International Journal of Mathematical Archive-2(11), 2011, Page: 2270-2280
Available online through www.ijma.info ISSN 2229 – 5046

MATHEMATICAL MODEL FOR MULTI-PHASE MICROCHANNEL BIOREACTORS

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(Received on:14-10-11; Accepted on: 01-11-11)

ABSTRACT

A mathematical model of multi-phase microchannel bioreactor is presented. Further, the effect of oxygen diffusion on the concentration profile and effectiveness response was examined. Analytical expression pertaining to the oxygen concentration profile and effectiveness responses was reported for all possible values of reaction diffusion parameter ϕ_{cc}^2 and the saturation parameter β. These analytical results were found to be in good agreement with numerical simulations. Moreover, herein we employ Adomian decomposition method (ADM) to solve the non-linear reaction/diffusion equation.

Keywords: *Bioreactors, Immobilization of Gluconobacter; Adomian decomposition method, Reaction/Diffusion equation, Mathematical modeling.*

1. INTRODUCTION:

G. oxydans was chosen as a model for investigating the effects of latex coating microstructure, thickness, and drying properties on the preservation of cell viability at ambient temperature and oxidation reactivity. The oxidation of D-sorbitol to L-sorbose by bilayer coatings was studied in a non-growth sorbitol, phosphate, pyruvate medium. Intrinsic kinetic parameters of suspended cells (K_0, k_{cat}) and catalytic parameters of the matrix ($D_{eff,cc}$, $D_{eff,TC}$, X_{cat}) were estimated from independent experiments and used with a diffusion-reaction model to predict the effectiveness factor and the effective reaction rate as a function of cellcoat thickness (L_{cc}), topcoat thickness (L_{TC}), and dissolved oxygen concentration in the liquid medium (CB) (Fidaleo and Flinckinger, 2011). Simulation of there activity of a multi-phase microchannel bioreactor for the oxidation of D-sorbitol to L-sorbose by viable Gluconobacter oxydans entrapped in an adhesive, bilayer, nano-porous latex coating indicates that very high reaction rates may be achieved. These high reaction rates are strongly dependent on the reactivity of the biocatalytic coating which is affected by the nano-porous sealant topcoat thickness and the cellcoat active G. oxydans concentration (Fidaleo and Flinckinger, 2011). Thin, adhesive, nanoporous bilayer diffusive latex coating are significantly more reactive and more stable for whole-cell oxidations than any previously reported viable microbial immobilization method (Flinckinger et al., 2006). Cryogenic scanning electron microscopy has been shown to be a powerful and versatile tool for studying film formation and microstructure in yet another type of latex coating biocatalytic coatings containing E. coli cells (Flinckinger et al., 1999). The monolith loop reactor eliminates the disadvantages of other configurations, such as separation of solvent and/or catalyst, deactivation due to catalyst separation outside the reactor and side reactions with solvents. The main advantages of using a monolith for this process are Low pressure drop, which is especially beneficial because of the high recycle ratio, high mass transfer, which reduces reactor volume and deactivation and Plug flow. Although the reaction runs to completion, the reaction can be carried out in a small reactor because of the limited extent of back mixing in monolith reactors (Kreutzer, Kapteijn and Moulijn, 2005).

However, to the best of our knowledge, there were no analytical results available till date that corresponds to the steady-state substrate concentration and effectiveness factor for all possible values of diffusion parameter ϕ_{cc}^2 and the saturation parameter β. Therefore, herein, we employ Adomian decomposition method to evaluate the steady-state substrate concentration and effectiveness factor for all values of diffusion parameter ϕ_{cc}^2 and the saturation parameter β.

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2. MATHEMATICAL FORMULATION OF THE PROBLEM AND ANALYSIS:

In a multi-phase microchannel bioreactor, the oxidizing D-sorbitol reacts with oxygen producing L-sorbose. A general scheme that represents the reaction occurring at a multi-phase microchannel bioreactor is shown below (Fidaleo and Flinckinger, 2011):

$$D-sorbitol+(1/2))O_2 \rightarrow L-sorbose+H_2o \tag{1}$$

Resting cells of G. oxydans are capable of oxidizing D-sorbitol to L-sorbose. In a non-growth medium, if oxygen is the only rate liming substrate, the kinetics of oxidation can be described by the following Michaelis–Menten equation: The steady state elemental balance for oxygen in the nanoporous latex cellcoat can be written as

$$r_p = \frac{k_{cat} c_0}{K_0 + c_0} X_{cat} \tag{2}$$

where r_p is the L-sorbose formation rate, k_{cat} is the rate constant for L-sorbose, c_o and X_{cat} are the dissolved oxygen and active G. oxydans concentrations, respectively and K_0 is the saturation constant for oxygen. The mass balance equation for oxygen in cellcoat can be written as follows:

