



ANALYTICAL SOLUTION OF STEADY STATE SUBSTRATE CONCENTRATION OF AN IMMOBILIZED ENZYME KINETICS BY ADOMIAN DECOMPOSITION METHOD (ADM)

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Abstract

The nonlinear dynamical system modeling the immobilized enzyme kinetics with Michaelis-Menten mechanism for an irreversible reaction without external mass transfer resistance is considered. Adomian decomposition method (ADM) is used to obtain the approximate solution of the governing nonlinear differential equation, which consists in determining the series solution convergent to the exact solution or enabling to build the approximate solution of the problem. The method allows determining the solution in form of the continuous function, which is significant for the analysis of the steady state dimensionless substrate concentration with dimensionless distance on the different support materials.

1. Introduction

Immobilization of enzymes on suitable support materials has resulted in their extended use in batch and continuous bio-reactors due their significant advantage like re-utilization of enzymes and purification of enzymes from the source. Also it increases the quality of the enzymatic activities. The immobilized enzymes have been used extensively as bio sensors in the form of analytical tool in both online/off-line sensors. Further, immobilized enzymes

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have found way in medical or therapeutic applications also. Thus immobilized enzyme solutions are of great interest in many biological and engineering applications whose reactions are described by the steady state, nonlinear diffusion equations. Exact analytical solutions of the nonlinear equations are difficult to obtain in many cases. Hence numerical or approximate solutions help us to understand the phenomena of the nonlinear differential equations. Recently, many authors paid attention on the various numerical methods such as Adomain decomposition method, Legendre wavelet method. The homotopy perturbation method (HPM) is a combination of the traditional perturbation method and homotopy in topology which eliminates the limitation of the small parameter assumed in the perturbation methods. HPM is a parameter free method, whose suitable choice provides us a simple way to adjust and control the convergence region of solution series, which leads to fast convergence [7]. HPM has been widely used to obtain analytical or approximate solution of linear and nonlinear differential equations. Recently, HPM has been used to study the solution of system of nonlinear equations like Ebola epidemic model [3], Diabetes [1], Dengu Model with Maturation Delay [4]. HPM has also been used to find the solution of boundary value problems [2]. Laplace transform (LT) has wide applications in solving the nonlinear ordinary and partial differential equations. The combination of Homotopy Perturbation Method (HPM) and the Laplace transform (LT), in order to obtain highly accurate solutions for these equations was reported [5]. The approximate solution of oxygen diffusion problem, a reversible reaction, in a spherical cell including nonlinear Michaelis Menten uptake kinetics was obtained by Laplace transform homotopy perturbation method (LT-HPM) [6]. To best our knowledge, Laplace transform homotopy perturbation method (LT-HPM) has not been used to obtain the approximate solution of the nonlinear dynamical system modeling the immobilized enzyme kinetics with Michalis-Menten mechanism for an irreversible reaction without external mass transfer resistance. We investigate the effects of the dimensionless substrate concentration with the dimensionless distance on the slab, cylindrical and spherical pellets. The reveals that the steady state substrate concentration for an immobilized enzyme kinetics of an irreversible reaction on different support material exhibit rich dynamics.

2. Mathematical Formulation

Kinetic modeling for immobilized enzymes: The following assumptions are made in the development of the kinetic model for immobilized enzymes:

(i) The kinetics of the free enzyme is described by the Michaelis Menten equation for irreversible reactions.

(ii) The enzyme is uniformly distributed over the support material.

(iii) The partition effect between the support and bulk fluid phase is neglected.

(iv) Temperature and effective diffusivity are constant within the support.

(v) Steady-state conditions are developed.

(vi) Enzyme deactivation is neglected.

