

Analytical Solution of Steady State Substrate Concentration of an Immobilized Enzyme Kinetics by Laplace Transform Homotopy Perturbation Method

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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. Laplace transform homotopy perturbation method 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 built the approximate solution of the problem. Numerical solutions are obtained and the results are discussed graphically. The method allows to determine 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.

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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 has been used extensively as bio sensors in the form of analytical tool in both online/off-line

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sensors. Further, immobilized enzymes 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 [9]. 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], Dengue Model with Maturation Delay [4]. HPM has also been used to find the solution of boundary value problems [2, 8]. 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 Michaelis-Menten mechanism for an irreversible reaction without external mass transfer resistance.

In this paper, the mathematical model has been formulated in section 2. In section 3, the approximate solution of the model is obtained by Laplace Transform Homotopy Perturbation Method. In section 4, numerical simulations are obtained. We investigate the effects of the dimensionless substrate concentration with the dimensionless distance on the slab, cylindrical and spherical pellets. The analysis and simulations 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:

$$\nu = \frac{V_m S}{K_m + S}$$

where ν 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

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

with boundary conditions

$$x=0, \frac{dY}{dx} = 0; \quad x=1, Y=1 \quad (2)$$

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:

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

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. Laplace transform homotopy perturbation method

In this section, we find the approximate solution of the following equation by Laplace transform homotopy perturbation method. Consider the equation

$$\frac{d^2 Y}{dx^2} + \frac{g-1}{x} \frac{dY}{dx} = \phi^2 \frac{Y}{1+bY} \quad (3)$$

It can be rewritten as

$$x \frac{d^2 Y}{dx^2} + bxY \frac{d^2 Y}{dx^2} + (g-1) \frac{dY}{dx} + (g-1)bY \frac{dY}{dx} - \phi^2 xY = 0 \quad (4)$$

By the homotopy technique let us construct the homotopy $y(x, p) : \Omega \times [0, 1] \rightarrow \mathcal{R}$ as

$$H(y, p) = (1 - p) \left[x \frac{d^2 y}{dx^2} - x \frac{d^2 y_0}{dx^2} \right] + p \left[x \frac{d^2 y}{dx^2} + bxy \frac{d^2 y}{dx^2} + (g - 1) \frac{dy}{dx} + (g - 1)by \frac{dy}{dx} - \phi^2 xy \right] = 0, p \in [0, 1]$$

or

$$H(y, p) = x \frac{d^2 y}{dx^2} - x \frac{d^2 y_0}{dx^2} - p \left[x \frac{d^2 y_0}{dx^2} + bxy \frac{d^2 y}{dx^2} + (g - 1) \frac{dy}{dx} + (g - 1)by \frac{dy}{dx} - \phi^2 xy \right],$$

(5)

where $p \in [0, 1]$ is an embedding parameter. The changing process of p from zero to unity is just that of $y(x, p)$ from $y_0(x)$ to $Y(x)$. In topology, this is called homotopy. According to the HPM, we can first use the embedding parameter p as a small parameter, and assume that the solution of (3) can be written as a power series in p :

$$y(x) = \sum_{n=0}^{\infty} p^n v_n(x) \quad (6)$$

and choose

$$v_0(x) = \frac{Ax^2}{2} \quad (7)$$

as the first approximation for the solution of (3) that satisfies the boundary condition $\frac{dy(0)}{dx} = 0$. Applying Laplace transform

$$\begin{aligned} \mathcal{L} \left(x \frac{d^2 y}{dx^2} \right) &= \mathcal{L} \left(x \frac{d^2 y_0}{dx^2} - p \left[x \frac{d^2 y_0}{dx^2} + bxy \frac{d^2 y}{dx^2} + (g - 1) \frac{dy}{dx} + (g - 1)by \frac{dy}{dx} - \phi^2 xy \right] \right) \\ -\frac{d}{ds} \left(s^2 \mathcal{L}(y) - sy(0) - y'(0) \right) &= \mathcal{L} \left(x \frac{d^2 y_0}{dx^2} - p \left[x \frac{d^2 y_0}{dx^2} + bxy \frac{d^2 y}{dx^2} + (g - 1) \frac{dy}{dx} + (g - 1)by \frac{dy}{dx} - \phi^2 xy \right] \right) \\ -\frac{d}{ds} \left(s^2 \mathcal{L}(y) - sA \right) &= \mathcal{L} \left(x \frac{d^2 y_0}{dx^2} - p \left[x \frac{d^2 y_0}{dx^2} + bxy \frac{d^2 y}{dx^2} + (g - 1) \frac{dy}{dx} + (g - 1)by \frac{dy}{dx} - \phi^2 xy \right] \right) \end{aligned} \quad (8)$$

