<th>Error %</th>
<th>$S(x)$ (when $\delta = 3$)</th>
<th>Simulation</th>
<th>Error %</th>
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<td>0.4815</td>
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<td>0.5000</td>
<td>0.5000</td>
<td>0.0000</td>
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</tbody>
</table>

Average 0.0309

**Table 2.** Comparison of normalized steady-state concentration $S(x)$ with simulation results for various values of $x$ and for some fixed values of $S_L = 5$.

<table>
<thead>
<tr>
<th>$x$</th>
<th>$S(x)$ (when $\delta = 1$)</th>
<th>Simulation</th>
<th>Error %</th>
<th>$S(x)$ (when $\delta = 5$)</th>
<th>Simulation</th>
<th>Error %</th>
<th>$S(x)$ (when $\delta = 10$)</th>
<th>Simulation</th>
<th>Error %</th>
</tr>
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<td>4.6500</td>
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<td>3.4520</td>
<td>3.4500</td>
<td>0.0579</td>
<td>2.3330</td>
<td>2.4000</td>
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<tr>
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<td>4.6700</td>
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<td>3.5100</td>
<td>0.0854</td>
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<td>2.4450</td>
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</tr>
<tr>
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<td>3.6950</td>
<td>0.1081</td>
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</tr>
</tbody>
</table>

Average 0.0571

**Figure 2.** Normalized concentration profile $S(x)$ as a function of dimensionless distance $x$. The concentrations were computed using Eq.11 for various values of the $\delta$ when $S_L = 0.5$, (−) denotes Eq.11 and (…) denotes the numerical simulation.

**Figure 3.** Normalized concentration profile $S(x)$ as a function of dimensionless distance $x$. The concentrations were computed using Eq.11 for various values of the $\delta$ when $S_L = 5$, (−) denotes Eq.11 and (…) denotes the numerical simulation.
Figure 4. Normalized concentration profile \( S(x) \) as a function of dimensionless distance \( x \). The concentrations were computed using Eq.11 for various values of the \( S_L \) when \( \delta = 10 \). \((-\)) denotes Eq.11 and \((\ldots)\) denotes the numerical simulation.

Figure 5. Normalized concentration profile \( S(x) \) as a function of dimensionless distance \( x \). The concentrations were computed using Eq.11 for various values of the \( S_L \) when \( \delta = 1 \). \((-\)) denotes Eq.11 and \((\ldots)\) denotes the numerical simulation.

concentration is uniform and the uniform value depends upon \( S_L \). It is clear that as dimensionless substrate concentration outside the biofilm \( S_L \) increases when the value of dimensionless concentration \( S(x) \) increases. Eq.12 represents the normalized concentration flux into the biofilm. Figure 6 represents flux versus \( S_L \) (dimensionless substrate concentration outside the biofilm). From this figure, it is inferred that the value of concentration flux decreases when the thickness of biofilm increases. Figure 7 represents flux versus \( \log \delta \). From this figure, it is inferred that, the value of the flux is high when \( S_L \) is large and then decreases slowly and reaches the minimum value when \( \log \delta = 10^2 \).

6. CONCLUSION

This paper reports a mathematical treatment for analyzing biofilm for a square law of microbial death rate. In this paper, we have evaluated a theoretical model for an investigation of the dynamic behavior of substrate consumption by a biofilm. The approximate analytical expressions for the steady state substrate concentrations for all values of biochemical parameters (\( \delta \) and \( S_L \)) were obtained using Adomian decomposition method. Further-
more, an analytical expression corresponding to the steady state flux response is also presented. A satisfactory agreement with the existing results is noted. This theoretical result is useful to further develop the model involving the balance of production of active biomass and biofilm erosion.

7. ACKNOWLEDGEMENTS

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REFERENCES


APPENDIX A

Basic Concept of the Adomian Decomposition Method (ADM)

Adomian decomposition method \[9-13\] depends on the non-linear differential Equation

\[ F(x, y(x)) = 0 \]  

(A.1)

into the two components

\[ L(y(x)) + N(y(x)) = 0 \]  

(A.2)

where \( L \) and \( N \) are the linear and non-linear parts of \( F \) respectively. The operator \( L \) is assumed to be an invertible operator. Solving for \( L(y) \) leads to

\[ L(y) = -N(y) \]  

(A.3)

Applying the inverse operator \( L \) on both sides of Eq. A.3 yields

\[ y = -L(N(y)) + \varphi(x) \]  

(A.4)

where \( \varphi(x) \) is the constant of integration which satisfies the condition \( L(\varphi) = 0 \). Now assuming that the solution \( y \) can be represented as infinite series of the form

\[ y = \sum_{n=0}^{\infty} y_n \]  

(A.5)

Furthermore, suppose that the non-linear term \( N(y) \) can be written as infinite series in terms of the Adomian polynomials \( A_n \) of the form

\[ N(y) = \sum_{n=0}^{\infty} A_n \]  

(A.6)

where the Adomian polynomials \( A_n \) of \( N(y) \) are evaluated using the formula:

\[ A_n(x) = \frac{1}{n!} \frac{d^n}{dx^n} N\left( \sum_{k=0}^{\infty} \lambda^k y_k \right) \bigg|_{\lambda=0} \]  

