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Solving free boundary problem for an initial cell layer in multispecies biofilm formation by Newton-Raphson method

Karim Ivaz*
Faculty of Mathematical sciences,
University of Tabriz, Tabriz, Iran.
E-mail: ivaz@tabrizu.ac.ir

Mohammad Asadpour Fazlallahi
Faculty of Mathematical sciences,
University of Tabriz, Tabriz, Iran.
E-mail: asadpour.m2020@gmail.com

Abstract The initial attached cell layer in multispecies biofilm growth is studied in this paper. The corresponding mathematical model leads to discuss a free boundary problem for a system of nonlinear hyperbolic partial differential equations, where the initial biofilm thickness is equal to zero. No assumptions on initial conditions for biomass concentrations and biofilm thickness are required. The data that the problem needs are the concentration of biomass in the bulk liquid and biomass flux from the bulk liquid. The differential equations are converted into an equivalent system of Volterra integral equations. We use Newton-Raphson method to solve the nonlinear system of Volterra integral equations (SVIEs) of the second kind. This method converts the nonlinear system of integral equations into a linear integral equation at each step.

Keywords. Biofilm, Newton-Raphson method, Free boundary problem, Nonlinear system of Volterra integral equations.

2010 Mathematics Subject Classification. 65R20, 35Q92, 35E99, 92B05.

1. Introduction

Jones [12], by using electron microscope, discovered in 1969 that a biofilm is characterized by several kinds of cells. Since then, the combination of high resolution three-dimensional imaging techniques, specific molecular fluorescent stains, molecular reporter technology, and biofilm-culturing apparatus have shown that biofilms are not simply a passive assemblage of cells that are stuck to surfaces, but structurally and dynamically complex biological systems [11].

Mathematical modelling of biofilm growth was extensively performed during the past decades. Essentially, two different classes of models have been developed: continuum models, e.g. among others [8, 14], and differential-discrete models, e.g. [2, 13]. In principle, methods of statistical mechanics can be used to derive macroscopic equations from the underlying description at the cellular scale [6].

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∗ corresponding.

Usually, an initial nonzero thickness in biofilm growth is assumed, and the formation of an attached cell layer is neglected, Figure. 1(a) and (b). Nevertheless, this biological process can last several days or months, since it depends on many factors such as physical and chemical characteristics of substratum, nutrient concentration, hydrodynamic conditions and concentration of planktonic bacteria in the bulk. Therefore, the formation of an attached cell layer is very important in environmental industrial application for wastewater treatment, in particular in the start-up of fixed-growth treatment reactors.

Berardino D'Acunto and Luigi Frunzo, in 2012 [7], show that this biological process is described by a free boundary problem for nonlinear hyperbolic equations where the initial biofilm thickness is zero.

The mathematical model, introduced by Berardino D'Acunto and Luigi Frunzo, in 2012, described the complete free boundary problem [7]. The differential equations are converted into an equivalent system of Volterra integral equations. Subsequently, an existence and uniqueness theorem is proved by the classical fixed point theorem and suitable weighted norms. They show that the solutions are positive and the sum of fraction volumes is equal to 1. In addition, it is proved that the free boundary is an increasing function of time [7] (see Fig. 2).

The application of some numerical method in solving nonlinear system of equation analyzed in [1, 4, 5, 9, 10]. In this paper, we solve free boundary problem for an initial cell layer in multispecies biofilm formation by the Newton-Raphson method. At first, we introduce the linear operator F on the system of integral equations, then obtain Frechet derivative. Therefore, one can write the iterative formula of Newton-Rafson Method. We show that Kantorovich theorem's conditions satisfy on Newton-Rafson formula.

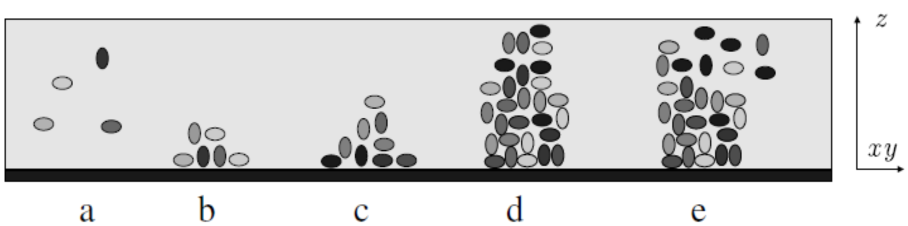

FIGURE 1. Schematic biofilm formation. (a) Planktonic cells; (b) Attached cell layer; (c) Cell proliferation; (d) Mature biofilm; (e) Detachment.

