

## Mathematical modeling of substrate consumption in a biofilm: Solutions arrived using Akbari-Ganji method

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This paper reports the mathematical modelling of substrate consumption by a biofilm. This model is based on a nonlinear equation comprising a nonlinear term connected to a square law of microbial death rate. This paper applies a powerful analytical method to solve the nonlinear equation, known as Akbari-Ganji's method. A simple closed-form of analytical expression concentration of substrate and flux in the biofilm has been derived. The impact of several parameters on concentration and flux is explored, including biofilm thickness and bulk concentration. Numerical simulation for the concentration profile for steady-state conditions was compared with our analytical results. It is also observed that a satisfactory agreement has been obtained.

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**Keywords:** Nonlinear equations, Mathematical modeling, Numerical simulation, biofilm, Akbari-Ganji's method.

### 1. INTRODUCTION

Microorganisms (bacteria, algae, and unicellular organisms) form biofilms when they attach to the interfaces between gas and liquid phases (e.g., the water surface), liquid and solid phases (e.g., the rocky bottom), or two liquid phases (e.g., an oil drop in water) [1]. The microorganisms attach themselves to the object's surface by secreting a slimy, glue-like substance. Biofilms can grow on almost any surface, including metals, plastics, natural materials, medical implants, kitchen counters, contact lenses, hot tub or swimming pool walls, human and animal tissue, and so on. Biofilms will most likely grow anywhere there is a combination of moisture, nutrients, and a surface. The primary mechanism for the transport of reactants in the biofilm's microporous matrix is diffusion.

The rate at which the substratum is transferred to microorganisms inside the biofilm affects the macro kinetics method. The condition is like heterogeneous reactions in a porous layer. Consumption of substrates is only possible when the biofilm has a sufficiently high concentration of biologically active microorganisms, which is determined by microbial reproduction and death rates. Mirgolbabaee et al. [2,3], solving the Duffing equation with cubic nonlinearities, assumed a trial function up to three terms to obtain an accurate result.

The steady-state problem of substrate consumption in a biofilm was investigated by Min'kov et al. [4] for the established square law of microbial death rate [5–7]. The purpose of this work is to obtain the approximate simple and closed-form analytical expression of the steady-state concentration of substrate and flux into the biofilm using Akbari-Ganji’s method. Analytical results are compared with previous and numerical results, in agreement.

## 2. MATHEMATICAL FORMULATION OF THE PROBLEM.

It is assumed that the Michaelis-Menten kinetics describes substrate consumption. Schematic representation of the biofilm is given in Fig-1. The equation of which is derived based on the theory of enzymatic reactions [8,9] on the particle surface of biofilm is of the following form [4]:

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

The boundary conditions are

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

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

The biomass balance [4] is

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

The concentration of active biomass can be represented as substrate concentration using Eq. (4).

Eq. (1) can now be written in the following format:

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

where  $S_f$  is the biofilm's substrate concentration,  $D_f$  is the diffusion coefficient within the biofilm,  $q$  is the substrate consumption rate constant,  $Y$  is the yield biomass,  $b$  is the Microbial death constant,  $K$  is the Michaelis- Menten constant.  $S_1$  is the concentration of substrate outside the biofilm and  $L_f$  is the biofilm thickness,  $X_f$  is the Concentration of physiologically active micro organism. By introducing the following dimensionless parameters

$$S = \frac{S_f}{K}, x = \frac{z}{L_f}, \delta = \frac{Y q^2 L_f^2}{b K D_f}, S_L = \frac{S_1}{K} \tag{6}$$

the above eq. (5) reduces to the following dimensionless form.

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

The initial and boundary conditions in dimensionless form are as follows:

$$x = 0, \frac{dS(x)}{dx} = 0 \tag{8}$$

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

where  $S(x)$  denotes the dimensionless concentration of substrate,  $x$  represents the dimensionless distance, and  $\delta$  and  $S_L$  are dimensionless biofilm thickness and substrate concentration outside the biofilm. The dimensionless concentration flux into the biofilm is given by [4]

$$\psi = \frac{1}{\sqrt{\delta}} \left( \frac{dS(x)}{dx} \right)_{x=1} \tag{10}$$

