



Development and evaluation of a two-dimensional microscale transport and biofilm process model
by Ernest Jay Visser

A thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in
Civil Engineering

Montana State University

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Abstract:

A mathematical model describing the interactions of fluid dynamics, substrate transport, and biofilm reaction is formulated. Equations modeling the processes of fluid dynamics, substrate transport, and biofilm reaction are solved. The Finite Difference method is used to solve coupled partial differential equations. A perturbation scheme is formulated that can account for the influence of thin biofilms on the boundaries. This model is compared with available experimental dissolved oxygen data.

Application of the model demonstrates the influence that biofilm distribution can have on biofilm system performance. Simulation of capillary tubes demonstrates the influence of domain geometry on local velocity and concentration distributions.

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Doctor of Philosophy

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MONTANA STATE UNIVERSITY-BOZEMAN
Bozeman, Montana

July 1998

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APPROVAL

of a thesis submitted by

Ernest Jay Visser

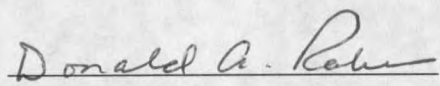
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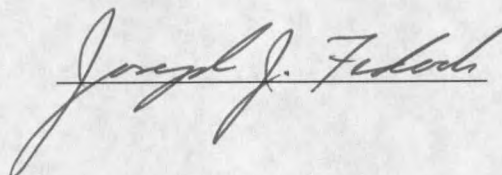
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ACKNOWLEDGEMENTS

I would like to say thank you to my committee members who contributed advice and insight into my research. Special thanks for patience and advice goes to my thesis adviser Dr. Al Cunningham, and Dr. Benito Chen and Dr. Marty Hamilton for their patience and perseverance in helping me complete my graduate work. Thanks also to Brian Goldstein for computer related support and putting up with my computational requirements. I would like to say thank you to all the people at the Center for Biofilm Engineering who made my stay a pleasant time and also supplied many interesting discussions of related research.

A special thanks also to my parents for their support while I was a student.

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ABSTRACT

A mathematical model describing the interactions of fluid dynamics, substrate transport, and biofilm reaction is formulated. Equations modeling the processes of fluid dynamics, substrate transport, and biofilm reaction are solved. The Finite Difference method is used to solve coupled partial differential equations. A perturbation scheme is formulated that can account for the influence of thin biofilms on the boundaries. This model is compared with available experimental dissolved oxygen data. Application of the model demonstrates the influence that biofilm distribution can have on biofilm system performance. Simulation of capillary tubes demonstrates the influence of domain geometry on local velocity and concentration distributions.

CHAPTER 1

INTRODUCTION

Biofilms can be found in most natural and industrial aquatic systems and can account for significant microbial activity in these systems (Characklis and Marshall, 1990). Biofilms are becoming recognized as a prominent mode of growth for bacteria (Potera, 1996). Biofilms can be beneficial or detrimental in environmental systems (Mattila-Sandholm and Wirtanen, 1992; Jass and Lappin-Scott, 1997). For example, biofilm play a substantial role in degrading xenobiotic compounds in groundwater and soil. Significant problems caused by biofilms include: biofouling in cooling towers which costs more than \$7 billion U.S. Dollars for biocides to control (Lappin-Scott et al., 1992); biofilms found on medical implants, poses serious health risks (Lappin-Scott et al., 1992); biofilm plaque on teeth, which can increase risk of cavities (Marsh, 1995); and biofilm growth in drinking water systems, which can present a health risk (Camper, 1994; Camper et al., 1994; Mittleman, 1995; Gagnon et al., 1997). Biofilms can cause significant pressure losses in industrial pipeline processes (Picologlou et al., 1980; Butterworth, 1981; Lira and Sengupta, 1990) and increased heat transfer resistance (Lira and Sengupta, 1990). Biofilms may be found in harsh environments, including those contaminated by acid mine drainage (Boult et al., 1997).

In porous media biofilm growth can cause permeability reduction through pore blocking. The growth of sulfate reducing bacteria in oil bearing formations may cause souring of petroleum reservoirs through sulfide production. Conversely, beneficial aspects of biofilms in porous media include bioremediation of contaminant plumes.

