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Non-Linear Reaction Diffusion Equation with Michaelis-Menten Kinetics and Adomian Decomposition Method

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Abstract The mathematical model of reaction diffusion problem with Michaelis-Menten kinetics in a solid of planar and spherical shape is discussed. A simple series solution for the substrate concentration is obtained as a function of the Thiele modulus, modified Sherwood number, and the Michaelis constant. Here the Adomian decomposition method (ADM) is used to find the analytical expressions for the concentration of substrate and effectiveness factor. The numerical simulation of non-linear equations was carried out using the Matlab program. A comparison of the analytical approximation and numerical simulation is also presented. A good agreement between analytical and numerical results is observed.

Keywords Mathematical Modeling, Non-Linear Diffusion-Reaction Equation, Michaelis-Menten Kinetics, The Adomian Decomposition Method

1. Introduction

The modern theory of the nonlinear processing is an important field of today science. The nonlinear system and coherent structures represent an interdisciplinary area with many nonlinear applications in physics (nonlinear optics, nonlinear electric circuits, hydrodynamics, plasmas and states of solid), general relativity, chemistry (chemical reactions), biology (atmosphere and oceans, animal dispersal), random media and modern telecommunications. A great variety of phenomena in physics, chemistry or biology can be described by nonlinear PDEs and particularly by reaction-diffusion equations. For these reasons, the theory of the analytical solutions of the reaction-diffusion equations is considered. The general form of nonlinear parabolic reaction diffusion equation

$$\frac{\partial u(x,t)}{\partial t} = D\Delta^2 u(x,t) + f(u(x,t)) \tag{1}$$

describes density/concentration of substrate fluctuations in a material undergoing reaction-diffusion. A reaction-diffusion equation comprises a reaction term and a diffusion term. Δ^2 denotes the Laplace operator. So the first term on the right hand side describes the diffusion, including D as diffusion coefficient. The second term, $f(u)$ is a smooth function $f: R \to R$ and describes the processes with really "change" the present u, i.e. something happens to it (birth, death, chemical reaction), not just diffuse in the space. It is also possible, that the reaction term depends not only u but also on the first derivative of u. It appears in population dynamics, combustion theory and chemical kinetics. Reaction-diffusion equations are closely connected to the large deviation problems for diffusion processes.

Many problems in theoretical and experimental biology involve the solution of the steady-state reaction diffusion equation with nonlinear chemical kinetics. Such problems arise in the formulation of substrate and product material balances for enzymes immobilized within particles [1, 2], in the description of substrate transport into microbial cells [3-5], in membrane transport, in the transfer of oxygen to respiring tissue [6, 7] and in the analysis of any artificial kidney system [8]. For such cases, the problem is often well poised as a two-point nonlinear boundary –value problem because of the saturation, Michaelis-Menten, or Monod expression used to describe consumption of the substrate.

The Michaelis-Menten kinetics [9] is the one of the simplest and best-known model for the non-linear reaction diffusion process. It takes the form of an equation relating reaction velocity to substrate concentration for a system where the substrate S binds reversibly to an enzyme E to form an enzyme-substrate complex ES, which then reacts irreversibly to generate a product P and regenerate to free

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enzyme E. This system can be represented schematically as follows:

$$E+S \underset{k_{off}}{\overset{k_{on}}{\leftrightarrow}} ES \xrightarrow{k_{cat}} E+P \tag{2}$$

For the above described scheme, k_{on} is the bimolecular association rate constant of enzyme-substrate binding; k_{off} is the unimolecular rate constant of the ES complex dissociating to regenerate free enzyme and substrate; and k_{cat} is the unimolecular rate constant of the ES complex dissociating to give the free enzyme and product P. The Michaelis-Menten equation for this system is:

$$v=\frac{d[P]}{dt}=\frac{V_{\max}[S]}{K_M+[S]} \tag{3}$$

Here, $V_{\max}$ represents the maximum velocity achieved by the system, at maximum (saturating) substrate concentrations. K_M (The Michaelis constant; sometimes represented as K_S instead) is the substrate concentration at which the reaction velocity is 50% of the $V_{\max}$. $[S]$ is the concentration of the substrate S. The Michaelis-Menten equation has been used to predict the rate of product formation in enzymatic reactions for more than a century. Reuvei et al. [10] mathematically analyzed the effect of enzyme-substrate unbinding on enzymatic reactions at the single - molecule level.

Tosaka et al. [11] analyzed mathematical model for oxygen diffusion in a spherical cell with Michaelis-Menten oxygen uptake kinetics by means of an integral equation method. Maalmi et al. [12] analyzed steady-state reactant diffusion followed by uptake at a small active site on a larger macromolecule or cell by Michaelis-Menten kinetics. Marchant et al. [13] described the cubic-autocatalysis with Michaelis-Menten kinetics in a one-dimensional reaction-diffusion cell. Indira et al. [14] discussed mathematical model based on catechol polyphenol oxidase as a prototype electro enzymatic system. Bucolo et al. [15] analyzed substrate removal from the extravascular compartment by Michaelis-Menten saturation type kinetics with negligible diffusion in the axial and instantaneous diffusion in the transverse directions. Do et al. [16] used the approximate analytical technique employing a finite integral transform to solve the reaction diffusion problem with Michaelis-Menten kinetics in a solid of general shape.

Chapwanya and Lubuma [17] have presented the basic SIR epidemiological model with the Michaelis-Menten formulation of the contact rate. Bucolo et al. [15] analyzed the steady-state solution of the equations governing the substrate exchange between vascular and extravascular compartments separated by a membrane with finite, symmetrical substrate permeability. Napper et al. [19] discussed the Michaelis-Menten kinetics model of oxygen transport to heart tissue. A method for obtaining good approximate solutions to nonlinear diffusion-reaction boundary value problems based on the maximum principle are presented in [20]. Rajendran et al. [21] discussed mediated bioelectrocatalysis in very useful to build bioreactors, biofuel cells and biosensors. The purpose of this work is to obtain a simple closed approximate expression of concentration of substrate using the Adomian decomposition method for all values of Thiele modulus h, dimensionless Michaelis constant α_1 and modified Sherwood number S_h.