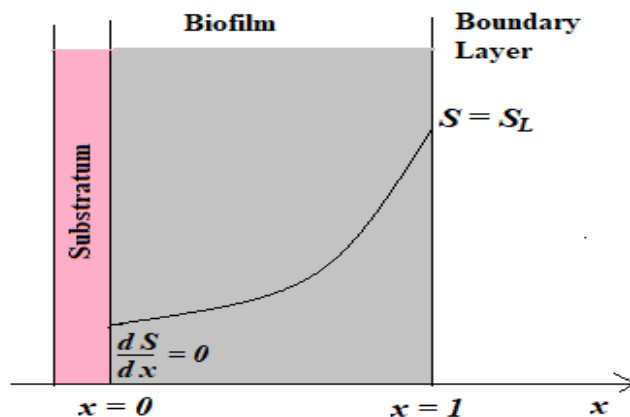


Figure 1. Schematic representation of biofilm

### 3. APPROXIMATE ANALYTICAL EXPRESSION OF THE CONCENTRATION USING AKBARI-GANJI'S METHOD.

Recently some asymptotic methods such as the homotopy perturbation method [10,11], new approach of homotopy perturbation method [12,13], Variational iteration method [14,15], Taylor series method [16-18], Adomian decomposition method [19,20], and Padé approximants method [21] and Akbari- Ganji's method [22-27], are used to solve the nonlinear equations. Akbari- Ganji's method (AGM) might be considered an effective algebraic (semi-analytic) approach for solving such problems. In the AGM, the differential equation and initial conditions are supposed to be satisfied by a solution function with unknown constant coefficients (IC). The unknown coefficients are then calculated using equations derived from IC and derivatives. We can assume that the trial solution of Eq. (7) is

$$S(x) = \sum_{i=0}^2 S_i x^i = S_0 + S_1 x + S_2 x^2 \tag{11}$$

where  $S_0, S_1$  and  $S_2$  are constants. Using the boundary conditions (8) and (9) we get

$$S_1 = 0, \quad S_0 + S_2 = S_L \tag{12}$$

Now define the function  $H$  by

$$H(z) = \frac{d^2 S(x)}{d x^2} - \delta \left( \frac{S(x)}{1+S(x)} \right)^2 = 0 \tag{13}$$

Using Eq. (11) and Eq. (13) at  $x = 1$  becomes

$$H(x = 1) = S_2 - \frac{\delta}{2} \left( \frac{S_L}{1+S_L} \right)^2 = 0 \tag{14}$$

Using Eq. (12) in Eq. (14), gives

$$S_2 = \frac{\delta}{2} \left( \frac{S_L}{1+S_L} \right)^2, \quad S_0 = S_L - \frac{\delta}{2} \left( \frac{S_L}{1+S_L} \right)^2 \tag{15}$$

Eq. (15) and (12) into Eq. (11) gives the closed form of analytical expression of a substrate concentration  $S(x)$  for all dimensionless parameters  $\delta$  and  $S_L$ .

$$S(x) = S_L + \frac{\delta}{2} \left( \frac{S_L}{1+S_L} \right)^2 (x^2 - 1) \tag{16}$$

The concentration at the substratum is

$$S(x = 0) = S_L - \frac{\delta}{2} \left( \frac{S_L}{1+S_L} \right)^2$$

The current becomes

$$\psi = \sqrt{\delta} \left( \frac{S_L}{1+S_L} \right)^2 \tag{17}$$

When  $S_L \gg 1$ , the concentration and the flux becomes

$$S(x) = S_L + \frac{\delta}{2} (x^2 - 1) \tag{18}$$

$$\psi = \sqrt{\delta}. \tag{19}$$

#### 4. PREVIOUS ANALYTICAL RESULT

Very recently Rajendran et al. [19] used the Taylor series method (TSM) to solve Eq. (7) with boundary conditions (8)-(9). They obtained that the analytical expression of a substrate concentration and flux biofilm

$$S(x) = S(0) + \frac{\delta(S(0))^2}{(1+S(0))^2} \frac{x^2}{2!} + \frac{2\delta^2(S(0))^3}{(1+S(0))^5} \frac{x^4}{4!} + \frac{2\delta^3(S(0))^4[5-6S(0)]}{(S(0)+1)^8} \frac{x^6}{6!} \tag{20}$$

where  $S(0)$  can be obtained from boundary conditions. The flux of the substrate to the biofilm becomes

$$\psi = \frac{1}{\sqrt{\delta}} \left[ \frac{\delta(S(0))^2}{(1+S(0))^2} + \frac{\delta^2(S(0))^3}{3(1+S(0))^5} + \frac{\delta^3(S(0))^4[5-6S(0)]}{60(S(0)+1)^8} \right] \tag{21}$$

#### 5. DISCUSSION

Equation (16) are the new closed and simple approximate analytical expressions of substrate concentration for all parameter values  $\delta \left( = \frac{Yq^2L_f^2}{bKD_f} \right)$  and  $S_L \left( = \frac{S_1}{K} \right)$ .

