CHAPTER – V

MATHEMATICAL MODELING OF A BIOFILM; THE ADOMIAN DECOMPOSITION METHOD

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5.1 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 chapter 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.
5.2 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:

\[ D_f \frac{d^2 S_f}{dz^2} = q \frac{S_f}{K + S_f} X_f \] (5.1)

The boundary conditions are

\[ z = 0, \quad \frac{dS_f}{dz} = 0 \] (5.2)

\[ z = L_f, \quad S_f = S_1 \] (5.3)

The biomass balance [10]

\[ Y_q \frac{S_f}{K + S_f} X_f = b X_f^2 \] (5.4)

From equation (5.4), the concentration of active biomass can be expressed through the substrate concentration. Now the equation (5.1) can be written in the form

\[ D_f \frac{d^2 S_f}{dz^2} = \frac{q^2 Y}{b} \left( \frac{S_f}{K + S_f} \right)^2 \] (5.5)

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 (equation(5.5)) is made dimensionless by defining the following parameters:

\[ S = \frac{S_f}{K}, x = \frac{z}{L_f}, \delta = \frac{Yq^2L_f^2}{bKD_f}, S_L = \frac{S_i}{K} \]  \hspace{1cm} (5.6)

The above equation (5.5) reduces to the following dimensionless form:

\[ \frac{d^2S}{dx^2} = \delta \left( \frac{S}{1+S} \right)^2 \]  \hspace{1cm} (5.7)

where \( \delta \) is the dimensionless biofilm thickness, \( S \) is the dimensionless concentration and \( x \) is the dimensionless distance.

The corresponding boundary conditions are

\[ x = 0, \quad \frac{dS}{dx} = 0; \]  \hspace{1cm} (5.8)

\[ x = 1, \quad S = S_L \]  \hspace{1cm} (5.9)

The dimensionless concentration flux into the biofilm is given by

\[ \psi(x) = \frac{1}{\sqrt{\delta}} \left. \frac{dS}{dx} \right|_{x=1} \]  \hspace{1cm} (5.10)

5.3 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 [12]. However, in this method, some modifications are proposed by several authors [13-17]. By applying the Adomian’s decomposition method, a new iterative method to
compute nonlinear equations is developed. The Adomian decomposition method is an extremely simple method [13-17] 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 (5.A) and (5.B)), the solution of equation (5.7) becomes:

\[
S(x) = S_L + \frac{\delta}{2} \left( \frac{S_L}{1 + S_L} \right)^2 (x^2 - 1) + \frac{\delta^2 S^3_L}{(1 + S_L)^5} \left( \frac{x^4}{12} - \frac{x^2}{2} + \frac{5}{12} \right) + \frac{\delta^2 S^2_L}{4(1 + S_L)^6} \left( \frac{x^6}{30} - \frac{x^4}{6} + \frac{x^2}{2} \right) \\
- \frac{\delta^2 S^5_L}{(1 + S_L)^5} \left( \frac{x^6}{30} - \frac{x^4}{6} + \frac{x^2}{2} \right) + \frac{2\delta^2 S^2_L}{(1 + S_L)^7} \left( \frac{x^6}{360} - \frac{x^4}{24} + \frac{5x^2}{24} \right) + \frac{3\delta^2 S^6_L}{4(1 + S_L)^8} \left( \frac{x^6}{360} - \frac{x^4}{6} + \frac{x^2}{2} \right) \\
- \frac{2\delta^2 S^5_L}{(1 + S_L)^8} \left( \frac{x^6}{360} - \frac{x^4}{24} + \frac{5x^2}{24} \right) + \frac{\delta^2 S^4_L}{360(1 + S_L)^8} (-155 + 66S_L) \\
\] (5.11)

The solution of concentration flux into the biofilm is obtained as

\[
\psi = \frac{1}{\sqrt{\delta}} \left[ \frac{\delta}{3} \left( \frac{S_L}{1 + S_L} \right)^2 - \frac{2\delta^2 S^3_L}{3 (1 + S_L)^5} + \frac{2\delta^2 S^2_L}{15 (1 + S_L)^6} - \frac{8\delta^2 S^5_L}{15 (1 + S_L)^7} \right] \\
+ \frac{8\delta^2 S^2_L}{15 (1 + S_L)^7} + \frac{2\delta^2 S^6_L}{5 (1 + S_L)^8} - \frac{8\delta^2 S^5_L}{15 (1 + S_L)^8} \right] (5.12)
\]

