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 SL. 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 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:

$$D_f \frac{d^2 S_f}{dz^2} = q \frac{S_f}{K+S_f} X_f$$  \hspace{1cm} (1)

The boundary conditions are

$$z = 0, \quad \frac{dS_f}{dz} = 0$$  \hspace{1cm} (2)

$$z = L_f, \quad S_f = S_1$$  \hspace{1cm} (3)

The biomass balance [10].

$$Y_e \frac{S_f}{K+S_f} X_f = bX_f^2$$  \hspace{1cm} (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

$$D_f \frac{d^2 S_f}{dz^2} = \frac{q^2 Y}{b} \left( S_f \right)^2$$  \hspace{1cm} (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:

\[
S = \frac{S_f}{K}, \quad x = \frac{2}{L_f}, \quad \delta = \frac{Yq^2L_f^2}{bKD_f}, \quad S_L = \frac{S_L}{S_f}
\]

(6)

The above Eq.5 reduces to the following dimensionless form:

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

(7)

\[
x = 0, \quad \frac{dS}{dx} = 0
\]

(8)

\[
x = 1, \quad S = S_L
\]

(9)

The dimensionless concentration flux into the biofilm is given by

\[
\psi(x) = \frac{1}{\sqrt{\delta}} \frac{dS}{dx}
\]

(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:

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

\[
+ \frac{\delta^2 S_L^3}{(1+S_L)} \left( \frac{x^6}{12} - \frac{x^4}{2} + \frac{5x^2}{12} \right) + \frac{\delta^2 S_L^2}{4(1+S_L)} \left( \frac{x^6}{30} - \frac{x^4}{6} + \frac{x^2}{2} \right)
\]

\[
- \frac{\delta^2 S_L^3}{(1+S_L)} \left( \frac{3x^6}{30} - \frac{x^4}{6} + \frac{5x^2}{2} \right) + \frac{2\delta^2 S_L^2}{(1+S_L)} \left( \frac{x^6}{360} - \frac{x^4}{24} + \frac{5x^2}{24} \right)
\]

\[
+ 3\delta^2 S_L^3 \left( \frac{x^6}{30} - \frac{x^4}{6} + \frac{x^2}{2} \right) - 2\delta^2 S_L^2 \left( \frac{x^6}{360} - \frac{x^4}{24} + \frac{5x^2}{24} \right)
\]

\[
+ \frac{\delta^2 S_L}{360(1+S_L)} (-155 + 66S_L)
\]

(11)

The solution of concentration flux into the biofilm is obtained as

\[
\psi = \frac{1}{\sqrt{\delta}} \left[ \delta \left( \frac{S_L}{1+S_L} \right)^2 \left( \frac{2\delta^2 S_L^3}{3(1+S_L)} \right) + \frac{2\delta^2 S_L^2}{15(1+S_L)^6} \right]
\]

\[
- \frac{8\delta^2 S_L^5}{15(1+S_L)^6} + \frac{8\delta^2 S_L^7}{15(1+S_L)^6} \]

(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 \( \delta \) 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 this figures it is observed that, the value of the concentration increases when \( S_L \) increases. When \( \delta \geq 1 \), 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 \( \delta \) when \( S_L = 0.05 \), (—) denotes Eq.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 $S_L = 0.5$.