$$D_{eff.cc} \frac{d^2 c_0}{dx^2} = \frac{1}{Y_{P/0}} \frac{k_{cat} X_{cat} c_0}{K_0 + c_0} \tag{3}$$

where c_o is the dissolved oxygen concentration at depth x in the cellcoat, $D_{eff.cc}$ is the effective diffusivity of oxygen in the cellcoat, $Y_{P/O}$ is the yield of L-sorbose on oxygen and X_{cat} is the concentration of viable cells in the cellcoat. The boundary conditions are**:**

$$\frac{dc_0}{dx} = 0 \text{ at } x = 0; \tag{4}$$

$$c_0 = c_1 \text{ at } x = L_{cc}; \tag{5}$$

where L_{cc} is the thickness of the cellcoat and c_1 is the dissolved oxygen concentration at the interface of cellcoat and topcoat. Solution of the above equations requires that the value of c_1 is known. An additional condition can be obtained by imposing the continuity of oxygen flux at the interface between the cellcoat and the topcoat:

$$c_1 = c_{0.c} - L_{TC} \frac{D_{eff.cc}}{D_{eff.TC}} \left(\frac{dc_0}{dx} \right)_{x=L_{cc}} \tag{6}$$

The oxygen volumetric consumption rate of the coating can be reported in terms of the effectiveness factor, which in the case under study can be expressed as:

$$\eta_{cc} = \frac{(1 + c_{0.c} / K_0)}{\phi_{cc}^2} \left(\frac{L_{cc}}{c_{0.c}} \right) \left(\frac{dc_0}{dx} \right)_{x=L\,cc} \tag{7}$$

where ϕ_{cc} is the Thiele modulus:

$$\phi_{cc} = L_{cc} \sqrt{\frac{k_{cat} X_{cat}}{Y_{P/0} K_0 D_{eff.cc}}} \tag{8}$$

2.1 Normalised form:

By introducing the following dimensionless variables

$$U = \frac{c}{c_1} \text{ and } X = \frac{x}{L_{cc}} \tag{9}$$

the non-linear equation (3) becomes as follows:

$$\frac{d^2U}{dX^2} = \phi_{cc}{}^2 \frac{U}{(1+\beta U)} \tag{10}$$

where

$$\phi_{cc}{}^2 = \frac{k_{cat} X_{cat} L_{cc}{}^2}{K_0 Y_{P/0} D_{eff,cc}} \quad \text{and} \quad \beta = \frac{c_1}{K_0} \tag{11}$$

The boundary conditions are:

$$\frac{dU}{dX} = 0 \text{ at } X = 0 \tag{12}$$

$$U = 1 \text{ at } X = 1 \tag{13}$$

The dimensionless effectiveness factor is

$$\eta = \frac{1+\beta}{\phi_{cc}{}^2}\left(\frac{dU}{dX}\right)_{X=1} \tag{14}$$

3. ANALYTICAL SOLUTION OF THE CONCENTRATION 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 (Adomian, 1984; Mohamed, 2010; Jaradat, 2008; Sergio and Serrano, 2011; Ghori et al., 2010). The ADM yields, without linearization, perturbation, transformation or discretisation, 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 expression of concentration (see Appendix B) is as follows:

$$U(X) = \left[1 - \frac{\phi_{cc}{}^2}{2(1+\beta)} + \frac{\phi_{cc}{}^4}{12(1+\beta)^3}\right] + \left[\frac{\phi_{cc}{}^2}{2(1+\beta)} - \frac{\phi_{cc}{}^4}{4(1+\beta)^3}\right] X^2 + \frac{\phi_{cc}{}^4}{(1+\beta)^3}\frac{X^4}{24} \tag{15}$$

The effectiveness factor is:

$$\eta(\phi_{cc}, \beta) = \left[1 - \frac{\phi_{cc}{}^2}{3(1+\beta)^2}\right] \tag{16}$$

4. NUMERICAL SIMULATION:

The diffusion equation (9) for the boundary conditions (Eqs. (11) and (12)) are also solved numerically. We have used the function pdex4 in SCILAB software to solve numerically the initial-boundary value problems for parabolic-elliptic partial differential equations. This numerical solution is compared with our analytical result in Figs. (1) and (2). Upon comparison, it gives a satisfactory agreement for all values of the reaction/diffusion parameter $\phi_{cc}{}^2$ and the saturation parameter β.

