Alexandria Engineering Journal (2014) 53, 917–928

Alexandria University

Alexandria Engineering Journal

www.elsevier.com/locate/aej
www.sciencedirect.com

ORIGINAL ARTICLE

A new mathematical model for effectiveness factors in biofilm under toxic conditions

V. Meena [b], K. Indira [b], Sunil Kumar [a], L. Rajendran [b,*]

[a] Department of Mathematics, National Institute of Technology, Jamshedpur, Jharkhand, India
[b] Department of Mathematics, The Madura College, Madurai 625011, Tamil Nadu, India

Received 27 January 2014; revised 12 August 2014; accepted 4 September 2014
Available online 27 September 2014

KEYWORDS

Biofilms;
New approach to Homotopy perturbation method;
Mathematical modeling;
Non-linear reaction/diffusion equations;
Simulation

Abstract A mathematical model for biofilms inhibition for steady-state conditions is discussed. The model involves the reaction–diffusion equations which have variety of non-linear reaction rate functions for various types of inhibition. Simple and an approximate polynomial expression of concentration and effectiveness factor are derived for general non-linear monod kinetics models. Comparison of the analytical results and numerical simulation is also presented. A good agreement between theoretical predictions and numerical results is observed. The concentrations and the effectiveness factors are also computed for the limiting cases of monod kinetics models. The optimum value of the parameters for effectiveness factors is also discussed.

1. Introduction

Biofilms play a very important role in many scientific and technological areas. Consequently, they are studied in many disciplines. Biofilm research is a truly interdisciplinary research topic. A biofilm is a well-organized, cooperating community of microorganisms attached to an environmental surface [1–3]. These surfaces include biological tissues, water surfaces and solid substrates which can be located in marine or freshwater environments. These film-forming microorganisms secrete extracellular polymers which anchor the cells to each other as well as to the surfaces on which the film is formed. Once anchored to a surface, biofilm microorganisms carry out a variety of detrimental or beneficial reactions, depending on the surrounding conditions [4–6].

Biofilms can be used for treating wastewater [7], creating barriers to protect soil and groundwater from contamination or the bioremediation of hazardous waste sites. For wastewater treatment, biofilms can be grown on filters to be used in the treatment process. Although biofilms are beneficial in waste water management [8], the study demonstrates that the biofilm structure is highly stratified and characterized by an increase of biofilm density, a decrease of metabolically active biomass and a decrease of porosity with biofilm depth. Both the effective diffusivity for dissolved oxygen, the effectiveness factor decrease with biofilm depth [9]. Difficulties for the treatment of these types of wastewaters are mostly related to the high organic strength, the toxic compound load, or extreme environmental conditions encountered (e.g., pH, temperature and salinity, which are no longer diluted with domestic wastewater) [10]. The toxic compounds are present in the waste water and

* Corresponding author.
Peer review under responsibility of Faculty of Engineering, Alexandria University.

http://dx.doi.org/10.1016/j.aej.2014.09.003

Nomenclature

Symbols

D_s	diffusion coefficient of substrate in biofilms (L^2T^{-1})
D_I	diffusion coefficient of inhibitor in biofilm (L^2T^{-1})
D_P	diffusion coefficient of product in biofilm (L^2T^{-1})
I	inhibitor concentration in biofilm (ML^{-3})
I^*	normalized inhibitor concentration in biofilm (dimensionless)
I_b	inhibitor concentration in bulk liquid (ML^{-3})
K_S	half saturation constant (ML^{-3})
K_i	inhibition constant (ML^{-3})
K_C	product substrate ratio at which reaction rate is half maximum value when Substrate limitation is neglected (K_P/K_S) (dimensionless)
L	biofilm thickness (L)
r_{vf}	volumetric reaction rate in biofilms ($ML^{-2}T^{-1}$)
S	substrate concentration in biofilms (ML^{-3})
S_b	substrate concentration in bulk liquid (ML^{-3})
S^*	normalized substrate concentration in biofilm (dimensionless)
P	product concentration in biofilm (ML^{-3})
P_b	product concentration in bulk liquid (ML^{-3})
P^*	normalized product concentration in biofilm (dimensionless)
x	biofilm depth (L)
X	biomass concentration (ML^{-3})
x^*	normalized biofilm depth (dimensionless)
Y_P	stoichiometric ratio of conversion of substrate to product (dimensionless)

