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MATHEMATICAL MODELING FOR SOLVING NONLINEAR BOUNDARY VALUE PROBLEM FOR THE PHENOL HYBRID BIO REACTOR

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Abstract. This research article focuses on the mathematical model for phenol concentration and the approximate analytical solution is brought out for the analytical expression of concentration of phenol in hybrid bioreactor for the treatment of wastewater and effectiveness of the factors pertaining to hybrid bioreactor were discussed .The model is based on system of reaction diffusion equation containing a non linear term related to the specific growth rate of biomass. A new approach of the Homotopy perturbation method is successfully employed in the development of non linear steady state phenol concentration. Our analytical results are compared with the numerical simulation and a satisfactory agreement is arrived.

Key Words: Chemical reaction; Bioreactor; Diffusion equation; Biomass; Non-linear ordinary differential equations; New Homotopy.

1. Introduction

Chemical and petroleum industries generate a wide variety of higher toxic organic wastes. The effluents of these industries often contain aromatic compounds that are resistant to natural degradation and therefore persist in the environment. One of the major organic pollutants found in these waste waters is phenol. Process industries, which are major sources of phenolic discharges, are petroleum refineries, coal carbonization units, gas and coke industries and fiberglass units [1].

Madhuri et al. [2] has been chosen hybrid treatment system work, because of its potential to reduce investment costs through the use of cheaper local media and also its flexibility to deal with almost all kinds of waste water. An anaerobic hybrid reactor (AHR) which combines advantages of both anaerobic filter and up flow anaerobic sludge blanket designs, operates with a sludge blanket in the lower zone and packing media forming a filter in the upper zone, was first developed by Maxham and Wakamiya in 1981.Biological waste water treatment based on microorganisms or their aggregates is a widely applied environmental-friendly method in waste water treatment and can be divided into aerobic and anaerobic treatment processes according to the relationship between microorganisms and oxygen. It can also be divided into activated. Sludge and biofilm treatment processes based on microbial suspension or fixation in treatment facilities [3-5]. Phenol which is a significant industrial feed found in myriad industrial products are produced mainly from fossil fuels. Phenol resins are typically cross-linked polymeric resins, and because phenol price and availability are linked to that of petroleum, industrial products using phenol as feed such as phenol-formaldehyde or phenol resins are relatively expensive. Attempts have been made to substitute petroleum-based phenol in phenol resins with cost effective phenols derived from lingo cellulosic materials. Phenols are priority pollutants because they are harmful to organisms at low concentrations, and many of them have been classified as hazardous pollutants because they are harmful to human health [6, 7]. Araujo et al. [8] studies was to evaluate the anaerobic treatment of waste water from the household and personal products industry in a hybrid bioreactor containing immobilized microorganisms as granular sludge and biofilm and to determine the feasibility of applying this process on a commercially successful basis. Mazumder et al.[9] to increase the treatment capacity of activated sludge process by making it shaft-type reactor with the addition of some inert carrier materials and also developed applying the tyre tube beads as bio-carriers to evaluate the performance for carbonaceous oxidation. Xia et al. [10] analyzed whether the microorganism would maintain bioactivity degrading phenol or change under UV irradiation. Mohammad et al. [11] investigated two dimensional incompressible flow and mass transfer in a lid driven cavity of annular geometry accompanied by enzymatic surface reactions. Recently, Sudipta et al. [12] has developed a mathematical model to study the biological treatment of wastewater using biofilm. To the best of our knowledge, no rigorous analytical solutions for the steady state concentration of phenol and the effectiveness factor for hybrid bioreactor for all values of the parameters have been published. The purpose of this chapter is to evaluate the steady-state substrate concentration and effectiveness factor for all values of diffusion parameter $\boldsymbol{\varphi^2}$ and the saturation parameter $\boldsymbol{\beta}$ using new approach of Homotopy perturbation method.

2. Mathematical formulation of the problem

The general equation of mass transfer of substrate in biofilm are described by the following nonlinear equation [12]

$$D_{fz}\frac{d^2S}{dZ^2}+\zeta\frac{ds}{dz}=\frac{\mu_{max}SX_{av}}{Y_{x/s}(K+S)} \quad (1)$$

Where effective diffusivity gradient $\zeta = dD_{fz}/dZ$ and D_{fz} is the diffusivity of the substrate in biofilm in the Z-direction. D_{fav} , X_{av} are average diffusivity and biofilm concentration respectively. μ_{max} is the specific growth rate, $Y_{x/s}$ is the yield coefficient, K is the substrate concentration at which specific substrate degradation rate is half. We introduce following set of dimensionless variables,

