

# Two-Dimensional Modeling of Microscale Transport and Biotransformation in Porous Media

**B. Chen**

*Department of Mathematics, University of Wyoming, Laramie, Wyoming 82071-3036*

**A. Cunningham**

*Center for Biofilm Engineering at Montana State University, Bozeman, Montana 59717*

**R. Ewing**

*Departments of Mathematics, Chemical Engineering, and Petroleum Engineering, University of Wyoming, Laramie, Wyoming 82071-3036*

**R. Peralta\***

*Unite de Formation et de Recherche de Mathematiques, University of Paris VII, Paris, France*

**E. Visser**

*Center for Biofilm Engineering at Montana State University, Bozeman, Montana, 59717*

*Received 20 August 1992; revised manuscript received 23 June 1993*

We develop a model for simulating the growth of a biofilm in a tortuous tube. The solutions to the Navier-Stokes equations and the advection-diffusion equation are calculated numerically using finite differences. These solutions are then coupled with a biofilm growth model. © 1994 John Wiley & Sons, Inc.

## I. INTRODUCTION

Biofilm growth in porous media is an important mechanism for many processes, from the detrimental permeability reduction through pore blocking or the souring of petroleum reservoirs through sulfide production to the beneficial aspects of bioremediation of contaminant plumes. Although some of the growth mechanisms in pipes are beginning to be fairly well understood [1], the growth process in a tortuous porous media is considerable more complicated. Due to this complexity, we feel that we must try to understand the basic process first at the pore level together with the most important mechanisms and their rates. Only then can we scale this nonlinear information up to field-scale knowledge.

\*Current address: Instituto de Investigaciones en Matemáticas Aplicadas y en Sistemas, National University of Mexico, Mexico City, Mexico.

When physical processes are nonlinear and are coupled to other nonlinear processes, the ability to first understand the coupled phenomena at a local level and then to scale this knowledge up to longer length scales is extremely important. However, numerical simulations hold enormous promise for this difficult problem. First, numerical simulations can be used to separate the processes so that we can understand each specific phenomena by itself. Then the processes can be coupled in various ways to build the intuition of the modeler as to the effects of the various couplings. This separation of processes is difficult if not totally impossible in the laboratory. However, the "computational laboratory" is the basis of a third new methodology, taking its place along side analysis and laboratory experimentation as a powerful new scientific tool. Once a model is chosen, computer simulations can predict sensitivities of various parameters and coupled interactions. Finally, the simulations can be compared with laboratory experiments to support important phenomenological models and to determine reaction rates. In this paper, we use scientific computation and simulations to assess models and try to develop a better understanding of the coupled, nonlinear properties of biotransformations in porous media.

Computer models have already been utilized very effectively to help in developing an understanding of the basic biofilm growth process. A code entitled BIOSIM has been developed [2] and used extensively to study various biofilm systems with fairly simple fluid flow regimes. For example, this model has been used to model flow and growth in pipes or conduits, along river beds, and on the surface of tanks or large containers.

Since such a model already exists and had been used successfully for some applications, one of the first goals of our study was to see if this model could be adapted to understand the more complex regime of tortuous flow in a heterogeneous porous media domain. First, we had to clearly specify the major assumptions of this model and see if these assumptions were too restrictive for the porous media applications. For example, basic assumptions of uniform, average flow, and concentration of species made in BIOSIM are clearly not totally appropriate for tortuous flow at the pore level. Other assumptions such as the existence of a small diffusive boundary layer with no advective flow in the layer were also considered.

Once we understood the model and the effects of its basic assumptions, we needed to couple this with other models that could hopefully aid in overcoming the more restrictive assumptions. For example, we coupled BIOSIM with a Navier-Stokes code which can produce the variable velocity distribution in a tortuous pore-level model of a porous medium. This addressed the assumption of a uniform flow in BIOSIM. Then we also coupled a species-transport model to the system that can utilize the flow from the Navier-Stokes code to describe the coupled advection-diffusion-reaction properties of the variable flow field. This model allows both advection and diffusion of the cells and nutrients to the biofilm surface.

Coupling the Navier-Stokes flow model with species transport equations and the BIOSIM growth/decay model was a difficult modeling and computational task. This task is the focus of this article, describing some novel algorithms for the coupling. We then tried to assess the capabilities of this coupled system to treat the complex biofilm process with sufficient accuracy to yield basic understanding of the underlying process.

The outline of the article is as follows. We first give a brief description of the basic problem to be addressed: (a) a description of the basic microbial processes as we currently understand them; (b) an indication of the need for microscale modeling; and (c) a more detailed discussion of the coupled model mentioned above. Then in Sec. III we present the basic mathematical models used to describe the complex process. We first discuss the Navier-Stokes equations together with the advective-diffusive transport equation. Then we present the mathematical model for the biofilm process that is used in BIOSIM.

Finally, we discuss the coupling process of the models. In Sec. IV, we describe how the models are discretized and how these discretizations are coupled. In Sec. V, we present some numerical computational results and difficulties. Finally, in Sec. VI we discuss the conclusions of our study and outline the next step in the modeling process to understand the physical phenomena.

## II. PROBLEM DESCRIPTION

### A. Microbial Processes

In saturated porous media, processes governing mass transport, biofilm accumulation, and the biotransformation of organic constituents are intrinsically interrelated. As shown in Fig. 1, suspended cells are transported to the porous media surface where they may adsorb. Some fraction of these adsorbed cells desorb and return into suspension perhaps through some diffusion-like process. If environmental conditions are favorable, the adsorbed cells grow, replicate, and form a matrix composed of extracellular polymer substance (EPS) which binds the cells together. The aggregate of attached cells, EPS, and other particulate matter is termed a biofilm [3]. Once the biofilm is established, additional cells and particulate matter may attach to and detach from the biofilm surface. If biofilm thickness bridges across the pore channel, the accumulation of biofilm may be enhanced further by the filtration of particulate matter from suspension. The net accumulation of biofilm in porous media is therefore the result of biomass added to the surface from the processes

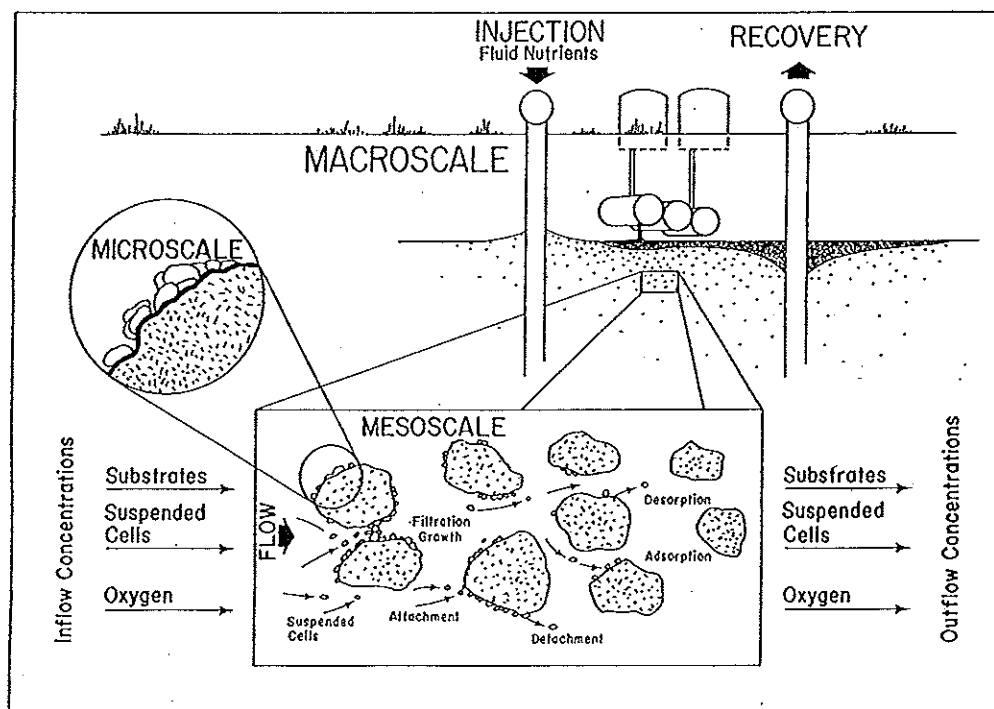


FIG. 1. Microbial processes in saturated porous media flow.

of adsorption, growth, attachment, and filtration less the amount of mass removed by the processes of desorption and detachment.

