Global Journal of Pure and Applied Mathematics (GJPAM) ISSN 0973-1768 Volume 12,Number 4 (2016)
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Analytical solutions of coupled non-linear reaction diffusion equations for substrate and Hydrogen ion concentrations in immobilized enzyme system

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***Abstract*—A mathematical model describing the effects of electrostatic interaction with reaction generated pH change on the kinetics of immobilized enzyme has been discussed for both large and small pore cases. This model contains the system of non-linear reaction diffusion equations. Approximate analytical solutions of non-linear reaction diffusion equations containing non-linear terms related to rate of reaction mechanism are solved using Adomian decomposition method. The relevant analytical expressions for the substrate and hydrogen ion concentration profiles are discussed in terms of dimensionless reaction diffusion parameters α, β and γ. The numerical solutions are also obtained using MATLAB program. While comparing our analytical solutions with the numerical estimation a good agreement is noted.**

Keywords*— Mathematical modeling; non-linear reaction diffusion equations; immobilized enzyme system; hydrogen ion; electrostatic interaction.

I. INTRODUCTION

Immobilization is one of the efficient methods to improve enzyme stability [1]. The main aim of immobilization is to obtain stable and reusable enzymes with resistance to different environmental factors [2, 3].The main objective of the immobilization of enzymes is to enhance the economics of bio catalytic processes. Immobilization allows one to re-use the enzyme for an extended period of time and enables easier separation of the catalyst from the product. Additionally, immobilization improves many properties of enzymes such as performance in organic solvents, pH tolerance, heat stability or the functional stability. Many enzyme-catalyzed reactions involve the production or consumption of hydrogen ions and this is expressed by the change in the binding of hydrogen ions in the biochemical reactions as written in terms of reactants [4]. The change in the binding of hydrogen ions in an enzyme catalyzed reaction is noteworthy as it determines the effect of pH on the thermodynamics of the reaction which has been catalyzed [5]. In many biochemical reactions the produced hydrogen ions can alter the micro environment considerably [6].

A mathematical model based on immobilized enzyme catalysis with reaction-generated pH change was investigated by Bailey and Chow [7] and their study is restricted mainly to the large pore case. The electrostatic effects in immobilized enzyme system in terms of apparent Michaaelis-Menten constants were first discussed by Goldstein et al. [8]. A mathematical frame work was established by Bhalla and Deen [9] to evaluate the electrostatic interaction energy between a charged sphere and a charged pore by solving the nonlinear Poisson Boltzmann equations. Gupta and Ramachandran[10] have analyzed the effect of both internal and external diffusion resistances together with electrostatic interaction not only for the small pore case and also for large pore case .

In this study, the effect of interactions between the charged carrier and the hydrogen ion has been analyzed analytically for both small and large pore cases. The nonlinear equations depicted by the mathematical model discussed here have been solved by Adomian decomposition method [10-15] and the analytical expressions corresponding to the steady state concentrations of the substrate and hydrogen ion, have been derived. These analytical results are useful to understand and optimize the behavior of electrostatic interaction in the kinetics of immobilized enzymes. The information gathered from the theoretical modeling is fruitful in experimental design, optimization and prediction of the enzyme kinetics.

II. MATHEMATICAL FORMULATION OF THE PROBLEM

The system under consideration consists of enzyme immobilized on a plain porous charge support. The enzyme catalyses the reaction

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This paper was presented by the first author in the National Conference on AMASE-2016 conducted in Department of Mathematics, University College of Engineering Pattukkottai, Thanjavur, Tamil Nadu, India, on 22nd January 2016.

$$E + S \rightarrow P^{-} + H^{+} + E \qquad (1)$$

The rate expression for the above enzyme catalyzed reaction based on the effect of hydrogen ion concentration is given by

$$r(s,h)=\left[\frac{V_m s}{s+K_m}\right]\left[\frac{1}{1+h/K_1+K_2/h}\right]$$

Small pore case:

In this small pore case the analysis is done for supports having pores of very small diameter of the order of the characteristic dimensions of the electrostatic double layer and the electrostatic potential due to charged support will be uniform within the pore. The transport of hydrogen ion from the pore mouth to the exterior of the bulk will be affected by the electrostatic interaction.