2. Preliminaries

2.1. Mathematical modelling of an initial cell layer. Consider the initial phase in one-dimensional multispecies biofilm growth. Let $f_i(z,t)$ be the volume fraction of the microbial species i, $\sum_{i=1}^{n} f_i = 1$, ρ_i the constant density, $X_i = \rho_i f_i(z,t)$ the concentration of the microorganism i such that $X = (X_1, \ldots, X_n)$, $r_{M,i}(z,t,X_i)$ the specific growth rate, and $u(z,t)$ the velocity of the microbial mass, $L(t)$ biofilm

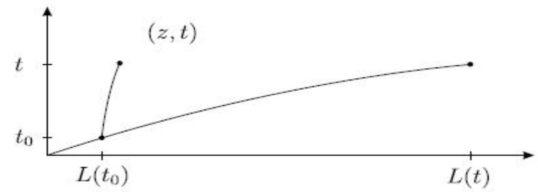

FIGURE 2. Free boundary problem.

thickness. In addition, the biomass flux from bulk liquid to biofilm is denoted by $\sigma(t)$. This is the most used convention. On the other hand, if an opposite definition is adopted, as in [6], $\sigma(t)$ must be replaced by $-\sigma(t)$ and must represent the biomass flux from biofilm to bulk liquid. The initial growth process for multispecies biofilms in one space dimension may be described by the following free boundary problem

$$\frac{\partial X_i(z,t)}{\partial t} + u(z,t)\frac{\partial X_i(z,t)}{\partial z} = \rho_i r_{M,i}(z,t,X) - X_i(z,t)\frac{\partial u(z,t)}{\partial z},$$

$$\frac{\partial u(z,t)}{\partial z} = \sum_{i=1}^{n} r_{M,i}(z,t,X), \quad 0 < z \le L(t), \quad t > 0,$$

$$\dot{L}(t) = u(L(t),t) - \sigma(t), \quad t > 0.$$

The following boundary conditions will be associated to the above system:

$$X_i(L(t),t) = \psi_i(t), \qquad i = 1,2,...,n, \qquad u(0,t) = 0, \qquad \sigma(t) \ge \sigma_L > 0,$$

$$L(0) = 0.$$

Consider the following relations (similar to [7]):

$$x_i(t_0,t) = X_i(c(t_0,t),t), X = (x_1, x_2, \cdots, x_n), \tag{2.1}$$

$$\Phi_i(X(t_0,t), c(t_0,t), t) = F_i(c(t_0,t), t, X(t_0,t)), \; i = 1, \cdots, n, \tag{2.2}$$

$$\Phi_{n+1}(X(t_0,t), c(t_0,t), c_{t_0}(t_0,t), t) = G(c(t_0,t), t, X(t_0,t))c_{t_0}(t_0,t), \tag{2.3}$$

$$\Phi_{n+2} = \Phi_{n+1}. \tag{2.4}$$

By using relations (2.1)-(2.4) and converting differential equations into an equivalent system of Volterra integral equations; one can rewrite it as follows:

$$x_i(t_0,t) = \psi_i(t_0) + \int_{t_0}^{t} \Phi_i(X(t_0,\tau), c(t_0,\tau), \tau)d\tau, \tag{2.5}$$

$$c(t_0,t) = \int_0^{t_0} \sigma(\theta)d\theta + \int_0^{t_0} d\theta \int_0^{\theta} \Phi_{n+1}(X(\tau,\theta), c(\tau,\theta), c_\tau(\tau,\theta), \theta)d\tau$$
$$+ \int_{t_0}^{t} d\theta \int_0^{t_0} \Phi_{n+1}(X(\tau,\theta), c(\tau,\theta), c_\tau(\tau,\theta), \theta)d\tau, \tag{2.6}$$

$$c_{t_0}(t_0,t) = \sigma(t_0) + \int_{t_0}^{t} \Phi_{n+2}(X(t_0,\theta), c(t_0,\theta), c_{t_0}(t_0,\theta),\theta)d\theta, \tag{2.7}$$

$$L(t_0) = \int_0^{t_0} \sigma(\theta)d\theta + \int_0^{t_0} d\theta \int_0^{\theta} G(c(\tau,\theta),\theta, X(\tau,\theta))c_\tau(\tau,\theta)d\tau, \tag{2.8}$$

where $i = 1, 2, \dots, n$ and $0 \le t_0 \le t \le T$. Note that equation (2.8) is separated from system (2.5), (2.6), (2.7). Thus, this system is solved firstly. Then, the solution is replaced in equation (2.8) to obtain $L(t)$. The following theorem holds for system (2.5), (2.6), (2.7).

