Mathematical modelling of a biofilm: The Adomian decomposition method

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ABSTRACT

A mathematical modelling by a biofilm under steady state conditions is discussed. The nonlinear differential Equations in biofilm reaction is solved using the Adomian decomposition method. Approximate analytical expressions for substrate concentration have been derived for all values of parameters δ and S_L . These analytical results are compared with the available numerical results and are found to be in good agreement.

Keywords: Mathematical Modeling; Simulation; Adomian Decomposition Method; Initial Boundary Value Problems

1. INTRODUCTION

Microorganisms biofilms adhere to the interfaces between gas and liquid phases, liquid and solid phases, or two liquid phases [1]. Their activity can have an adverse effect, e.g., biofilms damage materials [2], and water purification technology [3]. The situation is largely similar to the case of heterogeneous reaction in a porous layer [4,5]; however, for the biofilm kinetics, there are a number of specific features. The dependence of the biochemical reaction rate on a substrate concentration is described by a saturating curve and can not be characterized by a power function [3,6]. Dueck et al. [7-9] described the mathematical modeling of evaluation of biofilm with allowance for its erosion. Recently, Min kov et al. [10] obtained the analytical expression for the substrate flux in to the biofilm as the function of volumetric flow rate of the substrate solution. To my knowledge no rigorous analytical solution of concentration of substrate and flux into the biofilm for a square law of microbial death rate with steady-state conditions has been reported. The purpose of this communication is to derive approximate analytical expressions for the steady-state concentration of substrate and flux into the biofilm using the Adomian decomposition method for all values of biofilm thickness and substrate concentration outside the biofilm.

2. MATHEMATICAL FORMULATION OF THE PROBLEM

It is assumed that the substrate consumption is described by the Michaelis-Menten kinetics. The Equation of which are derived on the basis of the theory of enzymatic reactions [3,5] on the particle surface of biofilm [10] is of the following form:

$$D_f \frac{\mathrm{d}^2 S_f}{\mathrm{d}z^2} = q \frac{S_f}{K + S_f} X_f \tag{1}$$

The boundary conditions are

$$z = 0, \ \frac{\mathrm{d}S_f}{\mathrm{d}z} = 0 \tag{2}$$

$$z = L_f, \ S_f = S_1 \tag{3}$$

The biomass balance [10].

$$Y_q \frac{S_f}{K + S_f} X_f = b X_f^2 \tag{4}$$

From **Eq.4**, the concentration of active biomass can be expressed through the substrate concentration. Now the **Eq.1** can be written in the form

$$D_f \frac{\mathrm{d}^2 S_f}{\mathrm{d}z^2} = \frac{q^2 Y}{b} \left(\frac{S_f}{K + S_f}\right)^2 \tag{5}$$

where S_f is the substrate concentration in the biofilm, K is the Michaelis-Menten constant, z is the co-ordinate, L_f is the biofilm thickness, D_f is the diffusion coefficient within the biofilm, b is the Microbial death constant, q is the substrate consumption rate constant, S_1 is the substrate concentration outside the biofilm and Y is the biomass yield per unit amount of substrate consumed respectively. The non-linear ODE (**Eq.5**) is made dimensionless by defining the following parameters:

$$S = \frac{S_f}{K}, x = \frac{z}{L_f}, \delta = \frac{Yq^2L_f^2}{bKD_f}, S_L = \frac{S_1}{K}$$
(6)

The above **Eq.5** reduces to the following dimension-less form:

$$\frac{\mathrm{d}^2 S}{\mathrm{d}x^2} = \delta \left(\frac{S}{1+S}\right)^2 \tag{7}$$

$$x = 0, \ \frac{\mathrm{d}S}{\mathrm{d}x} = 0 \tag{8}$$

$$x = 1, \ S = S_L \tag{9}$$

The dimensionless concentration flux into the biofilm is given by

$$\psi(x) = \frac{1}{\sqrt{\delta}} \frac{dS}{dx}\Big|_{x=1}$$
(10)