Porous media biofilms may develop as patchy discontinuous colonies or the colonies may grow together and form a continuous film. As film thickness increases, the effective pore space of the media will decrease, thereby causing a corresponding decrease in media porosity and permeability [4, 5]. If piezometric gradient remains constant, 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 biomass specific growth rate and thus in the rate of biotransformation of organic material. Decreased pore velocities also reduce the rate of detachment. Both growth rate and detachment rate will continue to change unless a steady-state biofilm thickness is achieved. As a first approximation we will consider biofilm thickness which are sufficiently small so as not to affect the velocity distribution within the pore channel.

### B. Modeling Approach

As Fig. 1 indicates, the accumulation and activity of biofilms varies from point to point along individual porous media flow channels, and are thus considered to be microscale phenomena. The rate and extent of biofilm accumulation, as well as corresponding biotransformation of organic constituents, is influenced by the geometry and microscale transport environment along an individual pore channel. Phenomenological modeling must likewise be carried out at the microscale in order to adequately describe these processes. The modeling results developed herein will deal exclusively with microscale modeling of hydrodynamics, mass transport, and biotransformation. Once transport and microbial processes can be simulated adequately at the microscale, methods will be developed for making simulation predictions of transport and biotransformation in bulk media systems, i.e., at the mesoscale and macroscale.

The microscale model consists of the coupled processes of flow and transport and biofilm growth. The flow is modeled by the Navier-Stokes equations of motion coupled with equations describing the mass-transport processes of advection, diffusion, and reaction. The reaction process will be modeled by considering the presence of a thin biofilm attached to the walls of a single pore channel which is capable of metabolizing a single dissolved substrate from the bulk liquid phase. A biofilm process model will be used to describe the strength of the reaction term. This coupled system will be solved for the simplified model case of two-dimensional steady-state flow along an individual porous medium pore channel. A sample flow channel with both pore openings and throats is initially modeled by the geometry shown in Fig. 2.

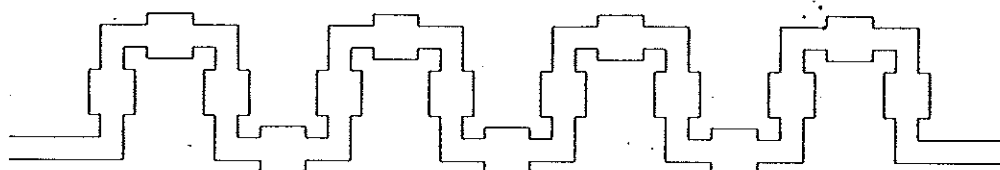


FIG. 2. Schematic of two-dimensional porous medium pore channel with expansions.

### C. Description of Coupled Model

Our main interest is to couple the flow through a porous medium with biofilm reactions and growth on the pore walls. 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.

As a first step we consider the scenario in which the porous medium is approximated by a series of rectangular cavities linked by straight tubes (see Fig. 2). This way we have a well-defined tortuous laminar flow field as an initial model to try to understand the complexities of the coupled processes. Calculations are done for the full tube, but in order to better understand the interaction between the flow and the biofilm reactions, we first concentrate our attention on only one cavity.

We perform numerical experiments on the flow in the cavity with two different Reynolds numbers, 1 and 10; these represent typical values for laminar flow in a porous medium. First we assume that there is no biofilm and solve the Navier-Stokes and concentration equations accordingly. The boundary value for the concentration at the walls is a zero-derivative condition.

Next we illustrate how the flow equation can be coupled in a simple way with the biofilm equations. We use the values for the flow and concentration distribution calculated with no biofilm present and then input the velocities and the concentration into the biofilm equations. Now we have a biofilm of a certain thickness that requires a flux of nutrients into it. This changes the domain for the flow and the boundary condition for the biofilm. Numerical experiments carried out show that for average values of the initial concentration, the growth of the biofilm is small compared with the diameter of the tubes. Thus as a first approximation we will take the size of the tubes to be constant in time. From the biofilm equations we get a value for the flux of nutrients into the biofilm. Using this new flux we again solve the concentration equation and input the newly calculated value into the biofilm, and we can keep iterating until the values of the concentration at the biofilm surface between two successive iterations is sufficiently small. Of course we must eventually shrink the size of the part of the tube available to flow to model the growth of the biofilm.

## III. MODEL EQUATIONS

### A. Navier-Stokes Equations

We consider a viscous incompressible fluid with dissolved nutrients moving through the two-dimensional domain defined by Fig. 2. The equations that model the movement of viscous fluids are the Navier-Stokes equations

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} + \nabla p = \frac{1}{\Re} \nabla^2 \mathbf{v}, \quad (3.1)$$

$$\nabla \cdot \mathbf{v} = 0, \quad (3.2)$$

and the concentration equations,

$$\frac{\partial}{\partial t}(c_i) + \nabla \cdot (c_i \mathbf{v}) = \frac{\nabla \cdot (\Gamma_i \nabla c_i)}{\Re \mathcal{C}} + R_i, \quad i = 1, \dots, n. \quad (3.3)$$

Here we denote by  $\mathbf{v}$  the velocity of the fluid,  $p$  the pressure,  $\Re$  the Reynolds number,  $c_i$  the mass concentration of species  $i$ ,  $\Gamma_i$  the diffusion coefficient of species  $i$ ,  $\mathfrak{Sc}$  the Schmidt number of species  $i$ ,  $R_i$  the generation rate of species  $i$ , and  $n$  the total number of dissolved species. Our present model does not consider transformation of any species in the fluid, so we assume that  $R_i \equiv 0$ . The boundary conditions are  $\mathbf{v}$  given at the inflow boundary,  $\partial \mathbf{v} / \partial n = 0$  at the outflow boundary, and  $\mathbf{v} = 0$  at the boundaries with the biofilm. For the  $c_i$ 's the conditions are value given at the inflow,  $\partial c_i / \partial n = 0$  at outflow, and  $\partial c_i / \partial n$  given at the biofilm. Here,  $\partial / \partial n$  denotes the normal derivative.

For computational considerations, it is more convenient to work with the stream function  $\psi$  and vorticity  $\omega$  as the fluid unknowns. Equations (3.1) and (3.2) are replaced by

$$\frac{\partial \omega}{\partial t} + u \frac{\partial \omega}{\partial x} + v \frac{\partial \omega}{\partial y} - \frac{1}{\Re} \nabla^2 \omega = 0, \quad (3.4)$$

$$\nabla^2 \psi + \omega = 0, \quad (3.5)$$

where  $u = \partial \psi / \partial y$ ,  $v = -\partial \psi / \partial x$ , and  $\omega = \partial v / \partial x - \partial u / \partial y$ . The boundary conditions are now  $\psi$  given at the inflow,  $\partial \psi / \partial n = 0$  at the outflow, and  $\psi = \text{const}$  on the biofilm boundaries. Conditions for the vorticity are obtained using (3.5) evaluated at the boundary. We will solve the Navier-Stokes equations (3.4) and (3.5) with no slip and no penetration boundary conditions at the walls, parabolic velocity profile at inlet, and zero derivatives in the axial direction at outflow. Since we assume that the thickness of the biofilm is small the velocity field will not change. Then we solve the concentration equation using the velocity field together with the boundary conditions: uniform concentration at entrance, zero derivative in the axial direction at outflow, and flux given at the walls. The flux is given by the biofilm-process model described in the following section. In writing the boundary conditions at the biofilm interface we have used the assumption that the velocity of the fluid in the biofilm is very small. We intend to develop various experimental flow tests to assess the validity of these assumptions. In this way we have a model for the fluid flow where we have advection and diffusion of nutrients and other organic and inorganic material to the biofilm.