5.4. NUMERICAL SIMULATION

The non-linear differential equation (5.7) 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 (5.C). Its numerical solution is compared with Adomian decomposition method in table 1 to 2 and figures 1 to 3 for various value of parameters.
5.5 RESULTS AND DISCUSSION

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

Figure 1. Normalized concentration profile $S(x)$ as a function of dimensionless distance $x$. The concentrations were computed using equation (5.11) for various values of the $\delta$ when $S_L = 0.05$, (—) denotes equation (5.11) and (…) denotes the numerical simulation.
Table 1: Comparison of normalized steady-state concentration $S(x)$ with simulation results for various values of $x$ and for some fixed values of $S_\tau = 0.5$.

<table>
<thead>
<tr>
<th>$x$</th>
<th>$S(x)$ (when $\delta = 0.5$)</th>
<th>$S(x)$ (when $\delta = 1$)</th>
<th>$S(x)$ (when $\delta = 3$)</th>
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</thead>
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<tr>
<td></td>
<td>This work Equation (11)</td>
<td>Simulation</td>
<td>Error %</td>
</tr>
<tr>
<td>0.0</td>
<td>0.4738</td>
<td>0.4738</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.2</td>
<td>0.4749</td>
<td>0.4748</td>
<td>0.0211</td>
</tr>
<tr>
<td>0.4</td>
<td>0.4781</td>
<td>0.4780</td>
<td>0.0209</td>
</tr>
<tr>
<td>0.6</td>
<td>0.4834</td>
<td>0.4831</td>
<td>0.0621</td>
</tr>
<tr>
<td>0.8</td>
<td>0.4904</td>
<td>0.4900</td>
<td>0.0816</td>
</tr>
<tr>
<td>1.0</td>
<td>0.5000</td>
<td>0.5000</td>
<td>0.0000</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td><strong>0.0309</strong></td>
<td><strong>Average</strong></td>
<td><strong>0.0572</strong></td>
</tr>
</tbody>
</table>
Table 2: Comparison of normalized steady-state concentration \( S(x) \) with simulation results for various values of \( x \) and for some fixed values of \( S_c = 5 \).

<table>
<thead>
<tr>
<th>( x )</th>
<th>Concentration ( S(x) )</th>
<th>Simulation</th>
<th>Error %</th>
<th>Concentration ( S(x) )</th>
<th>Simulation</th>
<th>Error %</th>
<th>Concentration ( S(x) )</th>
<th>Simulation</th>
<th>Error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>This work Equation (11)</td>
<td>4.6600</td>
<td>0.2146</td>
<td>This work Equation (11)</td>
<td>3.4520</td>
<td>0.0579</td>
<td>This work Equation (11)</td>
<td>2.3330</td>
<td>2.8718</td>
</tr>
<tr>
<td>0.2</td>
<td>Simulation</td>
<td>4.6500</td>
<td>0.2146</td>
<td>Simulation</td>
<td>3.4500</td>
<td>0.0579</td>
<td>Simulation</td>
<td>2.4000</td>
<td>2.8718</td>
</tr>
<tr>
<td>0.4</td>
<td>This work Equation (11)</td>
<td>4.7150</td>
<td>0.0636</td>
<td>This work Equation (11)</td>
<td>3.6990</td>
<td>0.1081</td>
<td>This work Equation (11)</td>
<td>2.7400</td>
<td>3.2847</td>
</tr>
<tr>
<td>0.4</td>
<td>Simulation</td>
<td>4.7120</td>
<td>0.0636</td>
<td>Simulation</td>
<td>3.6950</td>
<td>0.1081</td>
<td>Simulation</td>
<td>2.6500</td>
<td>3.2847</td>
</tr>
<tr>
<td>0.6</td>
<td>This work Equation (11)</td>
<td>4.7800</td>
<td>0.0000</td>
<td>This work Equation (11)</td>
<td>3.9920</td>
<td>0.0000</td>
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<td>3.2660</td>
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<td>0.0000</td>
<td>Simulation</td>
<td>3.9920</td>
<td>0.0000</td>
<td>Simulation</td>
<td>3.2600</td>
<td>0.1837</td>
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<tr>
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<td>0.0000</td>
<td>This work Equation (11)</td>
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<td>0.0000</td>
<td>This work Equation (11)</td>
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<tr>
<td>1.0</td>
<td>Simulation</td>
<td>5.0000</td>
<td>0.0000</td>
<td>Simulation</td>
<td>5.0000</td>
<td>0.0000</td>
<td>Simulation</td>
<td>5.0000</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