Theorem 2.1. [7]. *Assume $\psi_i, \sigma, i = 1, \dots, n,$ continuous and ϕ_j Lipschitz continuous $\psi_i, \sigma \in C([0,T]), i = 1, ..., n,$*

$$|\phi_i(x,c,t) - \phi_i(\tilde{x},\tilde{c},t)| \le L_i(\sum_{h=1}^{n} |x_h - \tilde{x}_h| + |c-\tilde{c}|), \qquad i = 1, ..., n, \tag{2.9}$$

$$|\phi_i(x,c,c_{t_0},t) - \phi_i(\tilde{x},\tilde{c},\tilde{c}_{t_0},t)| \le L_i(\sum_{h=1}^{n} |x_h - \tilde{x}_h| + |c-\tilde{c}| + |c_{t_0} - \tilde{c_{t_0}}|), \tag{2.10}$$

where $i = n+1, n+2$. Then, there exists a unique continuous solution $x_i, c, c_{t_0} \in C(I)$, to Volterra system (2.5), (2.6), (2.7), where $I = \{(t_0,t) : 0 \le t_0 \le t \le T\}, T > 0$.

Corollary 2.2. [7]. *Under the same hypotheses as Theorem 2.1 the function $L \in C([0,T])$.*

3. problem statement

Now according to nonlinear system of Volterra integral equations (2.5), (2.6), (2.7), we have

$$\vec{X} = G_0 + \int_{t_0}^{t} \kappa(t,\tau,\vec{X}(\tau))d\tau, \tag{3.1}$$

where

$$\vec{X} = \begin{bmatrix} x_1(c(t_0,t),t) \\ x_2(c(t_0,t),t) \\ \vdots \\ x_n(c(t_0,t),t) \\ c(t_0,t) \\ c_{t_0}(t_0,t) \end{bmatrix},$$

and

$$G_0 = \begin{bmatrix} \psi_1(c(t_0,t)) \\ \psi_2(c(t_0,t)) \\ \vdots \\ \psi_n(c(t_0,t)) \\ L(t_0) \\ \sigma(t_0) \end{bmatrix},$$

and

$$\kappa(t,\tau,\vec{X}(\tau)) = \begin{bmatrix} \Phi_1(\vec{X}(c(t_0,\tau),\tau),c(t_0,\tau),\tau) \\ \Phi_2(\vec{X}(c(t_0,\tau),\tau),c(t_0,\tau),\tau) \\ \vdots \\ \Phi_n(\vec{X}(c(t_0,\tau),\tau),c(t_0,\tau),\tau) \\ \int_0^{t_0} \Phi_{n+1}(\vec{X}(c(\theta,\tau),\tau),c(\theta,\tau),c_\theta(\theta,\tau),\tau)d\theta \\ \Phi_{n+2}(\vec{X}(c(t_0,\tau),\tau),c(t_0,\tau),c_{t_0}(t_0,\tau),\tau) \end{bmatrix}.$$

and $0 < \theta \leq t_0 < t$.

3.1. **Newton-Raphson method.** For applying Newton's method to linearize the problem, define

$$S = \{V : V \in C([0,T]^{n+2})\}. \tag{3.2}$$

Let U and V be two Banach spaces. Assume $F : U \to V$ is Fr'echet differentiable. We are interested in solving the equation $F(u) = 0$.
The Newton method reads as follows:

(1) Choose an initial guess $u_0 \in U$.
(2) For $n = 0, 1, \ldots,$ compute

$$u_{n+1} = u_n - [F(u_n)]^{-1}F(u_n). \tag{3.3}$$

One can show that the Newton method is locally convergent with quadratic convergence. The main drawback of the result is the dependence of the assumptions on the root of the equation, which is the quantity to be computed. The Kantorovich theory overcomes this difficulty. A proof of the following theorem can be found in [15].