In the small pore case the potential is uniform within the pore and the flux within the pore due to electrostatic effect becomes zero. Hence for such system the mass balance equations for the substrate and the hydrogen ion for the reaction following the kinetics given by equation can be written by the following equations [6]:

$$D_{es}\frac{d^2 s}{dx^2}=\left[\frac{V_m s}{s+K_m}\right]\left[\frac{1}{1+h/K_1+K_2/h}\right] \qquad (2)$$

$$D_{eh}\frac{d^2 h}{dx^2}=\left[\frac{-V_m s}{s+K_m}\right]\left[\frac{1}{1+h/K_1+K_2/h}\right] \qquad (3)$$

The corresponding boundary conditions are given by

$$\frac{ds}{dx}=0,\ \frac{dh}{dx}=0 \text{ at } x=0 \qquad (4)$$

$$D_{es}\frac{ds}{dx}=k_s(s_o-s),\quad D_{eh}\frac{dh}{dx}=Mk_h\left(h_0-\frac{h}{P}\right) \qquad (5)$$

at $x = L$, where s and h denote the concentration of substrate and hydrogen ion, V_m is the maximum rate of reaction, k_1 and k_2 are equilibrium constants, K_m is the Michaelis - Menten constant, h is the external mass transfer coefficient, x represents the distance from the center of the pore and P is the partition coefficient defined by $P=e^{-\lambda}$.

III. DIMENSIONLESS FORM OF THE PROBLEM

To compare the analytical results with simulation results, we make the above non-linear partial differential equations (3) and (4) in dimensionless form by defining the following parameters.

$$X=\frac{x}{L},\ S=\frac{s}{s_o},\ H=\frac{h}{h_o},\ \varphi=\frac{V_m L^2}{D_{es}K_m}, \qquad (6)$$

$$\alpha_1=\frac{h_o}{K_1},\ \alpha_2=\frac{h_0}{K_2},\ \gamma=\frac{s_0}{K_M},\ \beta_s=\frac{Lk_s}{D_{es}}$$

The dimensionless form of the equations (2) and (3) in terms of dimensionless quantities described in equation (6) can be written as

$$\frac{d^2 S}{dX^2}=\frac{\varphi S}{1+\gamma S}\left(\frac{1}{1+\alpha_1 H+1/\alpha_2 H}\right) \qquad (7)$$

$$\frac{d^2 H}{dX^2}=-\frac{D_{es}}{D_{eh}}\frac{s_0}{h_0}\frac{\varphi S}{1+\gamma S}\left(\frac{1}{1+\alpha_1 H+1/\alpha_2 H}\right)$$

The boundary conditions in dimensionless form will be as follows:

$$\frac{dS}{dX}=\frac{dH}{dX}=0 \quad \text{at} \quad X=0$$

$$\frac{dS}{dX}=\beta_s(1-S) \quad \text{at} \quad X=1$$

$$\frac{dH}{dX}=M\beta_s\frac{D_{es}}{D_{eh}}\frac{k_h}{k_s}\left(1-\frac{H}{P}\right) \quad \text{at} \quad X=1$$

Using the Adomian decomposition method (Appendix B) the non-linear equations (7) and (8) can be solved and the analytical expressions of substrate and hydrogen ion concentrations are given by

$$S(X)=1+\left(\frac{\varphi}{1+\gamma}\right)\left(\frac{1}{1+\alpha_1 P+1/\alpha_2 P}\right)\left(\frac{X^2}{2}-\frac{1}{2}-\frac{1}{\beta_s}\right) \qquad (12)$$

$$H(X)=P-\left(\frac{\beta_s PD}{M_h}\right)\left[\begin{array}{c}\left(\frac{\varphi}{1+\gamma}\right)\left(\frac{1}{1+\alpha_1 P+1/\alpha_2 P}\right)\\ \left(\frac{X^2}{2}-\frac{1}{2}-\frac{1}{\beta_s}\right)\end{array}\right] \qquad (13)$$

The basic concepts of Adomian decomposition method are given in Appendix A

The Thiele module is defined as

$$\varphi=\frac{V_m L^2}{D_{es}K_M} \qquad (14)$$

The effectiveness factor η, which is defined as the ratio of the actual reaction rate and Thiele modulus if the reaction took place at the bulk concentrations without the electrostatic effect in dimensionless form and its corresponding analytical expression are given below

$$\eta=\frac{1}{\varphi}(1+\gamma)(1+\alpha_1+1/\alpha_2)\left(\frac{dS}{dX}\right)_{X=1} \qquad (15)$$

$$\eta=(1+\alpha_1+1/\alpha_2)\left(\frac{1}{1+\alpha_1 P+1/\alpha_2 P}\right) \qquad (16)$$