2. Mathematical Formulation of the Problem

The problem of an enzymatic reaction occurring isothermally within a porous support particle will be considered. The shape of the particle is assumed to possess a sufficient symmetry to permit the composition at any point in space as a function of only one spatial variable (eg. slab and spherical enzyme support). The non-dimensional material balance of substrate species inside the support can be written as follows:

$$\frac{1}{x^s}\frac{d}{dx}\left(x^s\frac{dA}{dx}\right)-\frac{2h^2A}{\alpha_1+A}=0 \tag{4}$$

where

$$h=\left(V_m/2DS_0\right)^{1/2}L,\quad A=S/S_0,\quad \alpha_1=K_m/S_0 \tag{5}$$

The exponent s characterizes the shape of the immobilized catalyst with s =0, 2 for slab, sphere respectively. The boundary conditions applicable to Eqn. (4) are

$$x=0,\quad \frac{dA}{dx}=0 \text{ (symmetry condition),} \qquad 6)$$

$$x=1,\quad \frac{dA}{dx}=S_h(1-A) \tag{7}$$

Where $S_h=(k_mL/D)$ is a modified Sherwood number and k_m is a mass-transfer coefficient. The equation (4) can be written for slab and spherical enzyme support as follows:

Case (1): Planar particle ($s=0$)

In this case the Eqn. (4) was reduces to the following dimensionless form:

$$\frac{d^2A}{dx^2}-\frac{2h^2A}{\alpha_1+A}=0 \tag{8}$$

Case (2): Spherical particle ($s=2$)

In this case the Eqn. (4) was reduces to the following dimensionless form:

$$\left(\frac{d^2A}{dx^2}\right)+\frac{2}{x}\frac{dA}{dx}-\frac{2h^2A}{\alpha_1+A}=0 \tag{9}$$

Eqn. (6) and Eqn. (7) are the boundary conditions for the Eqns. (8) and (9). The Effectiveness factor is given by

$$Ef=\frac{(1+\alpha_1)}{2h^2}\left[\frac{dA}{dx}\right]_{X=1} \tag{10}$$

3. Analytical Expression of Substrate Concentration Using the Adomian Decomposition Method (ADM)

In this paper, the Adomian decomposition method is used to solve nonlinear differential equations (8) and (9). The ADM [21-25] yields without linearization, perturbation or transformation, an analytical solution in terms of a rapidly convergent infinite power series with easily computable terms. The technique is based on a decomposition of a solution of a nonlinear operator equation in a series of functions. Each term of the series is obtained from a polynomial generated from an expansion of an analytic function in a power series. The Adomian technique is very simple in an abstract formulation, but the difficulty arises in calculating the polynomials and in proving the convergence of the series of functions. Convergence of the Adomian method when applied to some classes of ordinary and partial differential equations is discussed by many authors. For example, Abbaoui and Cherrault [26, 27] had proved the convergence of the Adomian method for differential and operator equation. The basic concept of the Adomian decomposition method is given in Appendix A. The analytical expression of concentration (Appendix B) of the substrate for planar enzyme support is as follows:

$$A(x)=1+l(h)+m(h)x^2-2\frac{m(h)\alpha_1}{(\alpha_1+1)}\left[\frac{3l(h)}{2}+\frac{5m(h)}{12}-\frac{l(h)x^2}{2}-\frac{m(h)x^4}{12}\right] \tag{11}$$

For spherical enzyme support, the concentration of substrate become as follows:

$$A(x)=1+\frac{1}{3}\left[l(h)+m(h)\right]-2\frac{m(h)\alpha_1}{S_h(\alpha_1+1)}\left[\frac{l(h)}{9}+\frac{m(h)}{15}+\frac{S_hl(h)}{18}+\frac{S_hm(h)}{60}+\frac{S_hl(h)x^2}{18}+\frac{S_hm(h)x^4}{60}\right] \tag{12}$$

where

$$l(h)=-\left[\frac{h^2}{\alpha_1+1}+\frac{2h^2}{S_h(\alpha_1+1)}\right] \text{ and } m(h)=\frac{h^2}{\alpha_1+1} \tag{13}$$

4. Discussion

Eqn. (11) represents the new analytical expression of concentration of substrate A for the planar enzyme support. Concentration of substrate depends upon the parameter Thiele modulus h, dimensionless Michaelis constant α_1, and modified Sherwood number S_h. The Thiele modulus describes the relationship between diffusion and reaction rate in porous catalyst pellets with no mass transfer limitations. This value is generally used in determining the effectiveness factor for catalyst pellets. The Thiele modulus is represented by the symbols h as

$$h=\left(\frac{V_mL^2}{2DS_0}\right)^{1/2}=\frac{\text{diffusion time}}{\text{reaction time}} \tag{14}$$

The Sherwood number S_h (also called the mass transfer Nusselt number) is a dimensionless number used in mass-transfer operation. It represents the ratio of convective to diffusive mass transport, and is named in honor of Thomas Kilgore Sherwood. It is defined as follows:

$$S_h=\frac{k_mL}{D}=\frac{\text{convective mass transfer coefficient}}{\text{Diffusive mass transfer coefficient}} \tag{15}$$

where L is a characteristic length (m), D is the mass diffusivity (m^2s^{-1}), k_m is the mass transfer coefficient (ms^{-1}). Using dimensional analysis, it can also be further defined as a function of the Reynolds and Schmidt numbers $S_h=f(\mathrm{Re},Sc)$. Figures (1.a)-(1.c) represent the dimensionless concentration of substrate A versus dimensional position X for various values of Thiele modulus h, Michaelis-Menten constant α_1 and Sherwood number S_h. From the figure (1.a), it is evident that the concentration of the substrate increases when h decreases. Also, the concentration is maximum at $X=1$. From the figures (1.b) and (1.c), it is inferred that the concentration of the substrate increases when α_1 and S_h increases.

