NUMERICAL MODELING OF BIOFILM GROWTH AT THE PORE SCALE

B. Chen and Y. Li

Department of Mathematics, University of Wyoming, P.O. Box 3036, Laramie, WY 82071; Phone: (307)766-4221; Fax: (307)766-6838.

ABSTRACT

Biofilms play a very important role in porous media. The most useful application is the use of biofilms to form biobarriers to restrict the spread of contaminant plumes. They can also be used to consume the pollutants by interacting with them. Biofilms are still not well understood. Here we present a model for fluid flow, and contaminant and nutrient transport, coupled with biofilm growth. The model is complicated due to the effect of the flow on the biofilm growth and vice versa, so that all the effects are strongly coupled. The model is discretized using finite elements to take into account the pore geometry and the amount of biofilm growth. Results of different calculations are presented.

Key words: *biofilms, bioremediation, mathematical model*

INTRODUCTION

The main motivation of this paper is to develop a mathematical model of biofilm growth in porous media at the microscopic scale. Biofilms are found on essentially any environmental surface provided that sufficient moisture is present. Biofilms first start with some cells or bacteria being immobilized at a solid surface (substratum). After being adhered to the substratum for a while, the cells or bacteria may consume nutrients, and begin to grow, reproduce, and at the same time produce extracellular polymers and other byproducts.

The development of biofilms is most rapid in flowing systems where adequate nutrients are available. Biofilms are responsible for much of the transformation and degradation of natural and man-made organic compounds in the water. They can be beneficial or detrimental, depending on their location and on the biotransformation process.

Biofilms grow in porous media and play an important mechanism for many processes. For example, in porous media biofilm growth can cause detrimental permeability reduction through pore blocking or it can cause the souring of petroleum reservoirs through sulfide production. But there are beneficial aspects of biofilms like the bioremediation of contaminant plumes and the formation of biobarriers. The significance of biofilms makes it necessary to understand the processes associated with biofilm growth (Chen et al., 1994).

The growth of biofilms in porous media is a very complicated process. It involves fluid dynamics, mass transport, biofilm accumulation, and biotransformation of organic constituents. Due to its complexity, it is important to try to understand and model the basic processes occurring and their rates at the pore level. Fluid-biofilm modeling is fundamental in the understanding and the prediction of physical processes. A brief review some of biofilm models follows: Picologlou et al., 1980, dealt with the growth of biofilms in pipes. Cunningham et al., 1991, have studied the influence of biofilm

growth on the permeability and porosity of a porous medium. Sáez and Rittman, 1988, derived algebraic equations that approximate the growth of a biofilm. Reichert et al., 1990, developed a code called BIOSIM that models biofilm growth using units. Chen et al., 1994, presented a pore-scale model using a variation of BIOSIM for some irregular biofilm growth simulations.

In this paper, we will extend the results by implementing a better biofilm growth model in the sense that we will allow the biofilm to grow to any thickness in irregular domains.

MATHEMATICAL MODEL

In this paper, we have a microscopic model of the porous media using pore channels that are divided into fluid and biofilm regions. Along the walls of the pore channels, the biofilm grows, while the fluid flows through. The interface between the fluid and the biofilm separates the bulk fluid region from the biofilm region.

Bacteria will attach to solid surfaces to take advantage of the organic molecules adsorbed there. After being attached for some time, the microorganisms start to consume nutrients, grow, reproduce, and also produce extracellular polymeric substances (referred to as EPS) which bind the cells together. This aggregate of attached microorganisms, EPS, and other particulate matter is termed as biofilm (Characklis and Marshall, 1990; Costerton and Lappin-Scott , 1995).

In saturated porous media, processes governing fluid dynamics, mass transport, biofilm accumulation, and the biotransformation of organic constituents are intrinsically interrelated (Chen et al., 1994). The net accumulation of biofilm in porous media is the result of biomass added to the surface from the processes of adsorption, growth, attachment, and filtration less the amount of mass removed by the processes of desorption and detachment.

As the film thickness increases, the effective pore space of the media will decrease, thereby causing a corresponding decrease in media porosity and permeability. If the piezometric gradient remains constant, the pore velocity will also decrease thereby reducing both advective and diffusive transport of nutrients through the system. Decreased nutrient transport results in a corresponding reduction in the biomass specific growth rate and thus in the rate of biotransformation of organic material. Decreased pore velocities also reduce the rate of detachment.