Biofilm Processes in Uniform Flow Systems

Processes governing fluid dynamics, mass transport, biofilm accumulation, and the biotransformation of organic constituents are intrinsically interrelated. Suspended cells are transported to the substratum 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 cells and extracellular polymeric substance (EPS), which binds the cells together. The aggregate of attached cells, EPS, and other particulate matter is termed a biofilm (Characklis and Marshall, 1990; Costerton and Lappin-Scott, 1995). Once a biofilm is established, additional cells and particulate matter may attach to and detach from the biofilm surface.

Biofilm Processes in Porous Media

In porous media, biofilm accumulation may cause bridging across the pore channel, thereby further enhancing accumulation by the filtration of particulate matter from suspension. The net accumulation of biofilm in porous media is defined by the difference between biomass added to the surface from the processes of adsorption, growth, attachment, and filtration and 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. The nature of the accumulation pattern may have a strong impact on behavior of microbial biofilm processes in porous media (Baveye and Valocchi, 1989). As film thickness increases, the effective pore space of the media will decrease, thereby causing a corresponding decrease in media porosity and permeability (Cunningham et al., 1991; Taylor et al., 1990). If the piezometric gradient remains constant, pore velocity will also decrease, thereby

reducing both advective and dispersive transport of nutrients through the system. Decreased nutrient transport results in a corresponding reduction in biofilm cell specific growth rate, and thus, in the rate of biotransformation of organic material. Decreased pore velocities reduce the shear rate, which could reduce the rate of detachment. Both biofilm growth rate and detachment rate will continue to change, unless a steady state biofilm thickness is achieved.

If the flow rate is held constant, the shear stress will increase as the biofilm grows and restricts the cross sectional area available for fluid flow. This increase in effective pore velocity will increase the shear stress, which can increase the detachment rate. Shear stress and biofilm detachment loss rates have together been the subjects of biofilm research, with both strong and weak correlations being reported (Peyton, 1996; Peyton and Characklis, 1993; Rittmann, 1982; Lau, 1995; Cao and Alaerts, 1995). A biofilm may slough and adjust to higher shear with a stronger biofilm matrix. In the case of porous media, the change in shear rate with time is small; and the biofilm could dynamically adapt.

Review of Biofilm System Models

Biofilm modeling started with trickling filters for which empirical models, experimental investigations, and conceptual models were applied to the attached biofilms (Atkinson and Daoud, 1968; Atkinson et al., 1968; Atkinson and Daoud, 1970; Atkinson and Davies, 1974; Atkinson and How, 1974; Atkinson et al., 1967).

Atkinson et al. (1967) were some of the early researchers to attempt modeling of microbial films. In this work, a *pseudo-homogeneous* and a *heterogeneous* model were analyzed. Conclusions resulting from this work were: 1) mathematical models derived on a heterogeneous basis are applicable to the biological film reactor, and 2) liquid phase diffusion resistance has considerable influence on the performance of a

continuous flow biological reactor. This work was extended, and diffusion limitations within the biofilm was found to be important. Atkinson and Daoud (1968) suggested that a model based on the catalytic nature of microbial biomass might help to clarify the importance of diffusional limitation. Atkinson and Daoud (1968) went on to develop model equations for biofilms and "flocs" in terms of a characteristic thickness and concentration of reactant in adjacent solution.

Williamson and McCarty (1976a) presented a model of substrate utilization by bacterial films using Monod kinetics (Monod, 1949) for a single substrate. This model was limited to a single substrate and it was necessary to determine which substrate limited overall biofilm uptake. This could be performed using model and stoichiometric coefficients in the biochemical transformation equation representing the metabolic reaction within a biofilm. An allowance for mass transfer was included using a defined liquid film thickness outside the biofilm as a model parameter. In experimental work Williamson and McCarty (1976b) found that the liquid layer could not be completely removed and attributed this to the uneven or sponge like nature of the liquid-biofilm interface. Solutions were found for thick biofilms, which are limited by mass transfer (diffusion). In subsequent experimental verification studies of their biofilm model (Williamson and McCarty, 1976b), the model was extended to include thin biofilms. In their experimental work they found that diffusion coefficients for substrates (ammonia, nitrite, nitrate, and oxygen) moving through the biofilms of nitrifying bacteria were approximately 80 to 100 percent of corresponding values in water (Williamson and McCarty, 1976b).