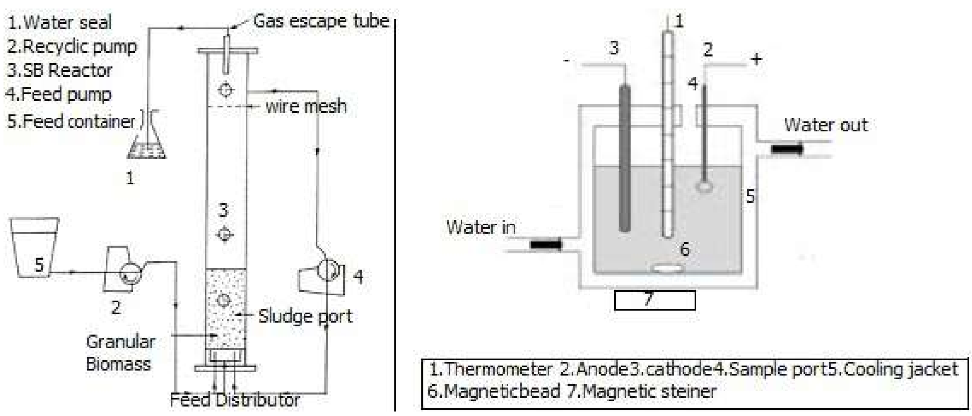

Fig.1.Schematic diagram of reaction set up

$$Z^* = \frac{Z}{L_f}, S^* = \frac{S}{S_s}, \alpha = \frac{\zeta S_s}{D_{fz} L_f}, \beta = \frac{K}{S}, \varphi = \sqrt{\frac{\mu_{max} L_f^2 X_{av}}{Y_{x/s} S_s D_{fav}}} \quad (2)$$

Where L_f is biofilm thickness, S_s and S are phenol concentration at the surface of biofilm and within the biofilm. Z^* is the dimensionless distance and S^* is the dimensionless substrate concentration, α and β are relation diffusion and saturation parameters respectively. By using these dimensionless parameters,The following nonlinear Equation $\frac{du}{dx} = u^2$ can be reduced to dimensionless form as follows:

$$\frac{d^2 S^*}{dZ^{*2}} + \alpha \frac{dS^*}{dZ^*} = \varphi^2 \frac{S^*}{\beta + S^*} \quad (3)$$

The boundary conditions are

$$Z^* = 1, S^* = 1 \quad (4)$$

$$Z^* = 0, \frac{dS^*}{dZ^*} = 0 \quad (5)$$

The dimensionless effectiveness factor is [12],

$$\eta = \frac{(\beta+1)}{\varphi^2} \left(\frac{dS^*}{dZ^*}\right)_{at\, Z^*=1} \quad (6)$$

3. Anaytical expressions of the concentrations and

Effectiveness factor

By solving Eqn. (3), using new approach of Homotopy perturbation method [13-18], the analytical expression for the concentration of phenol is obtained as follows:

$$S^*(Z^*) = \frac{\exp(aZ^*) + (a/b)\exp(-bZ^*)}{\exp(a) + (a/b)\exp(-b)} \quad (7)$$

Where: $\mathbf{a} = \frac{-\alpha + \sqrt{\alpha^2 + 4(\phi^2/(\beta+1))}}{2}$ and $\mathbf{b} = \frac{\alpha + \sqrt{\alpha^2 + 4(\phi^2/(\beta+1))}}{2}$ (8)

Using Eqn. (6), the dimensionless effectiveness factor is,

$$\eta = \frac{ab(\beta+1)}{\varphi^2} \left[\frac{\exp(a) - \exp(-b)}{b\exp(a) + a\exp(-b)} \right] \quad (9)$$

4. Limiting case

4.1 Zero order kinetics

In this case, the dimensions substrate concentration $\mathbf{S}^*$ is greater than Monod half rate constant β. When $\beta \ll S^*$, Eqn. (3) reduces to

$$\frac{d^2S^*}{dZ^{*2}} + \alpha\frac{dS^*}{dZ^*} - \varphi^2 = 0 \qquad (10)$$

By solving the Eqn. (10), we obtain the concentration of substrate as follows:

$$S^*(Z^*) = C_3 e^{m_1 Z^*} + C_4 e^{-m_2 Z^*} \qquad (11)$$

Now by using the boundary conditions (Eqn. 4 and Eqn. 5), we can obtain constants as follows

$$C_3 = \frac{m_2}{m_1 e^{-m_2} + m_2 e^{m_1}} \qquad (12)$$

$$C_4 = C_3 \frac{m_1}{m_2} \qquad (13)$$

Now the effectiveness factor becomes as follows:

$$\eta = \left(\frac{\beta+1}{\varphi^2}\right)\left(\frac{ds^*}{dZ^*}\right)_{Z^*=1} = \left(\frac{\beta+1}{\varphi^2}\right)\left(C_3 m_1 e^{m_1} - C_4 m_2 e^{-m_2}\right) \qquad (14)$$

4.2 First order kinetics

In this case, the dimensionless substrate concentration is less than Monod half rate constant β. When $\beta \ll S^*$, Eqn. (3) reduces to

$$\frac{d^2S^*}{dZ^{*2}} + \alpha\frac{dS^*}{dZ^*} - \frac{\varphi^2 S^*}{\beta} = 0 \qquad (15)$$

By solving the Eqn. (15), we obtain the concentration of substrate as follows:

$$S^*(Z^*) = C_1 e^{n_1 Z^*} + C_2 e^{n_2 Z^*} \qquad (16)$$

Now by using the boundary conditions (i.e.) Eqn. (4) and Eqn.(5), we can obtain constants,

$$C_2 = [e^{n_2} - (n_2/n_1)e^{n_1}]^{-1} \qquad (17)$$

$$C_1 = -C_2\left(\frac{n_2}{n_1}\right) \qquad (18)$$

$$\eta = \left(\frac{\beta+1}{\varphi^2}\right)\left(\frac{dS^*}{dZ^*}\right)_{Z^*=1} = \left(\frac{\beta+1}{\varphi^2}\right)(C_1 n_2 e^{n_2} + C_2 n_1 e^{n_1}) \qquad (19)$$