The significance of biofilms motivates us to understand the processes associated with biofilm growth (Visser, 1998). These processes need to be understood at the pore scale before scaling up to laboratory and field scales can be done.

A biofilm system consists of different compartments including the substratum, the biofilm, and bulk water. In these compartments different phases can be distinguished (Gujer and Wanner 1990):
1. A continuous liquid phase, usually water, which fills the connected fraction of the biofilm volume and contains dissolved species.
2. Solid phases composed of a species of microorganism and extracellular material. The solids cannot move freely as they are attached to each other.

The concentration of a certain component in the liquid phase is simply the mass of component contained in one unit volume of the liquid phase. The density of the solid phase will be the density of the major or bulk component in that phase. The volume fraction refers to the fraction of the volume that each of the phases occupies in the biofilm matrix.

Our main interest is to couple the flow through a porous medium with biofilm reactions and growth on the pore walls. The dynamics of biofilm formation is a complex process which involves fluid dynamics, mass transfer, chemical reactions, and biochemical reactions (Brading et al., 1995). The fluid will bring nutrients to the biofilm, which will grow and gradually change the geometry and flow properties of the medium. This will affect the flow pattern, which in turn will change the availability of nutrients to the biofilm. The strong interaction of these processes is modeled via a coupling of the flow, transport, and growth processes.

Bulk Fluid Region

The bulk fluid region is defined as the region outside the biofilm regions depicted in Figure 1. Here we assume that the concentrations of dissolved constituents in the bulk fluid are small enough so that the solution can be considered dilute. That means the properties of the fluid are not influenced by the presence of dissolved species, but only by the geometry of the fluid region. The transport of liquid and dissolved constituents is interrelated. The flow of the fluid will certainly affect the concentration of the dissolved constituents through a flux-like process. Although the concentration of the nutrients will not affect the fluid velocity directly, it will surely influence the growth of biofilms. The gradually changing geometries of our domain due to the biofilm growth will in turn affect the fluid velocity.

Navier-Stokes Equations

Since the fluid with which we are concerned is Newtonian flow with constant viscosity, the bulk fluid dynamics can be modeled by the Navier-Stokes equations. The continuity equation obtained from a mass balance on the fluid (Girault and Raviart, 1986) gives

$$\nabla \cdot \mathbf{u} = 0. \tag{1}$$

While the balance of momentum gives the equations (Girault and Raviart, 1986)

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta \mathbf{u} + \nabla \mathrm{P} = \mathbf{f}, \tag{2}$$

where $\mathbf{u}(x,t) = (u_1,u_2)$ is the bulk fluid velocity and $P(x,t)$ is the pressure of the flow. $\mathbf{f}$ is external force acting the on fluid and $\nu > 0$ is the kinematic viscosity.

The gradient and Laplacian of a vector in two dimensions are defined by

$$\nabla \mathbf{u} = \left(\frac{\partial u_i}{\partial x_j} \right)_{2x2}$$

$$\Delta \mathbf{u} = \left(\Delta u_1, \Delta u_2 \right).$$

Species Balance Equations

The species balance equation for dilute concentrations of dissolved species in the bulk fluid is given by Bird et al., 1960, and Probstein, 1989,

$$\frac{\partial C_i}{\partial t} = -\nabla \cdot \mathbf{J}_i + r_i, \tag{3}$$

where $C_i = C_i(\mathbf{X},t)$ is the concentration of species *i* and r_i is the production rate of species *i*. $\mathbf{J}_i$ is the total mass flux of species *i* and is given by

$$\mathbf{J}_i = \mathbf{u} \cdot \nabla C_i - D_i(\mathbf{X}) \nabla C_i. \tag{4}$$

The first term on the right hand side of above equation represents the convective flux due to bulk fluid flow. The second term represents the diffusive flux which is assumed to obey Fick's first law (Characklis and Marshall, 1990). $D_i(\mathbf{X})$ is the diffusion coefficient for species *i*.
Insertion of (4) into (3) gives

$$\frac{\partial C_i}{\partial t} + \mathbf{u} \cdot \nabla C_i = \nabla \cdot \left(D_i(X) \nabla C_i \right) + r_i \qquad i = 1, \ldots\ldots, N_s. \tag{5}$$

Here N_s is the total number of dissolved species. Our current model does not consider transformation of any species in the fluid, so we assume that $r^i \equiv 0$.