3. SOLUTION OF BOUNDARY VALUE PROBLEM BY THE ADOMIAN DECOMPOSITION METHOD

The Adomian's decomposition method has been successfully applied to linear and nonlinear problems. One of its advantages is that it provides a rapid convergent series solution. However, in this method, some modifications are proposed by several authors [11-15]. By applying the Adomian's decomposition method, a new iterative method to compute nonlinear Equations are developed. The Adomian decomposition method is an extremely simple method [11-15] to solve the non-linear differential Equations. First iteration is enough. Furthermore, the obtained result is of high accuracy. Using this Adomian decomposition method (see Appendix A and B), the solution of **Eq.7** becomes:

$$S(x) = S_{L} + \frac{\delta}{2} \left(\frac{S_{L}}{1+S_{L}} \right)^{2} \left(x^{2} - 1 \right)$$

+ $\frac{\delta^{2} S_{L}^{3}}{\left(1+S_{L}\right)^{5}} \left(\frac{x^{4}}{12} - \frac{x^{2}}{2} + \frac{5}{12} \right) + \frac{\delta^{2} S_{L}^{2}}{4\left(1+S_{L}\right)^{6}} \left(\frac{x^{6}}{30} - \frac{x^{4}}{6} + \frac{x^{2}}{2} \right)$
- $\frac{\delta^{2} S_{L}^{5}}{\left(1+S_{L}\right)^{7}} \left(\frac{x^{6}}{30} - \frac{x^{4}}{6} + \frac{x^{2}}{2} \right) + \frac{2\delta^{2} S_{L}^{2}}{\left(1+S_{L}\right)^{7}} \left(\frac{x^{6}}{360} - \frac{x^{4}}{24} + \frac{5x^{2}}{24} \right)$
+ $\frac{3\delta^{2} S_{L}^{6}}{4\left(1+S_{L}\right)^{8}} \left(\frac{x^{6}}{30} - \frac{x^{4}}{6} + \frac{x^{2}}{2} \right) - \frac{2\delta^{2} S_{L}^{5}}{\left(1+S_{L}\right)^{8}} \left(\frac{x^{6}}{360} - \frac{x^{4}}{24} + \frac{5x^{2}}{24} \right)$
+ $\frac{\delta^{2} S_{L}^{4}}{360\left(1+S_{L}\right)^{8}} \left(-155 + 66S_{L} \right)$ (11)

The solution of concentration flux into the biofilm is obtained as

$$\psi = \frac{1}{\sqrt{\delta}} \left[\delta \left(\frac{S_L}{1 + S_L} \right)^2 - \frac{2}{3} \frac{\delta^2 S_L^3}{\left(1 + S_L \right)^5} + \frac{2}{15} \frac{\delta^2 S_L^2}{\left(1 + S_L \right)^6} - \frac{8}{15} \frac{\delta^2 S_L^5}{\left(1 + S_L \right)^7} + \frac{8}{15} \frac{\delta^2 S_L^2}{\left(1 + S_L \right)^7} + \frac{2}{5} \frac{\delta^2 S_L^6}{\left(1 + S_L \right)^8} - \frac{8}{15} \frac{\delta^2 S_L^5}{\left(1 + S_L \right)^8} \right]$$
(12)

4. NUMERICAL SIMULATION

The non-linear differentials **Eq.7** is also solved by numerical methods. The function bvp4c in Matlab software which is a function of solving two-point boundary value problems (BVPs) for ordinary differential equations is used to solve this equation. The Matlab program is also given in Appendix C. Its numerical solution is compared with Adomian decomposition method in **Tables 1** and **2** and **Figures 1-3** for various value of parameters.

5. RESULTS AND DISCUSSION

An approximate analytical expression of concentrations S is given in the **Eq.11**. The concentration S(x)is plotted in **Figures 1-3** for various values of δ and S_L . From these figures, it is evident that the value of concentration gradually increases as the dimensionless biofilm thickness δ decreases. **Figures 4** to **5** represent the concentration S(x) for various values of S_L . From these this figures it is observed that, the value of the concentration increases when S_L increases. When $\delta \leq 1$, the



Figure 1. Normalized concentration profile S(x) as a function of dimensionless distance *x*. The concentrations were computed using **Eq.11** for various values of the δ when $S_L = 0.05$, (—) denotes **Eq.11** and (...) denotes the numerical simulation.

Table 1. Comparis	on of normaliz	ed steady-state	concentration S	S(x) with	simulation	results for	various v	alues of :	x and t	for some	fixed
values of $S_L = 0.5$.											