where $y(0) = A$, where A is a constant to be determined.

$$y = \mathcal{L}^{-1} \left\{ \frac{A}{s} - \frac{1}{s^2} \int \mathcal{L} \left(x \frac{d^2 y_0}{dx^2} - p \left[x \frac{d^2 y_0}{dx^2} + bxy \frac{d^2 y}{dx^2} + (g-1) \frac{dy}{dx} + (g-1)by \frac{dy}{dx} - \phi^2 xy \right] \right) ds \right\}. \tag{9}$$

Substituting (6) and (7) in (9), we get

$$\begin{aligned} \sum_{n=0}^{\infty} p^n v_n(x) = \mathcal{L}^{-1} \left\{ \frac{A}{s} - \frac{1}{s^2} \int \mathcal{L} \left(Ax - p \left[Ax + bx \sum_{n=0}^{\infty} p^n v_n(x) \sum_{n=0}^{\infty} p^n v_n''(x) \right. \right. \right. \\ \left. \left. \left. + (g-1) \sum_{n=0}^{\infty} p^n v_n'(x) + (g-1)b \sum_{n=0}^{\infty} p^n v_n(x) \sum_{n=0}^{\infty} p^n v_n'(x) \right. \right. \right. \\ \left. \left. \left. - \phi^2 x \sum_{n=0}^{\infty} p^n v_n(x) \right] \right) ds \right\} \end{aligned} \tag{10}$$

Equating the coefficients of p , with the same power leads to

$$\begin{aligned} p^0 : v_0 &= \mathcal{L}^{-1} \left[\frac{A}{s} - \frac{1}{s^2} \int \mathcal{L}(Ax) ds \right] \\ p^1 : v_1 &= \mathcal{L}^{-1} \left[- \int \mathcal{L} \left(Ax + xbv_0v_0'' + (g-1)v_0' + (g-1)v_0v_0' - \phi^2 xv_0 \right) ds \right] \\ p^2 : v_2 &= \mathcal{L}^{-1} \left[- \int \mathcal{L} \left(xb(v_0v_1'' + v_1v_0'') + (g-1)v_1' + (g-1)(v_0v_1' + v_1v_0') \right. \right. \\ &\quad \left. \left. - \phi^2 xv_1 \right) ds \right] \\ p^3 : v_3 &= \mathcal{L}^{-1} \left[- \int \mathcal{L} \left(xb(v_0v_2'' + v_1v_1'' + v_2v_0'') + (g-1)v_2' + (g-1)(v_0v_2' + v_1v_1' \right. \right. \\ &\quad \left. \left. + v_2v_0') - \phi^2 xv_2 \right) ds \right] \end{aligned}$$

and so on. Solving the above equations we get the solution of (3) as

$$Y(x) = \lim_{p \rightarrow 1} y(x) = v_0 + v_1 + v_2 + v_3 + \dots \tag{11}$$

4. Numerical results

Solving the above equations for A we obtain $A = 32.34$. The substrate concentration y versus the dimensionless radial distance x for the irreversible reactions without external mass transfer is plotted for the various values of the Thiele modulus ϕ and b for the slab, cylindrical and spherical pellet shapes.