(A.7)

Then substituting Eqs.A.5 and A.6 in Eq.A.4 gives

\[ \sum_{n=0}^{\infty} y_n = \varphi(x) - L^{-1}\left( \sum_{n=0}^{\infty} A_n \right) \]  

(A.8)

Then equating the terms in the linear system of Eq. A.8 gives the recurrent relation

\[ y_0 = \varphi(x), \ y_{n+1} = -L^{-1}(A_n), \quad n \geq 0 \]  

(A.9)

However, in practice all the terms of series in Eq.A.7 cannot be determined, and the solution is approximated by the truncated series \( \sum_{n=0}^{\infty} y_n \). This method has been proven to be very efficient in solving various types of non-linear boundary and initial value problems.

APPENDIX B

Analytical Solutions of Concentrations of Substrate Using ADM

In this appendix, we derive the general solution of nonlinear Eq.11 by using Adomian decomposition method. We write the Eq.11 in the operator form,

\[ L(S) = \delta\left( \frac{S}{1+S} \right)^2 \]  

(B.1)

where \( L = x^{-1} \frac{d^2}{dx^2} x \) and \( N(S) = \left( \frac{S}{1+S} \right)^2 \). Applying the inverse operator \( L^{-1} \) on both sides of Eq.B.1 yields

\[ S(x) = Ax + B + \delta L^{-1}\left( \frac{S}{1+S} \right)^2 \]  

(B.2)

where \( A \) and \( B \) are the constants of integration. We let,

\[ S(x) = \sum_{n=0}^{\infty} S_n(x) \]  

(B.3)

\[ N\left[ S(x) \right] = \sum_{n=0}^{\infty} A_n \]  

(B.4)

In view of Eqs.B.2-B.4, gives

\[ \sum_{n=0}^{\infty} S_n(x) = Ax + B + \delta L^{-1}\sum_{n=0}^{\infty} A_n \]  

(B.5)

We identify the zeroth component as

\[ S_0(x) = Ax + B \]  

(B.6)

and the remaining components as the recurrence relation

\[ S_{n+1}(x) = \delta L^{-1} A_n, \quad n \geq 0 \]  

(B.7)

where \( A_n \) are the Adomian polynomials of \( S_1, S_2, \ldots, S_n \). We can find the first few \( A_n \) as follows:

\[ A_0 = N(S_0) = \left( \frac{S_L}{1+S_L} \right)^2 \]  

(B.8)

\[ A_1 = \frac{d}{d\lambda} \left[ N(S_0 + \lambda S_1) \right] = \delta \left( \lambda^2 - 1 \right) S_1^3 \]  

(B.9)

\[ \left( 1+S_L \right)^3 \]
\[ A_2 = \frac{d^2}{dx^2} \left[ N \left( S_0 + \lambda S + \lambda^2 S_i \right) \right] \]
\[ = \frac{3S_i}{4(1 + S_i)} \left( x^2 - 1 \right) - \frac{\delta^2 S_i}{(1 + S_i)} \left( x^2 - 1 \right)^2 \]
\[ + \frac{2\delta^2 S_i}{(1 + S_i)} \left( \frac{x^6}{30} - \frac{x^4}{6} + \frac{5x^2}{24} \right) \]
\[ + \frac{3\delta^2 S_i}{(1 + S_i)} \left( \frac{x^6}{30} - \frac{x^4}{6} + \frac{x^2}{2} \right) \]
\[ + \frac{\delta^2 S_i}{360(1 + S_i)} \left( -155 + 66S_i \right) \]  
(E.10)

The remaining polynomials can be generated easily, and so,
\[ S_0 = S_i \]  
(E.11)
\[ S_1(x) = \frac{\delta}{2} \left( \frac{S_i}{1 + S_i} \right)^2 \left( x^2 - 1 \right) \]  
(E.12)
\[ S_2(x) = \frac{3S_i}{(1 + S_i)} \left( \frac{x^6}{30} - \frac{x^4}{6} + \frac{x^2}{2} \right) \]  
(E.13)
\[ S_3(x) = \frac{3\delta^2 S_i}{(1 + S_i)} \left( \frac{x^6}{30} - \frac{x^4}{6} + \frac{x^2}{2} \right) \]
\[ + \frac{2\delta^2 S_i}{(1 + S_i)} \left( \frac{x^6}{30} - \frac{x^4}{6} + \frac{5x^2}{24} \right) \]
\[ + \frac{3\delta^2 S_i}{(1 + S_i)} \left( \frac{x^6}{30} - \frac{x^4}{6} + \frac{x^2}{2} \right) \]
\[ + \frac{\delta^2 S_i}{360(1 + S_i)} \left( -155 + 66S_i \right) \]  
(E.14)

Adding (E.11) to (E.14) we get Eq.11 in the text.

**APPENDIX C**

Scilab/Matlab Program to Find the Numerical Solution of Eqs.7-9

```matlab
function pdex4
m = 0;
end
```

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