Biofilm Region

The biofilm model used in this dissertation is based on the multi- species biofilm model given by Wanner and Gujer, 1986. The model is a one-dimensional model in space with biofilm growth only normal to the substratum. A biofilm consists of different compartments including the substratum, the biofilm, and water. Assume *k* different phases can be distinguished in the biofilm matrix. Each phase occupies a fraction e_k of the total biofilm volume. We will consider that we have only one liquid phase and all the other phases are solid phases. Using the index *l* for the liquid phase and index *s* for the biofilm solid phases, we will have

$$\sum_k e_k = e_l + \sum_s e_s = 1. \tag{6}$$

Liquid Phase

The mass balance of dissolved species in liquid phase in the biofilm is given by

$$\frac{\partial e_l C_{l,i}}{\partial t} = -\nabla \cdot \mathbf{J}_{l,i} + r_{l,i}, \tag{7}$$

where $C_{l,i}$, $r_{l,i}$ are the concentration and the production rate of the dissolved species *i* in liquid phase *l*.

The flux $\mathbf{J}_{l,i}$ of species *i* in the biofilm, due to diffusion, is assumed by Fick's first law as

$$\mathbf{J}_{l,i} = -D_{l,i}(\mathbf{X}) \nabla C_{l,i}, \tag{8}$$

where $D_{l,i}$ is the diffusion coefficient of dissolved species *i* in the biofilm. Estimating Jl,i in the biofilm is similar to that of $\mathbf{J}_i$ in the bulk fluid, except that the effect of the flux due to the movement of the fluid in the biofilm is regarded as negligible. Insertion of (8) into (7) gives

$$\frac{\partial e_l C_{l,i}}{\partial t} = \nabla \cdot \left(D_{l,i}(\mathbf{X}) \nabla C_{l,i} \right) + r_{l,i}. \tag{9}$$

Solid Phase

Under the same assumptions, the mass balance for the solid phase in the biofilm is given by

$$\frac{\partial e_s \rho_s}{\partial t} = -\nabla \cdot \mathbf{J}_s + r_s, \tag{10}$$

where ρ_s is the density of the only solid phase; r_s is the production rate of the solid cells; and $\mathbf{J}_s$ is the flux of the only solid component within the solid phase *s*. Since the solid biofilm phase is mainly subject to a common advection process (Characklis and Marshall, 1990), i.e., if any one attached particle moves, it causes displacement of its neighboring particles. The $\mathbf{J}_s$ will be an advective flux and is given by

$$\mathbf{J}_s = \mathbf{v}_s \rho_s e_s, \tag{11}$$

where $\mathbf{v}_s = \mathbf{v}_s(\mathbf{X},t)$ is the velocity vector of the solid phase in biofilm.

Since we assume that the biofilm growth is predominantly normal to the substratum, it implies that

$$\nabla \cdot \mathbf{J}_s = \frac{\partial \mathbf{J}_s}{\partial \eta} = \frac{\partial}{\partial \eta}(\mathbf{v}_s \rho_s e_s), \tag{12}$$

where we use η to denote the direction perpendicular to the substratum. Insertion of (12) into (10) gives

$$\frac{\partial e_s \rho_s}{\partial t} = -\frac{\partial}{\partial \eta}(\mathbf{v}_s \rho_s e_s) + r_s. \tag{13}$$

We now further assume constant density r_s and volume fraction e_s so equation (13) simplifies to

$$\frac{\partial \mathbf{v}_s}{\partial \eta} = \frac{r_s}{e_s \rho_s}. \tag{14}$$