The dimensionless reaction rate and its corresponding analytical solution are given by

$$V=\left(\frac{dS}{dX}\right)_{X=1}=\left(\frac{\varphi}{1+\gamma}\right)\left(\frac{1}{1+\alpha_1 P+1/\alpha_2 P}\right) \qquad (17)$$

Large pore case:

In artificial immobilized enzyme systems, the pores can be significantly larger than the electrostatic double layer thickness. For these cases, the effects can be taken into account by lumping them into the partitioning coefficient *P*. For this case the mass balance equation for substrate and hydrogen ion can be obtained by replacing H by PH and defining the partition coefficient as $P = e^{\lambda}$. Hence the boundary condition for hydrogen ion becomes

$$\frac{dH}{dX} = M\beta_s \frac{D_{es}}{D_{eh}} \frac{k_h}{k_s}(1-H) \quad at \quad X = 1 \quad (18)$$

Hence the analytical expression for hydrogen ion in large pore case is given by

$$H = P - \left(\frac{\beta_s PD}{M_h}\right)\left[\begin{array}{c}\left(\frac{\varphi}{1+\gamma}\right)\left(\frac{1}{1+\alpha_1 P + 1/\alpha_2 P}\right) \\ \left(\frac{x^2}{2} - \frac{1}{2} - \frac{1}{\beta_s}\right)\end{array}\right] \quad (19)$$

Table: 1 Parameters used in this work and Ramachandran et. al work

Para meter	Values used in this work	Parameter	Values used in previous work
$K1$	5x10^{-5} M	$\alpha_1 = \frac{h_o}{K_1}$	0.01 - 0.5
K_2	10^{-5} M	$\alpha_2 = \frac{h_0}{K_2}$	0.01-0.5
K_M	10^{-5} M	$\gamma = \frac{s_0}{K_M}$	1
k_h / k_s	1	$\beta_s = \frac{Lk_s}{D_{es}}$	100
D_{es} / D_{eh}	0.25	$X = \frac{x}{L}$	0 - 1
$s0$	10^{-4} M, 10^{-6}M	s_0	10^{-4} M, 10^{-6}M
h_0	10^{-4} M, 10^{-7}M	h_0	10^{-4} M, 10^{-7}M
λ	-1, 0, 1	λ	-1,0,1
β	10,100, 1000	β	10,100,1000

IV. NUMERTICAL SIMULATION

The non-linear differential equations (4) and (12) for the given initial – boundary conditions are being solved numerically. The function pdex, in MATLAB software which is a function of solving the initial – boundary value problems for non-linear ordinary differential equations is used to solve these equations. The numerical solutions are compared with analytical results using Adomian decomposition method as shown in figures 1, 2 and 3 and it gives a satisfactory result. The MATLAB program is also given in Appendix C.

V. RESULTS AND DISCUSSION

The proposed mathematical model for small pore and large pore cases consists of coupled non - linear equations for substrate and hydrogen ion concentrations. They are solved by adomian decomposition method to obtain analytical solutions for the both concentrations as well as for Thiele module and effectiveness factors. These analytical results are discussed graphically as shown in figures. Fig. 1 shows the time independent evolution of normalized concentration profiles for the substrate. Fig. 1(a) - 1(d) shows the dimensionless concentration S versus the dimensionless Length L. Fig. 1(a) indicates that the value of the concentration increases when then value of the Thiele modulus is being decreased and from Fig. 1(b) it is evident that as the value of the equilibrium constant α_1 increases the concentration also increases. Fig. 1 (c) denotes the concentration increases with the increase in the value of reaction diffusion parameter γ. From Fig. 1(d) it is obvious that the Sherwood number β does not play a significant role in the concentration of the substrate as there is no change when the number is being increased. Fig. 2 demonstrates steady state normalized profiles of hydrogen ion concentration. In Fig. 2(b) and (c), it is understood there is remarkable increase in the concentration when the Sherwood number β as well as the Thiele modulus are being increased. Fig. 2(a) and (d) exhibits that the concentration increases when the parameter M_h and reaction diffusion parameter γ are being decreased. Fig.3 indicates the concentration profiles of hydrogen ion for large pore case. It is noteworthy that same results are obtained in both the cases for varying the parameters β and γ. Fig.4 illustrates that there is a linear relationship between the reaction rate and Thiele modulus for various values of the parameters.