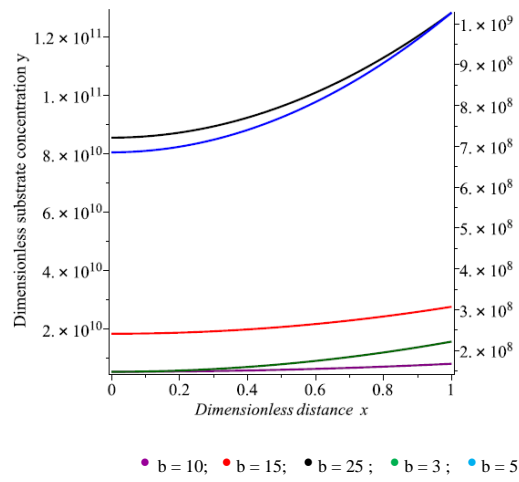


Figure 1. In the slab pellet for various values of b and for fixed value of Thiele modulus $\phi = 1$.

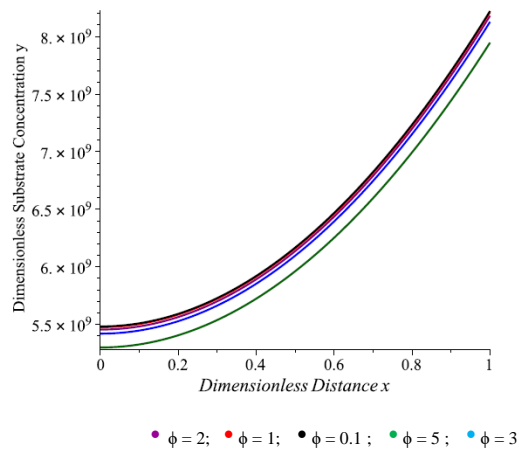


Figure 2. In the slab pellet for various values of Thiele modulus ϕ and for a fixed value of $b = 10$.

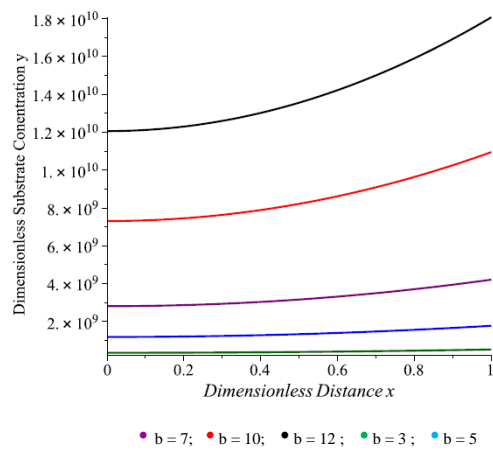


Figure 3. In the cylindrical pellet for various values of b and for fixed value of Thiele modulus $\phi = 1$.

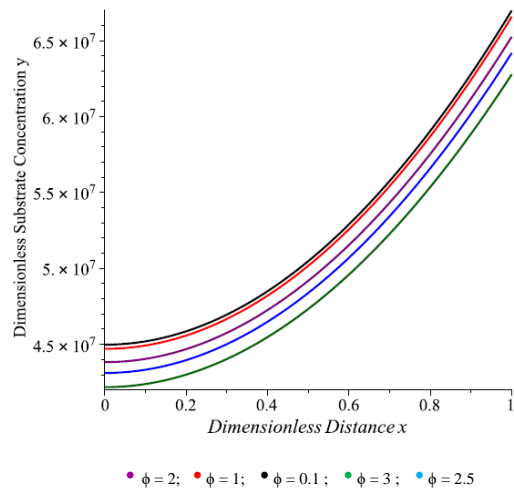


Figure 4. : In the cylindrical pellet for various values of Thiele modulus ϕ and for a fixed value of $b = 1$.

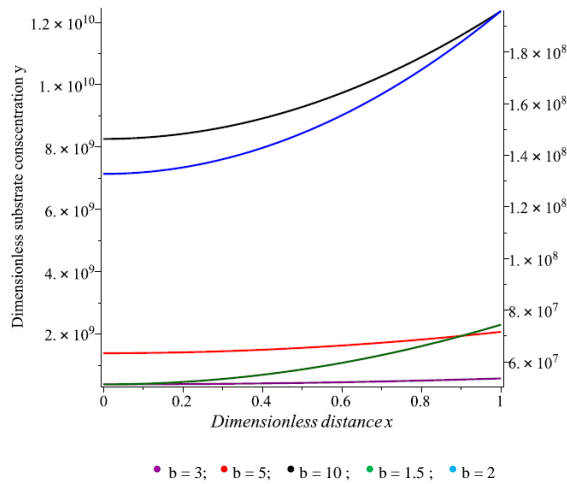


Figure 5. In the spherical pellet for various values of b and for fixed value of Thiele modulus $\phi = 10$.