Rittmann and McCarty (1978) developed expressions to provide a more convenient and easily used biofilm model based on the biofilm substrate removal model provided by Williamson and McCarty (1976a). This work provided a variable-order model that yields an approximate analytical solution for the flux of limiting substrate

into a fixed bacterial film, that is "deep". This worked to simplify application of the model of Williamson and McCarty (1976a) and aided application of fundamental, fixed-film kinetics to practical reactor problems.

Rittmann and McCarty (1980b) further extended the biofilm modeling of Williamson and McCarty (1976a) to include the mass of the biofilm, coupling the steady-state flux of substrate into a biofilm to the mass (or thickness) of the biofilm for a given bulk substrate concentration. In this analysis, a first-order decay term was used, which defined a minimum substrate concentration below which no significant biofilm activity should occur. This model provided substrate flux and biofilm thickness for bulk substrate concentrations greater than the minimum substrate concentration. Biofilm thickness was based on the total amount of biofilm mass which which could be supported by the substrate flux. Experimental evaluation of this steady-state biofilm model was performed (Rittmann and McCarty, 1980a), which confirmed the hypothesis that, for a single substrate limitation there exists a predictable steady-state concentration, below which no significant biofilm activity occurs. It was also noted that the steady-state model of biofilm kinetics successfully predicted substrate utilization in a steady-state reactor at maximum utilization rates; however, predicted biofilm thickness tended to be overestimated relative to those achieved experimentally.

A model for estimating substrate flux into a biofilm of any thickness was developed by Rittmann and McCarty (1981) as an extension of previous work (Atkinson and Daoud, 1968; Atkinson and Davies, 1974) by including external mass transfer resistance. The external mass transfer resistance was lumped into an effective stagnant layer through which all diffusional resistance takes place. With this model, the flux became a direct function of the bulk substrate concentration, which is typically the measured concentration and is often the concentration of interest. An explicit solution was available for thick biofilms, and a simple iterative solution was used for

thin biofilms. This model had the ability to predict the flux of a single, rate-limiting substrate when the biofilm thickness was independently known.

The steady-state biofilm model of Rittmann and McCarty (1980b) was criticized by Arcuri and Donaldson (1981) for only including decay as a loss mechanism when decaying cells would be trapped under the young cells. Arcuri and Donaldson (1981) argue that substrate uptake rate predicted by steady-state biofilm model (Rittmann and McCarty, 1980b) may not be realistic since the major mechanism for loss of biomass is probably sloughing of outer cells or cell aggregates as film becomes large and unstable. In response to this criticism, Rittmann (1982) presented a procedure to implement shear loss from biofilm by incorporating loss into a first order decay term in the steady-state biofilm model.

The steady-state biofilm model of Rittmann and McCarty (1980b) later was improved by correcting an error in the pseudo-analytical solution (Sáez and Rittmann, 1988). Additional work was performed to estimate error associated with limiting cases of the steady-state biofilm model (Sáez and Rittmann, 1990). Heath et al. (1990) provided a procedure for design of biofilm processes using normalized loading curves based on the steady-state biofilm model (Rittmann and McCarty, 1980b) and the improved solution technique (Sáez and Rittmann, 1988). This process was based on families of normalized loading curves allowing simple and rapid computation of required design volume for biofilm reactors. An improved pseudo-analytical solution (Sáez and Rittmann, 1992) to the steady-state biofilm model (Rittmann and McCarty, 1980b) was used to eliminate some inaccuracies (Cannon, 1991).

Benefield and Molz (1985) developed a mathematical model for fixed-film biological process (film flow over a flat plate) which described bulk liquid transport, diffusional transport of oxygen and organics across a stagnant film, diffusional transport of oxygen and organics into the biofilm, biochemical reactions by the individual

cells within the biofilm, biofilm growth, and cell density change within the biofilm due to cellular decay. Kinetics were modeled as double Monod for oxygen and one organic (electron donor and carbon source). This model was solved numerically with a grid of points in the flow direction and a grid of points within the biofilm. Some shortcomings of this model included lack of a general detachment expression accounting for erosion and sloughing type losses and a relationship between flow velocity and diffusion layer thickness used in the film type diffusional resistance from bulk model.