	Concentration of $S(x)$									
x	$S(x)$ (when $\delta = 0.5$)			S	$\delta(x)$ (when $\delta = 1$))	$S(x)$ (when $\delta = 3$)			
	This work Eq.11	Simulation	Error %	This work Eq.11	Simulation	Error %	This work Eq.11	Simulation	Error %	
0.0	0.4738	0.4738	0.0000	0.4506	0.4506	0.0000	0.3785	0.3785	0.0000	
0.2	0.4749	0.4748	0.0211	0.4523	0.4520	0.0663	0.3831	0.3831	0.0000	
0.4	0.4781	0.4780	0.0209	0.4581	0.4579	0.0437	0.3971	0.3969	0.0504	
0.6	0.4834	0.4831	0.0621	0.4678	0.4670	0.1710	0.4211	0.4210	0.0237	
0.8	0.4904	0.4900	0.0816	0.4818	0.4815	0.0623	0.4559	0.4557	0.0439	
1.0	0.5000	0.5000	0.0000	0.5000	0.5000	0.0000	0.5000	0.5000	0.0000	
	Ave	rage	0.0309 Avera		age 0.0572		Average		0.0197	

Table 2. Comparison of normalized steady-state concentration S(x) with simulation results for various values of x and for some fixed values of $S_L = 5$.

	Concentration of $S(x)$										
x	$S(x)$ (when $\delta = 1$)			S	$\delta(x)$ (when $\delta = 5$))	$S(x)$ (when $\delta = 10$)				
	This work Eq.11	Simulation	Error %	This work Eq.11	Simulation	Error %	This work Eq.11	Simulation	Error %		
0.0	4.6600	4.6500	0.2146	3.4520	3.4500	0.0579	2.3330	2.4000	2.8718		
0.2	4.6730	4.6700	0.0642	3.5140	3.5110	0.0854	2.4340	2.4450	0.4519		
0.4	4.7150	4.7120	0.0636	3.6990	3.6950	0.1081	2.7400	2.6500	3.2847		
0.6	4.7800	4.7800	0.0000	3.9920	3.9920	0.0000	3.2660	3.2600	0.1837		
0.8	4.8760	4.8760	0.0000	4.4530	4.4530	0.0000	4.0310	4.0020	0.7194		
1.0	5.0000	5.0000	0.0000	5.0000	5.0000	0.0000	5.0000	5.0000	0.000		
	Ave	rage	0.0571	0.0571 Average 0.041		0.0419	Average		1.2519		



5.5 5 Dimensionless concentration S(x) $\delta = 1$ 4.5 $\delta = 3$ $\delta = 5$ 3.5 $\delta = 8$ 3 $S_{L} = 5$ 2.5 = 10δ 2 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1 Dimensionless distance x

Figure 2. Normalized concentration profile S(x) as a function of dimensionless distance *x*. The concentrations were computed using **Eq.11** for various values of the δ when $S_L = 0.5$, (—) denotes **Eq.11** and (…) denotes the numerical simulation.

Figure 3. Normalized concentration profile S(x) as a function of dimensionless distance *x*. The concentrations were computed using **Eq.11** for various values of the δ when $S_L = 5$, (—) denotes **Eq.11** and (…) denotes the numerical simulation.



Figure 4. Normalized concentration profile S(x) as a function of dimensionless distance *x*. The concentrations were computed using **Eq.11** for various values of the S_L when $\delta = 10$, (—) denotes **Eq.11** and (…) denotes the numerical simulation.



Figure 5. Normalized concentration profile S(x) as a function of dimensionless distance *x*. The concentrations were computed using **Eq.11** for various values of the S_L when $\delta = 1$, (—) denotes **Eq.11** and (...) denotes the numerical simulation.

concentration is uniform and the uniform value depends upon S_L . It is clear that as dimensionless substrate concentration outside the biofilm S_L increases when the value of dimensionless concentration S(x) increases. **Eq.12** represents the normalized concentration flux into the biofilm. **Figure 6** represents flux versus S_L (dimensionless substrate concentration outside the biofilm). From this figure, it is inferred that the value of concentration flux decreases when the thickness of biofilm increases. **Figure 7** represents flux versus $\log \delta$. From this figure, it is inferred that, the value of the flux is high when S_L is large and then decreases slowly and reaches



Figure 6. Normalized concentration flux into the biofilm ψ as a function of dimensionless substrate concentration outside the biofilm S_L . The concentrations were computed using **Eq.12** for various values of the δ (—) denotes **Eq.12** and (...) denotes the numerical solution.