The above assumptions are employed to develop the governing differential equations for irreversible reactions as follows. The Michaelis-Menten equation for irreversible reactions is given by:

$$v = \frac{V_m S}{K_m + S}, \quad (1)$$

where v is the reaction rate, V_m is the maximum reaction rate, K_m is the Michaelis constant, and S is the substrate concentration [10]. The following differential equation and associated boundary conditions express the dimensionless substrate concentration, Y , in the pellet

$$\frac{d^2 Y}{dx^2} + \frac{g-1}{x} \frac{dY}{dx} = \phi^2 \frac{Y}{1+bY} \quad (2)$$

with Y boundary conditions

$$x = 0, \frac{dY}{dx} = 0; \quad x = 1, Y = 1, \quad (3)$$

where Y represents the dimensionless substrate concentration, x represents the dimensionless distance to the center or the surface of symmetry of the pellet, b is the dimensionless parameter in irreversible reaction for bulk fluid phase and g is the pellet shape factor for slab, cylindrical and spherical

respectively. The dimensionless parameters are defined as follows:

$$Y = \frac{S}{S_b}, \quad x = \frac{X}{R}, \quad b = \frac{S_b}{K_m}, \quad \phi \sqrt{\frac{RV_m}{K_m D_e}} \quad (\text{Thiele modulus}). \quad (4)$$

Here, S represent the irreversible substrate concentration inside the pellet, S_b is the irreversible substrate concentration in the bulk fluid phase, X represent the distance to the center, R is half thickness of the pellet, K_m is the irreversible reaction Michaelis constant, V_m irreversible maximum reaction rate, D_e is the effective diffusivity of the substrate in the pellet.

3. Analytical Expressions of Concentration of an Immobilized Enzyme Kinetics using Adomian Decomposition Method

In the recent years, much attention is devoted to the application of the Adomian decomposition method to the solution of various scientific models [16-20]. The ADM yields, without linearization, perturbation, transformation or discrimination, an analytical solution in terms of a rapidly convergent infinite power series with easily computable terms. In this paper, Adomian decomposition method (see Appendix A) is used to solve non-linear differential equation. The analytical expressions of concentration of immobilized enzyme kinetics, (see Appendix B) are obtained as follows:

$$Y(X) = 1 + \frac{\phi^2}{(1+b)} \left(\frac{X^2}{4} - \frac{1}{4} \right) + \frac{\phi^4}{(1+b)^3} \left(\frac{X^4}{64} - \frac{X^2}{16} + \frac{3}{64} \right) \quad (5)$$

4. Discussion and Numerical Simulation

In order to investigate the accuracy of the ADM solution with a finite number of terms, the system of differential equations were solved numerically. The substrate concentration Y versus the dimensionless radial distance x for the irreversible reactions without external mass transfer is for the various values of the Thiele modulus ϕ and b .

In Figures 1-2, we notice that when dimensionless parameter increases the substrate concentration is also increases and when the Thiele modulus for thickness of the pellet increases, the substrate concentration with the catalyst

decreases. From the Figure we infer that the decrease in substrate concentration implies the increase in the end product when increases which exhibit rich dynamics as desired. To show the efficiency of the present method, our results are analytical results graphically. The analytical solution of concentrations in dimensionless substrate concentration in Figures (1) to (2). A satisfactory agreement is noted.

6. Conclusion

Approximate analytical solutions to the non-linear reaction equations are presented using Adomian decomposition method. A simple, straight forward and a new method of estimating the concentrations of substrate, enzyme-substrate complex and free enzyme are derived. The pertinent analytical solutions for the substrate, substrate-enzyme complex and free enzyme are discussed in terms of dimensionless parameters ϕ and b .