Kissel et al. (1984) started work on numerical simulation of mixed culture biofilms. Some of their assumptions prompted a discussion (Gujer and Wanner, 1985; Kissel et al., 1985). Wanner and Gujer (1986) developed a multispecies biofilm model to model biofilm processes. This model formulation and background also appears in a later publication (Gujer and Wanner, 1990). This model was adopted in a technical report on biofilm modeling (Characklis et al., 1989) and has been used to model spatial dynamics (Wanner, 1989; Wanner, 1994). A computer software package BIOSIM (Ruchti et al., 1991; Reichert et al., 1990) utilized this biofilm model in conjunction with CSTR's for modeling biofilm systems. With this model the significance of spatial distributions in mixed culture biofilm was simulated (Fruhen et al., 1991). BIOSIM has been used in modeling of biofilms systems (Drury et al., 1993; van Loosdrecht et al., 1994; Arcangeli and Arvin, 1995; Okabe et al., 1995; Okabe et al., 1997) The BAM (Camper et al., 1994) computer software package also uses this mathematical biofilm model. The BAM computer software package was developed at the Center for Biofilm Engineering and has been used for simulation of biofilm systems (Stewart, 1994).

Rittmann and Manem (1992) looked at steady-state solutions to the multi-species biofilm model. In this approach, detachment was lumped into a first order decay parameter.

Szego et al. (1993a) developed and solved a model for simulation of biofilm processes in pipelines. This model was restricted to circular pipes of constant cross section and allowed for both laminar and turbulent flow (Szego et al., 1993b). Wend (1994) extended the use of biofilm modeling by including a gas phase for use in modeling vapor-phase bioreactors.

Computer models have already been utilized very effectively to help in developing an understanding of the basic biofilm growth process. The BIOSIM code has been 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. BIOSIM has been used effectively to describe and explain experimental data (Okabe et al., 1995; Okabe et al., 1997; Drury et al., 1993; van Loosdrecht et al., 1994; Arcangeli and Arvin, 1995).

A newer version of this biofilm system model called AQUASIM (Reichert, 1994b; Reichert, 1994a) has recently been developed. It models mixed culture biofilms and has some added features over BIOSIM (Wanner and Reichert, 1996). For example, it allows for movement of solids in biofilm in the liquid phase (Reichert and Wanner, 1997). AQUASIM has been used to model biofilm in porous media (Wanner et al., 1995), biofilm systems (Janning et al., 1995; Arcangeli and Arvin, 1997; Horn and Hempel, 1997; Beaudoin et al., 1998), and activated sludge (Reichert et al., 1995).

This review of biofilm system modeling has shown that modeling of systems is typically one dimensional steady uniform flow. In the case of porous media, the biofilm models are typically based on bulk media properties. These models do not consider microscale flow/transport effects. Experimental research into biofilm systems shows that in some situations they have some heterogeneity associated with them. Experimental research into the structure of the biofilm community and local transport

variations in mass and momentum transfer provide new insight into the biofilm processes (de Beer, Stoodley, Roe and Lewandowski, 1994; de Beer and Stoodley, 1995; de Beer, Stoodley and Lewandowski, 1994; Lewandowski et al., 1993; Lewandowski and Stoodley, 1995; Lewandowski et al., 1995; Lewandowski et al., 1994; Bishop et al., 1995). This is a local phenomenon and biofilm systems modeling should reflect the local flow/transport conditions. While not all processes are well understood at this point, some of these processes can now be simulated. In some situations it is not necessary to model all processes associated with biofilm system (Bishop and Rittmann, 1995).

Research Goals and Objectives

At the microscale, biofilm formation is a complex problem involving fluid dynamics, mass transfer, chemical reactions and biochemical reactions (Brading, Jass and Lappin-Scott, 1995). To understand the interaction of these different processes, it is useful to use a mathematical model to describe these processes. The goal of this research is to couple equations describing fluid flow, mass transport, and biofilm processes at the microscale to more accurately describes bulk fluid transport processes at the micro scale and the subsequent effect on the associated biofilm processes at the microscale. The resulting model is applied to different distributions of biomass and porous media capillary model. Results of these simulations demonstrate the coupled behavior of fluid dynamics, substrate transport, and biofilm reaction.