5. Homogeneous biofilm

For the homogeneous biofilm (where $\alpha = 0$ or $\zeta = 0$ or $a = b$), Eqn. (3) is simplified to the form

$$\frac{d^2S^*}{dZ^{*2}} = \varphi^2 \frac{S^*}{\beta + S^*} \qquad (20)$$

The analytical expressions for the concentration from Eqn. (20) as follows:

$$S^*(Z^*) = \frac{\cosh\left(\sqrt{\varphi^2/(\beta+1)Z^*}\right)}{\cosh\left(\sqrt{\varphi^2/(\beta+1)}\right)} \tag{21}$$

The dimensionless effectiveness factor is,

$$\eta = \frac{(\beta+1)}{\varphi^2}\left(\frac{dS^*}{dZ^*}\right)_{\text{at } Z^*=1} = \sqrt{\frac{\beta+1}{\varphi^2}}\ \tanh\left(\sqrt{\varphi^2/(\beta+1)}\right) \tag{22}$$

5.1 First order kinetics for homogeneous biofilm

In this case, the dimensionless substrate concentration is less than Monod half rate constant β, When $\beta \gg S^*$, Eqn. (20) reduce to

$$\frac{d^2S^*}{dZ^{*2}} - \frac{\varphi^2 S^*}{\beta} = 0 \tag{23}$$

Now the equation of substrate becomes,

$$S^*(Z^*) = \frac{\cosh\left(\sqrt{\varphi^2/\beta}Z^*\right)}{\cosh\left(\sqrt{\varphi^2/\beta}\right)} \tag{24}$$

The dimensionless effectiveness factor is,

$$\eta = \frac{(\beta+1)}{\varphi^2}\left(\frac{dS^*}{dZ^*}\right)_{\text{at } Z^*=1} = \left(\frac{\beta+1}{\varphi\sqrt{\beta}}\right)\tanh\left(\sqrt{\varphi^2/\beta}\right) \tag{25}$$

5.2 Zero order kinetics for homogeneous biofilm

In this case, the dimensionless substrate concentration is greater than Monod half rate constant β, when $\beta \ll S^*$ Eqn. (20) reduces to

$$\frac{d^2S^*}{dZ^{*2}} - \varphi^2 = 0 \tag{26}$$

Now the concentration $\mathbf{S}^*$ becomes,

$$S^*(Z^*) = \frac{\cosh(\varphi Z^*)}{\cosh(\varphi)} \tag{27}$$

Analytical expression for effectiveness factor is,

$$\eta = \frac{(\beta+1)}{\varphi^2}\left(\frac{dS^*}{dZ^*}\right)_{\text{at } Z^*=1} = \left(\frac{\beta+1}{\varphi}\right)\tanh(\varphi) \tag{28}$$

6. Numerical simulation

The non-linear differential equation (20) for the given initial- boundary conditions is being solved numerically. The function pdex, in MATLAB software which is a function of solving the initial-boundary value problems for non-linearOrdinary differential equations are used to solve this equation. Its numerical solution is compared with analytical results using new approach of Homotopy perturbation method and it gives a satisfactory result. The MATLAB program is also given in Appendix 1.B.

7. Result and discussion

The approximate analytical expressions of concentration of substrate and effectiveness factor using new approach of Homotopy perturbation technique. Fig. 2 represents the dimensionless concentration of substrate S^* versus dimensionless distance Z^*. From this figure, it is confirmed that for all large values of β the concentration of substrate reaches constant level. The concentration increases when saturation parameter β increases. From Fig. 3 we can see that the value of the concentration S^* increases when α increases. The concentration of substrate S^* increases slowly and rises abruptly when $Z^* \geq 0.3$ and all values ofa.

Fig.4 describes the dimensionless concentration S^* versus dimensionless distance Z^* for various values of φ. The concentration profile within the biofilm is plotted. The phenolic substrates penetrated to the whole depth, did not reduce to zero concentration in the biofilm which indicated that increase in diffusion rate was higher than the increase in rate of reaction. It was also observed that, the substrate concentration at the innermost layer of biofilm ($Z^* = 0$) was lowest for total influent phenolic concentration. Therefore it can be concluded that at low concentration of influent substrate, the culture consumed the substrate quickly showing low S^* value within the biofilm. The concentration decreases when the Thiele modulus increases.Effectiveness factor η versus Thiele modulus φ is plotted in Fig.5(a)-5(f).

From Fig. 5(a)-5(f), it is evident that the value of the effectiveness factor decreases when β decreases and effectiveness factor decreases when α increases. From Fig. 6(a)-6(f), it is evident that the effectiveness factor increases when α decreases and effectiveness factor increases φ decreases. From Fig. 7(a)-7(c), it is inferred that, the value of the effectiveness factor increases β increase and effectiveness factor increases φ decreases.

8. Conclusion

In this paper the analytical expression of concentration $\mathbf{S}^*(\mathbf{Z}^*)$ is reported. The primary result of this work is simple approximate calculations of dimensionless concentration $\mathbf{S}^*(\mathbf{Z}^*)$ for different values of parameters. This is an extremely simple method and it is also a promising method to solve the non-linear equations. This method can be easily extended to all kinds of non-linear equations.

9. Appendix A:

In this appendix, we derive the solution of non-linear equation (3) using new Homotopy perturbation method.