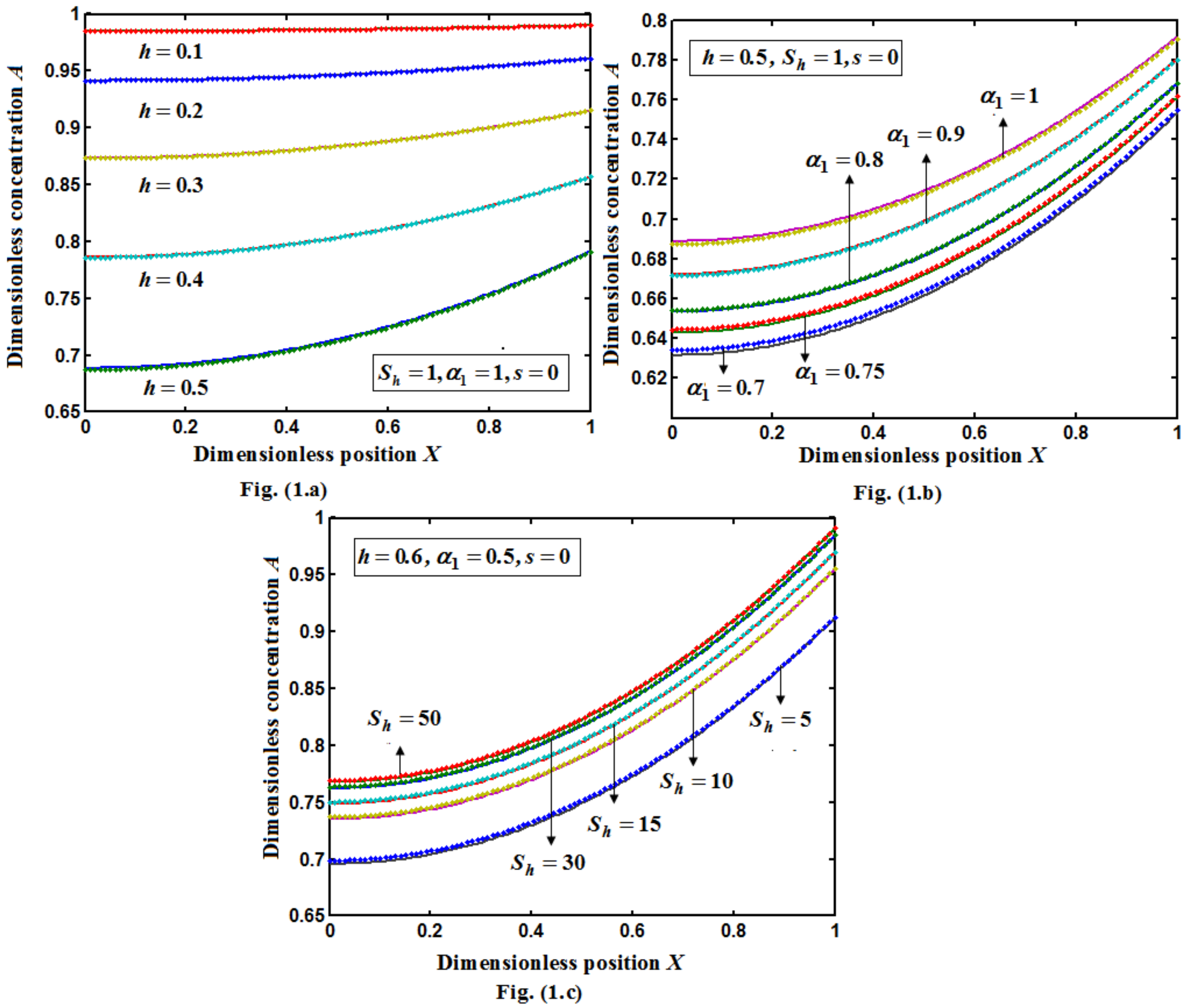

Figure 1. The influence of (a) Thiele modulus h, (b) dimensionless Michaelis constant α_1, (c) modified Sherwood number S_h on the concentration profile of the substrate A obtained in this work (equation (11)) and from the simulation result. Solid lines represent the analytical solution whereas the dotted lines in the numerical solution

Eqn. (12) represents the new analytical expression of concentration of substrate A for spherical enzyme support. Figures (2.a)-(2.c) represent the dimensionless concentration of substrate A versus dimensional position X for various values of Thiele modulus h, Michaelis-Menten constant α_1 and Sherwood number S_h. From the figure (2.a), it is obvious that the concentration of the substrate increases when h decreases. From the figures (2.b) and (2.c), it is evident that the concentration of the substrate increases when Michaelis-Menten constant α_1 and Sherwood number S_h increases. The concentration of substrate attains the maximum value when

$$x=\sqrt{\frac{-3}{m(h)}\left[l(h)+\frac{\alpha_1+1}{\alpha_1}\right]} \text{ and } x=\sqrt[3]{\frac{-5l(h)}{3m(h)}} \quad (16)$$

for planar and spherical enzyme support respectively. Figures (3) and (4) represent the normalized three dimensions substrate concentration profiles A versus(a) Thiele modulus h, (b) dimensionless Michaelis constant α_1, (c) modified Sherwood number S_h calculated using equations (11) and (12) for slab and spherical geometry respectively. All the results discussed above are confirmed in this three dimensional figures.

The concept of effectiveness factor is an important one in heterogeneous catalysis and solid fuel. The effectiveness factor is widely used to account for the interaction between pore diffusion and reactions on pore walls in porous catalytic pellets and solid fuel particles. The effectiveness factor is defined as the ratio of the reaction rate actually observed in the reaction rate calculated if the surface reactant concentration persisted throughout the interior of the particle, that is, no reactant concentration gradient within the particle. The reaction rate in a particle can therefore be conveniently expressed by its rate under surface conditions multiplied by the effectiveness factor. Also, it is evident that the Effectiveness factor Ef for various values of h, α_1 and S_h is plotted in figures (5) to (7). From the figure (5), it is inferred that the Effectiveness factor Ef decreases when modified Sherwood number S_h decreases for various values of α_1. From the figure (6), it is evident that the Effectiveness factor Ef decreases for certain value and then increases when modified Sherwood number S_h decreases for various values of h. From the figure (7. a), it is obvious that the Effectiveness factor Ef decreases when dimensionless Michaelis constant α_1 decreases. From the figure (7. b), it is evident that the Effectiveness factor Ef decreases for certain value and then increases when the Thiele modulus h decreases.