5. DISCUSSION:

5.1 Concentration profile:

The kinetic response of a multi-phase microchannel bioreactor depends on the concentrations of oxygen. The concentrations of oxygen depends on the following two factors $\phi_{cc}{}^2$, β. Thiele modulus ϕ^2, represents the ratio of the characteristic time of the enzymatic reaction to that of substrate diffusion. The variation in the Thiele modulus $\phi_{cc}{}^2$ can be achieved by varying either the thickness of the enzyme layer or the amount of enzyme immobilized in the multi-phase microchannel bioreactor. The Thiele modulus $\phi_{cc}{}^2$ is indicative of the competition between the diffusion and

reaction in the enzyme layer. When $\phi_{cc}^{\ 2}$ is small, the kinetics dominate and the uptake of oxygen in the multi-phase microchannel bioreactor is kinetically controlled. Under these conditions, the substrate concentration profile across the membrane is essentially uniform. The overall kinetics are governed by the total amount of active enzyme. Diffusion limitations are the principal determining factor when Thiele modulus is large.

Figs. 1(*a*)-(*d*) and 2(*a*)-(*d*) represent the normalized steady state substrate dissolved oxygen concentration U in the nono-porus cellcoat. The concentration of substrates were calculated for the various values of saturation parameter values β and reaction diffusion parameter $\phi_{cc}^{\ 2}$ respectively using the (Eq 10). From the figures 1(*a*)-(*d*), it is evident that when the value concentration decreases when $\phi_{cc}^{\ 2}$ increases. The concentration of oxygen *U* equal to 1 when $\phi_{cc}^{\ 2} \le 0.01$ and *U* becomes zero when $\phi_{cc}^{\ 2} > 180$ for all values of parameters. From the figure 2(*a*)-(*d*), it is observed that the oxygen concentration *U* increases when the saturation parameter value β increases. We can conclude that the results are in satisfactory agreement with simulation results for all possible values of β and $\phi_{cc}^{\ 2}$.

5.2 Effectiveness factor:

The variation in effectiveness factor η is obtained for various values of β is shown in Figs. 3 and 4. From these figures, it is evident that the effectiveness factor decreases when the saturation parameter β increases.

5.3 Volumetric formation rate:

Figs. 5 and 6, represents the L-sorbose volumetric formation rate r_p. These figures are computed using the Equation 2. The formation rate r_p increases when the active G.oxydans concentration X_{cat} increases for all the values of rate constant. In fig. 6 volumetric formation rate r_p decreases as Michaelis-Menten constant for oxygen K_0 increases.

6. CONCLUSIONS:

We have presented a theoretical model describing the process of reaction and diffusion of steady state elemental balance for oxygen concentration in the nano-porous latex cellcoat. We have derived the transport and kinetics in terms of the reaction/diffusion parameter $\phi_{cc}^{\ 2}$ and the saturation parameter β. An approximate analytical expressions of substrate concentration profile for all possible values of the reaction/diffusion parameter $\phi_{cc}^{\ 2}$ and the saturation parameter β are derived using Adomian decomposition method. Our approximate analytical results offer more advantages over traditional methods for an efficient operation on multiphase microchannel bioreactor. Information gained from this theoretical model is providing basis for engineering of channel geometry, channel coating, reactive density, coating stability and nano-porosity, multi-phase channel properties and thickness for monolithic microchannel bioreactors. Further based on the outcome of this work. It is possible to extend the procedure to improve the vitrification of the carbohydrates in the pore space to a uniform glassy state which stabilizes the viability of the entrapped G.oxydans at ambient temperature during drying. Moreover, we have also presented an analytical expression for the steady-state effectiveness factor.

ACKNOWLEDGEMENT:

This work was supported by the Department of Science and Technology (DST), Government of India. The authors are grateful to Dr. R. Murali, The Principal, The Madura College, Madurai, and Mr. M. S. Meenakshi sundaram, The Secretary, The Madura College Board, Madurai, for their encouragement. We thank the reviewers for their valuable coments to improve the quality of the manuscript

APPENDIX A:

Basic concept of the Adomian decomposition metho (ADM)

Adomian decomposition method depends on decomposing the non-linear differential equation

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

into the two components

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

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

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

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

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

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

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

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

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

where the Adomian polymomials A_n of *N*(y) are evaluated using the formula:

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

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

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

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

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

However, in practice all the terms of series in Eq. (A. 7) cannot be determined, and the solution is approximated by the truncated series $\sum_{n=0}^{N} y_n$. 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 concentration of dissolved oxygen in the nano-porous latex cellcoat

The solution of Eq. (10) allows us to predict the concentration profiles of the oxygen. To solve Eq. (10) using the Adomian decomposition method, we write the Eq. (10) in the operator form,

$$LU = \phi_{cc}{}^2 \frac{U}{(1+\beta U)} \text{ where } L = \frac{d^2}{dX^2} \tag{B. 1}$$