VI. SENSITIVITY ANALYSIS

Equation (12) represents the analytical expression for the concentration of the substrate in dimensionless form in terms of the parameters $\alpha_1, \alpha_2, \beta, \gamma$, and P. From the spread sheet analysis given in Figure 5 it is understood that the parameter α_1 has the greater impact than all other factors. The parameters α_2, γ and the Thiele modulus φ, partition coefficient P have more or less equal impact whereas the parameter β has very less impact in the substrate concentration. It is evident from the spread sheet analysis exhibited in Figure 6, the influence of the partition coefficient P is very high whereas influence of the diffusion coefficient D is very low in the hydrogen ion concentration H . It is noteworthy that the Thiele modulus φ as well as the diffusion parameter β have similar impact .The parameter M_h also has significant impact in H whereas the influence of other parameters such as α_1, α_2 and γ are comparatively less. On the whole, the sensitivity analysis described in this paper will be fruitful to evaluate the significance of each parameter to the simulation‗s accuracy.

VII. CONCLUSION

A mathematical model based on the effects of electrostatic interaction with reaction generated pH change on the kinetics of immobilized enzymes has been discussed here. The analytical expressions for the concentrations of the substrate and hydrogen ion concentration have been derived by making use of Adomian Decomposition Method. It is noteworthy that there is a good agreement between the analytical and numerical simulations. The analytical results derived by making use of this described model are used to determine the influence of effectiveness factor as well as Thiele modulus in the electrostatic interaction without using any experimental techniques. The importance of partition coefficient in selecting a carrier for enzyme immobilization is also shown graphically. This theoretical model can also be used to optimize the performance of the electrodes.

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APPENDIX - A

Basic concepts of the modified Adomian decomposition method

The modified 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 the nonlinear parts of F respectively. The operator L is assumed to be an invertible operator. Solving for $L(y)$ leads to

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

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

$$y(x) = -L^{-1}[N(y)] + \varphi(x) \tag{A.4}$$

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

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

The modified Adomian decomposition method assumes that the nonlinear term $N(y)$ can be written as an infinite series in terms of the Adomian polynomials A_n :

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

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 (28).
Substituting Eqs.(A.5) and (A.6) in (A.4) gives

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

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

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

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

Approximate analytical solution of Eqn. (7) using ADM method

In this appendix, we indicate how Eq. (12) in this paper has been derived. Furthermore, an ADM was constructed to determine the solution of Eq. (7) for $(a=1)$ in the operator form,

$$Ls = \frac{\varphi S}{1+\gamma S}\left(\frac{1}{1+\alpha_1 P+1/\alpha_2 P}\right) \tag{B.1}$$

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

$$s(x) = Ax + B + \frac{\varphi S}{1+\gamma S}\left(\frac{1}{1+\alpha_1 P+1/\alpha_2 P}\right) \tag{B.2}$$

Where *A* and *B* are the constants of integration. We let,

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

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

where $N[s(x)] = \frac{\varphi S}{1+\gamma S}\left(\frac{1}{1+\alpha_1 P+1/\alpha_2 P}\right)$ (B.5)

From the Eqns (B.3), (B.4) and (B.5), Eq. (B.2) gives

$$\sum_{n=0}^{\infty} s_n(x) = Ax + B + \frac{S}{1+\gamma S}\left(\frac{1}{1+\alpha_1 P+1/\alpha_2 P}\right) \tag{B.6}$$

We identify the zeroth component as

$$s_0(x) = Ax + B \tag{B.7}$$

And the remaining components as the recurrence relation

$$s_{n+1} = \varphi L^{-1} A_n \,;\, n \geq 0 \tag{B.8}$$

where A_n are the Adomian polynomials of $s_{0,}\, s_{1,}\, \ldots, s_n$. We can find the first few A_n as follows:

$$s_0(x) = 1 \tag{B.9}$$

$$s_1(x) = \left(\frac{\varphi S}{1+\gamma S}\right)\left(\frac{1}{1+\alpha_1 P+1/\alpha_2 P}\right)\left(\frac{x^2}{2}-\frac{1}{2}-\frac{1}{\beta_s}\right) \tag{B.10}$$

Adding (B.9) and (B.10), we get the concentration substrate Eqn.(12). Similarly, we can obtain the concentration of hydrogen ion (13) by solving Eqns. (8), (9) and (11).