## B. Biofilm-Process Model

Figure 3 illustrates the conditions near the interface between fluid and biofilm. Mass transport of bulk fluids constituents to (and from) the biofilm surface occurs by the process of diffusion. Net growth of biofilm is presently described by Monod kinetics with a first-order decay term. Net biofilm accumulation rate is considered as the difference between net growth rate and the net rate of detachment from the biofilm surface. In this investigation net detachment rate is assumed to be a second-order function of biofilm thickness ( $L_f$ ). Equations for each of these processes are as follows.

- Bulk fluid transport:

$$\frac{d}{dt}(VC) = \underbrace{Q_{in}(C_{in} - C)}_{\text{advection}} + \underbrace{J_B A_F}_{\text{diffusion to biofilm}} + \underbrace{Vr}_{\text{reaction}}. \quad (3.6)$$

- Diffusion (bulk fluid and biofilm):

$$J = -D \frac{\partial C_s}{\partial y}. \quad (3.7)$$

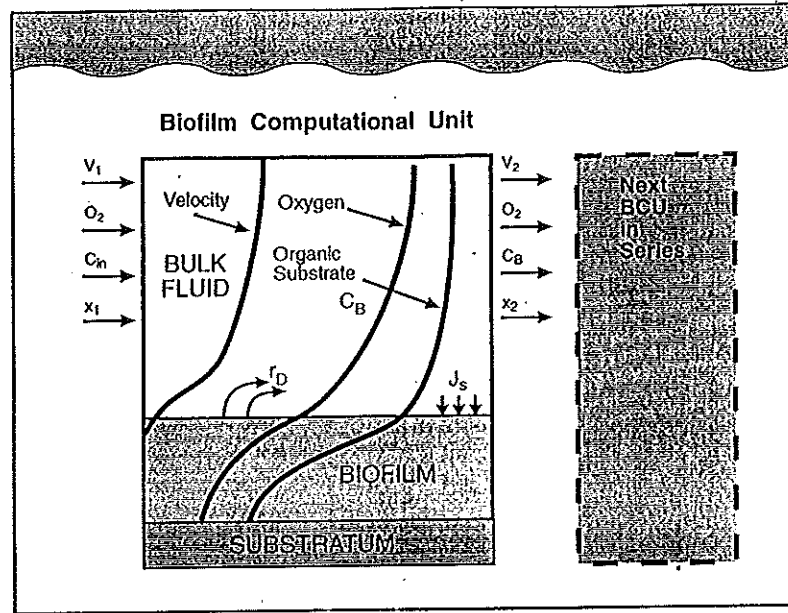


FIG. 3. Mass transport and biofilm accumulation in a biofilm computational unit.

- Biochemical transformation (net cell growth):

$$\frac{dX}{dt} = \mu_{\max} \frac{XC}{K + C} - bX \quad (\text{net cell growth}), \quad (3.8)$$

$$\frac{dC}{dt} = -\frac{\mu_{\max}}{Y_{x/c}} \frac{XC}{K + C} \quad (\text{substrate utilization}). \quad (3.9)$$

- Net detachment:

$$r_D = -k_D L_f^2, \quad (3.10)$$

where

$C$  = constituent concentration,

$C_s$  = substrate concentration,

$C_{in}$  = inlet concentration,

$V$  = bulk fluid volume,

$Q_{in}$  = volumetric flow rate,

$J_B$  = mass flux to the biofilm surface,

$J$  = mass flux,

$D$  = diffusivity,

$X$  = biofilm mass per unit volume,

$b$  = endogenous decay coefficient,

$K$  = monod rate (saturation) coefficient,

$L_f$  = biofilm thickness,

$k_D$  = detachment coefficient,

$\mu_{\max}$  = maximum specific growth rate,

$Y_{x/c}$  = yield of X from C,

$y$  = coordinate in direction of growth, and

$A_F$  = biofilm surface area.

The biofilm processes described by Eqs. (3.6)–(3.10) are used in the BIOSIM model [2]. BIOSIM is well documented and has been previously used to analyze various biofilm systems including river beds and surfaces of tanks and conduits. BIOSIM performs mass balances on all system constituents including substrate(s) electron acceptor(s), multiple species, and attached and suspended biomass.

The geometry of the biofilm system is described in a simplified way as a series of one or more boxes, which are called "units." As shown in Fig. 3, a unit consists of a biofilm compartment, a liquid boundary layer, and a bulk fluid compartment. It is assumed that the bulk fluid in the unit is completely mixed. Consequently, it is assumed that the properties of the biofilm, which form in the unit, are equal over the whole area  $A_F$  and that gradients in directions other than perpendicular to the solid surface can be neglected. If this last assumption is not valid, more than one unit is needed to model the biofilm system. BIOSIM allows for up to 12 units, which are arranged in series. These units are automatically coupled by the program such that the effluent of the previous unit becomes the influent of the next one. The area of biofilm,  $A_F$ , the liquid boundary-layer thickness  $L_L$ , the length  $L_{un}$  of the unit, and either thickness  $L_B$  of the bulk fluid compartment or the volume  $V_{un}$  of the unit are constant parameters of the units. Since the two parameters  $L_B$  and  $V_{un}$  are not independent from each other, only one of them can be specified by the user and the other one is calculated by the program from  $V_{un} = (L_F + L_L + L_B)A_F$ . The volumetric inflow rate  $Q_{in}$  and the inflow concentrations  $C_{in}$  may vary with time and are specified by the user. The biofilm thickness  $L_F$  in subsequent units is calculated by BIOSIM. Significant results include computed spatial gradients in key system variables including biofilm thickness, bulk concentrations of substrate and electron acceptor, and substrate flux into the biofilm surface.

### C. Coupled Biofilm Accumulation Model

Results from previous modeling scenarios define velocity  $v$  and concentration  $c$  fields within the single-cavity domain. For the lowest  $\mathfrak{N}$  condition (Fig. 4) we observe significant variation in the computed  $v$  values for near-substratum nodes along the flow path through the cavity. If we consider the product of  $c \times v$  to be an indicator of mass (i.e., substrate/nutrient) transport near the substratum, it is obvious that, for conditions in Fig. 4, the surface of an attached biofilm will experience significant variations in substrate/nutrient flux depending on flow path position. Plots of the velocity profiles for  $\mathfrak{N} = 10$  are shown in Fig. 5. Regions of high/low near-surface transport for the low- $\mathfrak{N}$  scenario are shown in Fig. 6.

Following is the procedure used to couple the biofilm process model with the Navier-Stokes-solute transport model.