Appendix A: Basic concept of the Adomian decomposition method (ADM)

Adomian decomposition method depends on the non-linear differential equation

$$F(x, y(x)) = 0. \quad (\text{A.1})$$

Into the two components

$$L(y(x)) + N(y(x)) = 0, \quad (\text{A.2})$$

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

$$L(y) = -N(y). \quad (\text{A.3})$$

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

$$y = -L(N(y)) + \varphi(x), \quad (\text{A.4})$$

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

$$y = \sum_{n=0}^{\infty} y_n. \quad (\text{A.5})$$

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

$$N(y) = \sum_{n=0}^{\infty} A_n. \quad (\text{A.6})$$

Where the Adomian polynomials A_n of $N(y)$ are evaluated using the formula:

$$A_n(x) = \frac{1}{n!} \frac{d^n}{d\lambda^n} N\left(\sum_{n=0}^{\infty} \lambda^n y_n\right) \Big|_{\lambda=0}. \quad (\text{A.7})$$

Then substituting Equations (A.5) and (A.6) in Equation (A.4) gives

$$\sum_{n=0}^{\infty} y_n = \varphi(x) - L^{-1}\left(\sum_{n=0}^{\infty} A_n\right). \quad (\text{A.8})$$

Then equating the terms in the linear system of Equation (A.8) gives the recurrent relation

$$y_0 = \varphi(x) y_{n+1} = -L^{-1}(A_n) n \geq 0. \quad (\text{A.9})$$

However, in practice all the terms of series in Equation (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 solution of non-linear reactions Equation (2) using the Adomian decomposition method

In this Appendix we derive the general solution of non linear Equation (2) by using Adomian decomposition method. We write the equations (2) in the operator form as

$$L(Y(X)) = \phi^2 \left(\frac{Y}{1 + bY} \right), \quad (\text{C.1})$$

where $L = X^{-1} \frac{d^2}{dx^2} X$

$$N(Y(X)) = \phi^2 \left(\frac{Y}{1 + bY} \right). \quad (\text{C.2})$$

Applying the inverse operator $L^{-1}(\cdot) = \int_0^X \int_0^X X^{-1} X(\cdot) dr dr$ on both sides of the equation (C.1) and (C.2) yield.

$$Y(X) = AX + B + \phi^2 L^{-1} \left(\frac{Y}{1 + bY} \right), \quad (\text{C.3})$$

Where A and B are constants of integration. Let

$$Y(X) = \sum_{n=0}^{\infty} Y_n(X) \quad (\text{C.4})$$

$$N[Y(X)] = \sum_{n=0}^{\infty} A_n. \quad (\text{C.5})$$

In view of Equation (C.4) and (C.5) gives

$$\sum_{n=0}^{\infty} Y(X) = AX + B + \phi^2 L^{-1}(A_n) \quad (\text{C.6})$$

we identify the zeroth component as

$$Y(X) = AX + B \quad (\text{C.7})$$

and the remaining components as the recurrence relation

$$Y_{n+1}(X) = \phi^2 L^{-1}(A_n), \quad n \geq 0 \quad (\text{C.8})$$

$$A_0 = N(Y_0) = \frac{\phi^2}{1 + b} \quad (\text{C.9})$$

$$A_1 = \frac{d}{d\lambda} N(Y_0 + \lambda Y_1) = \frac{\phi^3}{(1 + b)^3} \left(\frac{X^2}{4} - \frac{1}{4} \right). \quad (\text{C.10})$$

The remaining polynomials can be generated easily, and so

$$Y_0(X) = 1 \quad (\text{C.11})$$

$$Y_1(X) = \frac{\phi^2}{(1+b)} \left(\frac{X^2}{4} - \frac{1}{4} \right) \quad (\text{C.12})$$

$$Y_2(X) = \frac{\phi^4}{(1+b)^3} \left(\frac{X^4}{64} - \frac{X^2}{16} + 3 \right). \quad (\text{C.13})$$

Adding (C.11) to (C.13) we get the Eqn. (C.14). In the text

$$Y(X) = 1 + \frac{\phi^2}{(1+b)} \left(\frac{X^2}{4} - \frac{1}{4} \right) + \frac{\phi^4}{(1+b)^3} \left(\frac{X^4}{64} - \frac{X^2}{16} + \frac{3}{64} \right). \quad (\text{C.14})$$

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