This research couples the continuity equation for incompressible steady-state fluid flow

$$\nabla \cdot \mathbf{u} = 0 \quad (1.1)$$

with the steady-state momentum equations for an incompressible isothermal Newto-

nian fluid

$$\mathbf{u} \cdot \nabla \mathbf{u} = -\frac{\nabla p}{\rho} + \nu \nabla^2 \mathbf{u} + \frac{\mathbf{f}}{\rho} \quad (1.2)$$

and steady-state species balance equation for a dissolved constituent such as oxygen

$$\mathbf{u} \cdot \nabla O = \nabla \cdot (D(\mathbf{x}) \nabla O) + r_O \quad (1.3)$$

for the bulk fluid region. Equations (1.1)–(1.3) are solved in two dimensions with the boundary conditions arising from solution of the equations for the biofilm.

For the application and model evaluation a single species biofilm model is used for steady-state oxygen consumption

$$0 = D_f \frac{\partial^2 O}{\partial z^2} - V_{\max} \frac{O}{K_O + O} \quad (1.4)$$

which is applied for biofilm located on walls of simulation domain.

Due to nonlinearities and the multidimensional nature of the resulting mathematical model, it was necessary to use numerical techniques to obtain a solution. The resulting model allows simulations to be performed with flow tubes as shown in Figure 1. Tubes such as this one can be used to form *capillary* models of porous media (Dullien, 1991; Kaviani, 1995; Tiwari, 1997). This approach can determine the effect that system geometry and flow conditions have on biofilm accumulation and biotransformation in tortuous, laminar flow systems. In addition, the general flow and transport around patches of biofilm and subsequent development of the mass transfer boundary layer can be investigated with this computational mathematical modeling approach.

Baveye and Valocchi (1989) discuss the concept of a uniform biofilm vs. colonies in porous media. Using the above model, simulations can be performed describing local fluid velocity and transport variation to effects on various types of biofilm distributions (Figure 2). This allows different simulations to be performed, which can then be compared with laboratory experiments using biofilm reactors of similar geometry.

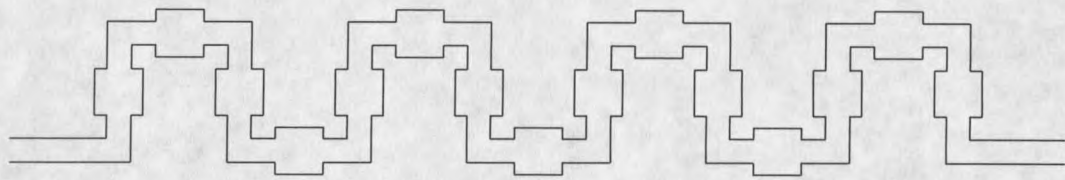


Figure 1. Two-dimensional model of a porous medium pore channel.

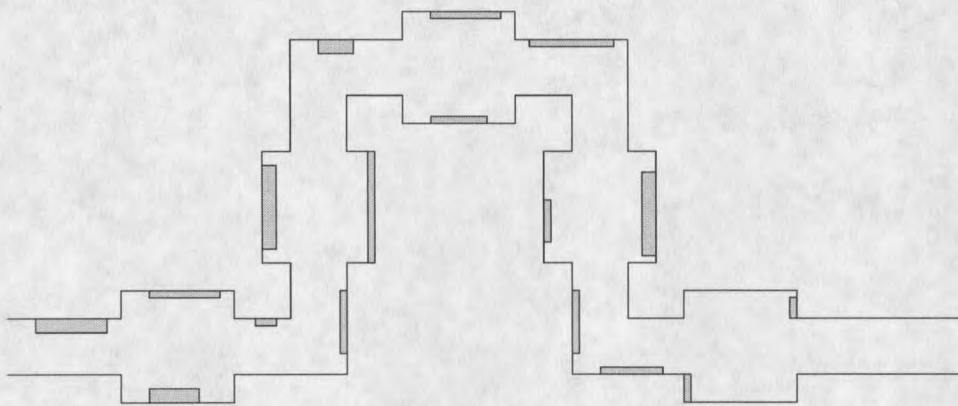


Figure 2. Tortuous tube with patchy biofilm.

The specific objectives of this thesis are to

- Formulate a mathematical microscale model.
- Solve the microscale mathematical model.
- Evaluate the model against experimental data.
- Apply the microscale model to biofilm systems.

Model Development Approach

Although some of the growth mechanisms in pipes are beginning to be fairly well understood (Picologlou et al., 1980), the growth process in a tortuous porous media is considerably more complicated. Due to this complexity, it is important to try to understand and model the basic processes occurring and their rates at the pore level. If the basic processes are understood and can be modeled at a small scale it is possible to scale up this nonlinear information to the field scale.