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

$$U(X) = AX + B + \phi_{cc}{}^2 \frac{U}{(1+\beta U)} \tag{B. 2}$$

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

$$U(X)=\sum_{n=0}^{\infty}U_n \tag{B. 3}$$

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

Where $N[U(X)]=\frac{U}{(1+\beta U)}$ (B. 5)

In view of Eqs. (B. 3), (B. 4) and (B. 5), Eq. (B. 2) gives

$$\sum_{n=0}^{\infty}U_n(X)=AX+B+{\phi_{cc}}^2\frac{U}{(1+\beta U)} \tag{B. 6}$$

We identify the zeroth component as

$$U_0(X)=AX+B \tag{B. 7}$$

and the remaining components as the recurrence relation

$$U_{n+1}={\phi_{cc}}^2L^{-1}A_n\;;\; n\geq 0 \tag{B. 8}$$

where A_n are the Adomian polynomials of $U_0,U_1,\ldots,U_n$

We can find the first few A_n as follows:

$$U_0(X)=1 \tag{B. 9}$$

$$U_1(X)=\frac{{\phi_{cc}}^2}{2(1+\beta)}\left[X^2+1\right] \tag{B.10}$$

$$U_2(X)=\frac{{\phi_{cc}}^2}{2(1+\beta)^3}\left[\frac{X^4}{12}-\frac{X^2}{2}\right]+\frac{5}{24}\frac{{\phi_{cc}}^2}{(1+\beta)^3} \tag{B. 11}$$

Adding (B. 9) to (B. 11) we get the oxygen concentration in the nano-porous latex cellcoat Eq.(13) in the text.

APPENDIX C:

```
function pdex1
m = 0;
x = linspace(0,1);
t = linspace(0,10000);
sol = pdepe (m,@pdex1pde,@pdex1ic,@pdex1bc,x,t);
% Extract the first solution component as u.
u = sol (,1);
figure
plot(x,u(end,:))
xlabel ('Distance x')
ylabel ('u(x, 2)')
% ---------------------------------------------------------------
function [c,f,s] = pdex1pde(x,t,u,DuDx)
c = 1;
f = DuDx;
r=;
a=;
s =-(r*u)/((1+(u*a)));
% ---------------------------------------------------------------
function u0 = pdex1ic(x)
u0 = 0;
```

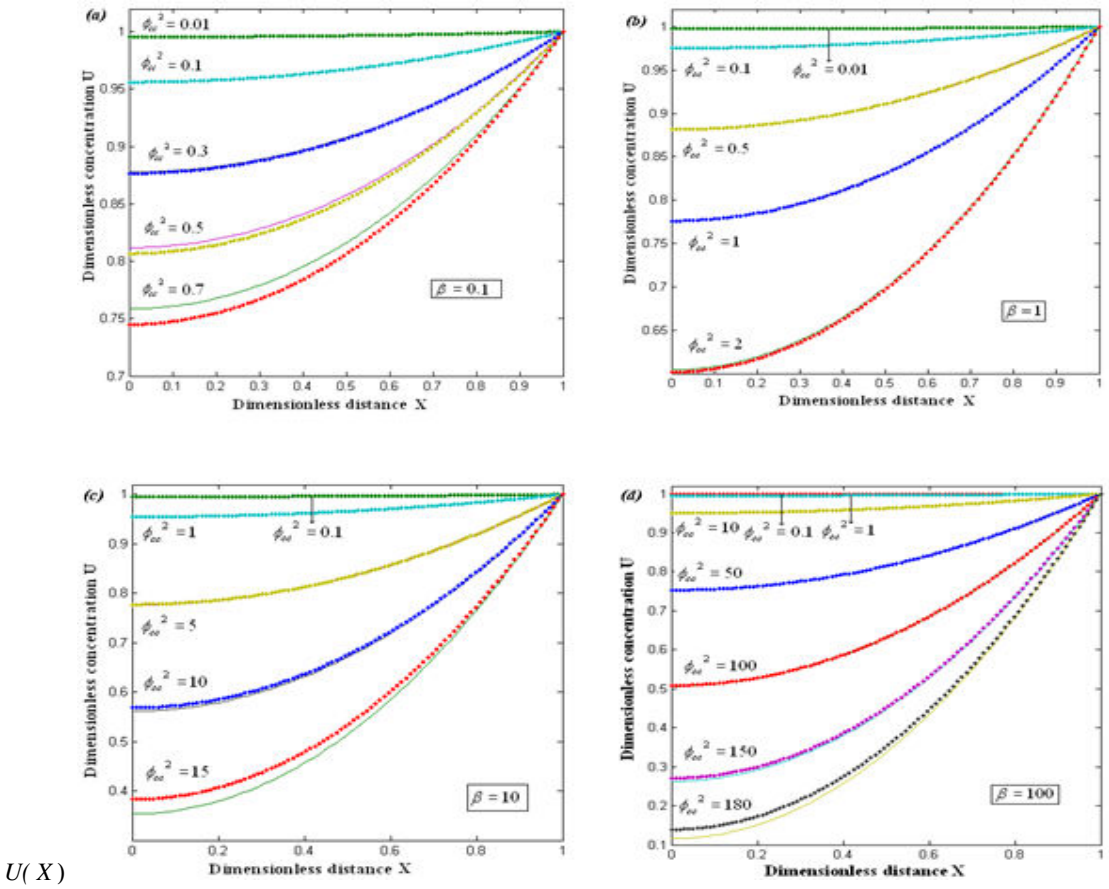


```
% ------------------------------------------------------------------
function [pl,ql,pr,qr] = pdex1bc(xl,ul,xr,ur,t)
pl = 0;
ql = 1;
pr = ur-1;
qr = 0;
```