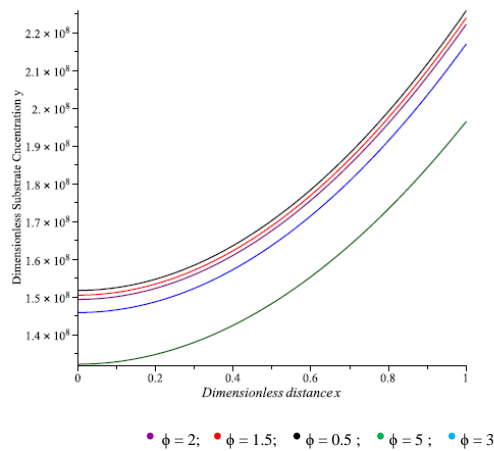


Figure 6. In the spherical pellet for various values of Thiele modulus ϕ and for a fixed value of $b = 1$.

In all the three cases, from the Figures 1-6, 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 exhibits rich dynamics as desired.

5. Conclusion

Laplace transform homotopy perturbation method is used to obtain the approximate solution of the nonlinear dynamical system modeling the immobilized enzyme kinetics with Michaelis-Menten mechanism for an irreversible reaction without external mass transfer resistance. Numerical solutions were obtained and the results discussed graphically, enable us to conclude the efficiency of the solution obtained which is much ideal. Laplace transform homotopy perturbation method is more reliable and require less computation costs and provides best results which could be utilized by the industry.

References

- [1] A. I. Enagi, M. Bawa and A. M. Sani, Mathematical Study of Diabetes and its Complication Using the Homotopy Perturbation Method, *Int. J. Math. Comput. Sci.* **12** (2017) 43-63.
- [2] M. A. Asadi, F. Salehi and M. M. Hosseini, Modified Homotopy Perturbation Method for nonlinear system of second-order BVPs, *Journal of Computer Science & Computational Mathematics*, **2** (2012) 23-28.
- [3] B. Ebenezer, A. Khan, M. A. Khan and S. Islam, Analytical Solution of the Ebola Epidemic Model by Homotopy Perturbation Method, *J. Appl. Environ. Biol. Sci.* **6** (2016) 41-49.
- [4] G. Devipriya, Analytical Solution of Dengue Model with Maturation Delay by Homotopy Perturbation Method, *Asia Matematika*, **1** (2017) 49-60.
- [5] Filobello-Nino et al, Nonlinearities distribution Laplace transform-homotopy perturbation method, SpringerPlus, doi: 10.1186/2193-1801-3-594.
- [6] Filobello-Nino et al, Extension of Laplace transform homotopy perturbation method to solve nonlinear differential equations with variable coefficients defined with Robin boundary conditions, *Neural Comput. & Applic.*, doi: 10.1007/s00521-015-2080-z.
- [7] J. H. He, Homotopy perturbation method: A new nonlinear analytical technique, *Appl. Math. Comput.* **135** (2003) 73-79.
- [8] K. P. T. V. Preethi, R. Poovazhaki and L. Rajendran, New Approach of Homotopy Perturbation Method for Solving the Equations in Enzyme Biochemical Systems, *Applied and Computational Mathematics*, **6** (2017) 161-166.
- [9] M. Salai Mathi Selvi et al, Two reliable computational methods pertaining to steady state substrate concentration of an immobilized enzyme system, *Alexandria Eng. J.*, doi: 10.1016/j.aej.2017.09.012.
- [10] F. Shiraishi, Substrate concentration dependence of the apparent maximum reaction rate and Michaelis-Menten constant in immobilized enzyme reactions, *Int. Chem. Eng.* **32** (1992) 140-147.