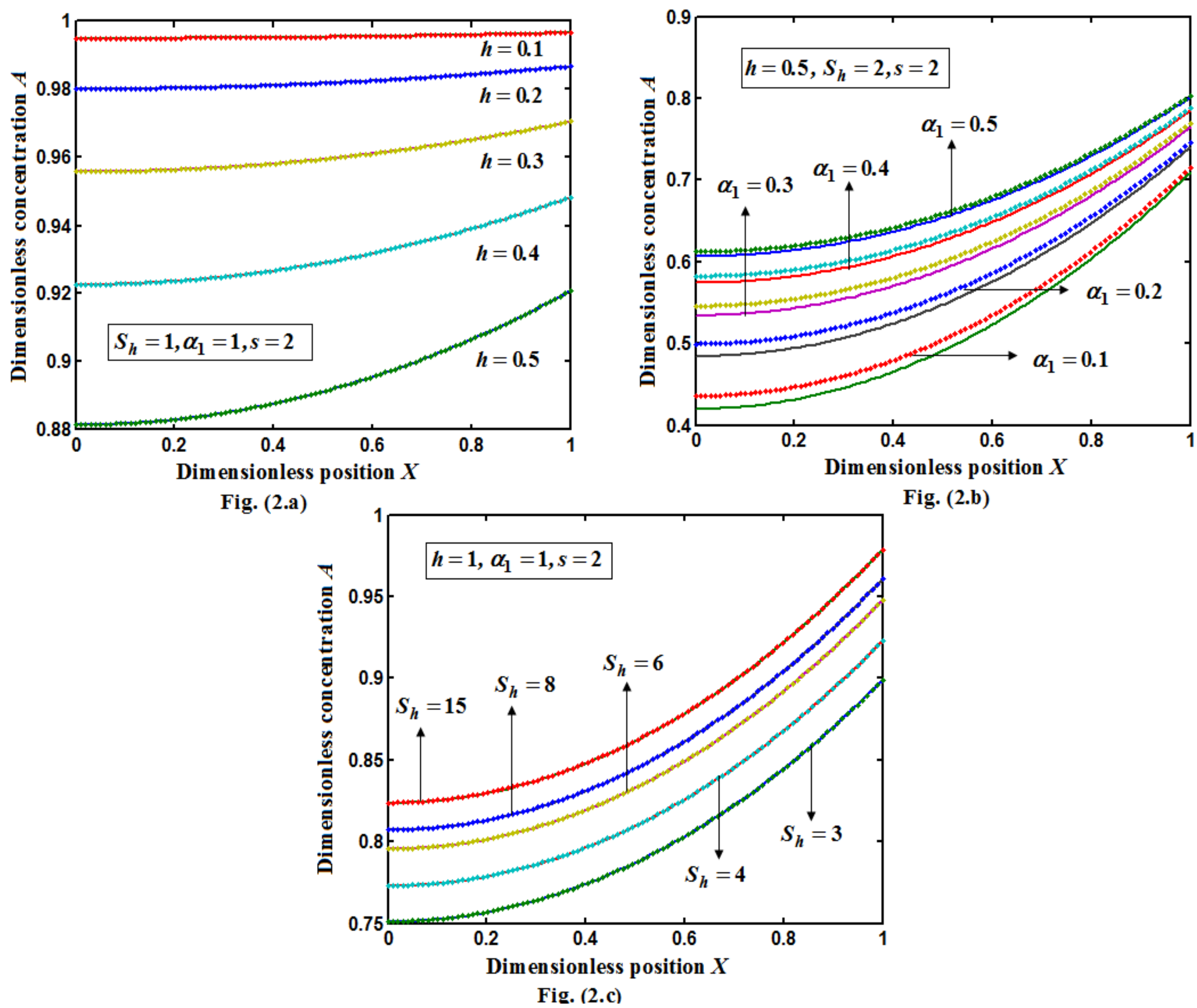

Figure 2. The influence of (a) Thiele modulus h, (b) dimensionless Michaelis constant α_1, (c) modified Sherwood number S_h on the concentration profile of substrate A obtained in this work (equation (12)) and from the simulation result. Solid lines represent the analytical solution whereas the dotted lines in the numerical solution

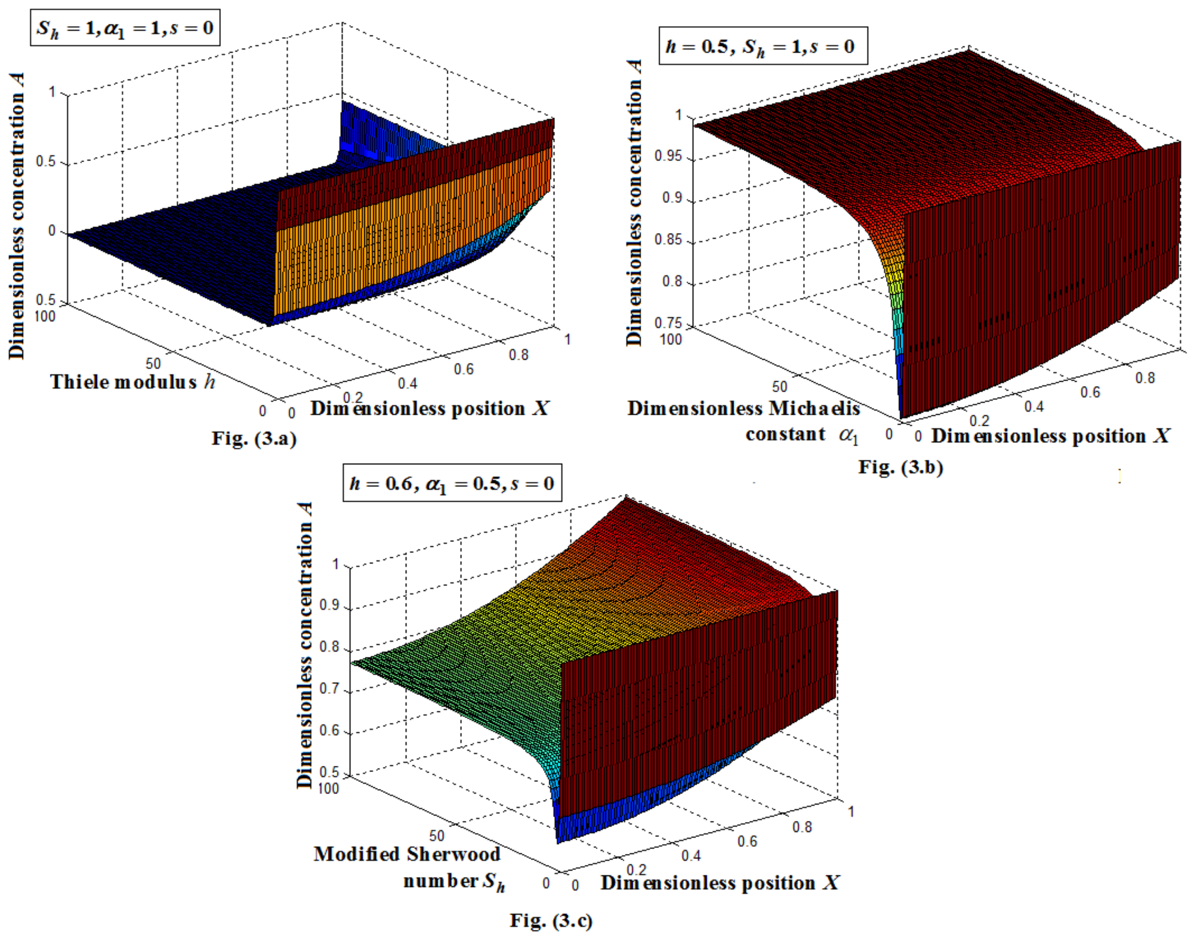

Figure 3. The normalized three dimensionless substrate concentration profiles A versus (a) Thiele modulus h, (b) dimensionless Michaelis constant α_1, (c) modified Sherwood number S_h calculated using equation (11) for slab geometry

5. Conclusions

An approximate analytical solution of the non-linear differential equation that arises from consideration of diffusion and reaction with Michaelis-Menten kinetics have been derived. Our analytical results are compared with the numerical results for various values of the Thiele modulus, the Michaelis constant and Sherwood number. Satisfactory agreement is noted. This method can be used to solve some nonlinear problems in physical and chemical sciences for various complex boundary conditions.