APPENDIX D:

Nomenclature

D_{eff}	oxygen effective diffusity ($m^2\ s^{-1}$)
c	dissolved oxygen concentration ($g\ l^{-1}$)
K_{cat}	reaction rate constant ($mol\ CFU^{-1}\ s^{-1}$)
X_{cat}	G.*oxydans* cell density in the cellcoat ($CFU\ m^{-3}$)
K_o	Michaelis-Menten constant for oxygen ($m\ g\ l^{-1}$)
$Y_{P/0}$	yield coefficient of L-sorbose on oxygen (dimensionless)
L_{cc}	cellcoat thickness (m)
η	effectiveness factor (dimensionless)
ϕ	Thiele modulus (dimensionless)
β	dimensionless oxygen concentration in the coating (C_0 / K_0) (dimensionless)
L_{TC}	topcoat thickness (m)



$U(X)$

Figure: 1(*a*)–(*d*): Normalised concentration profile $U(X)$ as a function of dimensionless parameter $X = x / L_{cc}$. The concentrations were computed using Eq. (11) for various values of the $\phi_{cc}^{\ 2}$ and for the values **(*a*)** $\beta = 0.1$ **(*b*)** $\beta = 1$ **(*c*)** $\beta = 10$ **(*d*)** $\beta = 100$.(——) denotes Eq. (11) and (●●●) denotes the numerical simulation.