##### 5.1 Numerical Simulation

Numerically, the non-linear Eq.(7) in biofilm are solved for the boundary condition (equations (8) and (9)). We have used the function pdex1 in Scilab/ Matlab (appendix) software to solve numerically with the initial-boundary value problems for the non-linear differential equations. The present and earlier analytical results are compared to this numerical solution in Tables (1-8). A satisfactory agreement is noted.

**Table 1.** Comparison of dimensionless concentration of substrate  $S(x)$  with simulation results for various values of parameter  $\delta$  when  $S_L = 100$ .

$x$	$\delta = 50$			$\delta = 100$			$\delta = 150$		
	Num.	Analytical Eq. (16)	Error % Eq. (16)	Num	Analytical Eq. (16)	Error % Eq. (16)	Num	Analytical Eq. (16)	Error % Eq. (16)
0	75.62	75.49	0.1719	51.67	50.99	1.3160	28.86	27.09	6.1330
0.2	76.61	76.49	0.1566	53.63	52.99	1.1934	31.73	30.80	2.9309
0.4	79.59	79.49	0.1256	59.53	58.99	0.9071	40.35	40.21	0.3473
0.6	84.57	84.49	0.0946	69.38	68.99	0.5621	54.79	54.39	0.7301
0.8	91.53	91.50	0.0328	83.19	82.99	0.2404	75.15	75.70	0.7319
1	100.00	100.00	0.0000	100.00	100.00	0.0000	100.00	100.00	0.0000
	Average error (%)		0.0423	Average error (%)		0.7032	Average error (%)		1.8122

**Table 2.** Comparison of dimensionless concentration of substrate  $S(x)$  with simulation results for various values of parameter  $\delta$  when  $S_L = 500$

$x$	$\delta = 300$			$\delta = 500$			$\delta = 800$		
	Num.	Analytical Eq. (16)	Error % Eq. (16)	Num	Analytical Eq. (16)	Error % Eq. (16)	Num	Analytical Eq. (16)	Error % Eq. (16)
0	350.8	350.6	0.0570	251.7	251.0	0.2781	105.4	101.6	3.6050
0.2	356.9	356.7	0.0560	261.9	261.2	0.2673	121.4	117.9	2.8830
0.4	375.1	375.0	0.0267	292.2	291.6	0.2053	169.5	166.6	1.7109
0.6	405.6	405.5	0.0246	342.9	342.5	0.1166	250.0	247.9	0.8400
0.8	448.2	448.2	0.0000	413.8	413.6	0.0483	362.8	361.8	0.2756
1	500.0	500.0	0.0000	500.0	500.0	0.0000	500.0	500.0	0.0000
	Average error (%)		0.0274	Average error (%)		0.1526	Average error (%)		1.5524

**Table 3.** Comparison of dimensionless concentration of substrate  $S(x)$  with simulation results for various values of parameter  $\delta$  when  $S_L = 1000$

$x$	$\delta = 500$			$\delta = 1000$			$\delta = 1500$		
	Num.	Analytical Eq. (16)	Error % Eq.(16)	Num	Analytical Eq. (16)	Error % Eq.(16)	Num	Analytical Eq. (16)	Error % Eq.(16)
0	750.6	750.5	0.0133	501.7	501.0	0.1395	254.4	251.5	1.1399
0.2	760.8	760.7	0.0131	522.1	521.4	0.1341	284.8	282.0	0.9831
0.4	791.3	791.2	0.0126	583.1	582.5	0.1029	375.9	373.7	0.5823
0.6	842.2	842.1	0.0119	684.7	684.3	0.0584	528.0	526.4	0.3030
0.8	913.5	913.4	0.0109	827.1	826.8	0.0363	741.1	740.3	0.1079
1	1000.0	1000.0	0.0000	1000.0	1000.0	0.0000	1000.0	1000.0	0.0000
	Average error (%)		0.0103	Average error (%)		0.0785	Average error (%)		0.5194