Integrating from 0 to η, with the boundary condition that the biofilm growth velocity v_s at the substratum equals zero, we have

$$\mathbf{v}_s = \frac{1}{e \rho_s} \int_0^{\eta} r_s d\eta. \tag{15}$$

Let $L_f = L_f(\xi,t)$ be the height of the biofilm growth at the space point ξ and time t. When we consider the moving of the interface, we also have to take into consideration effects of the detachment. Assume at each point ξ along the substratum, the interface is moving at velocity V_I normal to the substratum. Then the movement of the interface is due to the effect of the biofilm growth in terms of v_s as well as the effect of biofilm detachment in terms of the detachment rate γ_s:

$$V_I e_s \rho_s = \mathbf{v}_s(L_f) e_s \rho_s + \gamma_s, \tag{16}$$

where $v_s(L_f)$ is the biofilm growth velocity v_s at L_f. Here we mainly consider the erosion detachment. The detachment due to erosion has been studied by Peyton and Characklis, 1992, who indicate that nutrient supply, biofilm thickness, and hydraulic shear are important factors in the erosion. Furthermore, the shear stress apparently influences the rate and extent of erosion. Wanner and Gujer, 1986, in a theoretical study, used $-D_{etach} L_f^2$ as the detachment rate, where D_{etach} is a rate coefficient that may depend on local hydraulic shear and biofilm strength.

From (17) we obtain

$$V_I = \mathbf{v}_s(L_f) + \frac{\gamma_s}{e_s \rho_s} = \frac{1}{e_s \rho_s} \int_0^{L_f(\xi,t)} r_s d\eta + \frac{\gamma_s}{e_s \rho_s} \quad .$$

V_I is related to L_f by

$$V_I = \frac{dL_f(\xi,t)}{dt} \tag{17}$$

and therefore we obtain the biofilm growth equation

$$\frac{dL_f(\xi,t)}{dt} = \frac{1}{e_s \rho_s} \int_0^{L_f(\xi,t)} r_s d\eta + \frac{\gamma_s}{e_s \rho_s} \quad . \tag{18}$$

Notice that r_s depends on $C_{l,i}$, so the above biofilm growth equation is coupled with the concentration equation (9) in the liquid phase.

Biofilm Kinetics

We will model the cell growth rate r_s by Monod Kinetics (Characklis and Marshall, 1990)

$$r_s = \mu_{max} \frac{\rho_s C_{l,i}}{K + C_{l,i}} - b\rho_s \tag{19}$$

and the substrate utilization rate as

$$r_{l,i} = \frac{\mu_{max}}{Y} \frac{\rho_s C_{l,i}}{K + C_{l,i}} . \tag{20}$$

Here, μ_{max} is the maximum specific growth rate, K the Monod saturation coeeficient, b the endogenous decay coefficient, and Y the yield of cell material from $C_{l,i}$.

NUMERICAL SIMULATIONS OF THE TRANSPORT AND THE BIOFILM GROWTH

Numerical Simulations of Transport

The velocity profile in the fluid flow region is calculated by solving equations (1) and (2) using a mixed finite-element method with arbitrary quadrilateral elements (Li and Chen, 1998). We will use as an example of a pore region a sinusoidal domain with one expansion. The throat is fairly narrow to illustrate irregular flow regions.

The flow of the fluid carries nutrients to the biofilm and causes the biofilm to grow. The nutrient transport equations are given by equation (5) in the previous section.

As far as the boundary conditions, we have the concentration at the entrance of the pore, given to be constant. Along the interfaces that separate the bulk fluid and the biofilm, the normal derivatives are specified. At the exit of the flow, we assume there is no change, that is the normal derivative vanishes. We will use the finite element method over quadrilaterals to solve equation (5) with the same partition of the domain that we used when solving for the velocities.

Actually the equation for transport in the bulk fluid is coupled with the transport equations for concentration in the biofilm region. Although we distinguish the bulk fluid and the liquid phase in the biofilm, physically, it is natural to require the continuity of both the concentration and the flux of the concentration along the interfaces that separate the fluid and the biofilm regions. It is easy to enforce the continuity of one of the above quantities. However, we need the continuity of both quantities. We will illustrate how we achieve this after we present the transport equations in the biofilm region.

In the biofilm region, there are nutrients dissolved in the liquid phase of the biofilm. The concentration equations in the liquid phase of the biofilm region are given in the previous section.