Average 0.0571 Average 0.0419 Average 1.2519
Figure 2. Normalized concentration profile $S(x)$ as a function of dimensionless distance $x$. The concentrations were computed using equation (5.11) for various values of the $\delta$ when $S_L = 0.5$, (—) denotes equation (5.11) and (…) denotes the numerical simulation.

Figure 3. Normalized concentration profile $S(x)$ as a function of dimensionless distance $x$. The concentrations were computed using equation (5.11) for various values of the $\delta$ when $S_L = 5$, (—) denotes equation (5.11) and (…) denotes the numerical simulation.
Figure 4. Normalized concentration profile $S(x)$ as a function of dimensionless distance $x$. The concentrations were computed using equation (5.11) for various values of the $S_L$ when $\delta = 10$, (---) denotes equation (5.11) and (...) denotes the numerical simulation.

Figure 5. Normalized concentration profile $S(x)$ as a function of dimensionless distance $x$. The concentrations were computed using equation (5.11) for various values of the $S_L$ when $\delta = 1$, (---) denotes equation (5.11) and (...) denotes the numerical simulation.
Figure 6. Normalized concentration flux into the biofilm \( \psi \) as a function of dimensionless substrate concentration outside the biofilm \( S_L \). The concentrations were computed using equation (5.12) for various values of the \( \delta \) (—) denotes equation (5.12) and (...) denotes the numerical solution.

Figure 7. Normalized concentration flux into the biofilm \( \psi \) as a function of dimensionless biofilm thickness \( \delta \). The concentrations were computed using equation (5.12) for various values of the \( S_L \) (—) denotes equation (5.12) and (...) denotes the numerical simulation.
It is clear that as dimensionless substrate concentration outside the biofilm $S_L$ increases when the value of dimensionless concentration $S(x)$ increases. Equation (12) represents the normalized concentration flux into the biofilm. Figures 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 the minimum value when $\log \delta = 10^2$.

5.6 CONCLUSION

This chapter 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 ($\delta$ 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 biofilm erosion.
5.7 APPENDIX 5.A

Analytical solutions of concentrations of substrate using ADM

In this appendix, we derive the general solution of nonlinear equation (5.7) by using the Adomian decomposition method. We write the equation (5.7) in the operator form,

\[ L(S) = \gamma \left( \frac{S}{1 + S} \right)^2 \]  

(5.B1)

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 equation (5.B1) yields

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

(5.B2)

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

\[ S(x) = \sum_{n=0}^{\infty} S_n(x) \]  

(5.B3)

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

(5.B4)

In view of equations (5.B2) to (5.B4), gives

\[ \sum_{n=0}^{\infty} S_n(x) = Ax + B + \delta \sum_{n=0}^{\infty} A_n \]  

(5.B5)

We identify the zeroth component as

\[ S_0(x) = Ax + B \]  

(5.B6)

and the remaining components as the recurrence relation

\[ S_{n+1}(x) = \delta L^{-1} A_n, \quad n \geq 0 \]  

(5.B7)
where $A_n$ are the Adomian polynomials of $S_1, S_2, ..., S_n$. We can find the first few $A_n$ as follows:

$$A_0 = N(S_0) = \left(\frac{S_L}{1+S_L}\right)^2$$  \hspace{1cm} (5.B8)

$$A_1 = \frac{d}{d\lambda} \left[N(S_0 + \lambda S_1)\right] = \frac{\delta(x^2-1)S_L^2}{(1+S_L)^3}$$  \hspace{1cm} (5.B9)

$$A_2 = \frac{d^2}{d\lambda^2} \left[N(S_0 + \lambda S_1 + \frac{\lambda^2}{2} S_2)\right] = \frac{\delta^2 S_L^4}{4(1+S_L)^6} (x^2 - 1)^2 - \frac{\delta^2 S_L^4}{(1+S_L)^7} (x^2 - 1)^2 + \frac{2\delta^2 S_L^4}{360} \left(\frac{x^6 - x^4 + 5x^2}{24}\right) + \frac{3\delta^2 S_L^4}{4(1+S_L)^6} \left(\frac{x^6 - x^4 + 5x^2}{30 - 6 + 2}\right)$$

$$+ \frac{2\delta^2 S_L^4}{(1+S_L)^7} \left(\frac{x^6 - x^4 + 5x^2}{30 - 2 + 24}\right) + \frac{\delta^2 S_L^4}{360(1+S_L)^8} (-155 + 66S_L)$$  \hspace{1cm} (5.B10)