**Table 4.** Comparison of dimensionless concentration of substrate  $S(x)$  with simulation results for various values of parameter  $S_L$  when  $\delta = 100$

$x$	$S_L = 70$			$S_L = 100$			$S_L = 200$		
	Num.	Analytical Eq. (16)	Error % Eq. (16)	Num	Analytical Eq. (16)	Error % Eq. (16)	Num	Analytical Eq. (16)	Error % Eq. (16)
0	23.27	21.40	8.0361	150.6	150.5	0.0664	51.67	50.99	1.3160
0.2	25.15	23.38	7.6064	152.6	152.5	0.0655	53.63	52.99	1.1934
0.4	30.80	29.33	4.7727	158.7	158.6	0.0630	59.53	58.99	0.9071
0.6	40.29	39.25	2.5813	168.8	168.7	0.0592	69.38	68.99	0.5621
0.8	53.66	53.14	0.9691	182.9	182.8	0.0547	83.19	82.99	0.2404
1	70.00	70.00	0.0000	200.0	200.0	0.0000	100.0	100.0	0.0000
	Average error (%)		3.9943	Average error (%)		0.0515	Average error (%)		0.7032

**Table 5.** Comparison of dimensionless concentration of substrate  $S(x)$  with simulation results for various values of parameter  $S_L$  when  $\delta = 1000$

$x$	$S_L = 700$			$S_L = 1000$			$S_L = 1500$		
	Num.	Analytical Eq. (16)	Error % Eq. (16)	Num	Analytical Eq. (16)	Error % Eq. (16)	Num	Analytical Eq. (16)	Error % Eq. (16)
0	203.8	201.4	1.1776	501.7	501.0	0.1395	1001	1001	0000
0.2	224.0	221.8	0.9821	522.1	521.4	0.1341	1021	1021	0000
0.4	284.7	282.8	0.6674	583.1	582.5	0.1029	1082	1082	0000
0.6	385.9	384.6	0.3369	684.7	684.3	0.0584	1184	1184	0000
0.8	527.6	527.0	0.1137	827.1	826.8	0.0363	1327	1327	0000
1	700.0	700.0	0.0000	1000.0	1000.0	0.0000	1500	1500	0000
	Average error (%)		0.5463	Average error (%)		0.0785	Average error (%)		0000

**Table 6.** Comparison of dimensionless concentration of substrate  $S(x)$  with simulation results for various values of parameter  $S_L$  when  $\delta = 2000$

$x$	$S_L = 1500$			$S_L = 2000$			$S_L = 2500$		
	Num.	Analytical Eq. (16)	Error % Eq. (16)	Num	Analytical Eq. (16)	Error % Eq. (16)	Num	Analytical Eq. (16)	Error % Eq. (16)
0	503.0	501.3	0.3380	1002	1001	0.0998	1501	1501	0000
0.2	543.8	542.1	0.3126	1042	1042	0.0000	1542	1542	0000
0.4	665.8	664.4	0.2103	1165	1164	0.0858	1664	1664	0000
0.6	869.2	868.2	0.1150	1368	1368	0.0000	1868	1868	0000
0.8	1154	1153	0.0866	1654	1653	0.0604	2153	2153	0000
1	1500	1500	0.0000	2000	2000	0.0000	2500	2500	0000
	Average error (%)		0.1771	Average error (%)		0.0410	Average error (%)		0000

**Table 7.** Comparison of dimensionless concentration of substrate  $S(x)$  with simulation results for various values of parameter  $\delta$  when  $S_L = 5$