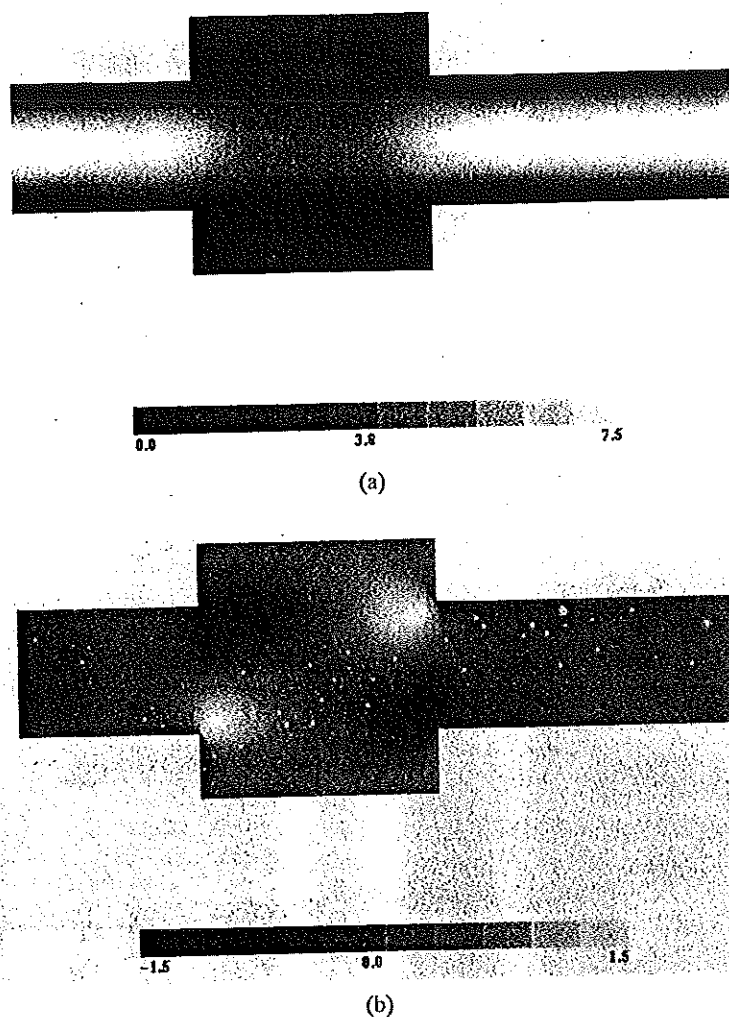


FIG. 4. Plots of velocity profiles for  $Re = 1$ . (a) shows the horizontal component  $u$ , and (b) the vertical component  $v$ .

The procedure for coupling the BIOSIM model with the results from the Navier-Stokes simulation is shown schematically in Fig. 7. The entire throat and cavity sections of the pore channel are treated as individual biofilm computational units (BCU). Initially we assume that the height of the BCU is equal to  $8\Delta y$ , where  $\Delta y$  is the vertical grid spacing used in Navier-Stokes simulation. As a consequence we compute the velocity and substrate concentration to the BCU as the numerical average of individual nodal values over the  $8\Delta y$  interval. Averages were computed at the  $x$  midpoint of each BCU. In our simulations we assumed the thickness of the liquid layer to be as follows:  $L_L = \Delta y - L_f$ .

The coupling procedure involving BIOSIM was as follows.

*Step 1.* Based on initial (nonreactive surface) simulations from Navier-Stokes and solute transport specify influent velocity and concentrations to BCU and assume an initial biofilm thickness of  $10 \mu\text{m}$ . Run BIOSIM until a steady-state thickness condition is achieved

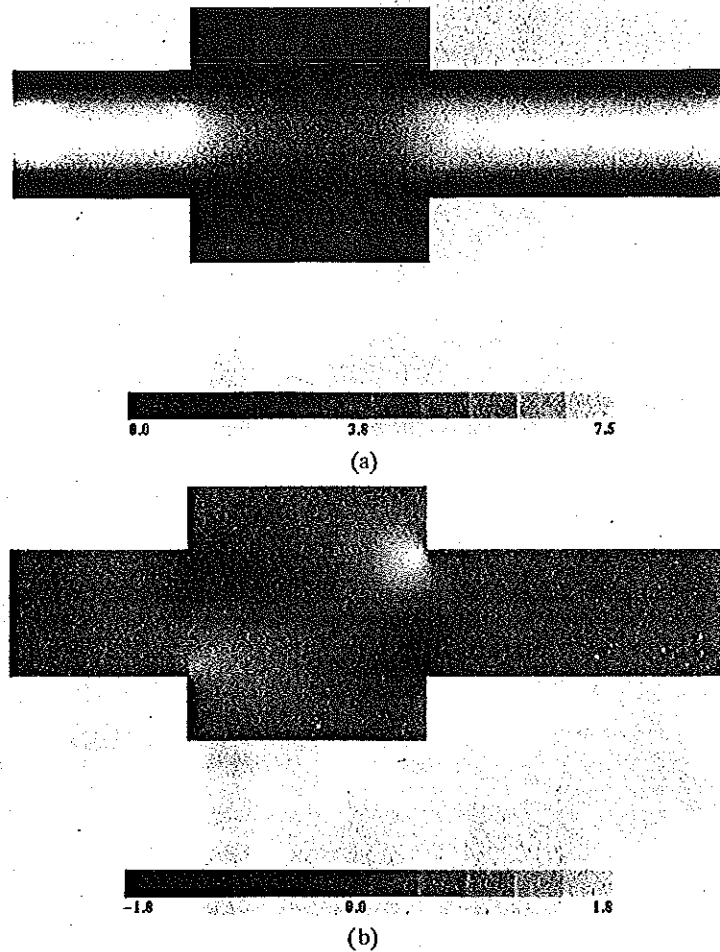


FIG. 5. Plots of velocity profiles for  $\beta = 10$ . (a) shows the horizontal component  $u$ , and (b) the vertical component  $v$ .

for the given influent conditions. This simulation results in the computed concentration of substrate at the biofilm surface and also the flux requirement needed to sustain the biofilm at steady-state thickness.

*Step 2.* Using the biofilm flux requirement from Step 1, repeat the solute-transport concentration simulation, which results in an updated concentration condition at each node. Velocity conditions, assuming small biofilm thickness, remain unchanged from the previous simulation.

*Step 3.* Repeat simulation with BIOSIM using updated concentration values from solute transport simulation. This BIOSIM iteration results in an updated biofilm thickness and also values for surface flux and substrate concentration at the fluid biofilm interface. We then check how close the BIOSIM computation of surface concentration ( $c_s$ ) agrees with the interpolated concentration value for the concentration profile from solute transport ( $c'_s$ ).

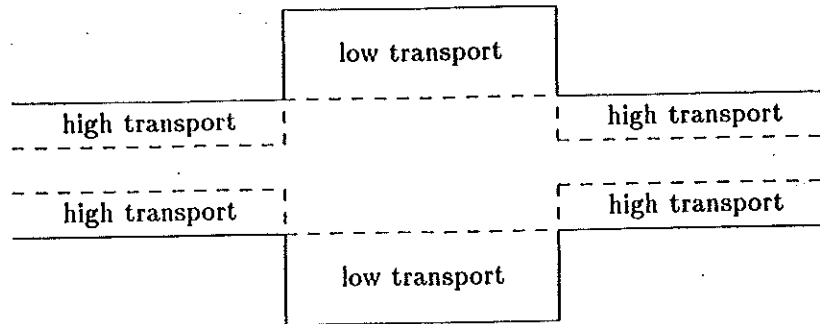


FIG. 6. Schematic showing regions of high and low near-surface transport as defined by product of  $c \times v$  from near-surface nodes in a nonreactive Navier-Stokes-solute transport model.