Notice that in the biofilm region, there is one concentration equation (9) associated with each point on the substratum. So each equation governing the concentration in the biofilm is one dimensional. As for the boundary conditions, for each equation (9), we specify the normal derivative at the end point on the substratum to be zero since there is no flux through the substratum. At the other end point on the interface with the bulk fluid, even though we do not know the real boundary value, we just assume a value for the normal derivative. To assure the continuity at the interface point with the bulk fluid, the outer normal derivative is enforced to be the same as the assumption of the normal derivative when we were solving the concentration equation (5) in the bulk fluid. To solve equations (9), since they are one dimensional, we use a finite difference method instead of a finite element method.

The resulting stiff matrix is a tridiagonal definite matrix. Solving the resulting algebraic system, we obtain the approximate solution of the concentration in the biofilm.

Now let us look at the real problem where we do not know the boundary values of the concentration and flux along the biofilm-liquid interfaces. We first assume the same flux along the

interfaces for the concentration equations (5) in the bulk fluid and (9) in the biofilm. Each time with the flux specified along the interface, we compute the concentration in both the bulk fluid region and the biofilm region. Along the interfaces, we expect a jump in values of concentration that are calculated from two different equations in two different domains. The secant method is applied to update the flux so that the jump of the boundary values will decrease until an acceptable value. We repeat the above steps until the desired continuity of the boundary values of the concentration is achieved.

Biofilm Growth Simulations

The biofilm growth equations (18) are given in the previous section. Approximating the integral in the above equation using the trapezoidal rule and replacing the derivative by the forward difference $\Delta L_f(\xi,t)/\Delta t$, we obtain the biofilm change $\Delta L_f(\xi,t)$ at spatial point ξ and time t.

When the biofilm has grown after a few time steps, we change our computational domains accordingly and recalculate the velocity and the concentration. Since the biofilm is subject to the detachment from the flow and the detachment is proportional to the biofilm thickness squared, at a certain time, when the biofilm reaches a certain height, the whole system will reach its steady state.

NUMERICAL TEST CASES

We have performed the simulation of the whole fluid-biofilm system in several representative regions and obtained very good results. Our simulation system can be used as an efficient tool for predicting concentration of nutrients and biofilm growths. In the example presented, we worked with the one-pore region illustrated in Figure 2. We also considered only one species of nutrient and one species of microbe. The parameters are assigned the following values: the initial concentration is set to be 100 gr/cm, e_l =0.8, e_s = 0.2, r_s = 0.8 gr/cm, μ_{max} = 7.0 1/sec, K = 1.0 gr/cm, b =1.0 1/sec, Y =.69, and the detachment coefficient D_{etach} to be 14.0 1/sec. The results for biofilm growth along the bottom wall are shown in Figure 4. If we check Figure 3 for the concentration profile, we will find out concentration is high in the narrow throat region and relatively low in the wide regions. This is because in the narrow regions the fluid flows faster so that it brings more nutrients to the biofilm, where in the wider regions, the flow is slow so that less nutrients are brought by the fluid to the biofilm. In our model the biofilm growth depends on the nutrients available, detachment rate, and the biofilm height. So with the same detachment rate, at first the biofilm growth will mainly depend on how much nutrients are available. This process will continue until the detachment balances with the biofilm growth and then the biofilm will reach its steady state.

CONCLUSIONS

In this paper, we implemented a working model of a fluid-biofilm system at the pore scale. The whole system is highly nonlinear and all the processes are coupled. The velocity profile, the concentration profile, and the biofilms growth profile were successfully obtained. The solutions are consistent with the physics of the problems.

We implemented an algorithm that allows the domains in our fluid-biofilm system to change with time as the biofilm grows. We applied the method to biofilm growth in several regions, all of which have narrow throats. These regions with varying thickness also appear in many aeronautical sciences, the petroleum industry, and fluid dynamics problems.