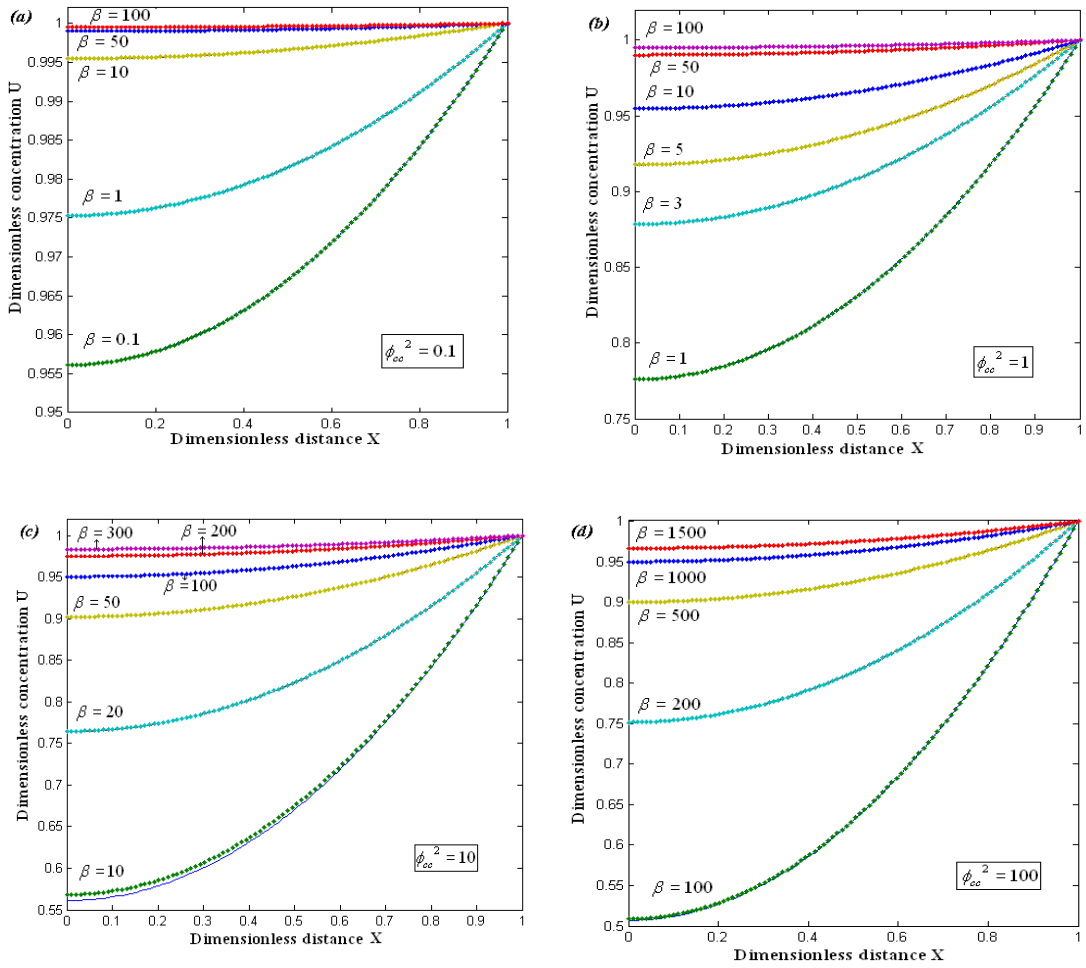
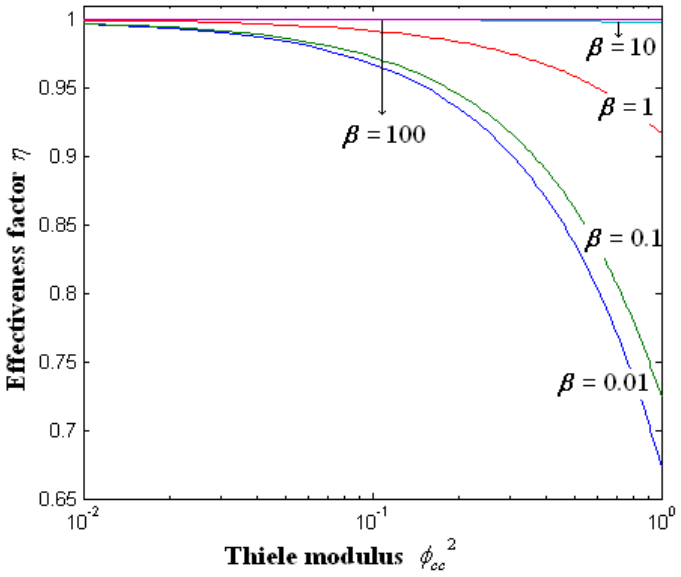


Figure: 2(a)–(*d*): Normalised concentration profile $U(X)$ as a function of dimensionless parameter $X = x / L_{cc}$. The concentrations are computed using Eq. (11) for various values of the β and for the values (a) $\phi_{cc}^2 = 0.1$ (b) $\phi_{cc}^2 = 1$ (c) $\phi_{cc}^2 = 10$ (d) $\phi_{cc}^2 = 100$. (——) denotes Eq. (11) and (●●●) denotes the numerical simulation.



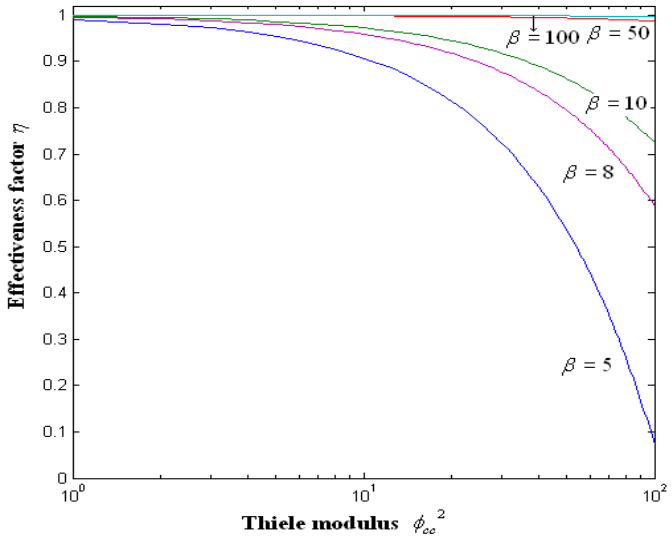


Figure: 3 & 4: The effectiveness factor η as a function of Thiele modulus $\phi_{cc} = L_{cc}\sqrt{\frac{k_{cat} X_{cat}}{K_0 Y_{P/0} D_{eff.cc}}}$. The effectiveness factor were computed using Eq.(14) for various values of the β by fixing $\phi_{cc}^2 = 0-100$ and $\phi_{cc}^2 = 0-1$.