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Appendix A

Basic concepts of the Adomian decomposition method

The Adomian decomposition method consists of decomposing the nonlinear differential equation

$$F[x, y(x)] = 0 \tag{A.1}$$

into two components

$$L[y(x)] + N[y(x)] = 0 \tag{A.2}$$

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

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

Applying the inverse operator to both sides of Eqn. (A.3) yields

$$y = -L^{-1}(N(y)) + \phi(x), \tag{A.4}$$

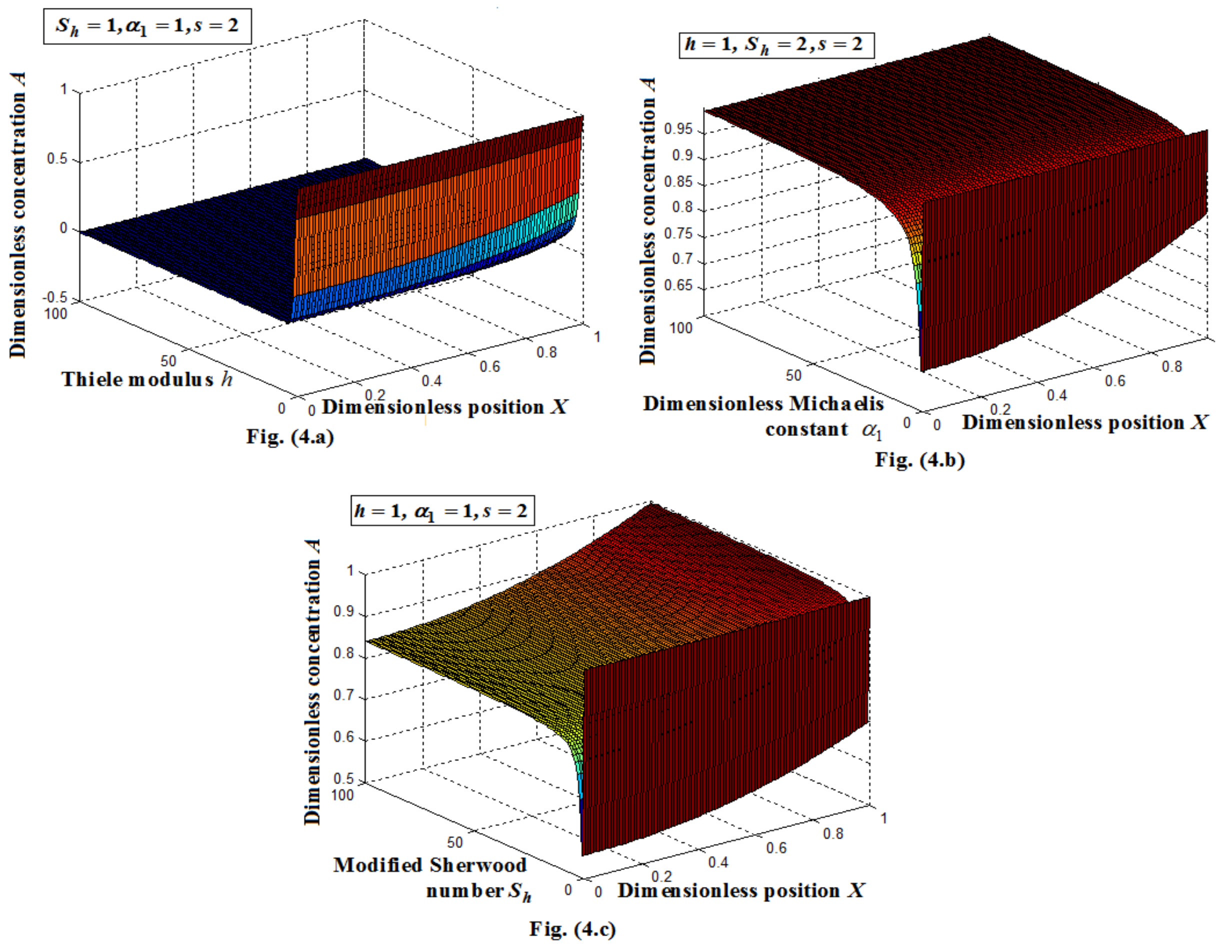

Figure 4. The normalized three dimensionless substrate concentration profiles A versus (a) Thiele modulus h, (b) dimensionless Michaelis constant α_1, (c) modified Sherwood number S_h calculated using equation (12) for spherical geometry

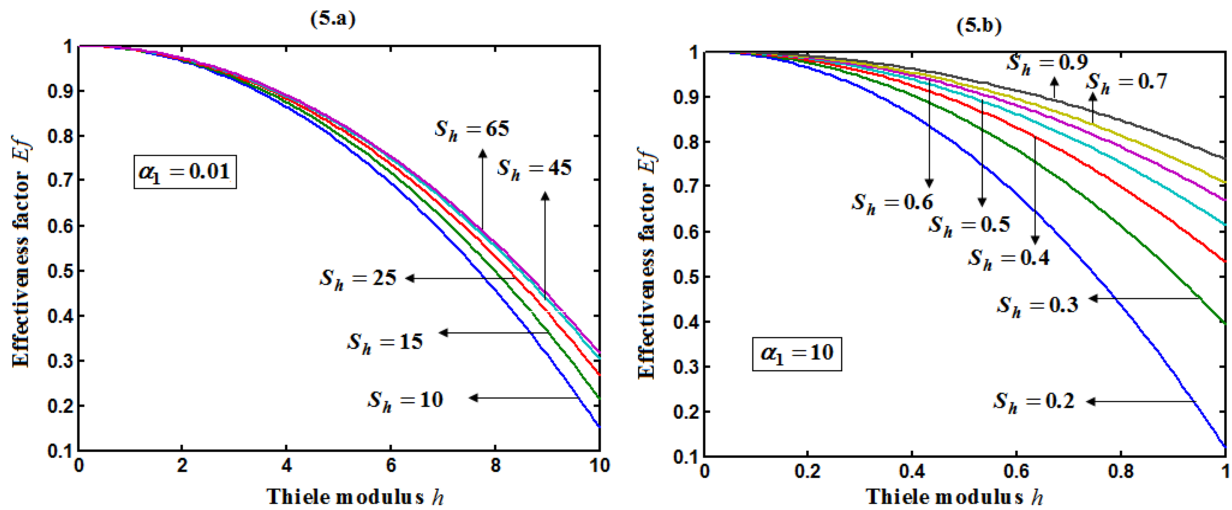

Figure 5. Dimensionless effectiveness factor Ef versus Thiele modulus h for various values of S_h and for the fixed value of (a) $\alpha_1 = 0.1$ and (b) $\alpha_1 = 10$.