Figure 7. Normalized concentration flux into the biofilm ψ as a function of dimensionless biofilm thickness δ . The concentrations were computed using **Eq12** for various alues of the S_L (—) denotes **Eq.12** and (…) denotes the numerical simulation.

the minimum value when $\log \delta = 10^2$.

6. CONCLUSION

This paper reports a mathematical treatment for analyzing biofilm for a square law of microbial death rate. In this paper, we have evaluated a theoretical model for an investigation of the dynamic behavior of substrate consumption by a biofilm. The approximate analytical expressions for the steady state substrate concentrations for all values of biochemical parameters (δ and S_L) were obtained using Adomian decomposition method. Furthermore, an analytical expression corresponding to the steady state flux response is also presented. A satisfactory agreement with the existing results is noted. This theoretical result is useful to further develop the model involving the balance of production of active biomass and bioilm erosion.

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APPENDIX A

Basic Concept of the Adomian Decomposition Method (ADM)

Adomian decomposition method [9-13] depends on the non-linear differential Equation

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

into the two components

$$L(y(x)) + N(y(x)) = 0$$
 (A.2)

where L and N are the linear and 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

$$y = -L(N(y)) + \varphi(x)$$
 (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 polynomials A_n of N(y) are evaluated using the formula:

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

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

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

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

$$y_0 = \varphi(x), \ y_{n+1} = -L^{-1}(A_n),$$

 $n \ge 0$ (A.9)

However, in practice all the terms of series in Eq.A.7 cannot be determined, and the solution is approximated

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by the truncated series $\sum_{n=0}^{\infty} y_n$. 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 Concentrations of Substrate Using ADM

In this appendix, we derive the general solution of nonlinear **Eq.11** by using Adomian decomposition method. We write the **Eq.11** in the operator form,

$$L(S) = \delta \left(\frac{S}{1+S}\right)^2 \tag{B.1}$$

where $L = x^{-1} \frac{d^2}{dx^2} x$ and $N(S) = \left(\frac{S}{1+S}\right)^2$. Applying

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

$$S(x) = Ax + B + \delta L^{-1} \left(\frac{S}{1+S}\right)^2$$
(B.2)

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

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

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

In view of Eqs.B.2-B.4, gives

$$\sum_{n=0}^{\infty} S_n(x) = Ax + B + \delta L^{-1} \sum_{n=0}^{\infty} A_n$$
 (B.5)

We identify the zeroth component as

$$S_0(x) = Ax + B \tag{B.6}$$

and the remaining components as the recurrence relation

$$S_{n+1}(x) = \delta L^{-1} A_n,$$

$$n \ge 0$$
(B.7)

where A_n are the Adomian polynomials of S_1, S_2, \dots, S_n . We can find the first few A_n as follows:

$$A_0 = N\left(S_0\right) = \left(\frac{S_L}{1+S_L}\right)^2 \tag{B.8}$$

$$A_{1} = \frac{d}{d\lambda} \Big[N \Big(S_{0} + \lambda S_{1} \Big) \Big]$$
$$= \frac{\delta \Big(x^{2} - 1 \Big) S_{L}^{3}}{\big(1 + S_{L} \big)^{5}}$$
(B.9)