The remaining polynomials can be generated easily, and so,

$$S_0 = S_L$$  \hspace{1cm} (5.B11)

$$S_1(x) = \frac{\delta}{2} \left(\frac{S_L}{1+S_L}\right)^2 (x^2 - 1)$$  \hspace{1cm} (5.B12)

$$S_2(x) = \frac{\delta S_L^2}{(1+S_L)^5} \left(\frac{x^4 - x^2}{12} + \frac{5}{12}\right)$$  \hspace{1cm} (5.B13)

$$S_3(x) = \frac{\delta^2 S_L^4}{4(1+S_L)^6} \left(\frac{x^6 - x^4 + 5x^2}{30 - 6 + 2}\right) - \frac{\delta^2 S_L^4}{(1+S_L)^7} \left(\frac{x^6 - x^4 + x^2}{30 - 6 + 2}\right)$$

$$+ \frac{2\delta^2 S_L^4}{(1+S_L)^7} \left(\frac{x^6 - x^4 + 5x^2}{30 - 2 + 24}\right) + \frac{3\delta^2 S_L^4}{4(1+S_L)^8} \left(\frac{x^6 - x^4 + x^2}{30 - 6 + 2}\right)$$

$$- \frac{2\delta^2 S_L^4}{(1+S_L)^8} \left(\frac{x^6 - x^4 + 5x^2}{30 - 2 + 24}\right) + \frac{\delta^2 S_L^4}{360(1+S_L)^8} (-155 + 66S_L)$$  \hspace{1cm} (5.B14)

Adding (5.B11) to (5.B14) we get equation (5.11) in the text.

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5.8 APPENDIX 5.B

Scilab/Matlab program to find the numerical solution of equations (5.7) to (5.9).

```matlab
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')

ylabel('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;

function [pl, ql, pr, qr] = pdex4bc(xl, ul, xr, ur, t)

pl = 0;
ql = 1;
pr = ur(1) - 0.5;
qr = 0;

5.9 APPENDIX 5.C

Nomenclature and Units

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<tr>
<th>Symbols</th>
<th>Meaning</th>
<th>Usual dimensions</th>
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<tr>
<td>b</td>
<td>Microbial death constant</td>
<td>cm³/(mg day)</td>
</tr>
<tr>
<td>$D_f$</td>
<td>Diffusion coefficient within the biofilm</td>
<td>cm²/day</td>
</tr>
<tr>
<td>J</td>
<td>Substrate flux into the biofilm</td>
<td>(mg cm²)/day</td>
</tr>
<tr>
<td>K</td>
<td>Michaelis-Menten constant</td>
<td>mg/cm³</td>
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<tr>
<td>$L_f$</td>
<td>Biofilm thickness</td>
<td>cm</td>
</tr>
<tr>
<td>q</td>
<td>Substrate consumption rate constant</td>
<td>day⁻¹</td>
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<tr>
<td>S</td>
<td>Dimensionless substrate in the biofilm</td>
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</tr>
<tr>
<td>$S_f$</td>
<td>Substrate concentration in the biofilm</td>
<td>mg/cm³</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
</tr>
<tr>
<td>--------</td>
<td>--------------------------------------------------</td>
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</tr>
<tr>
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<td>Time</td>
<td>days</td>
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<td>$x, y$</td>
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</tr>
<tr>
<td>$Y$</td>
<td>Biomass yield per unit amount of substrate consumed</td>
<td>mg/mg</td>
</tr>
<tr>
<td>$z$</td>
<td>Co-ordinate</td>
<td>cm</td>
</tr>
<tr>
<td>$X_f$</td>
<td>Concentration of physiologically active micro-organisms</td>
<td>mg/cm$^3$</td>
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<tr>
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<td>$\psi$</td>
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