The Homotopy for the non-linear equation (3) can be constructed as follows:

$$(1-p)\left\{\frac{d^2S^*}{dZ^{*2}} + \alpha\frac{dS^*}{dZ^*} - \frac{\phi^2S^*}{\beta+1}\right\} + p\left\{\alpha\frac{d^2S^*}{dZ^{*2}} + S^*\frac{d^2S^*}{dZ^{*2}} + \alpha\beta\frac{dS^*}{dZ^*} + \alpha S^*\frac{dS^*}{dZ^*} - \phi^2S^*\right\} = 0 \tag{A1}$$

Supposing the approximate solutions of Eq. (A1) has the form

$$S^* = S_0^* + pS_1^* + p^2S_2^* + \cdots \tag{A2}$$

Substituting Eq.(A2) into Eq. (A1) and equate the terms with the identical powers of p, we obtain

$$p^0: \frac{d^2S^*}{dZ^{*2}} + \alpha\frac{dS^*}{dZ^*} - \frac{\phi^2S^*}{\beta+1} = 0 \tag{A3}$$

$$p^1: \frac{d^2S_1^*}{dx^{*2}} + \alpha\frac{dS^*}{dZ^*} - \frac{\phi^2S_1^*}{\beta+1} + \frac{\beta\phi^2S_0}{\beta+1} + S_0^*\frac{d^2S_0^*}{dZ^{*2}} + \alpha S_0^*\frac{dS_0^*}{dZ^*} - \phi_s^2S_0^* = 0 \tag{A4}$$

The initial conditions are as follows:

$S_0^*(Z^* = 1) = 1;\ \frac{dS_0^*}{dZ^*}(Z^* = 0) = 0$ (A5)

$S_i^*(Z^* = 1) = 1;\ \frac{dS_i^*}{dZ^*}(Z^* = 0) = 0$ for all $i = 1,2,3,\ldots$ (A6)

Solving the Eq. (A3) using the boundary conditions Eq. (A5) gives the satisfactory result. Therefore, the solution of the substrate concentration as follows:

$$S_0^*(Z^*) = \frac{\exp(aZ^*)+(a/b)\exp(-bZ^*)}{\exp(a)+(a/b)\exp(-b)} \quad \text{(A7)}$$

Where $a = \frac{-\alpha+\sqrt{\alpha^2+4(\phi^2/(\beta+1))}}{2}$ and $b = \frac{\alpha+\sqrt{\alpha^2+4(\phi^2/(\beta+1))}}{2}$ (A8)

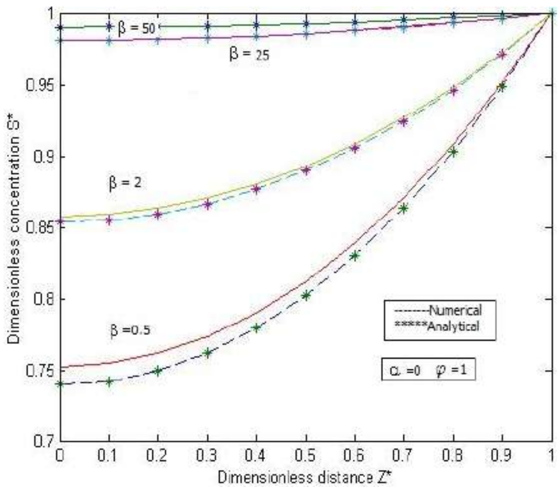

Fig.2.Plot the dimensionless concentration S* versus dimensionless distance Z* .The concentrations are computed by using Eqn.(7) for various values of β and some fixed values of parameters $\varphi = 1, \alpha = 0$

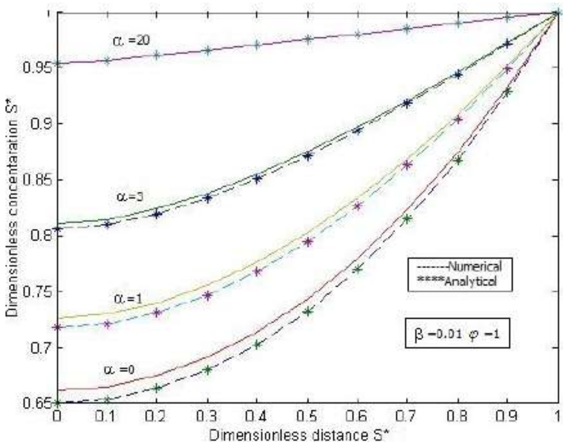

Fig.3.Plot the dimensionless concentration S* versus dimensionless distance Z* .The concentrations are computed by using Eqn.(7) for various values of φ and some fixed values of parameters $\varphi = 1, \beta = 0.01$

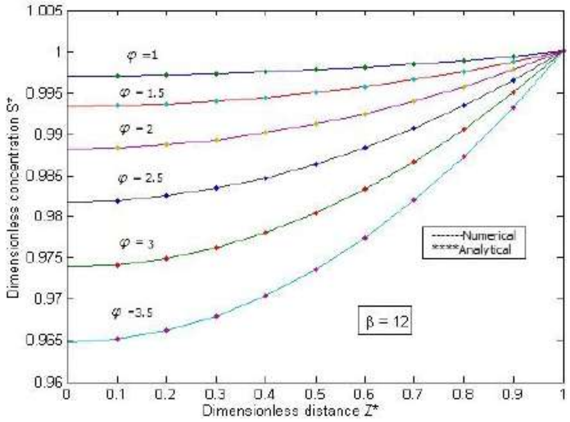

Fig.4(a).Plot the dimensionless substrate concentration S* versus dimensionless distance Z* .The concentrations are computed by using Eqn.(21) for various values of dimensionless parameters φ and some fixed values of parameters $\beta = 12$