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$$\begin{split} A_{2} &= \frac{d^{2}}{d\lambda^{2}} \Big[N \Big(S_{0} + \lambda S + \lambda^{2} S_{2} \Big) \Big] \\ &= \frac{\delta^{2} S_{L}^{4}}{4 \big(1 + S_{L} \big)^{6}} \Big(x^{2} - 1 \Big)^{2} - \frac{\delta^{2} S_{L}^{5}}{\big(1 + S_{L} \big)^{7}} \Big(x^{2} - 1 \Big)^{2} \\ &+ \frac{2\delta^{2} S_{L}^{2}}{\big(1 + S_{L} \big)^{7}} \Big(\frac{x^{6}}{360} - \frac{x^{4}}{24} + \frac{5x^{2}}{24} \Big) \\ &+ \frac{3\delta^{2} S_{L}^{6}}{4 \big(1 + S_{L} \big)^{8}} \Big(\frac{x^{6}}{30} - \frac{x^{4}}{6} + \frac{x^{2}}{2} \Big) \\ &- \frac{2\delta^{2} S_{L}^{5}}{\big(1 + S_{L} \big)^{8}} \Big(\frac{x^{6}}{360} - \frac{x^{4}}{24} + \frac{5x^{2}}{24} \Big) \\ &+ \frac{\delta^{2} S_{L}^{4}}{360 \big(1 + S_{L} \big)^{8}} \big(-155 + 66S_{L} \big) \end{split}$$
(B.10)

The remaining polynomials can be generated easily, and so,

$$S_0 = S_L \tag{B.11}$$

$$S_1(x) = \frac{\delta}{2} \left(\frac{S_L}{1 + S_L} \right)^2 (x^2 - 1)$$
 (B.12)

$$S_{2}(x) = \frac{\delta^{2} S_{L}^{3}}{(1+S_{L})^{5}} \left(\frac{x^{4}}{12} - \frac{x^{2}}{2} + \frac{5}{12}\right)$$
(B.13)

$$S_{3}(x) = \frac{\delta^{2} S_{L}^{2}}{4(1+S_{L})^{6}} \left(\frac{x^{6}}{30} - \frac{x^{4}}{6} + \frac{x^{2}}{2} \right) - \frac{\delta^{2} S_{L}^{5}}{(1+S_{L})^{7}} \left(\frac{x^{6}}{30} - \frac{x^{4}}{6} + \frac{x^{2}}{2} \right) + \frac{2\delta^{2} S_{L}^{2}}{(1+S_{L})^{7}} \left(\frac{x^{6}}{360} - \frac{x^{4}}{24} + \frac{5x^{2}}{24} \right) + \frac{3\delta^{2} S_{L}^{6}}{4(1+S_{L})^{8}} \left(\frac{x^{6}}{30} - \frac{x^{4}}{6} + \frac{x^{2}}{2} \right) - \frac{2\delta^{2} S_{L}^{5}}{(1+S_{L})^{8}} \left(\frac{x^{6}}{360} - \frac{x^{4}}{24} + \frac{5x^{2}}{24} \right) + \frac{\delta^{2} S_{L}^{4}}{360(1+S_{L})^{8}} \left(-155 + 66S_{L} \right)$$
(B.14)

Adding (B.11) to (B.14) we get **Eq.11** in the text.

APPENDIX C

Scilab/Matlab Program to Find the Numerical Solution of Eqs.7-9

function pdex4 m = 0;

x = linspace(0,1);t=linspace(0,1000);sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);u1 = sol(:,:,1);figure plot(x,u1(end,:)) title('u1(x,t)')xlabel('Distance x') vlabel('u1(x,2)')function [c,f,s] = pdex4pde(x,t,u,DuDx)c = 1;f = 1.* DuDx: $y = (u(1)/(1+u(1)))^{2};$ d=0.5: s=-d*y;function u0 = pdex4ic(x); u0 = 1:

APPENDIX D

Nomenclature

Symbols

b : Microbial death constant, $cm^3/(mg day)$

 D_f : Diffusion coefficient within the biofilm, cm²/day

J: Substrate flux into the biofilm, (mg cm²)/day

K: Michaelis-Menten constant, mg/cm³

 L_f : Biofilm thickness, cm

q: Substrate consumption rate constant, day⁻¹

S : Dimensionless substrate in the biofilm

 S_f : Substrate concentration in the biofilm, mg/cm³

 $S_{L}^{'}$: Dimensionless substrate concentration outside the bioflim

 S_1 : Substrate concentration outside the biofilm, mg/cm³ T: Time, days

x, *y* : Dimensionless co-ordinates

Y: Biomass yield per unit amount of substrate consumed, mg/mg

z : Co-ordinate, cm

 X_f : Concentration of physiologically active microorganisms, mg/cm³

 δ : Dimensionless biofilm thickness

 ψ : Concentration flux into the biofilm