When physical processes are nonlinear and are coupled to other nonlinear processes, the ability to understand the coupled phenomena at a local level and then to scale this knowledge up to longer length scales is extremely important. For example, typical length scale for pore scale flow governed by Navier-Stokes (10^{-4} – 10^{-3} meters) is quite different from the scale required by field-scale simulations (10 – 10^3 meters) (Ewing, 1997). 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 as powerful new scientific tool (Chen et al., 1994; Ewing, 1997). Simulations can

be compared with laboratory experiments to support important phenomenological models and to determine reaction rates. Once a model is chosen, computer simulations can predict sensitivities of various parameters and coupled interactions in the complex set of partial differential equations used in simulators for porous media can then be scaled up (Ewing, 1997).

Biofilm modeling can be a useful aid in designing experimental systems and scaling-up of biofilm processes and reactors. There has been some discussion in the literature on the scale up issues associated with of biofilm reactors and their nonlinear processes (Manem and Rittmann, 1990). Scale up issues in porous media applications are inherently nonlinear. When biological processes are added, the scale up process becomes much harder.

One component of biofilm modeling is the mass transfer to the biofilm from the bulk fluid to the biofilm. This process is often modeled using mass transfer coefficients. Average mass transfer coefficients are typically found in the literature for simplified geometries. Mass transfer correlation equations for common flow system geometries such as circular tube, flat duct, and flat plate are available (Cussler, 1984; Weber and DiGiano, 1996). These correlations typically have some simplifying assumptions related to uniform geometry and a uniform flux or concentration boundary conditions. In this thesis, the approach is to formulate equations describing the flow and transport of dissolved substrates and consumption by biofilm, and solve them using established computational fluid dynamics (CFD) techniques. The use of CFD techniques allows different geometries to be simulated where changes in reactor geometry lead to changing of local flow characteristics which can influence mass transfer to the biofilm surface. This approach will allow one dimensional patches of biofilm to be coupled with a two dimensional transport model for fluid velocity and mass transport outside the biofilm region, thereby facilitating a investigation of biofilm patchiness

and biomass distribution for conditions of interest.

The outline of this thesis is as follows. Chapter 2 contains the conceptual view of biofilm and bulk fluid processes with assumptions made to obtain a mathematical model describing the biofilm system. In Chapter 2, I discuss the Navier-Stokes equations and advective-diffusion-reaction equation describing transport in the bulk fluid region and the biofilm process model. Coupling of the mathematical equations is also discussed. In Chapter 3, I present a numerical scheme for solving the model equations presented in Chapter 2 in two spatial dimensions for the fluid dynamics and one dimension for the biofilm. Discretization of mathematical equations and resolution of nonlinear equations are examined. Chapter 4 contains an model evaluation using experimental data taken from an open channel reactor using an artificial biofilm. Application of the model to relevant biofilm systems is presented in Chapter 5. Conclusion are contained in Chapter 6 and future work in Chapter 7.

CHAPTER 2

MATHEMATICAL MODEL DEVELOPMENT

It is convenient to separate the domain of interest into a bulk fluid region and a biofilm region. These regions are depicted in Figure 3.