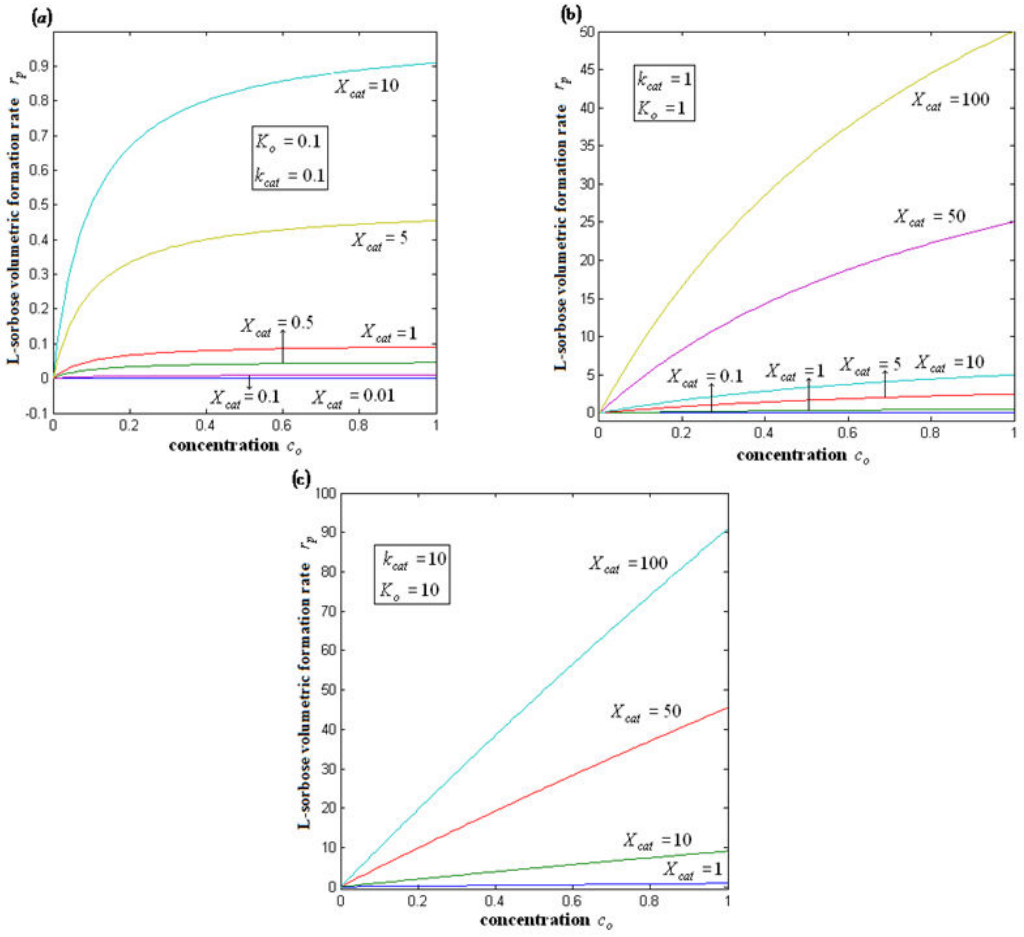


Figure: 5(*a*)-(*c*): The L-sorbose formation rate, r_p plotted as a function of the concentration C_0. The L-sorbose formation rate were computed using Eq. 2 for various values of the rate constant for L-sorbose k_{cat} and for the Michaelis–Menten constant K_0 (*a*) $X_{cat} \geq 0.01$, (*b*) $X_{cat} \geq 0.1$, and (*c*) $X_{cat} \geq 1$.