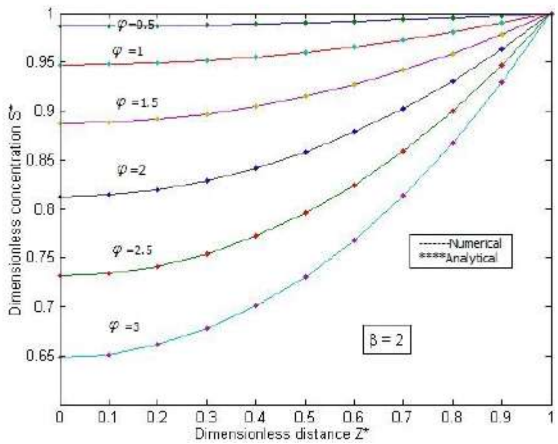

Fig.4(b).Plot the dimensionless substrate concentration S* versus dimensionless distance Z* .The concentrations are computed by using Eqn.(21) for various values of dimensionless parameters φ and some fixed values of parameters $\beta = 2$.

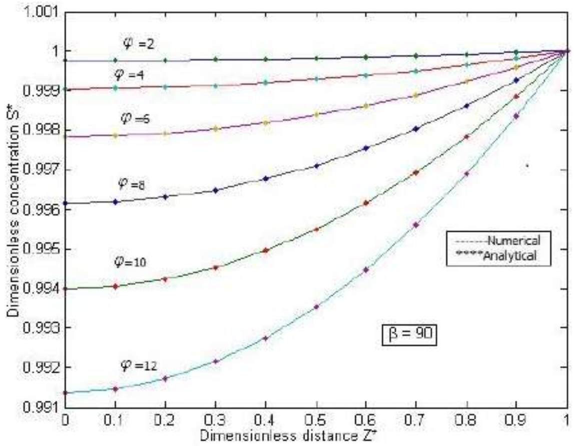

Fig.4(c).Plot the dimensionless substrate concentration S* versus dimensionless distance Z* .The concentrations are computed by using Eqn.(21) for various values of dimensionless parameters φ and some fixed values of parameters $\beta = 90$.

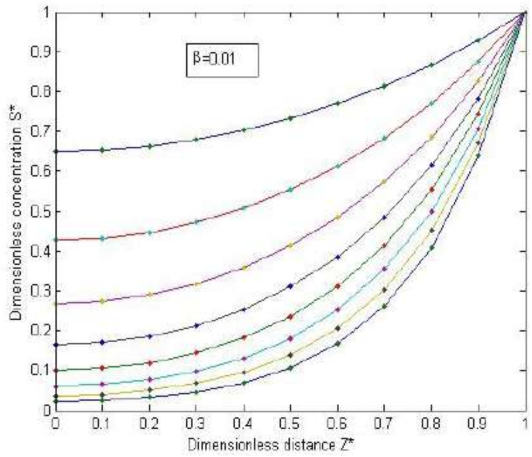

Fig.4(d).Plot the dimensionless substrate concentration S* versus dimensionless distance Z* .The concentrations are computed by using Eqn.(21) for various values of dimensionless parameters φ and some fixed values of parameters $\beta = 0.01$.

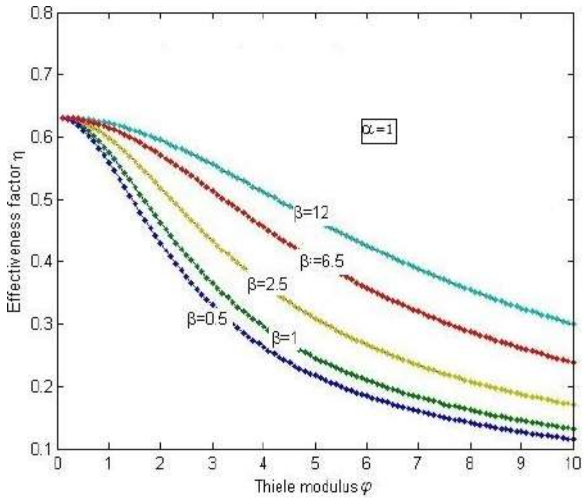

Fig5(a).The effectiveness factor η versus Thiele modulus φ is plotted.The effectiveness η is computed by (9) for various values of α

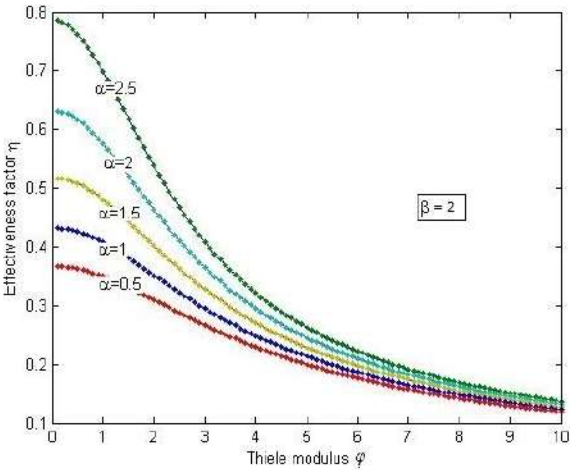

Fig.5(c).The effectiveness factor η versus Thiele modulus φ is plotted.The effectiveness η is computed by (9) for various values of β