**BCU Height Adjustment.** A problem arises in this coupling procedure due to the need to specify the height of the biofilm computational unit (BCU) in BIOSIM. Because advective transport in BIOSIM is one dimensional, the BCU height controls the amount of substrate flux entering the bulk fluid compartment inside the BCU. Diffusion from the well-mixed bulk compartment through the liquid layer transports substrate into the biofilm compartment, thereby reducing the substrate concentration in the bulk liquid compartment. This condition may result in BIOSIM bulk liquid concentrations which are significantly lower than the corresponding concentration, computed from the solute-transport model, for the same nodal locations. It may therefore be necessary to vary the BCU height as part of the iterative coupling procedures in order that  $|c_s - c'_s|$  reaches the desired tolerance.

Two cases were run to demonstrate the effect of varying BCU height: (1) BCU height set to  $8\Delta y$  for units 1, 2, and 3; and (2) BCU height raised to  $12\Delta y$  in units 1 and 3 and  $24\Delta y$  in unit 2.

#### IV. NUMERICAL SOLUTION OF COUPLED SYSTEM

The equations for the flow (3.3)–(3.5) are discretized using finite differences. Both centered differences and upwind differences were implemented. Since we are interested in low Reynolds numbers of this application, centered differences perform very well.

A uniform grid in both  $x$  and  $y$  is drawn over a rectangle that contains the region of interest, taking care that all corners correspond to a grid point. Equations are written only for the points internal to the flow region. A preprocessor program was written to describe the domain, the boundaries, and the discretization in a straightforward way. Details are given in [6]. The program stores in a database the information on all the boundary and internal nodes and the coordinates of neighboring points: it also checks for inconsistencies. If necessary, local grid refinement can be used, but all the examples in this article were run using a uniform mesh.

The equations and boundary conditions are described by giving the coefficients of the node point and all of its neighbors. For example, for Laplace's equation using a uniform mesh, a second-order difference approximation evaluated at  $(x, y)$  is

$$\begin{aligned} & \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \\ &= \frac{\phi(x+h, y) + \phi(x-h, y) + \phi(x, y+h) + \phi(x, y-h) - 4\phi(x, y)}{h^2} \end{aligned} \quad (4.1)$$

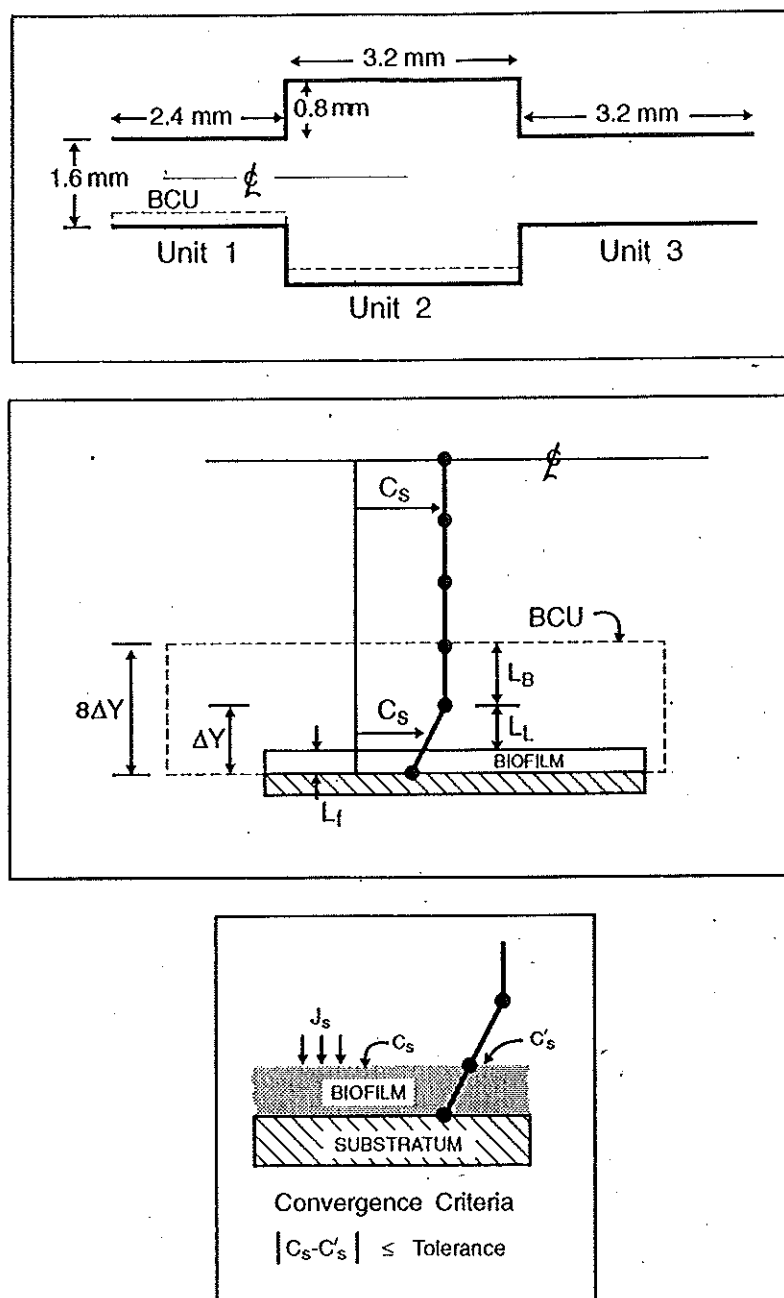


FIG. 7. Schematic showing the procedure for coupling the BIOSIM model with the results from the Navier-Stokes simulation.

To specify the corresponding equation for this point  $(x, y)$ , we will simply say that the coefficient at the point is  $-4/h^2$  and that at the coefficients its neighbors to the north, south, east, and west are  $1/h^2$ .

The program will then use (3.4) and (3.5) information on the grid to construct the discretized equations. For the Navier-Stokes equations, we will get two systems, one from the continuity equation for the stream function and the other for the vorticity,

$$\frac{\psi_{i+1,j}(t) + \psi_{i-1,j}(t) + \psi_{i,j+1}(t) + \psi_{i,j-1}(t) - 4\psi_{i,j}(t)}{h^2} + \omega_{ij}(t) = 0, \quad (4.2)$$

$$\begin{aligned} \frac{\partial \omega_{ij}(t)}{\partial t} + \frac{\psi_{i+1,j}(t) - \psi_{i-1,j}(t)}{2h} \frac{\omega_{i+1,j}(t) - \omega_{i-1,j}(t)}{2h} \\ + \frac{\psi_{i,j+1}(t) - \psi_{i,j-1}(t)}{2h} \frac{\omega_{i,j+1}(t) - \omega_{i,j-1}(t)}{2h} \\ - \frac{1}{\Re} \frac{\omega_{i+1,j}(t) + \omega_{i-1,j}(t) + \omega_{i,j+1}(t) + \omega_{i,j-1}(t) - 4\omega_{ij}(t)}{h^2} = 0, \end{aligned} \quad (4.3)$$

where  $\psi_{i,j}(t) = \psi(ih, jh, t)$ . The notation for  $\omega_{i,j}(t)$  is analogous.

We are assuming that the growth of the biofilm is sufficiently small that it does not affect the velocity field. This allows us to consider only stationary solutions.

Two different methods were implemented for calculating the steady solutions. In the first one, we take the time derivative in Eq. (4.3) equal to zero, and solve the resulting elliptic system. The discretized continuity equation for  $\psi$  depends on  $\omega$ , and the coefficients of the vorticity equation depend on the stream function. If we know the vorticity, (4.2) is a linear system for  $\psi$ . We solve it using a Successive Over Relaxation iteration [7]. The acceleration parameter  $\lambda$  was determined empirically.  $\lambda = 1.6$  worked well. Also, if we know the values of the stream function, (4.3) is a linear system for the vorticity that can be solved using SOR, now with  $\lambda = 1.1$ .