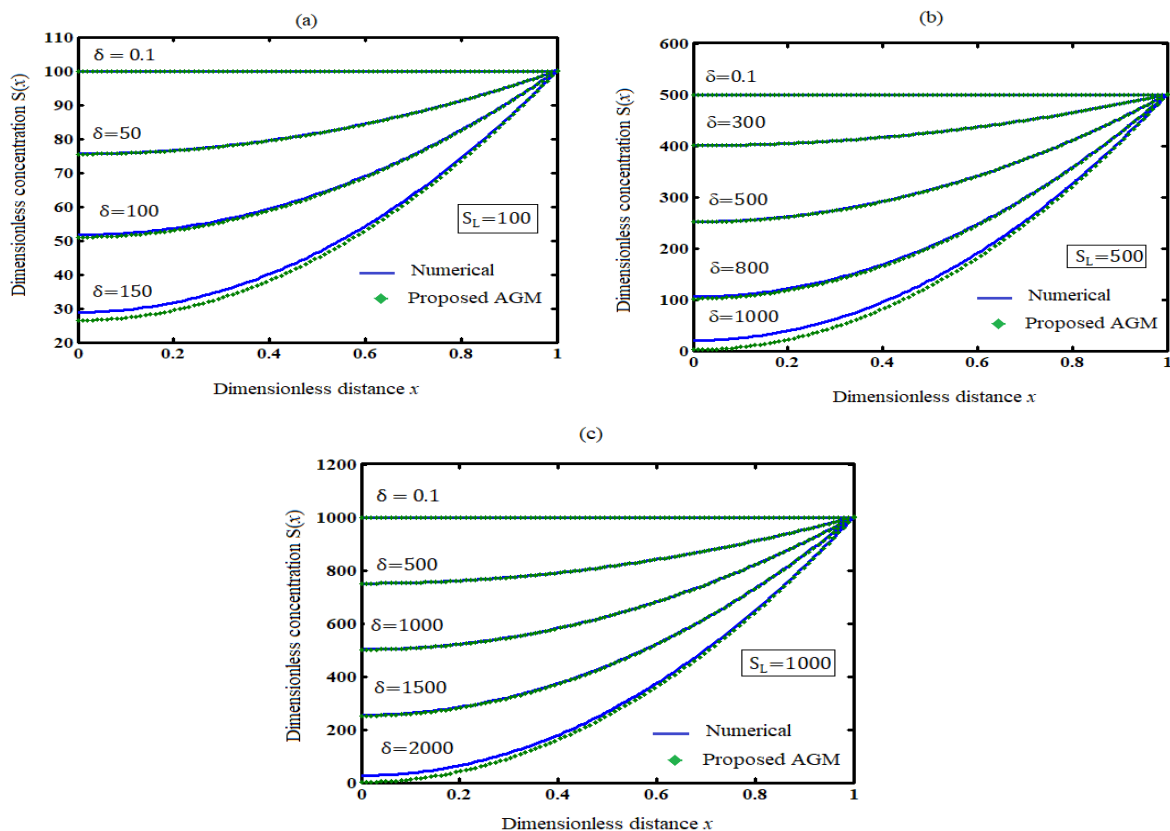
$x$	$\delta = 0.1$					$\delta = 0.5$				
	Num.	AGM Eq. (16)	TSM Eq. (18) [19]	Error % AGM Eq. (16)	Error % TSM [19] Eq. (18)	Num	AGM Eq. (16)	TSM [19] Eq. (18)	Error % AGM Eq. (16)	Error % TSM [19] Eq. (18)
0	4.9650	4.9650	4.9650	0.0000	0.0000	4.8280	4.8270	4.8280	0.0207	0.0000
0.2	4.9670	4.9670	4.9670	0.0000	0.0000	4.8350	4.8340	4.8340	0.0207	0.0207
0.4	4.9710	4.9710	4.9700	0.0000	0.0201	4.8560	4.8550	4.8530	0.0206	0.0618
0.6	4.9780	4.9780	4.9770	0.0000	0.0201	4.8910	4.8900	4.8910	0.0204	0.0000
0.8	4.9880	4.9880	4.9880	0.0000	0.0000	4.9400	4.9400	4.9400	0.0000	0.0000
1	5.0000	5.0000	5.0000	0.0000	0.0000	5.0000	5.0000	5.0000	0.0000	0.0000
	Average error (%)			0.0000	0.0067	Average error (%)			0.0137	0.0138

**Table 8.** Comparison of dimensionless concentration of substrate  $S(x)$  with simulation results for various values of parameter  $S_L$  when  $\delta = 1$