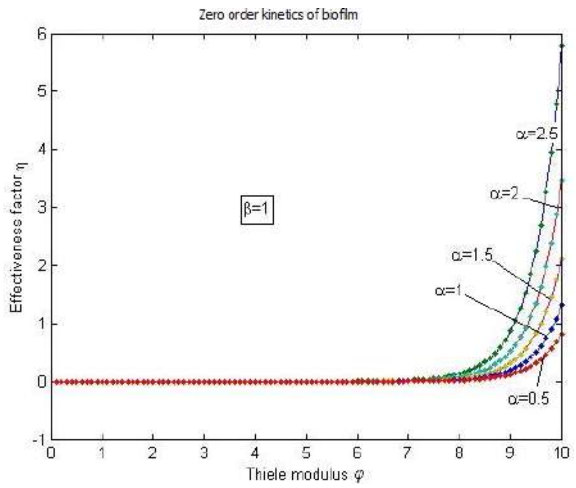

Fig5(c).The effectiveness factor η versus Thiele modulus φ is plotted.The effectiveness η is computed by (14) for various values of α

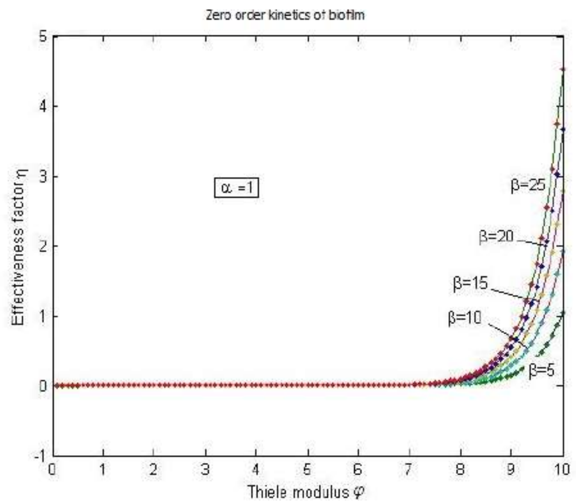

Fig.5(d).The effectiveness factor η versus Thiele modulus φ is plotted.The effectiveness η is computed by (14) for various values of β .

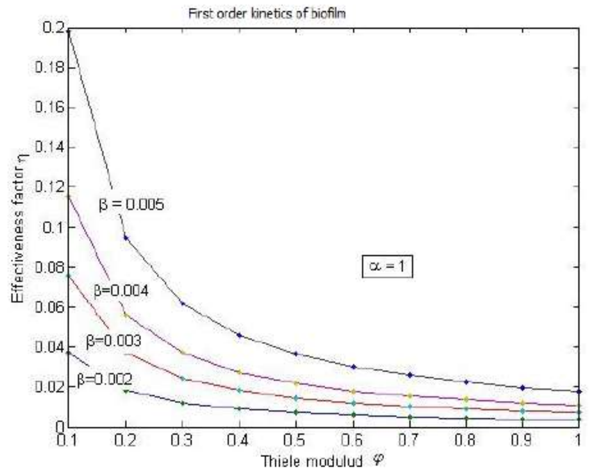

Fig5(e).The effectiveness factor η versus Thiele modulus φ is plotted.The effectiveness η is computed by (19) for various values of β .

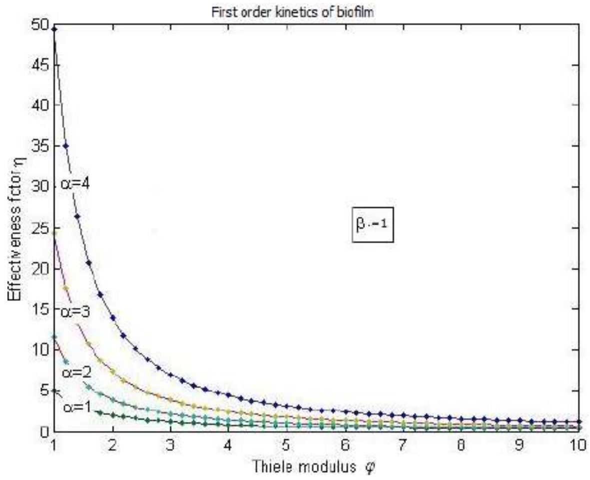

Fig.5(f).The effectiveness factor η versus Thiele modulus φ is plotted.The effectiveness η is computed by (14) for various values of α .

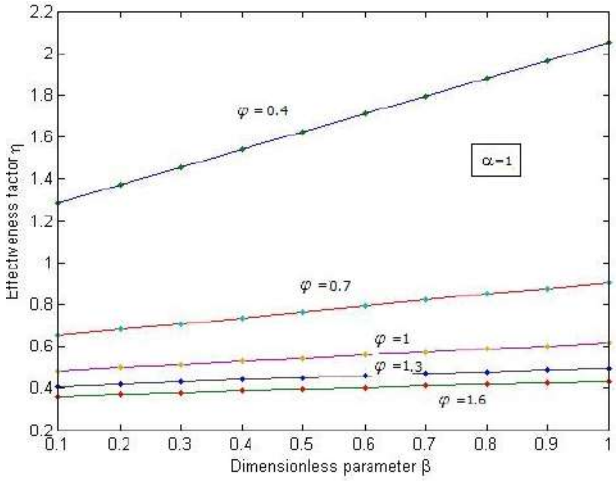

Fig6(a).The effectiveness factor η versus dimensionless parameter β is plotted.The effectiveness factor η is computed by (9) for various values of φ .