To account for the dependence of the equation for one variable on the other, an outer iteration scheme was set (the inner iteration is the SOR):

1. Give an initial guess for the vorticity and solve (4.2) for  $\psi$ .
2. Obtain the boundary conditions for the vorticity by applying the equivalent of (4.2) with one-sided derivatives at the boundary. Relax the boundary values for  $\omega$ .
3. Solve (4.3) using the values of  $\psi$  obtained from Step 1 and the boundary conditions obtained from Step 2.
4. Relax the vorticity.
5. Use the new vorticity to solve (4.2) and repeat until the change in the solution is less than the desired tolerance.

The vorticity needs to be relaxed for the above scheme to converge.

The relaxation procedure is

$$\omega^{(i)} = (1 - \lambda_\omega) \omega^{(i-1)} + \lambda_\omega \hat{\omega}^{(i)}$$

where  $\omega^{(i)}$  is the value of  $\omega$  at the  $i$ th iteration,  $\hat{\omega}^{(i)}$  is the solution of the vorticity equation at the  $i$ th iteration, and  $\lambda_\omega$  is a relaxation parameter.

Peyret and Taylor [8] recommend using a different parameter to relax the boundary values of  $\omega$ . In practice this will speed up the convergence.

The second method to calculate the steady velocities consists of giving an initial value for the stream function and vorticity and following the solution in time until a steady

solution is obtained. Explicit, semi-implicit, and completely implicit methods were tried. The semi-implicit method described below worked best.

Initial values for the stream function and vorticity were given. These values were either for no flow or the values for a different Reynolds number already calculated. The vorticity equation is advanced one time step using the stream-function values at the previous step. This way we do not have to solve a linear system. The vorticity at the new time is calculated by solving the continuity equation, which implies using SOR. The time stepping is continued until the solution at two consecutive times varies less than  $\epsilon$ .

Once we have the steady velocities, they were used in the discretized, time dependent concentration equations. We have to solve only one linear system for each concentration equation. The velocities and concentrations can then be used as input for the equations for the biofilm.

## V. COMPUTATIONAL RESULTS

For the computational scenario a single cavity was chosen. The first step was to solve the Navier-Stokes equations (3.1) and (3.2) in the stream-function vorticity formulation (3.4) and (3.5) for the steady-state solution for  $\mathfrak{R} = 1$  and  $\mathfrak{R} = 10$ . For the boundary conditions at the inlet, a parabolic velocity profile was used with average velocity  $u_{ave} = 48.4$  m/day ( $\mathfrak{R} = 1$ ) and  $u_{ave} = 484$  m/day ( $\mathfrak{R} = 10$ ). A uniform mesh was used for both Reynolds numbers with  $h = \Delta x = \Delta y = 0.04$  cm and  $\Delta t = 123.3$  days ( $\mathfrak{R} = 1$ ) and  $\Delta t = 49.32$  days ( $\mathfrak{R} = 10$ ). Velocity contour plots of solutions for  $\mathfrak{R} = 1$  and  $\mathfrak{R} = 10$  are shown in Figs. 4 and 5, respectively.

The next step was solving the concentration equation (3.3) for the concentration with a uniform inlet concentration of  $0.5$  g/m<sup>3</sup> and zero flux wall boundary conditions for fixed walls. Now the biofilm-process model (BIOSIM) was applied to the tube and cavity by using symmetry and defining three units shown in Fig. 6, where units were described in Sec. III.B.

For the biofilm process, one biofilm species, *Pseudomonas aeruginosa*, was used with glucose as the limiting substrate. *Pseudomonas aeruginosa* has kinetic parameters [1]:  $\mu_{max} = 0.37$  h<sup>-1</sup>,  $K = 1.6$  g m<sup>-3</sup>, and  $Y_{xlc} = 0.69 \frac{\text{g Biomass}}{\text{g Glucose}}$ . No endogenous respiration was used for this simulation (i.e.,  $b = 0$ ). A detachment coefficient of  $2 \times 10^5$  was used. Glucose diffusivity was set at  $3.09 \times 10^{-2}$  m<sup>2</sup>/day based on procedures suggested by Wilson *et al.* [10]. Diffusivity in the biofilm was  $0.64$  cm<sup>2</sup>/day. Inlet concentration of glucose in the bulk was  $0.5$  g/m<sup>3</sup>.

Three different cases were run. In case 1 we have  $\mathfrak{R} = 1$  and a BCU for all units of  $2\Delta y$ . Results are given in Table I. From this table we can see that only three iterations between the solute transport and the biofilm models are needed. The values of  $|c_s - c'_s|$  are not very good. The difficulty is due to the fact that for biofilm model all nutrients enter the unit only through the left side of the bulk layer. For case 2, the thickness of the BCU's was increased to  $12\Delta y$  for units 1 and 3, and to  $24\Delta y$  for unit 2, to get a closer agreement between the results of the two models. From Table II, we see that now the values are much closer. Table II is also for  $\mathfrak{R} = 1$ . A plot of the concentration profiles from the solute transport model is given in Fig. 8.

We also ran a third case with  $\mathfrak{R} = 10$ , and the thickness of the BCUs the same as for case 2. Results for case 3 are shown in Table III and Fig. 9.

TABLE I. Results for  $\mathfrak{R} = 1$ , and BCU thickness of  $2\Delta y$  for all units.

| Iter. 1                            | Unit 1 | Unit 2 | Unit 3 |
|------------------------------------|--------|--------|--------|
| $\bar{c}$ (g/m <sup>3</sup> )      | 0.500  | 0.500  | 0.500  |
| $\bar{v}$ (10 <sup>-4</sup> m/s)   | 3.240  | 0.7234 | 3.234  |
| $c'_s$ (g/m <sup>3</sup> )         | 0.500  | 0.500  | 0.500  |
| $J$ (g/m <sup>2</sup> day)         | 0.5580 | 0.2020 | 0.4891 |
| $c_{sout}$ (g/m <sup>3</sup> )     | 0.3498 | 0.1764 | 0.3221 |
| $L_f$ ( $\mu$ m)                   | 13.401 | 8.092  | 12.661 |
| $c_b$ (g/m <sup>3</sup> )          | 0.3505 | 0.1766 | 0.3221 |
| $ c_s - c'_s $ (g/m <sup>3</sup> ) | 0.1502 | 0.3236 | 0.1779 |
| Iter. 2                            | Unit 1 | Unit 2 | Unit 3 |
| $\bar{c}$                          | 0.4811 | 0.4562 | 0.4292 |
| $\bar{v}$                          | 3.240  | 0.7234 | 3.234  |
| $c'_s$                             | 0.4776 | 0.4546 | 0.4251 |
| $J$                                | 0.5328 | 0.1815 | 0.4123 |
| $c_{sout}$                         | 0.3379 | 0.1655 | 0.2816 |
| $L_f$                              | 13.104 | 7.655  | 11.531 |
| $c_b$                              | 0.3384 | 0.1657 | 0.2819 |
| $ c_s - c'_s $                     | 0.1397 | 0.2891 | 0.1435 |
| Iter. 3                            | Unit 1 | Unit 2 | Unit 3 |
| $\bar{c}$                          | 0.4820 | 0.4593 | 0.4372 |
| $\bar{v}$                          | 3.240  | 0.7234 | 3.234  |
| $c'_s$                             | 0.4786 | 0.4579 | 0.4337 |
| $J$                                | 0.5340 | 0.1829 | 0.4218 |
| $c_{sout}$                         | 0.3385 | 0.1665 | 0.2862 |
| $L_f$                              | 13.118 | 7.676  | 11.658 |
| $c_b$                              | 0.3390 | 0.1667 | 0.2866 |
| $ c_s - c'_s $                     | 0.1401 | 0.2914 | 0.1475 |

For all three cases the maximum growth of the biofilm was less than 13  $\mu$ m, which is very small compared to the width of the tube, 1600  $\mu$ m, so our assumption that the tube size did not change is very good.