APPENDIX - C

Scilab/Matlab program for the numerical solution of equation (4)

```
function pdex4
m = 0;
x = linspace(0,1);
t = linspace(0,100000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u1 = sol(:,:,1);
%————————————————————————————————
Figure
plot(x,u1(end,:))
title('u1(x,t)')
xlabel('Distance x')
ylabel('u1(x,1)')
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c =1;
f =1.* DuDx;
e=0.3;alpha=2;
F =-(e*u(1))/((1+(alpha*u(1))));
s =F;
% ———————————————————————————————
function u0 = pdex4ic(x);
  u0 = [0];
% ———————————————————————————————
function [pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
j=10;
pl = [0];
ql = [1];
pr = [-j*(1-ur(1))];
qr = [1];
```

APPENDIX - D

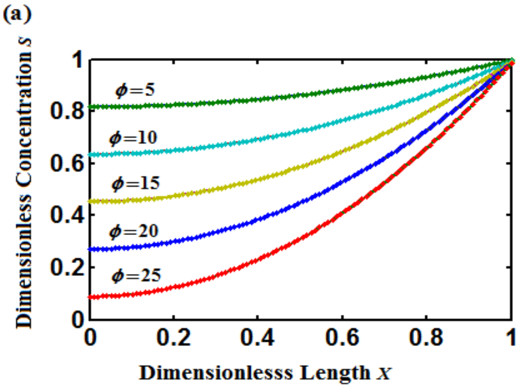
Nomenclature

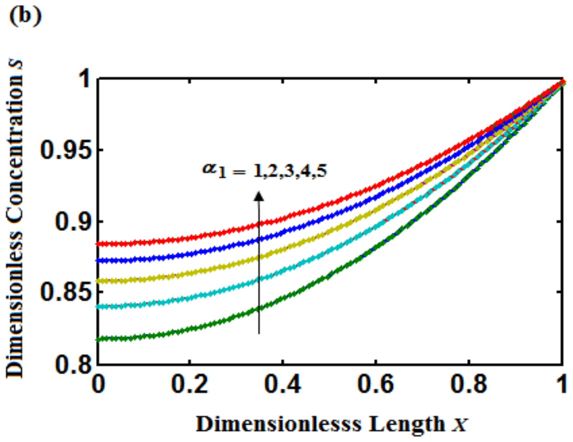
D_{es}	Effective diffusivity of substrate concentration
D_{eh}	Effective diffusivity of hydrogen ion concentration
e	Euler's Constant
h	Hydrogen ion Concentration
H	Dimensionless Hydrogen ion Concentration
$K_1,\, K_2$	Equilibrium constants
K_M	Michael-Menten Constant
L	Length of the pore
M	Dimensionless electro static potential modifier
P	Partition coefficient
s	Substrate Concentration
S	Dimensionless Substrate Concentration
V_m	Maximum rate of reaction
x	Distance from the center of the pore
X	Dimensionless Length

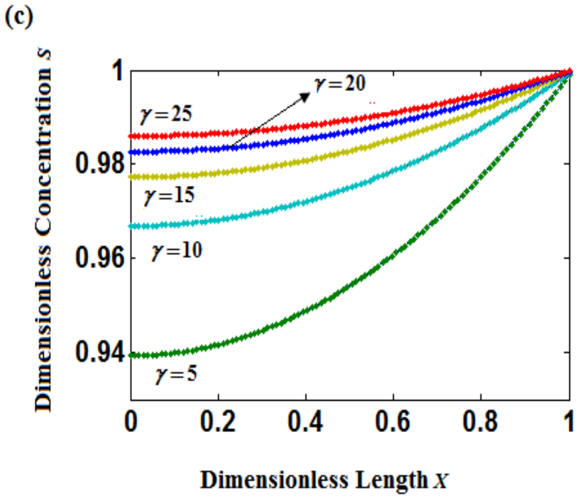
Greek symbols

α_1, α_2	Reduced equilibrium constant
β	Sherwood number
γ	Dimensionless Michaelis - Menten constant -
η	Effectiveness factor
λ	Dimensionless surface potential
φ	Thiele modulus