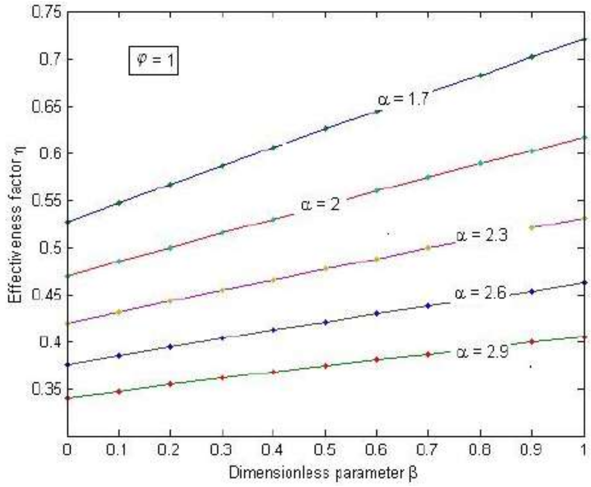

Fig.6(b).The effectiveness factor η versus dimensionless parameter β is plotted.The effectiveness factor η is computed by (9) for various values of α .

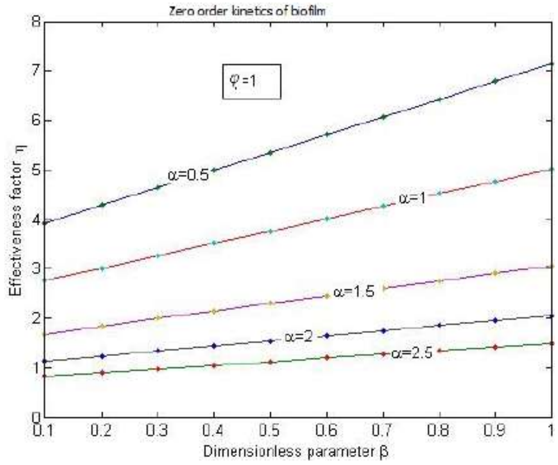

Fig.6(c).The effectiveness factor η versus dimensionless parameter β is plotted.The effectiveness factor η is computed by (14) for various values of φ.

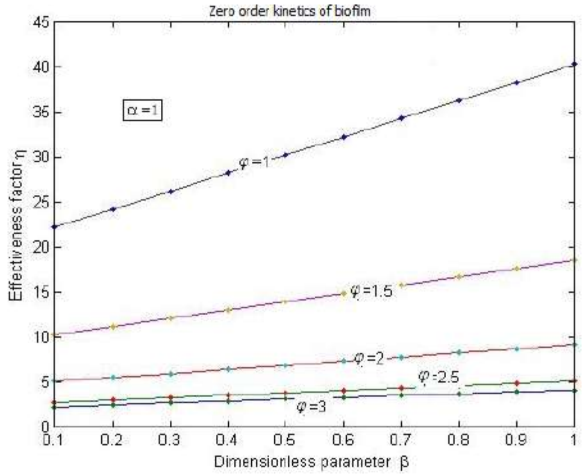

Fig.6(d).The effectiveness factor η versus dimensionless parameter β is plotted.The effectiveness factor η is computed by (14) for various values of α.

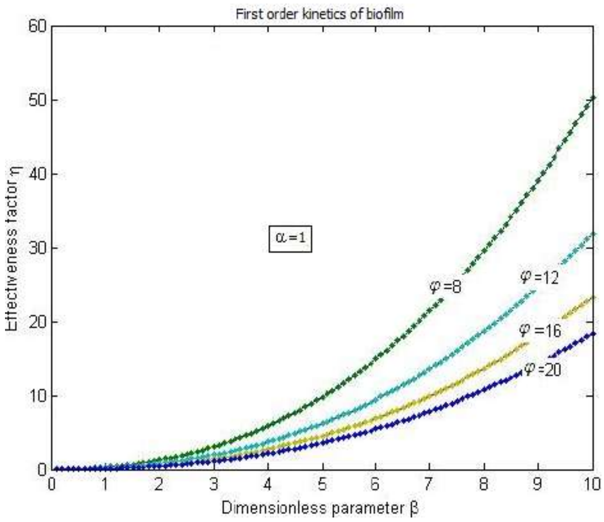

Fig.6(e).The effectiveness factor η versus dimensionless parameter φ is plotted.The effectiveness factor η is computed by (19) for various values of φ.

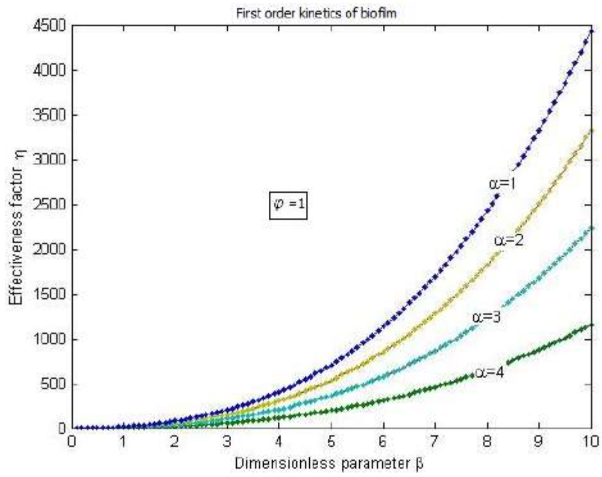

Fig.6(f).The effectiveness factor η versus dimensionless parameter β is plotted.The effectiveness factor η is computed by (19) for various values of α .