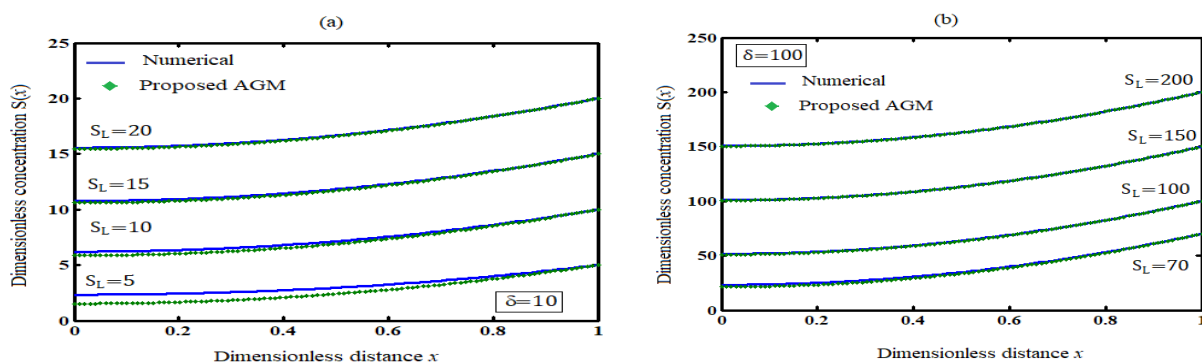
$x$	$S_L = 5$					$S_L = 10$				
	Num.	AGM Eq. (16)	TSM [19] Eq. (18)	Error % AGM Eq. (16)	Error % TSM [19] Eq. (18)	Num	AGM Eq. (16)	TSM [19] Eq. (18)	Error % AGM Eq. (16)	Error % TSM [19] Eq. (18)
0	4.6600	4.6590	4.6600	0.0214	0.0000	9.5890	9.5870	9.5880	0.0209	0.0104
0.2	4.6730	4.6720	4.6830	0.0214	0.0000	9.6060	9.6040	9.6080	0.0208	0.0208
0.4	4.7150	4.7150	4.7150	0.0000	0.0000	9.6560	9.6540	9.6560	0.0207	0.0000
0.6	4.7840	4.7850	4.7840	0.0209	0.0000	9.7400	9.7400	9.7500	0.0000	0.1027
0.8	4.8820	4.8810	4.8870	0.0205	0.1024	9.8570	9.8570	9.8570	0.0000	0.0000
1	5.0000	5.0000	5.0000	0.0000	0.0000	10.000	10.000	10.000	0.0000	0.0000
	Average error (%)			0.0140	0.0171	Average error (%)			0.0104	0.0223

Figs. 1 (a-c) displays the substrate concentration profiles for various values parameters. As the standardized parameter  $\delta$  or biofilm thickness decreases, the substrate concentration is decreases. From the figure 2(a-d) it is inferred that the concentration of substrate outside the biofilm  $S_L$  increases, the substrate concentration increases.

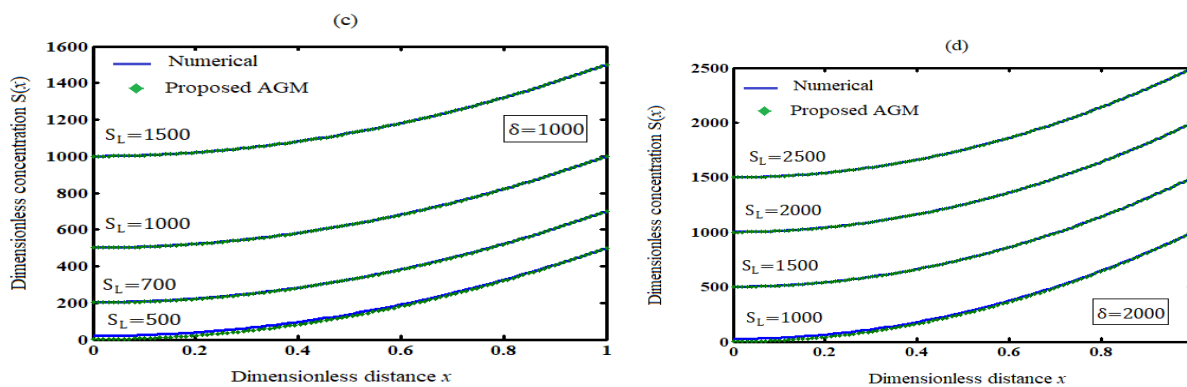
Equation (17) represents the normalized flux. The value of the flux increases as the biofilm thickness increases (refer Fig.3a). From Fig. 3b, it is inferred that flux increases as the parameter  $S_L$  increases.