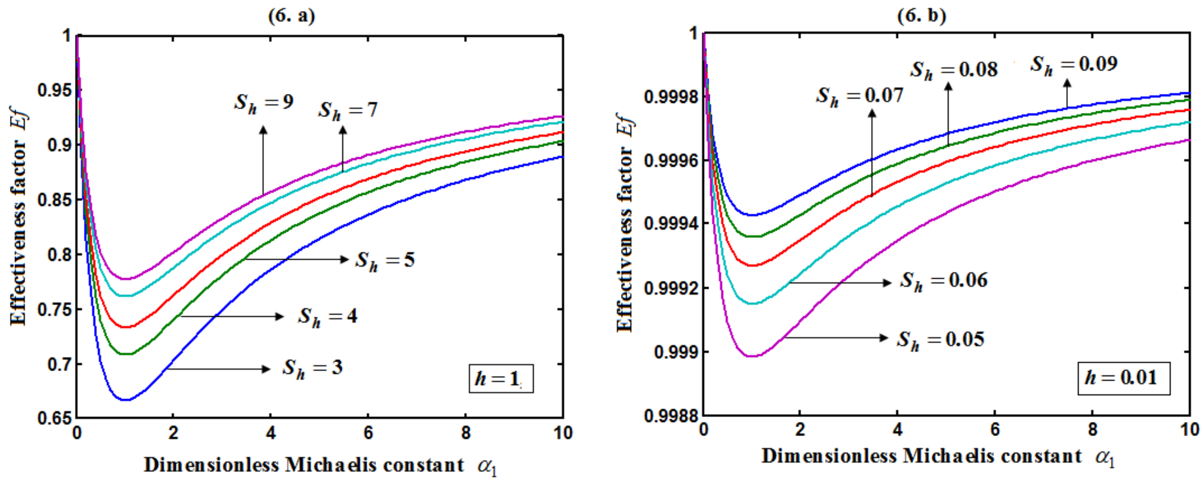

Figure 6. Dimensionless effectiveness factor Ef versus dimensionless Michaelis constant α_1 for various values of S_h and for the fixed value of (a) $h = 1$ and (b) $h = 0.01$.

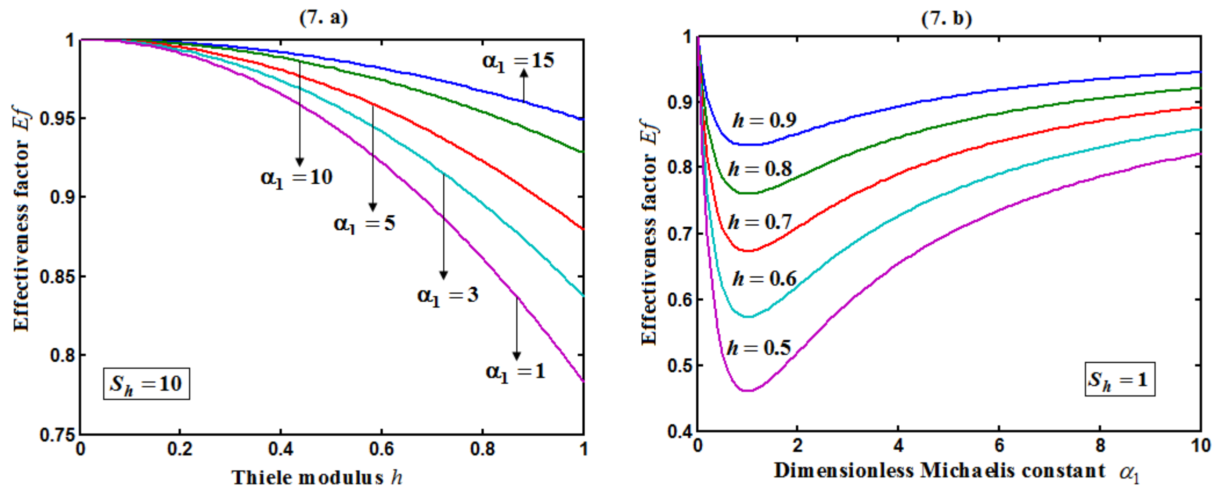

Figure 7. Dimensionless effectiveness factor Ef versus dimensionless (a) Thiele modulus h, (b) Michaelis constant α_1 for various values of α_1 and h respectively

where $\phi(x)$ is the function that satisfies the condition $L(\phi) = 0$. Now suppose that the solution y can be represented as an infinite series of the form

$$y = \sum_{n=0}^{\infty} y_n \tag{A.5}$$

Furthermore, suppose that the nonlinear term $N(y)$ can be written as infinite series in terms of the Adomain polynomials A_n of the form

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

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

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

where $\lambda \in [0,1]$ is a hypothetical parameter. Substituting Eqns. (A.5) and (A.6) in (A.4) gives

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

By equating the terms in the linear system of Eqns. (A.8) one obtains the recurrence formula

$$y_0 = \phi(x),\ y_{n+1} = -L^{-1}(A_n),\ n \ge 0 \tag{A.9}$$

However, in practice all terms of the series (A.6) cannot be determined, and the solution is approximated by the truncated series $\sum_{n=0}^{N} y_n$.

Appendix B

Analytical solutions of equation (8) using ADM (s=0)

In this appendix, we derive the general solution of nonlinear Eqn. (8) by using the Adomian decomposition method. We write the Eqn. (8) in the operator form,

$$L(A) = \frac{2h^2 A}{\alpha_1 + A} \tag{B.1}$$

where $L = \frac{d^2}{dx^2}$. Applying the inverse operator L^{-1} on both sides of Eqn. (B.1) yields

$$A(x) = Cx + D + 2h^2 L^{-1}\left(\frac{A}{\alpha_1 + A}\right) \tag{B.2}$$

where C and D are the constants of integration. We let,

$$A(x) = \sum_{n=0}^{\infty} A(x) \tag{B.3}$$

$$N[A(x)] = \sum_{n=0}^{\infty} U_{\mathrm{n}} \tag{B.4}$$

where

$$N[A(x)] = \left(\frac{A}{\alpha_1 + A}\right) \tag{B.5}$$

In view of Eqns. (B. 3-B. 5), Eqn. (B. 2) gives

$$\sum_{n=0}^{\infty} A_n(x) = Cx + \mathrm{D} + \gamma_E\, L^{-1} \sum_{n=0}^{\infty} U_{\mathrm{n}} \tag{B.6}$$

We identify the zeroth component as

$$U_0(x) = \mathrm{Cx} + \mathrm{D} \tag{B.7}$$

and the remaining components as the recurrence relation

$$A_{n+1}(x) = \gamma_E\, L^{-1} U_{\mathrm{n}} \quad n \ge 0 \tag{B.8}$$

where U_{n} are the Adomian polynomials of $A_1, A_2, \ldots, A_n$. We can find the first few U_{n} as follows:

$$U_0 = N(A_0) = \frac{1}{\alpha_1 + 1} \tag{B.9}$$

$$U_1 = \frac{d}{d\lambda}\left[N(A_0 + \lambda A_1)\right] = \frac{A_1}{\alpha_1 + A_0} \tag{B.10}$$