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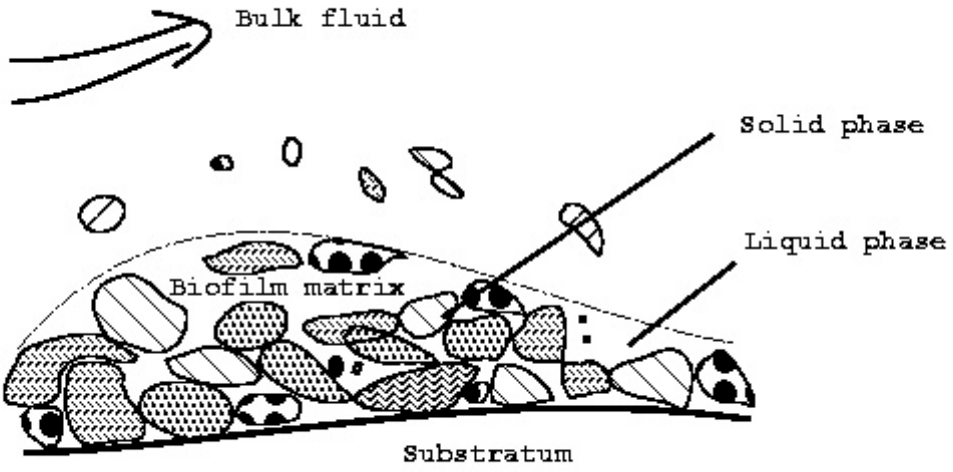

Figure 1. Compartments and phases of biofilms.