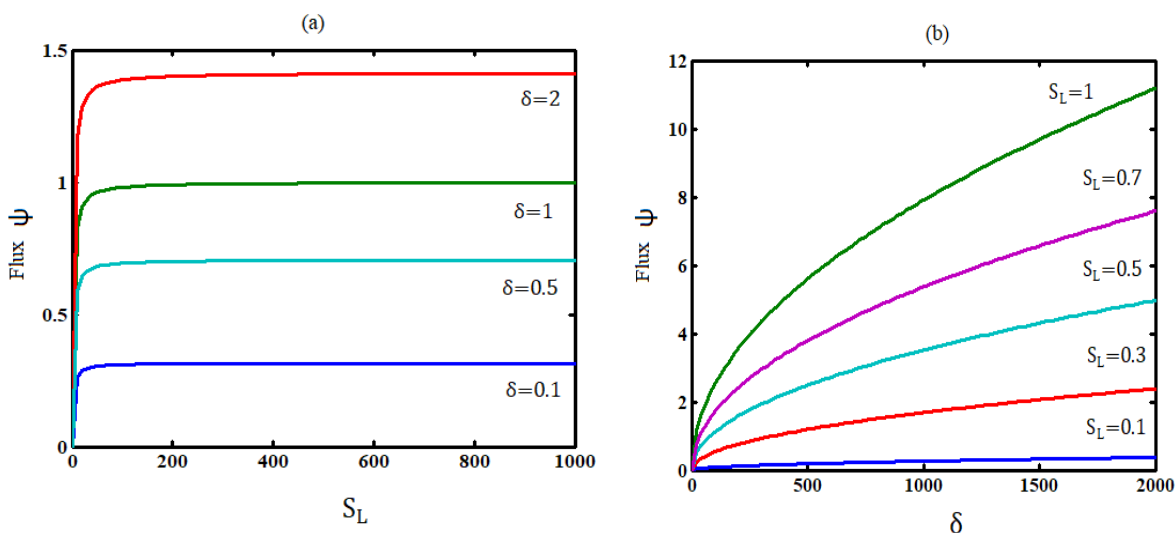
**Figure 1.** Comparison of concentration of substrate  $S(x)$  for different values of parameter  $\delta$  using eq. (16).







**Figure 2.** Comparison of concentration of substrate  $S(x)$  for different values of parameter  $S_L$  using eq. (16)



**Figure 3.** Normalized flux  $\psi$  for various values of  $S_L$  and  $\delta$  using Eq. (17).

## 6. CONCLUSIONS

The nonlinear differential equation in biofilm reaction was solved analytically. The Akbari-Ganji approach is used to develop an approximate analytical expression for substrate concentration for all experimental values of parameters. The impact of several parameters on concentration and flux, such as biofilm thickness and bulk concentration, is explored. Analytical results are compared with numerical and previous available analytical results. These analytical expressions can be used to analyze the effect of biofilm thickness. The influence of biofilm thickness can be studied using these analytical techniques.

**Appendix A:** Scilab/ Matlab program for the numerical solution of the system of nonlinear Eq.(7)

```
function pdex1
m = 0;
x = linspace(0,1);
t = linspace(0,100);
sol = pdepe(m,@pdex1pde,@pdex1ic,@pdex1bc,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] = pdex1pde(x, t, u, DuDx)
c = 1;
f = DuDx;
y = (u(1)/(1+u(1)))^2;
d=0.1;
s=-d*y;
% -----
function u0 = pdex1ic(x)
u0 = 1;
% -----
function [pl, ql, pr, qr] = pdex1bc(xl, ul, xr, ur, t)
pl = 0;
ql = 1;
pr = ur-0.5;
qr = 0;
    
```

Nomenclature

Symbols	Description	Units
<i>b</i>	Microbial death constant	$cm^3 / (mg \text{ day})$
<i>D<sub>f</sub></i>	Diffusion coefficient	$cm^2 / \text{day}$
<i>K</i>	Michaelis- Menten constant	$mg/cm^3$
<i>L<sub>f</sub></i>	Biofilm thickness	<i>cm</i>
<i>q</i>	Rate constant	$day^{-1}$
<i>S</i>	Dimensionless concentration of substrate	None
<i>S<sub>L</sub></i>	Dimensionless substrate concentration outside the biofilm	None
<i>S<sub>f</sub></i>	Substrate concentration in the biofilm	$mg/cm^3$
<i>S<sub>1</sub></i>	Substrate concentration outside the biofilm	$mg/cm^3$
<i>X<sub>f</sub></i>	Concentration of physiologically active microorganism	$mg/cm^3$
<i>x</i>	Dimensionless distance	None
<i>Y</i>	Yield biomass	$mg/mg$
<i>z</i>	Co-ordinate	<i>cm</i>

$\delta$	Dimensionless biofilm thickness	None
$\psi$	Concentration flux into the biofilm	None

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