<table>
<thead>
<tr>
<th>$x$</th>
<th>$S(x)$ (when $\delta = 0.5$)</th>
<th>Simulation</th>
<th>Error %</th>
<th>$S(x)$ (when $\delta = 1$)</th>
<th>Simulation</th>
<th>Error %</th>
<th>$S(x)$ (when $\delta = 3$)</th>
<th>Simulation</th>
<th>Error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.4738</td>
<td>0.4738</td>
<td>0.0000</td>
<td>0.4506</td>
<td>0.4506</td>
<td>0.0000</td>
<td>0.3785</td>
<td>0.3785</td>
<td>0.0000</td>
</tr>
<tr>
<td>0.2</td>
<td>0.4749</td>
<td>0.4748</td>
<td>0.0211</td>
<td>0.4523</td>
<td>0.4520</td>
<td>0.0663</td>
<td>0.3831</td>
<td>0.3831</td>
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</tr>
<tr>
<td>0.4</td>
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<td>0.4780</td>
<td>0.0209</td>
<td>0.4581</td>
<td>0.4579</td>
<td>0.0437</td>
<td>0.3971</td>
<td>0.3969</td>
<td>0.0504</td>
</tr>
<tr>
<td>0.6</td>
<td>0.4834</td>
<td>0.4831</td>
<td>0.0621</td>
<td>0.4678</td>
<td>0.4670</td>
<td>0.1710</td>
<td>0.4211</td>
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</tr>
<tr>
<td>0.8</td>
<td>0.4904</td>
<td>0.4900</td>
<td>0.0816</td>
<td>0.4818</td>
<td>0.4815</td>
<td>0.0623</td>
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<td>0.4557</td>
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</tr>
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<td>0.5000</td>
<td>0.0000</td>
<td>0.5000</td>
<td>0.5000</td>
<td>0.0000</td>
<td>0.5000</td>
<td>0.5000</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

Average 0.0309 Average 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 $S_L = 5$.

<table>
<thead>
<tr>
<th>$x$</th>
<th>$S(x)$ (when $\delta = 1$)</th>
<th>Simulation</th>
<th>Error %</th>
<th>$S(x)$ (when $\delta = 5$)</th>
<th>Simulation</th>
<th>Error %</th>
<th>$S(x)$ (when $\delta = 10$)</th>
<th>Simulation</th>
<th>Error %</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>4.6600</td>
<td>4.6500</td>
<td>0.2146</td>
<td>3.4520</td>
<td>3.4500</td>
<td>0.0579</td>
<td>2.3330</td>
<td>2.4000</td>
<td>2.8718</td>
</tr>
<tr>
<td>0.2</td>
<td>4.6730</td>
<td>4.6700</td>
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<td>4.7120</td>
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</tr>
<tr>
<td>0.6</td>
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<td>4.7800</td>
<td>0.0000</td>
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<td>3.9920</td>
<td>0.0000</td>
<td>3.2660</td>
<td>3.2600</td>
<td>0.1837</td>
</tr>
<tr>
<td>0.8</td>
<td>4.8760</td>
<td>4.8760</td>
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<td>4.4530</td>
<td>0.0000</td>
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<td>0.7194</td>
</tr>
<tr>
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<td>5.0000</td>
<td>0.0000</td>
<td>5.0000</td>
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<td>0.0000</td>
<td>5.0000</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 Eq.11 for various values of the $\delta$ 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 $\delta$ 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 $S_t$ 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 $S_t$ when $\delta = 1$, (—) denotes Eq.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 Eq.12 for various values of the $\delta$ (—) denotes Eq.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 Eq.12 for various values of the $S_t$ (—) denotes Eq.12 and (...) denotes the numerical simulation.

concentration is uniform and the uniform value depends upon $S_t$. 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 $S_t$ (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 $S_t$ is large and then decreases slowly and reaches 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 ($\delta$ and $S_t$) were obtained using Adomian decomposition method. Further-
more, 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.

7. ACKNOWLEDGEMENTS

This work was supported by the Council of Scientific and Industrial Research (CSIR No. 01(2442)/10/EMR-II), Government of India. The authors are thankful to Dr. R. Murali, the Principal, the Madura College, Madurai and Mr. S. Nataragobal, the Secretary, Madura College Board, Madurai for their encouragement. The author S. Muthukaruppan is very thankful to the Manonmanium Sundaranar University, Tirunelveli for allowing to do the research work.