Fig.1







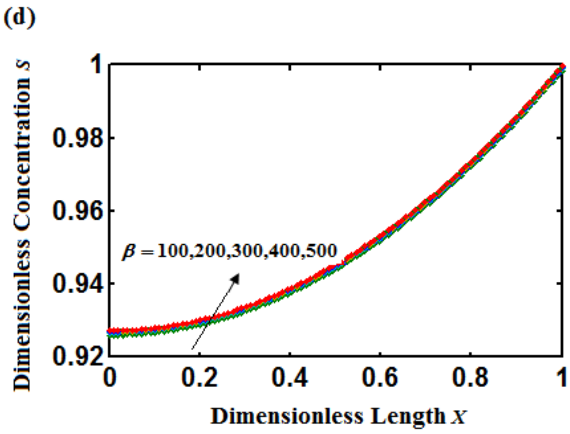


Fig.1. Plot of dimensionless concentration S versus dimensionless length X for various values of the parameters

a) $\alpha_1 = 1, \alpha_2 = 0.2, P = 1, \beta = 100$ *and* $\gamma = 1$

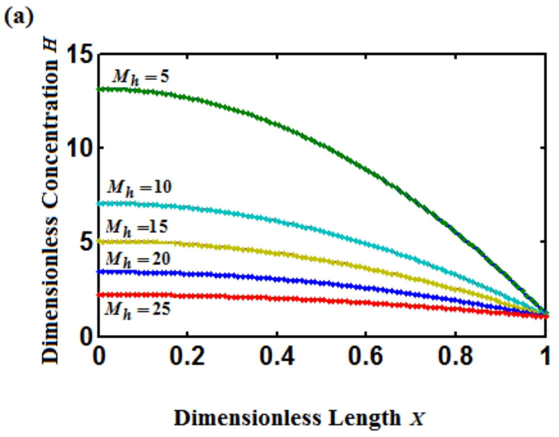
b) $\varphi = 5, \alpha_2 = 0.2, P = 1, \beta = 100$ *and* $\gamma = 1$

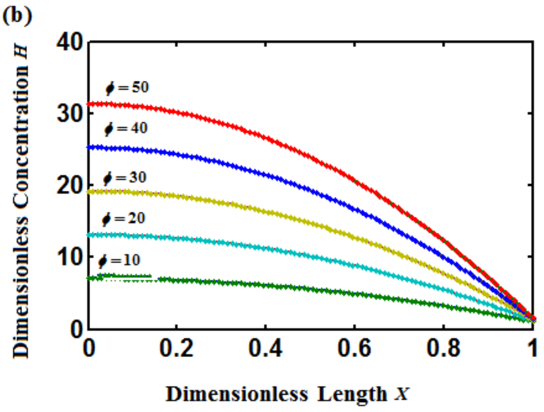
(c) $\alpha_1 = 1, \alpha_2 = 0.2, P = 1, \beta = 100$ *and* $\varphi = 5$

(d) $\alpha_1 = 1, \alpha_2 = 0.2, P = 1, \quad = 10$ *and* $\gamma = 5$

Solid lines represent numerical solutions whereas the dotted line represents analytical solutions.