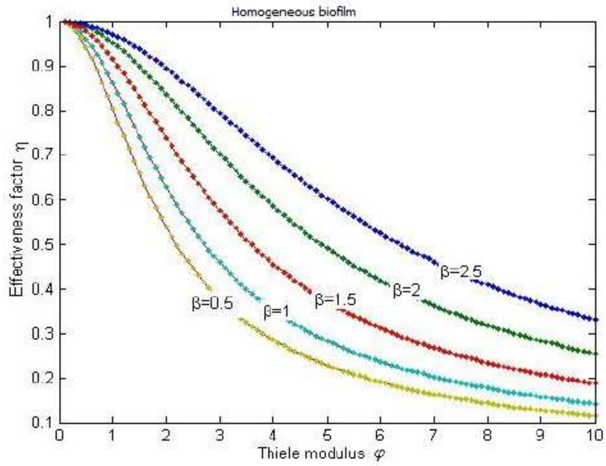

Fig.7(a).The effectiveness factor η versus Thiele modulus φ is plotted.The effectiveness factor η is computed by (22) for various values of β .

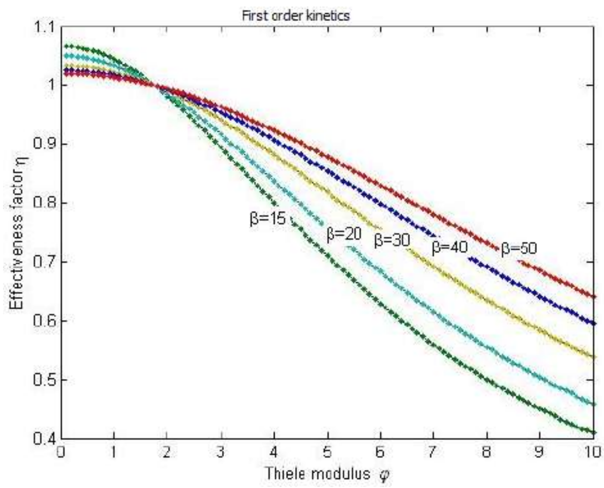

Fig.7(b).The effectiveness factor η versus Thiele modulus φ is plotted.The effectiveness factor η is computed by (25) for various values of β .

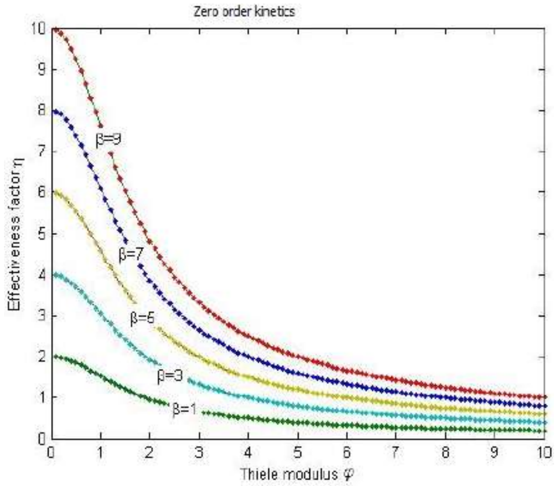

Fig.7(c).The effectiveness factor η versus Thiele modulus φ is plotted.The effectiveness factor η is computed by (28) for various values of β .

Table 1.1Nomenclatures

Symbols	Definitions	Units
D_{fav}	Average diffusivity in the biofilm	cm^2/day
D_{fv}	Diffusivity coefficient in the biofilm	m^2/sec
K	Substrate degradation rate	mg/L
J_f	Flux	kg/m^2day
L_f	Thickness of the biofilms	m
S	Substrate concentration	mg/L
S^*	Dimensionless substrate concentration	None
S_s	Substrate concentration at the biofilm surface	kg/m^3
S_f	Substrate concentration within the biofilm surface	kg/m^3
X_{av}	Average biofilm concentration	mg/L
$Y_{x/s}$	Yield coefficient	mg/L
Z	Distance	m
Z^*	Dimensionless distance	None

Table 1.2Greek Symbols

α	Dimensionless parameter	None
β	Dimensionless parameter	None
φ	Thiele Modulus	None
η	Effectiveness factor	None
μ_{max}	Maximum specific growth rate	day^{-1}

ζ	Effective diffusivity gradient	m^2/sec

CONSTANT PARAMETERS

$$m_1 = \frac{(-\alpha + \sqrt{\alpha^2 + 4\varphi^2})}{2}$$

$$m_2 = \frac{(\alpha + \sqrt{\alpha^2 + 4\varphi^2})}{2}$$

$$n_1 = \frac{(\alpha\beta + \sqrt{\beta^2\alpha^2 + 4\beta\varphi^2})}{2\beta}$$

$$n_2 = \frac{(\alpha\beta - \sqrt{\beta^2\alpha^2 + 4\beta\varphi^2})}{2\beta}$$

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