The remaining polynomials can be generated easily, and so,

$$A_0 = 1 \tag{B.11}$$

$$A_1(x) = -\left(\frac{h^2}{(\alpha_1 + 1)} + \frac{2h^2}{S_h(\alpha_1 + 1)}\right) + \frac{h^2}{(\alpha_1 + 1)} x^2 \tag{B.12}$$

$$\begin{aligned} A_2(x) = &-\left(\frac{2h^2\alpha_1}{(\alpha_1 + 1)^2}\right)\left(\frac{1}{2}\left(\frac{h^2}{(\alpha_1 + 1)} + \frac{2h^2}{S_h(\alpha_1 + 1)}\right) + \frac{h^2}{12(\alpha_1 + 1)}\right) \\ &- \frac{2h^2\alpha_1}{S_h(\alpha_1 + 1)^2}\left(\left(\frac{h^2}{(\alpha_1 + 1)} + \frac{2h^2}{S_h(\alpha_1 + 1)}\right) + \frac{h^2}{3(\alpha_1 + 1)}\right) \\ &\left(\frac{2h^2\alpha_1}{(\alpha_1 + 1)^2}\right)\left(\frac{1}{2}\left(\frac{h^2}{(\alpha_1 + 1)} + \frac{2h^2}{S_h(\alpha_1 + 1)}\right)x^2 + \frac{h^2}{12(\alpha_1 + 1)} x^4\right) \end{aligned} \tag{B.13}$$

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

Appendix C

Analytical solution of equation (9) using ADM (s=2)

In this appendix, we derive the general solution of nonlinear Eqn. (9) by using the Adomian decomposition method. We write the Eqn. (9) in the operator form,

$$L(A)=\frac{2h^2}{\alpha_1+1} \quad \text{(C.1)}$$

where $L=x^{-1}\frac{d^2}{dx^2}x$. Applying the inverse operator L on both sides of Eqn. (C.1) yields

$$A(x)=C+\frac{D}{x}+2h^2L^{-1}\left(\frac{A}{\alpha_1+A}\right) \quad \text{(C.2)}$$

where C and D are the constants of the integration. We let,

$$A(x)=\sum_{n=0}^{\infty}A(x) \quad \text{(C.3)}$$

$$N\left[A(x)\right]=\sum_{n=0}^{\infty}U_n \quad \text{(C.4)}$$

where

$$N[A(x)]=\left(\frac{A}{\alpha_1+A}\right) \quad \text{(C.5)}$$

In view of Eqns. (C.3-B.5), Eqn. (C.2) gives

$$\sum_{n=0}^{\infty}A_n(x)=C+\frac{D}{x}+\gamma_E L^{-1}\sum_{n=0}^{\infty}A_n(x) \quad \text{(C.6)}$$

We identify the zeroth component as

$$U_0(x)=C+\frac{D}{x} \quad \text{(C.7)}$$

and the remaining components as the recurrence relation

$$A_{n+1}(x)=\gamma_E L^{-1}U_n \quad n\geq 0 \quad \text{(C.8)}$$

where U_n are the Adomian polynomials of A_1, A_2 ,…., A_n. We can find the first few U_n as follows:

$$U_0=N(A_0)=\frac{1}{\alpha_1+1} \quad \text{(C.9)}$$

$$U_1=\frac{d}{d\lambda}\left[N(A_0+\lambda A_1)\right]=\frac{A_1}{\alpha_1+A_0} \quad \text{(C.10)}$$

The remaining polynomials can be generated easily, and so,

$$A_0=1 \quad \text{(C.11)}$$

$$A_1(x)=-\left(\frac{h^2}{3(\alpha_1+1)}+\frac{2h^2}{3S_h(\alpha_1+1)}\right)+\frac{h^2}{3(\alpha_1+1)}x \quad \text{(C.12)}$$

$$\begin{aligned}A_2(x)=&-\left(\frac{2h^2\alpha_1}{(\alpha_1+1)^2}\right)\left(\frac{1}{6}\left(\frac{h^2}{3(\alpha_1+1)}+\frac{2h^2}{3S_h(\alpha_1+1)}\right)+\frac{h^2}{60(\alpha_1+1)}\right)\\&-\frac{2h^2\alpha_1}{S_h(\alpha_1+1)^2}\left(\frac{1}{3}\left(\frac{h^2}{3(\alpha_1+1)}+\frac{2h^2}{3S_h(\alpha_1+1)}\right)+\frac{h^2}{15(\alpha_1+1)}\right)\\&+\left(\frac{2h^2\alpha_1}{(\alpha_1+1)^2}\right)\left(\frac{1}{6}\left(\frac{h^2}{3(\alpha_1+1)}+\frac{2h^2}{3S_h(\alpha_1+1)}\right)x^2+\frac{h^2}{60(\alpha_1+1)}x^4\right)\end{aligned} \quad \text{(C.13)}$$

Adding (C. 11) to (C. 13), we get the Eqn. (12) in the text.

Appendix D

Matlab program to find numerical solution of Eqns. (11) and (12)

```
function pdex1
m = 0;
x = linspace(0,1);
t = linspace(0,100);
sol = pdepe(m,@pdex1pde,@pdex1ic,@pdex1bc,x,t);
u = sol(:,:,1);
%surf(x,t,u)
%title('Numerical solution computed with 20 mesh points.')
%xlabel('Distance x')
%ylabel('Time t')
```

```
figure
plot(x,u(end,:))
title('Solution at t = 2')
xlabel('Distance x')
ylabel('u(x,2)')
% --------------------------------------------------------------
function [c,f,s] = pdex1pde(x,t,u,DuDx)
c = 1;
f = DuDx;
h =0.5;
alpha=10;
s = -2*h^2*u/alpha+u);
% --------------------------------------------------------------
function u0 = pdex1ic(x)
u0 = 1;
% --------------------------------------------------------------
function [pl,ql,pr,qr] = pdex1bc(xl,ul,xr,ur,t)
S = 1;
pl = 0;
ql = 1;
pr =-S*(1-ur);
qr = 1;
```

Appendix E

Nomenclature

A Dimensionless substrate concentration (= S/S_0) (None)

S Substrate concentration(mol/cm^3)

S_0 Bulk-substrate concentration(mol/cm^3)

K_m Michaelis constant (mol/cm^3)

k_m External mass-transfer coefficient (mol/cm^3)

D Effective diffusivity inside the particle (cm^2 s^{-1})

V_m Maximum reaction rate (mol/s cm^3)

x Spatial variable (cm)

L Half length of the particle (cm)

h Thiele modulus $\left(V_m/2DS_0\right)^{1/2}L$ (None)

α_1 Dimensionless Michaelis constant K_m/S_0 (None)

S_h Modified Sherwood number $k_m L/D$ (None)

REFERENCES

[1] R. Aris, The Mathematical theory of diffusion and reaction in permeable catalysts. Clarendon, Oxford, Volume 1, (1975).