Fig.2





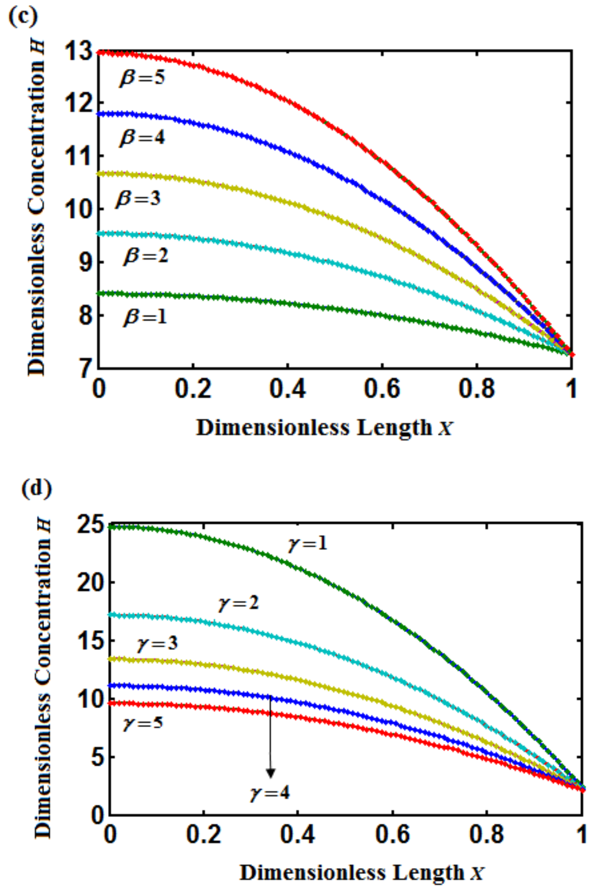


Fig.2. Plot of dimensionless concentration H versus dimensionless length X for various values of the other parameters

a) $\alpha_1 = 0.01, \alpha_2 = 0.05, P = 1, \beta = 100, \varphi = 10, D = 5$ and $\gamma = 1$

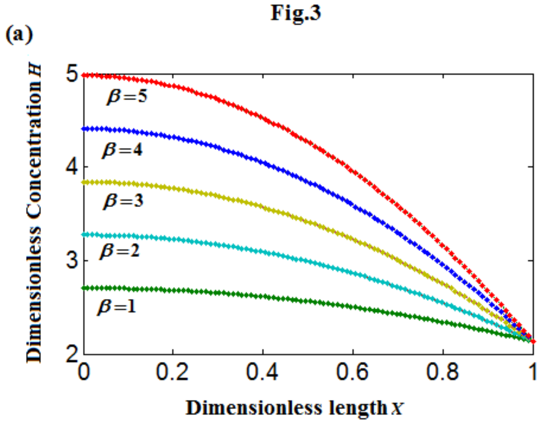
b) $\alpha_1 = 1, \alpha_2 = 5, P = 5, \beta = 100, M_h = 10, D = 5$ and $\gamma = 1$

c) $\alpha_1 = 0.01, \alpha_2 = 0.05, P = 5, M_h = 10, \varphi = 10, D = 5$ and $\gamma = 1$

d) $\alpha_1 = 0.01, \alpha_2 = 0.05, P = 5, M_h = 10, \varphi = 10, D = 5$ and $\beta = 100$

Solid lines represent numerical solutions whereas the dotted line represents analytical solutions.

Fig.3



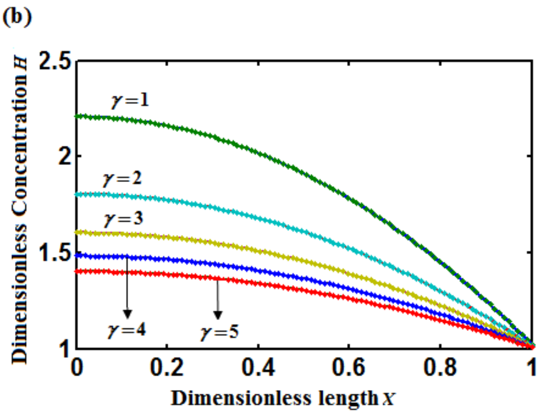


Fig.3. Plot of dimensionless concentration H versus dimensionless length X for various values of the parameters

a) $\alpha_1 = 1, \alpha_2 = 5, P = 1, M_h = 10, \varphi = 10, D = 5$ and $\gamma = 1$

b) $\alpha_1 = 1, \alpha_2 = 5, P = 1, M_h = 10, \varphi = 10, D = 5$ and $\beta = 100$