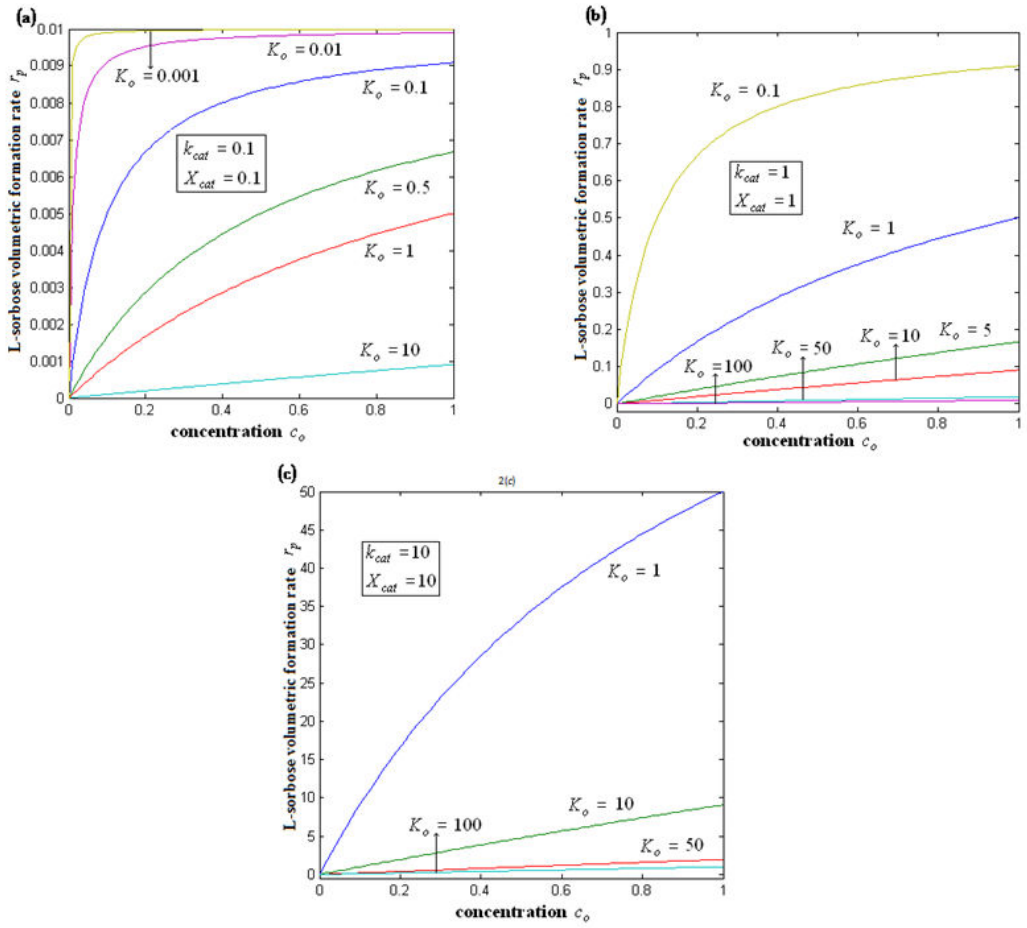


Figure: 6(*a*)-(*c*): The L-sorbose formation rate, r_p plotted as a function of the concentration C_0. The L-sorbose formation rate were computed using Eq. 2 for various values of the rate constant for L-sorbose k_{cat} and for the active G. oxydans concentration X_{cat} (*a*) $K_0 \geq 0.001$, (*b*) $K_0 \geq 0.1$, and (*c*) $K_0 \geq 1$.

REFERENCES:

[1] Adomian, G., Convergent series solution of nonlinear equations, J. Comp. App. Math. 11 (1984) 225-230.

[2] Fidaleo, M., Flickinger, M.C., Engineering and modeling of thin, adhesive, microbial biocatalytic coatings for high intensity oxidations in multi-phase microchannel bioreactors, Chemical Engineering Science 66 (2011), 3251-3257.

[3] Fidaleo, M., Charaniya ,S., Solheid, C., Diel, U., Laudon, M., Ge,H., Scriven, L.E., Flickinger, M.C., A model system for increasing the intensity of whole-cell biocatalysis: investigation of the rate of oxidation of D-sorbitol to L-sorbose by thin bi-layer latex coatings of non-growing gluconobacter oxydans, Biotechnology and Bioengineering 95, (2006), 446–458.

[4] Michiel T. Kreutzer , Freek Kapteijn, Jacob A. Moulijn., Fast gas–liquid–solid reactions in monoliths: A case study of nitro-aromatic hydrogenation, Catalysis Today 105 (2005) 421–428.

[5] Mohamed, M. A., Comparison Differential Transformation Technique with Adomian Decomposition Method for Dispersive Long-wave Equations in (2+1)-Dimensions, Appl. Appl. Math. 5 (2010) 148-166.

[6] Omar K. Jaradat, Adomian decomposition method for solving Abelian Differential Equations, J. Appl. Sci. 8 (2008) 1962-1966.

[7] Patel, A., Sergio E. Serrano, New approaches to the propagation of nonlinear transients in porous media, J. Hydrology 397 (2011) 202-209.

[8] Siddiqui, A.M., M. Hameed, B.M. Siddiqui, Q.K. Ghori, Use of Adomian decomposition method in the study of parallel plate flow of a third grade fluid, Commun Nonlinear. Sci. Numer. Simulat.15 (2010) 2388- 2399.

[9] Venkata S. Thiagarajan, Zhisong Huang, L. E. Scriven, Janet L. Schottel, and Michael C. Flickinger, Microstructure of a Biocatalytic Latex Coating Containing Viable Escherichia coli Cells, Journal of Colloid and Interface Science 215 (1999) 244–257.

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