[2] J. M. Engasser, C. Horvath, Effect of internal diffusion in heterogeneous enzyme systems: Evolution of true kinetic parameters and substrate diffusity, Journal of Theoretical Biology, 42, (1973), 137-155.

[3] P. Cheviollotte, Relation between the reaction cytochrom oxidase—Oxygenand oxygen uptake in cells in vivo- The role of diffusion. Journal of Theoretical Biology, 39, (1973) 277-295.

[4] D. L. S. McElwain, A re-examination of oxygen diffusion in a spherical cell with Michaelis-Menten oxygen uptake kinetics, Theoretical Biology, 71, (1978), 205-263.

[5] S. H. Lin, Oxygen diffusion in a spherical shell with nonlinear oxygen uptake kinetics, Journal of theoretical Biology, 60,(1976), 449-457.

[6] S. P. Ho and M. D. Kostin, Diffusion with irreversible chemical reaction in heterogeneous media, Application to oxygen transport in respiring tissue, Journal of theoretical Biology, 64,(1997), 237-251.

[7] A.S. Pope, Diffusion in tissue slices with metobolism obeying Michaelis-Menten kinetics, Journal of theoretical Biology, 80,(1979), 325-332.

[8] S. H. Lim, A modified model for predicting the performance of a compact artifical kidney, Journal of theoretical Biology, 77,(1972), 441-451.

[9] L. Michaelis, and M. Menten, Die kinetic der invertinwirkung, Biochemistry Zeitung 49, (1913), 333-369.

[10] R. Shlomi, U. Michael, K. Joseph, Role of substrate unbinding in Michaelis-Menten enzymatic reactions, Proceedings of the National Academy Sciences 111, (2012), 4391-4396.

[11] N. Tosaka, S. Miyale, Analysis of a nonlinear diffusion problem with Michaelis-Menten kinetics by an integral equation method, Bulletin of mathematical biology, Volume 44, issue 6, (1982), 841-849.

[12] M. Maalmi, W. Strieder, A. Varma, Ligand diffusion and receptor mediated internalization: Michaelis-Menten kinetics, Journal of chemical engineering science, Volume 56, issue 19, (2001), 5606-5616.

[13] T. R. Merchant, Cubic autocatalysis with Michaelis-Menten kinetics: Semi-analytical solutions for the reaction-diffusion cell, Journal of Chemical Engineering Science Volume 59, issue 16, (2004), 3433-3440.

[14] K. Indira, L. Rajendran, Analytical expression of the concentration of substrates and product in phenol-polyphenol oxidase system immobilized in laponite hydrogels; Michaelis-Menten formalism in homogeneous medium, Electrochimica Acta, Vol. 56, issue 18, (2011), 6411-6419.

[15] J. Bucolo, K. Tripathi, Steady-state analysis of a two-compartment barrier-limited capillary-tissue model with Michaelis-Menten saturation kinetics, Bulletin of Mathematical Biology, Vol. 42, Issue 5, (1980),691-700.

[16] D. Dang Do, F. Greenfield, A finite integral transform technique for solving the diffusion- reaction equation with Michaelis – Menten kinetics, Journal of Mathematical Biosciences, Vol. 54, Issues 1-2, (1981), 31-47.

[17] M. Chapwanya, S. Lubuma, E. Mickens, From enzyme kinetics to epidemiological models with Michaelis - Menten contact rate design of nonstandard finite difference schemes, Journal of Computers and Mathematics with Applications, Vol. 64, Issue 3, (2012), 201-213.

[18] A. Napper, W. Schubert, Michaelis – Menten kinetics as a

modeling assumption in a model of oxygen transport in heart, Proceedings of the first southern Biomedical Engineering conference, (1981), 201-204.

[19] C. Regalbuto, W. Strieder, A. Varma, Approximate solutions for nonlinear diffusion-reaction equations from the maximum principle, Journal of Chemical Engineering Science, Vol. 43, Issue 3, (1988), 513-518.

[20] L. Rajendran, K. Saravana kumar, Analytical expression of transient and steady-state catalytic current of mediated bioelectrocatalysis, Journal of Electrochimica Acta, Vol. 147, (2014), 678-687.

[21] M. A. Mohamed, Comparison differential transformation technique with Adomian decomposition method for dispersive long-wave equations in (2+1) dimensions, Applications and Applied Mathematics, Vol. 5, No. 1, (2010), 148-166.

[22] O. K. Jaradat, Adomian decomposition method for solving Abelian differential equations, Journal of Applied Sciences, Vol.8, No. 10, (2008), 1962-1966.

[23] A.M. Siddiqui, M. Hameed, B.M. Sidddiqui and Q. K. Ghori, Use of Adomian decomposition method for in the study of parallel plate flow of a Thir Grade Fluid, Communications and Nonlinear Science and Numerical Simulation, Vol. 15, No.9, (2010), 2388-2399.

[24] A. Majidwazwaz and A. Gorguis, An analytic study of Fisher's equation by Adomian decomposition method , Applied Mathematics and Computation, Vol.154, No.3, (2004), 609-620.

[25] H. Jafari and V. Daftardar-Gejji, Solving linear and nonlinear fractional diffusion and wave equation by Adomian decomposition method, Applied Mathematics and Computation, Vol.180, No.2, (2005), 488-497.

[26] K. Abbaoui, and Y. Cherruault, Convergence of Adomians method applied to differential equations, Computer Mathematical Application, 28, (1994a), 103-109.

[27] K. Abbaoui, and Y. Cherruault, Convergence of Adomians method applied to non-linear equations, Mathematical and Computer Modeling, 20, (1994b), 69-73.

[28] N.H. Sweilam and M. M. Khader, Approximate solutions to the nonlinear vibrations of multiwalled carbon nanotubes using Adomian decomposition method, Applied Mathematics and Computation, Vol. 217, No. 2, (2010), 495-505.

[29] G. Adomian, Solving the mathematical models of neurosciences and medicine, Mathematics and computers in simulation, Vol. 40, No. 1-2,(1995), 107-114.

[30] O. D. Makinde, Adomian decomposition approach to a SIR epidemic model with constant vaccination strategy, Applied Mathematics and Computation, Vol. 184, No. 2, (2007), 842-848.

[31] G. Adomian, Convergent series solution of nonlinear equations, Applied Mathematics and computations, 11, (1984), 225-230.

[32] G. Adomian, M. Witten, Computation of solutions to the generalized Michaelis-Menten equation, Applied Mathematics Lett, 7, (1994), 45-48.

[33] I. H. Sneddon, The use of integral transform, Mcgraw-Hill, New York, (1972).

[34] M. J. Abdekhodaie, X. Y. Wu, Modeling of cationic glucose sensitive membrane with consideration of oxygen limitation, Journal of Membrane Sciences, Volume 254, Issues 1-2, 254, (2005), 119-127.