REFERENCES

APPENDIX A

Basic Concept of the Adomian Decomposition Method (ADM)


\[ F(x, y(x)) = 0 \]  

(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

\[ L(y) = -N(y) \]  

(A.3)

Applying the inverse operator \( L^{-1} \) on both sides of Eq. A.3 yields

\[ y = L^{-1}(N(y)) + \phi(x) \]  

(A.4)

where \( \phi(x) \) is the constant of integration which satisfies the condition \( L(\phi) = 0 \). Now assuming that the solution \( y \) can be represented as infinite series of the form

\[ y = \sum_{n=0}^{\infty} y_n \]  

(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

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

(A.6)

where the Adomian polynomials \( A_n \) of \( N(y) \) are evaluated using the formula:

\[ A_n(x) = \frac{1}{n!} \frac{d^n}{dx^n} N \left( \sum_{m=0}^{\infty} A_m y_m \right) \bigg|_{x=0} \]  

(A.7)

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

\[ \sum_{n=0}^{\infty} y_n = \phi(x) - L^{-1} \left( \sum_{n=0}^{\infty} A_n \right) \]  

(A.8)

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

\[ y_0 = \phi(x), \ y_{n+1} = -L^{-1}(A_n), \quad n \geq 0 \]  

(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 \( \sum_{n=0}^{\infty} y_n \). 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,

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

(B.1)

where \( L = x^{-1} \frac{d^2}{dx^2} \) 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

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

(B.6)

and the remaining components as the recurrence relation

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

(B.7)

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

\[ A_0 = N(S_0) = \left( \frac{S_1}{1+S_1} \right)^2 \]  

(B.8)

\[ A_1 = \frac{d}{d\lambda} \left[ N(S_0 + \lambda S_1) \right] \bigg|_{\lambda=0} = \delta \left( x^2 - 1 \right) S_1^3 \]  

(B.9)
\[ A_2 = \frac{d^2}{dx^2} \left[ N(S_0 + \lambda S + \lambda^2 S_1) \right] \]

\[ = \frac{\delta^2 S_0^4}{4(1 + S_L)} (x^2 - 1)^2 \]

\[ + \frac{2 \delta^2 S_0^2}{(1 + S_L)^2} \left( \frac{x^6}{360} \right) \]

\[ + \frac{3 \delta^2 S_0^2}{4(1 + S_L)^2} \left( \frac{x^4}{30} - \frac{x^2}{6} + \frac{x^2}{2} \right) \]

\[ \frac{2 \delta^2 S_0^2}{(1 + S_L)^2} \left( \frac{x^6}{360} \right) \]

\[ + \frac{\delta^2 S_0^4}{360(1 + S_L)} (-155 + 66S_L) \]

\] 

The remaining polynomials can be generated easily, and so,

\[ S_0 = S_L \] (B.11)

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

\[ S_2(x) = \frac{\delta^2 S_L^3}{(1 + S_L)^2} \left( \frac{x^6}{12} - \frac{x^4}{2} + \frac{x^2}{12} \right) \] (B.13)

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

\[ - \frac{\delta^2 S_L^4}{(1 + S_L)^6} \left( \frac{x^6}{30} - \frac{x^4}{6} + \frac{x^2}{2} \right) \]

\[ + \frac{2 \delta^2 S_L^2}{(1 + S_L)^2} \left( \frac{x^6}{360} \right) \]

\[ + \frac{3 \delta^2 S_L^2}{4(1 + S_L)^2} \left( \frac{x^4}{30} - \frac{x^2}{6} + \frac{x^2}{2} \right) \]

\[ - \frac{2 \delta^2 S_L^2}{(1 + S_L)^2} \left( \frac{x^6}{360} \right) \]

\[ + \frac{\delta^2 S_L^4}{360(1 + S_L)^6} (-155 + 66S_L) \]

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

```matlab
function pdex4
m = 0;
```

The remaining polynomials can be generated easily, and so,

\[ S_0 = S_L \] (B.11)

**Symbols**

\[ b \]: Microbial death constant, cm³/(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

\[ S_1 \]: Substrate concentration outside the biofilm

\[ S_L \]: Dimensionless substrate concentration outside the biofilm

\[ S_I \]: Substrate concentration in 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

\[ \delta \]: Dimensionless biofilm thickness

\[ \psi \]: Concentration flux into the biofilm

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

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

```matlab
function pdex4
m = 0;
```