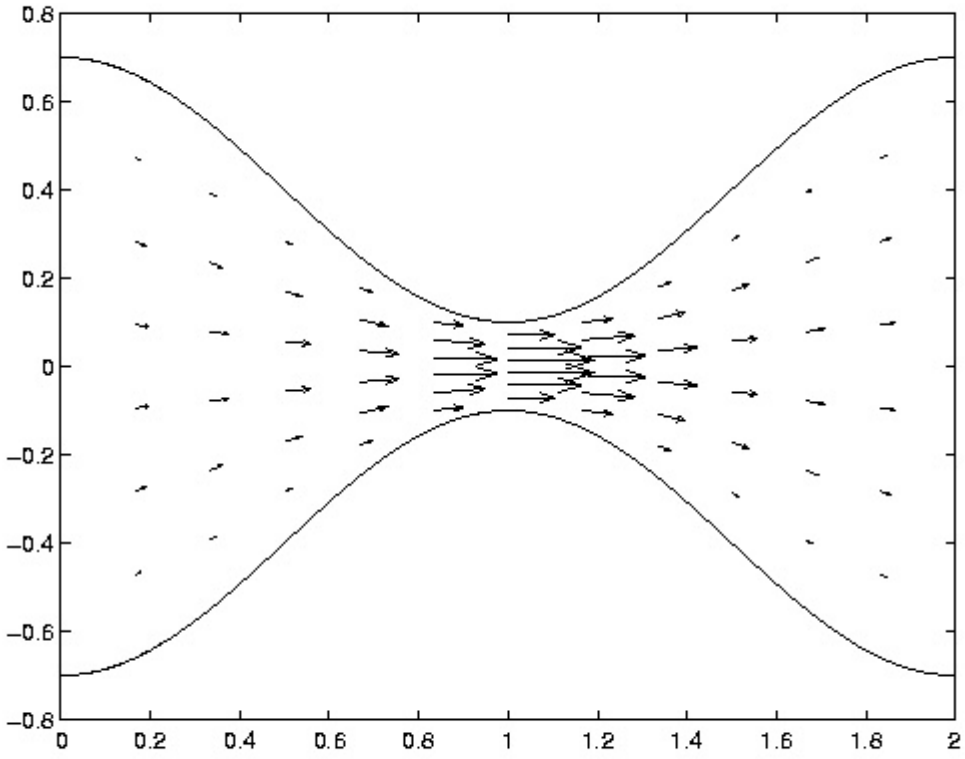

Figure 2. Velocity profile in the first type of pore region**.**

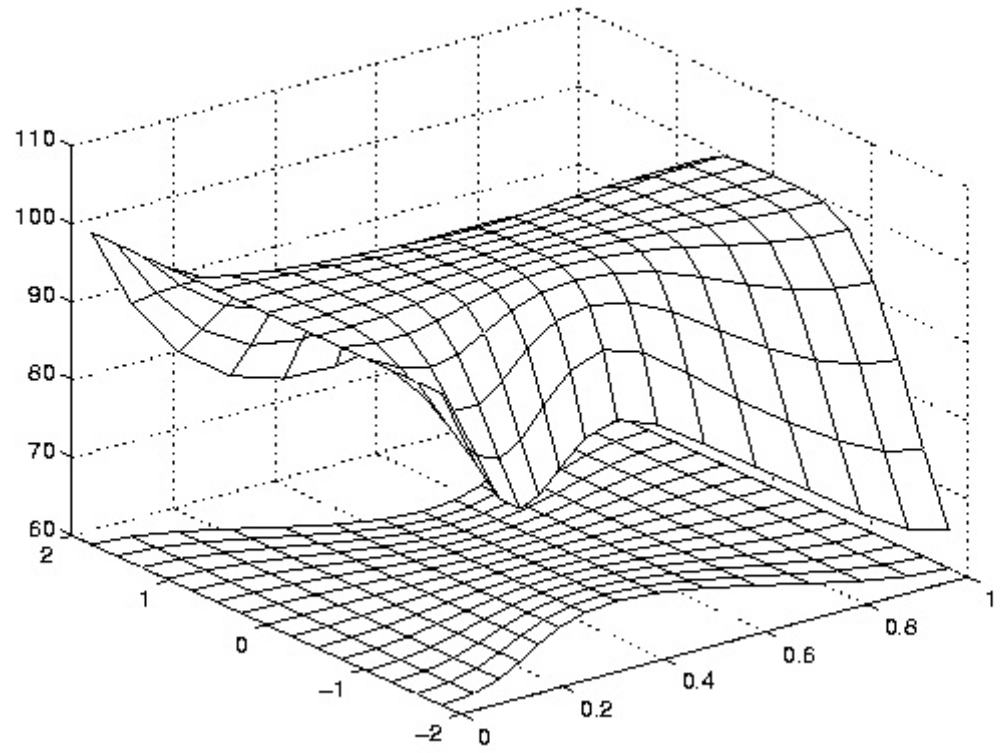

Figure 3. Steady state concentration profile in the first pore region.

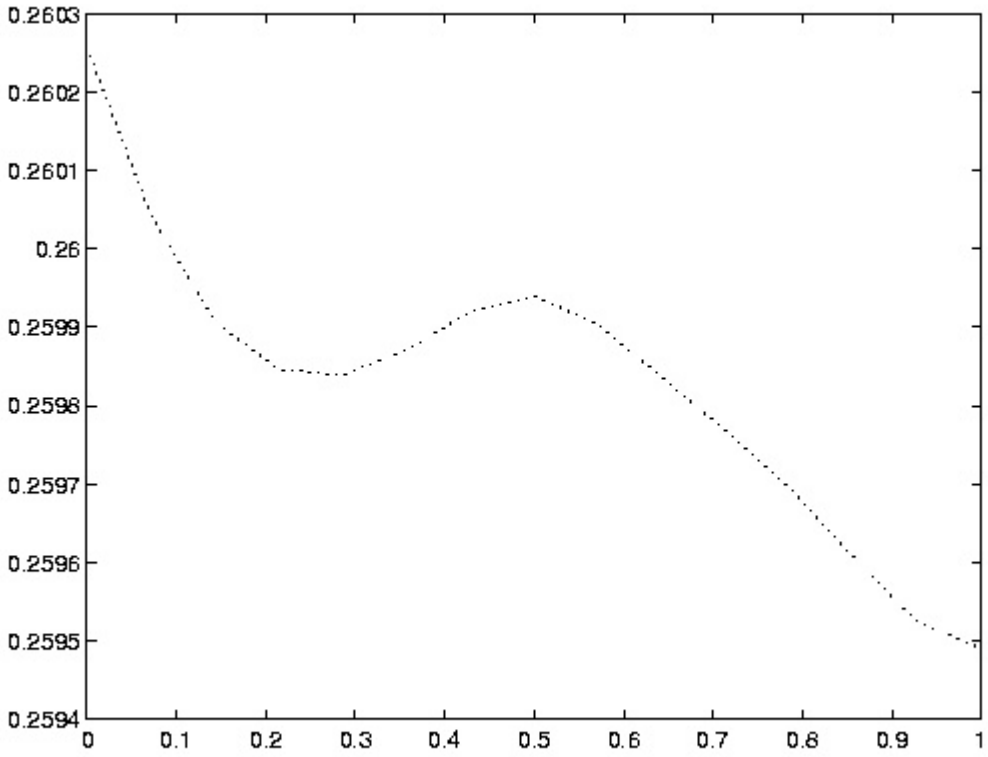

Figure 4. Interpolated biofilm growth in the first pore.