Theorem 3.1. *(Kantorovich) Suppose that*
(a) $F : D(F) \subset U \to V$ is differentiable on an open convex set $D(F)$, and the derivative is Lipschitz continuous:

$$\|F'(u) - F'(v)\| \leq L\|u - v\|, \quad \forall u, v \in D(F).$$

(b) For some $u_0 \in D(F)$, $[F'(u_0)]^{-1}$ exists and is a continuous operator from V to U, and such that $h = abL \leq \frac{1}{2}$ for some $a \geq \|[F'(u_0)]^{-1}\|$ and $b \geq \|[F'(u_0)]^{-1}F(u_0)\|$. Denote

$$t^* = \frac{1 - (1 - 2h)^{\frac{1}{2}}}{aL},$$

$$t^{**} = \frac{1 + (1 - 2h)^{\frac{1}{2}}}{aL}.$$

(c) u_0 is chosen so that $B(u_1, r) \subset D(F)$, where $r = t^* - b$.
Then the equation (3.3) has a solution $u^* \in B(u_1, r)$ and the solution is unique in $B(u_0, t^{**}) \cap D(F)$; the sequence u_n converges to u^*, and we have the error estimate

$$\|u_n - u^*\| \leq \frac{[1 - (1 - 2h)^{\frac{1}{2}}]^{2^n}}{2^n ah}, \qquad n = 0, 1, 2, \ldots.$$

The Kantorovich theorem provides sufficient conditions for the convergence of the Newton method.

We aim to solve (3.1) by Newton-Raphson method. We define linear operator F as follow:

$$F = \vec{X} - G_0 - \int_{t_0}^{t} \kappa(t, \tau, \vec{X}(\tau)) d\tau. \tag{3.4}$$

Now we obtain Fr'echet derivative of F. According to definition of Fr'echet derivative of F;

$$F'(\vec{X(t)})v(t) = \lim_{h \to 0} \frac{F(\vec{X(t)} + hv(t)) - F(\vec{X(t)})}{h}, \tag{3.5}$$

we have

$$F'(\vec{X(t)})v(t) = \lim_{h \to 0} \frac{1}{h}(hv(t) - \int_{t_0}^{t} \kappa(t, \tau, \vec{X}(\tau) + hv(t)) - \kappa(t, \tau, \vec{X}(\tau)) d\tau). \tag{3.6}$$

So,

$$F'(\vec{X(t)})v(t) = v(t) + \int_{t_0}^{t} \frac{\partial \kappa}{\partial \vec{X}}(t, \tau, \vec{X}(\tau)) v(\tau) d\tau. \tag{3.7}$$

By using Newton- Raphson's method we linearize the problem (3.1), and applying (3.7) and (3.4); we have:

$$\delta_n(t) + \int_{t_0}^{t} \frac{\partial \kappa}{\partial \vec{X}}(t, \tau, \vec{X_n}(\tau)) \delta_n(\tau) d\tau = -\vec{X_n}(t) + G_0 + \int_{t_0}^{t} \kappa(t, \tau, \vec{X_n}(\tau)) d\tau, \tag{3.8}$$

where $\delta_n(t) = \vec{X_{n+1}}(t) - \vec{X_n}(t)$ and $n = 0, 1, 2, \ldots$.

According to (3.8), $\delta_n(t)$ is only an unknown function. By choosing the suitable initial function $\vec{X_0}(t)$, the system of linear integral equations are solved by common numerical methods. Thus, one can obtain $\vec{X_1}(t)$ and similar to first step of method, $\vec{X_2}(t), \vec{X_3}(t), \ldots$ is obtainable.

3.2. **Checking convergence of Newton-Raphson's method.** In this section, we show that the Kantorovich theorem's conditions satisfy on linear operator F.

Remark 3.2.
(1) According to theorem 2.1, $\vec{X}_n(t)$ is continuous. Then, F is continuous.
(2) Iterration formula (3.8) will converge to the exact solution, if the initial function $\vec{X}_0(t)$, is satisfied in conditions of the Kantorovich theorem.

By choosing $D(F) = S$ in (3.2), it is clear that condition (c) of the Kantorovich theorem is automatically satisfied. For condition (b) it is sufficient to show that $abL \leq 0.5$. Purposely, we use the following theorems.

Theorem 3.3. ***Geometric series theorem:***
Let V be a Banach space, $F \in \mathbb{L}(V)$. Assume $\|F\| < 1$. Then $I - F$ is a bijection on V, its inverse is a bounded linear operator,

$$(I-F)^{(-1)} = \sum_{n=0}^{\infty} F^n,$$

and

$$\|(I-F)^{(-1)}\| \leq \frac{1}{1-\|F\|}. \tag{3.9}$$

Proof. see [3]. □

Corollary 3.4. *Let V be a Banach space, $F \in \mathbb{L}(V)$. Assume for some integer $m \geq 1$ that $\|F^m\| < 1$. Then $I - F$ is a bijection on V, its inverse is a bounded linear operator, and*

$$\|(I-F)^{(-1)}\| \leq \frac{1}{1-\|F^m\|} \sum_{i=0}^{m-1} \|F^i\|. \tag{3.10}$$