Greek symbols

α	substrate utilization kinetics (dimensionless)
β	magnitude of substrate inhibition (dimensionless)
γ	secondary substrate utilization kinetics (dimensionless)
φ_S^2	Thiele moduli of substrate concentration (dimensionless)
φ_I^2	Thiele moduli of inhibitor concentration (dimensionless)
φ_P^2	Thiele moduli of product concentration (dimensionless)
η	effectiveness factor (dimensionless)

the effect of their toxicity on the microorganisms would be reduced within the biofilm. Various inhibition mathematical models are used to describe the effect of toxicants on microorganisms [11]. The efficacy of a biofilm as compared to suspended growth systems is quantified using effectiveness factor. The effectiveness factor is defined as the ratio of the average reaction rate inside the biofilm to the reaction rate that would exist if the concentration in the film was equal to that in the surrounding water [12].

Biofilms are complex microbial ecosystems in which several physical, chemical and biological processes take place simultaneously. In order to evaluate such systems, mathematical models could be very helpful [13,14]. Miller et al. [15] present a mathematical model of mushroom-like architecture and cavity formation in Pseudomonas aeruginosa biofilms. A detailed study was conducted about the experimental studies and mathematical modeling of an up-flow biofilms reactor treating mustard oil rich wastewater [16]. Masic et al. [17] determine the oxygen profile in a biofilm on suspended carriers in two ways: firstly by microelectrode measurements and secondly by a simple mathematical model. Recently Rao et al. [18] developed mathematical and kinetic modeling of biofilm reactor based on ant colony optimization. Mannia et al. [19] describe the modeling and dynamic simulation of hybrid moving bed biofilm reactors. Wang and Zhang [20] briefly review the progress made in the mathematical modeling of biofilms. The models described in this review article have already been used to explain many complicated phenomena in the biofilm's dynamics.

Many important physical phenomena on the engineering and science fields are frequently modeled by nonlinear differential equations. Such equations are often difficult or impossible to solve analytically. Nevertheless, analytical approximate methods to obtain approximate solutions have gained importance in recent years [21]. There are several methods employed to find approximate solutions to nonlinear problems like Homotopy perturbation method (HPM) [22,23], Homotopy analysis method (HAM) [24,25], Adomian decomposition method (ADM) [26,27] and Picard's iterative method [28,29], etc.; Gheewala and Annachhatre [12] developed a mathematical model for effectiveness factors in biofilms and used the model to the various types of inhibition in biofilms. The purpose of this paper is to derive the analytical expressions of concentration of substrate, secondary substrate, product and effectiveness factor in biofilms by solving the nonlinear differential equations using the new approach to Homotopy perturbation method [30].

2. Mathematical formulation of the boundary value problem

Fig. 1 represents the schematic diagram of an ideal homogeneous biofilm with a typical substrate concentration profile [14]. A planar biofilm was considered with uniform density and diffusivity throughout the biofilm. The mass balance equation in biofilms using Fick's law is as follows [12]:

$$D\frac{d^2S}{dx^2} = r_{vf}. \tag{1}$$

where S [ML^{-3}] is the substrate concentration, D [$L^2\,T^{-1}$] is the diffusion coefficient of the substrate in a biofilm and r_{vf} [$ML^{-3}\,T^{-1}$] is the volumetric reaction rate. The reaction rate r_{vf} is a nonlinear term and it depends upon the types of inhibition in biofilm. Here Monod type inhibition models for inhibition due to (i) substrate (ii) secondary substrate (iii) product have been analyzed to predict the response of biofilm.