The BIOSIM model has capabilities which were not used in this study. For example, BIOSIM can predict the growth of multiple species each utilizing a different substrate. Alternative expressions for growth kinetics and net biofilm detachment can also be used. Because the individual biofilm processes are explicitly described in BIOSIM the coupling scheme developed herein provides a method for performing a detailed sensitivity analysis on many individual biofilm processes with reference to a specific flow path and geometry and mass transport regimen.

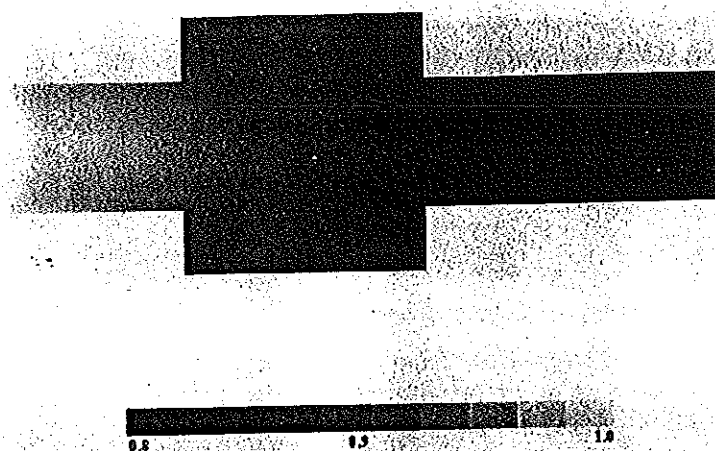
However, it is important to note that other published biofilm process models can also be used successfully. To demonstrate feasibility we replaced BIOSIM in our coupling scheme with a set of algebraic equations published by Sáez and Rittmann [11].

TABLE II. Results for  $\mathfrak{R} = 1$ , and BCU thickness of  $12\Delta y$  for units 1 and 3, and of  $24\Delta y$  for unit 2.

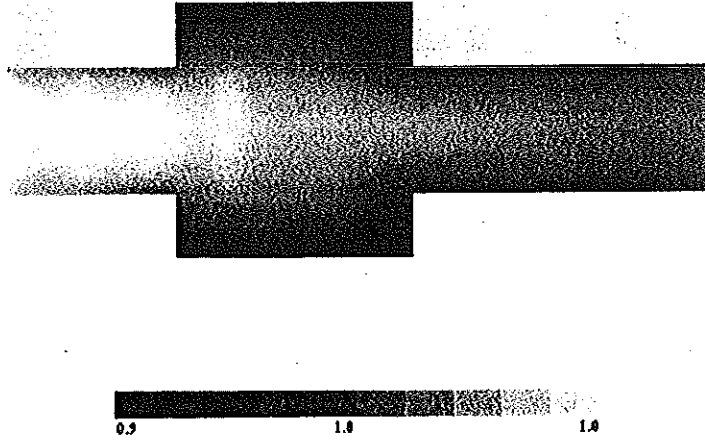
| Iter. 1                            | Unit 1 | Unit 2 | Unit 3 |
|------------------------------------|--------|--------|--------|
| $\bar{c}$ (g/m <sup>3</sup> )      | 0.50   | 0.50   | 0.50   |
| $\bar{v}$ (10 <sup>-4</sup> m/s)   | 4.320  | 1.903  | 4.316  |
| $c'_s$ (g/m <sup>3</sup> )         | 0.500  | 0.500  | 0.500  |
| $J$ (g/m <sup>2</sup> day)         | 0.6389 | 0.6128 | 0.6359 |
| $c_{sout}$ (g/m <sup>3</sup> )     | 0.4075 | 0.3750 | 0.3856 |
| $L_f$ ( $\mu$ m)                   | 14.084 | 14.044 | 14.307 |
| $c_b$ (g/m <sup>3</sup> )          | 0.4084 | 0.3757 | 0.3864 |
| $ c_s - c'_s $ (g/m <sup>3</sup> ) | 0.0925 | 0.1250 | 0.1144 |
| Iter. 2                            | Unit 1 | Unit 2 | Unit 3 |
| $\bar{c}$                          | 0.4775 | 0.4223 | 0.3829 |
| $\bar{v}$                          | 4.320  | 1.903  | 4.316  |
| $c'_s$                             | 0.4174 | 0.4110 | 0.3769 |
| $J$                                | 0.6468 | 0.4975 | 0.4545 |
| $c_{sout}$                         | 0.3903 | 0.3215 | 0.3013 |
| $L_f$                              | 14.438 | 12.666 | 12.112 |
| $c_b$                              | 0.3908 | 0.3219 | 0.2017 |
| $ c_s - c'_s $                     | 0.0811 | 0.0896 | 0.0756 |
| Iter. 3                            | Unit 1 | Unit 2 | Unit 3 |
| $\bar{c}$                          | 0.4789 | 0.4334 | 0.4045 |
| $\bar{v}$                          | 4.320  | 1.903  | 4.316  |
| $c'_s$                             | 0.4732 | 0.4239 | 0.4000 |
| $J$                                | 0.6492 | 0.5133 | 0.4875 |
| $c_{sout}$                         | 0.3914 | 0.3289 | 0.3169 |
| $L_f$                              | 14.465 | 12.861 | 12.533 |
| $c_b$                              | 0.3920 | 0.3294 | 0.3174 |
| $ c_s - c'_s $                     | 0.0818 | 0.0950 | 0.0831 |

The Sáez-Rittmann model consists of algebraic expressions for the flux of substrate into a steady-state biofilm. These expressions were developed based on an analysis of the numerical results from the numerical solution of differential equations similar to those in BIOSIM.

Because the Sáez-Rittmann model expresses flux into the biofilm as a function of substrate concentration at the diffusion layer/biofilm interface it was easily incorporated into our coupling scheme in the place of BIOSIM. The Sáez-Rittmann model does not deal explicitly with detachment as BIOSIM does but lumps detachment into the endogenous decay coefficient and calls it a biofilm shear loss and decay coefficient denoted by  $b'$ . The value used for this simulation was  $b' = 1.28 \text{ day}^{-1}$ . The other kinetic parameters were the same as used in the BIOSIM simulations. All other transport parameters and boundary conditions were the same for the  $\mathfrak{R} = 10$  run shown in Table II. Results of this simulation are shown in Table IV. Convergence criteria were satisfied after four iterations.