Proof. see [3]. □

By Kantorovich theorem F' must be satisfied Lipschitz continuous and F' must be a bounded and an invertible operator. For this purpose, we use geometric series theorem and corollary 3.4. Then by definition

$$M = \max_{0<t<T} |\frac{\partial \kappa}{\partial \vec{X}}(t, \tau, \vec{X}(\tau))|,$$

where T is final time, and (3.7), we have

$$(F'(\vec{X(t)}) - I)v(t) = \int_{t_0}^{t} \frac{\partial \kappa}{\partial \vec{X}}(t, \tau, \vec{X}(\tau))v(\tau)d\tau. \tag{3.11}$$

According to corollary 3.4, F' is an invertible operator and

$$\|(F'-I)^k\| \leq \frac{M^k T^k}{k!}.$$

If $\frac{M^k T^k}{k!} < 1$, then

$$\|(F')^{(-1)}\| \leq \frac{1}{1 - \|(F' - I)^m\|} \sum_{i=0}^{m-1} \|(F' - I)^i\|.$$

Therefore, $(F')^{(-1)}$ is a bounded operator.
Also, if we let $\vec{X}_0(t) \in S$ such that $\|F(\vec{X}_0(t))\| \leq 1$, then

$$\|[F'(\vec{X}_0(t))]^{(-1)} F(\vec{X}_0(t))\| \leq \|[F'(\vec{X}_0(t))]^{(-1)}\| \leq a.$$

Thus condition (b) is satisfied, by choosing a suitable value for $h = a^2 L \leq 0.5$ such that L is Lipschitz constant and $'a'$ define as follow:

$$\|(F'(\vec{X}_0(t)))^{(-1)}\| \leq \frac{1}{1 - \|(F' - I)^m\|} \sum_{i=0}^{m-1} \|(F' - I)^i\| = a.$$

Now, we investigate condition (a) of Kantorovich theorem. We show that F' is Lipschitz continuous. According to (3.7), we have

$$\begin{aligned} \|F'(\vec{X}_2) - F'(\vec{X}_1)\|_\infty &= |\int_{t_0}^{t} \frac{\partial \kappa}{\partial \vec{X}}(t, \tau, \vec{X}_1(\tau)) - \frac{\partial \kappa}{\partial \vec{X}}(t, \tau, \vec{X}_2(\tau)) v(\tau) d\tau| \\ &\leq \int_{t_0}^{t} |\frac{\partial^2 \kappa}{\partial \vec{X}^2}(t, \tau, \vec{X}_3(\tau))| \vec{X}_2 - \vec{X}_1 |v(\tau)| d\tau \\ &\leq L|\vec{X}_2 - \vec{X}_1|, \end{aligned}$$

where

$$L = \max_{\forall v \in D(F)} [\int_{t_0}^{t} |\frac{\partial^2 \kappa}{\partial \vec{X}^2}(t, \tau, \vec{X}_3(\tau)) v(\tau)| d\tau.$$

By choosing suitable initial function $\vec{X}_0(t)$, which is satisfied in $\frac{M^k T^k}{k!} < 1$, such that $M = \max_{0<t<T} |\frac{\partial \kappa}{\partial \vec{X}}(t, \tau, \vec{X}_0(\tau))|$ and choosing $h = abL \leq 0.5$ such that $'a'$ and $'b'$ as follows:

$$\|(F'(\vec{X}_0(t)))^{(-1)}\| \leq \frac{1}{1 - \|(F' - I)^m\|} \sum_{i=0}^{m-1} \|(F' - I)^i\| = a,$$

and

$$\|(F'(\vec{X}_0(t)))^{(-1)} F(\vec{X}_0(t))\| \leq b,$$

and realize condition (c) of Kantorovich theorem. We conclude the Newton-Raphson's method which used in (3.4), will converge to the exact solution of the system of integral equations (2.5), (2.6), (2.7).

4. Conclusions

We propose the Newton-Raphson method to solve the nonlinear system of Volterra integral equations (SVIEs) of the second kind. The advantage of this method is converting of the nonlinear system of integral equations into a linear integral equation at each step. The Kantorovich theorem provides sufficient conditions for the convergence of the Newton-Raphson method. Finally, we showed that the operator F is satisfied on Kantorovich theorem's conditions. In future work, we would present some numerical examples to verify the theoretical analysis which is announced in this paper.

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