For large pore case

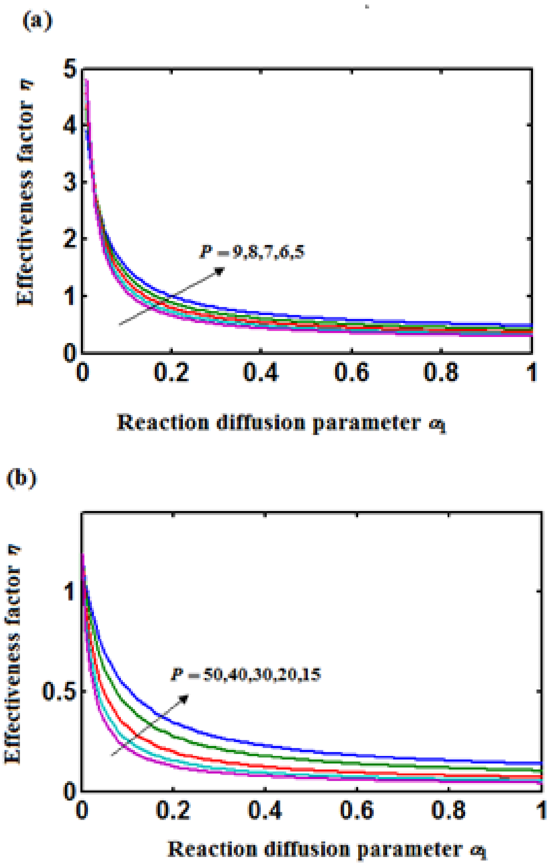


Fig.4. Plot of dimensionless effectiveness factor η versus dimensionless reaction diffusion parameter α_1 for various values of the other parameters.

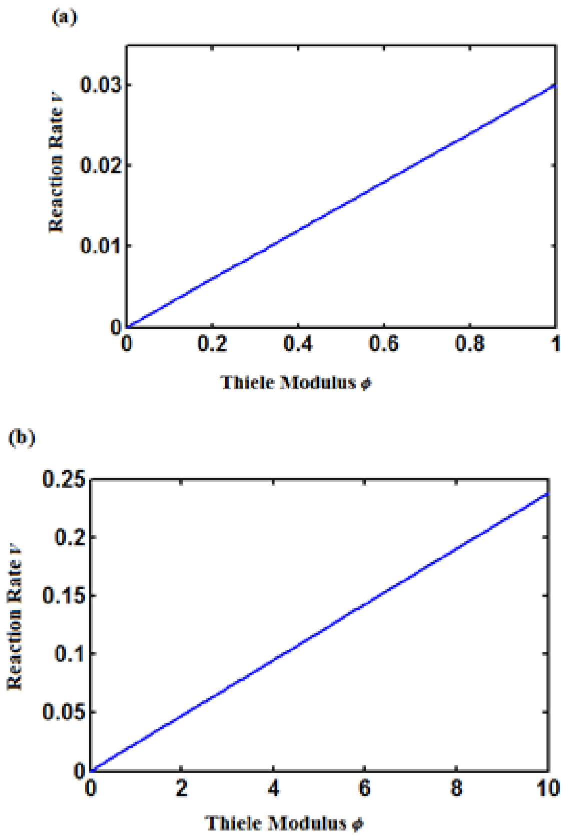


Fig.5.Plot of dimensionless reaction rate v versus dimensionless thiele modulus for various values of the parameters a) $\alpha_1 = 0.01, \alpha_2 = 0.05, P = 1$ *and* $\gamma = 1$
b) $\alpha_1 = 0.01, \alpha_2 = 0.05, P = 5$ and $\gamma = 10$

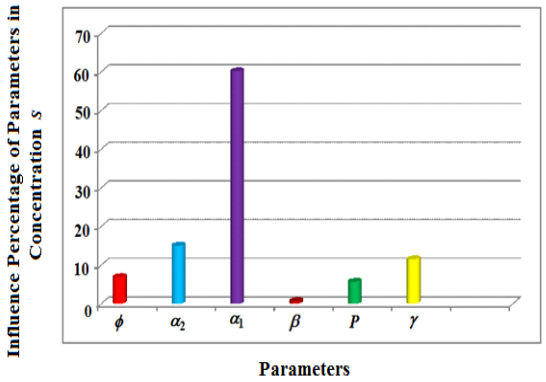


Fig.5. Sensitivity Analysis for evaluating the influence of parameters in Concentration S using equation (12)

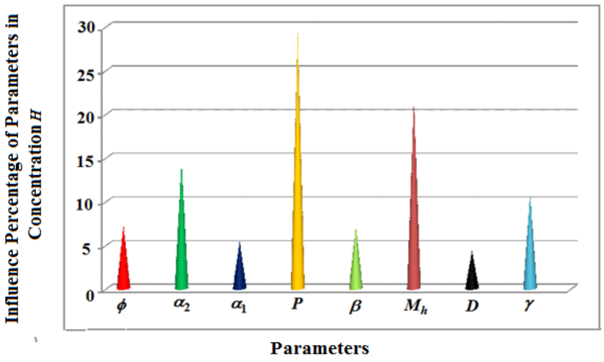


Fig.6. Sensitivity Analysis for evaluating the influence of parameters in Concentration H using equation (13).