FIG. 8. Plot of the concentration of glucose for  $\mathfrak{R} = 1$ .TABLE III. Results for  $\mathfrak{R} = 10$ , and BCU thickness of  $12\Delta y$  for units 1 and 3, and of  $24\Delta y$  for unit 2.

| Iter. 1                            | Unit 1 | Unit 2 | Unit 3 |
|------------------------------------|--------|--------|--------|
| $\bar{c}$ (g/m <sup>3</sup> )      | 0.500  | 0.500  | 0.500  |
| $\bar{v}$ (10 <sup>-3</sup> m/s)   | 4.320  | 1.903  | 4.316  |
| $c'_s$ (g/m <sup>3</sup> )         | 0.500  | 0.500  | 0.500  |
| $J$ (g/m <sup>2</sup> day)         | 0.8588 | 0.8465 | 0.8507 |
| $c_s$ (g/m <sup>3</sup> )          | 0.4784 | 0.4817 | 0.4837 |
| $L_f$ (μm)                         | 16.628 | 16.508 | 16.550 |
| $c_b$ (g/m <sup>3</sup> )          | 0.4885 | 0.4828 | 0.4848 |
| $ c_s - c'_s $ (g/m <sup>3</sup> ) | 0.0126 | 0.0183 | 0.0163 |
| Iter. 2                            | Unit 1 | Unit 2 | Unit 3 |
| $\bar{c}$                          | 0.4956 | 0.4860 | 0.4817 |
| $\bar{v}$                          | 4.320  | 1.903  | 4.316  |
| $c'_s$                             | 0.4886 | 0.4697 | 0.4741 |
| $J$                                | 0.8508 | 0.8186 | 0.8137 |
| $c_s$                              | 0.4835 | 0.4688 | 0.4666 |
| $L_f$                              | 16.559 | 16.243 | 16.194 |
| $c_b$                              | 0.4842 | 0.4694 | 0.4672 |
| $ c_s - c'_s $                     | 0.0051 | 0.0009 | 0.0075 |
| Iter. 3                            | Unit 1 | Unit 2 | Unit 3 |
| $\bar{c}$                          | 0.4956 | 0.4864 | 0.4823 |
| $\bar{v}$                          | 4.320  | 1.903  | 4.316  |
| $c'_s$                             | 0.4887 | 0.4706 | 0.4749 |
| $J$                                | 0.8508 | 0.8193 | 0.8148 |
| $c_s$                              | 0.4836 | 0.4691 | 0.4671 |
| $L_f$                              | 16.559 | 16.244 | 16.205 |
| $c_b$                              | 0.4842 | 0.4698 | 0.4677 |
| $ c_s - c'_s $                     | 0.0051 | 0.0015 | 0.0078 |

FIG. 9. Plot of the concentration of glucose for  $\mathfrak{R} = 10$ .TABLE IV. Results for  $\mathfrak{R} = 10$ , and BCU thickness of  $12\Delta y$  for units 1 and 3, and of  $24\Delta y$  for unit 2, using the Sáez-Rittmann model.

| Iter. 1                                       | Unit 1 | Unit 2 | Unit 3 |
|-----------------------------------------------|--------|--------|--------|
| $\bar{c}$ (g/m <sup>3</sup> )                 | 0.5000 | 0.5000 | 0.5000 |
| $c'_s$ (g/m <sup>3</sup> )                    | 0.5000 | 0.5000 | 0.5000 |
| $J$ (g/m <sup>2</sup> day)                    | 0.3487 | 0.3487 | 0.3487 |
| $c_s$ (g/m <sup>3</sup> )                     | 0.4991 | 0.4991 | 0.4991 |
| $L_f$ ( $\mu$ m)                              | 18.021 | 18.021 | 18.021 |
| $ c_s - c'_s $ ( $10^{-3}$ g/m <sup>3</sup> ) | 0.900  | 0.900  | 0.900  |
| Iter. 2                                       | Unit 1 | Unit 2 | Unit 3 |
| $\bar{c}$                                     | 0.4915 | 0.4765 | 0.4817 |
| $c'_s$                                        | 0.4911 | 0.4760 | 0.4795 |
| $J$                                           | 0.3298 | 0.2911 | 0.3006 |
| $c_s$                                         | 0.4911 | 0.4761 | 0.4796 |
| $L_f$                                         | 17.044 | 15.047 | 15.535 |
| $ c_s - c'_s $                                | 0.0200 | 0.0800 | 0.0600 |
| Iter. 3                                       | Unit 1 | Unit 2 | Unit 3 |
| $\bar{c}$                                     | 0.4923 | 0.4800 | 0.4827 |
| $c'_s$                                        | 0.4918 | 0.4795 | 0.4823 |
| $J$                                           | 0.3315 | 0.3004 | 0.3076 |
| $c_s$                                         | 0.4918 | 0.4795 | 0.4823 |
| $L_f$                                         | 17.133 | 15.527 | 15.899 |
| $ c_s - c'_s $                                | 0.0172 | 0.0129 | 0.0092 |
| Iter. 4                                       | Unit 1 | Unit 2 | Unit 3 |
| $\bar{c}$                                     | 0.4920 | 0.4793 | 0.4821 |
| $c'_s$                                        | 0.4915 | 0.4788 | 0.4817 |
| $J$                                           | 0.3308 | 0.2986 | 0.3061 |
| $c_s$                                         | 0.4915 | 0.4789 | 0.4817 |
| $L_f$                                         | 17.094 | 15.435 | 15.820 |
| $ c_s - c'_s $                                | 0.0037 | 0.0060 | 0.0096 |

Coupling using the Sáez-Rittmann or other similar model is an attractive alternative in simulation studies where substrate utilization and biofilm thickness along the flow path are the primary variables of interest.

## VI. CONCLUSIONS AND FUTURE DIRECTIONS

We simulated the growth of a biofilm in a tube with an expansion by solving the Navier-Stokes and the solute advection-diffusion equations using finite differences and coupling with a biofilm growth one-dimensional model. By changing the thickness of the BCU we showed that reasonable results are possible, even though there is the problem of BIOSIM considering that all nutrients enter only through the bulk layer. The coupling of the different processes works well. For the cases we treated, the growth of the biofilm was very small and therefore the hypothesis of a steady flow is satisfied.

Future work will try to solve the main difficulties in using the BIOSIM model. A better model can be obtained by writing biofilm equations at each node point, eliminating the bulk and diffusion layers, and by using directly the boundary conditions at the biofilm surface. A second point that has to be considered is how the growth of the biofilm changes the flow pattern by changing the physical regions for the fluid. These problems are much harder to deal with.

This research was supported by the National Science Foundation under Cooperative Agreement ECD-8907039 with Montana State University (MSU), the Center's Industrial Associates, the Montana Science & Technology Alliance, and MSU. Although the research described in this article has been funded in part by the U.S. Environmental Protection Agency under Assistance Agreement R-815709 to Montana State University through the Hazardous Substance Research Center for U.S. EPA Regions 7 and 8 headquartered at Kansas State University, it has not been subjected to the Agency's peer and administrative review and therefore may not necessarily reflect the views of the Agency, and no official endorsement should be inferred.

## References

1. B. F. Picologlou, N. Zelter, and W. G. Characklis, *J. Hyd. Div. ASCE* 106 733 (1980).
2. P. Reichert, J. Ruchti, and O. Wanner, BIOSIM, an interactive program for the simulation of the dynamics of mixed culture biofilm systems on a personal computer. Swiss Federal Institute for Water Resources and Water Pollution Control, Swiss Federal Institute of Technology, CH-8600 Dubendorf, Switzerland, 1990.
3. W. G. Characklis and K. C. Marshall, "Biofilms: A basis for and interdisciplinary approach," in W. H. Characklis and K. C. Marshall, Eds., *Biofilms*, Wiley-Interscience, New York, (1990).
4. A. B. Cunningham, W. G. Characklis, F. Abedeen, and D. Crawford, *Environ. Sci. Technol.* 25, 1305 (1991).
5. S. W. Taylor, P. C. D. Milly, and P. R. Jaffe, *Water Resour. Res.* 26, 2161 (1990).
6. R. Peralta and B. Chen, unpublished.
7. D. M. Young, *Iterative Solution of Large Linear Systems*, Academic, New York, 1971.
8. R. Peyret and T. Taylor, *Computational Methods for Fluid Flow*, Springer-Verlag, New York, 1983.
9. W. G. Characklis, "Kinetics of microbial transformations," in *Biofilms*, W. G. Characklis and K. C. Marshall, Eds., Wiley-Interscience, New York, 1990.
10. E. J. Wilson and C. J. Geankoplis, *Ind. Eng. Chem. Fund.*, 5, 9 (1966).
11. P. B. Sáez and B. E. Rittmann, *Biotechnol. Bioeng.*, 32, 379 (1988).