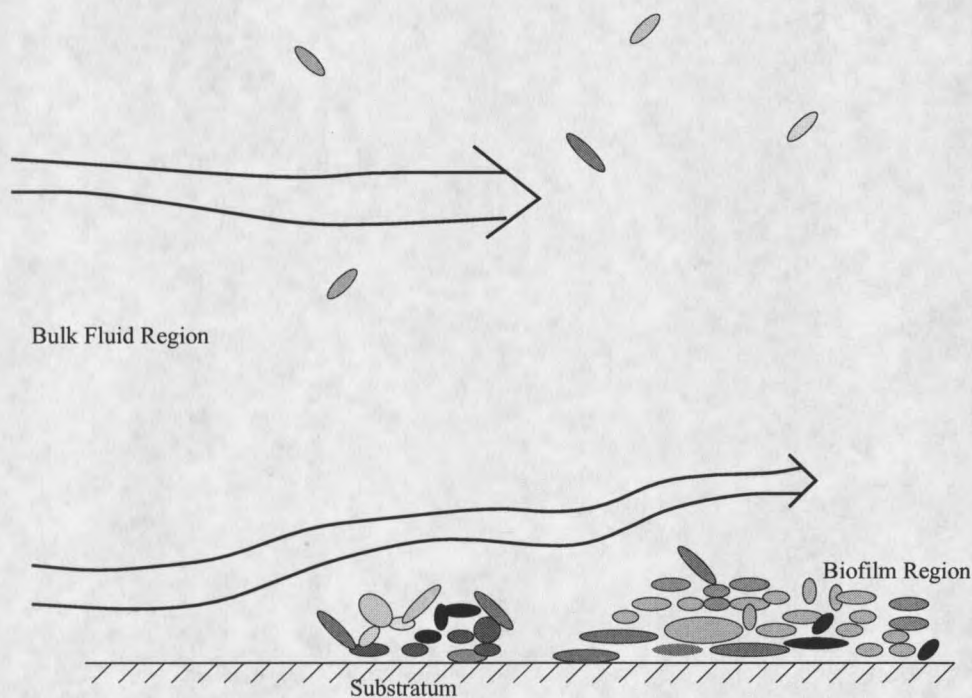


Figure 3. Sketch of bulk fluid and biofilm regions.

The bulk fluid region is characterized by dilute concentrations of suspended microorganisms and other dissolved constituents. The concentrations of these species is assumed to be small enough that their influence on the flow is negligible. The concentration of suspended microorganisms is typically small, so that the resulting reaction rate is small compared to reaction in the biofilm region. Conversely, the

biofilm region is characterized by high concentrations of biomass attached to a solid substratum. The biofilm region has a high concentration of biomass which leads to a higher substrate consumption than in the bulk.

These two regions are connected by an interface across which the dissolved and particulate components move. This interface region will have mathematical equations describing the transport of constituents across the interface and movement of the interface itself. Due to the high concentrations of biomass in the biofilm relative to the bulk fluid, sharp concentration gradients can develop near the biofilm bulk fluid interface.

Bulk Fluid

The bulk fluid region is defined as the region above the biofilm region as depicted in in Figure 3. Physical processes in the bulk fluid provide transport of nutrients and removal of biochemical transformation products from the biofilm. In addition, biomass can be transported to and from the substratum and biofilm surface. For dissolved species, transport processes are by fluid convection and diffusion/dispersion. Diffusion from high concentration to low concentration is typically modelled by Fick's law: the diffusive flux of a substance is proportional to the gradient of the concentration of that substance. Fick's law is mainly used for describing diffusion of soluble components, but can also be used for large molecules or small particles, such as microbial cells diffusing in water (Characklis, 1990a).

Microorganisms can be motile or nonmotile and thus different behavior is expected in bulk fluid for microorganisms possessing motility (Characklis and Marshall, 1990). Motile microorganisms can respond to concentrations of a substrate in which they move in increasing direction of substrate concentration which is termed *chemotaxis*. Movement away from an undesirable constituent would also be possible. Some

research has been done on determining chemotaxis coefficients (Ford et al., 1991) and single cell modeling with chemotaxis (Ford and Lauffenburger, 1991). Cellular dynamics simulations have been used to model large population of individual chemotactic bacteria in three dimensions (Frymier et al., 1993). In the case of a bare substratum, the physical process of interest is the transport of microorganisms to the surface and subsequent attachment of some microorganisms. The influence of hydrodynamics in movement of microorganisms in the vicinity of a boundary, between boundaries, and vicinity of another microorganism has been modeled by Ramia et al. (1993). Pedley and Kessler (1992) investigated hydrodynamics of suspensions of swimming microorganisms.

Dillon et al. (1995) developed a model including bacterial swimming, chemotaxis, and substrate consumption. This model was solved in two dimensions for a limited number of bacteria in the fluid. Fluid dynamic interaction of swimming bacteria was accounted for along with fluid force on bacteria. The ability to include a attachment term when bacteria come in proximity to a surface or other bacteria suggests this model might have potential for some initial events work. This model was extended in this way to model biofilm processes under laminar flow conditions (Dillon et al., 1996).

Quite often fluid dynamics of biofilm reactors are modeled with dispersed flow models (Muslu, 1990). Dispersed flow models such as continuously stirred tank reactor (CSTR) and plug flow reactor (PFR) represent average values in the bulk fluid. If mixing is high, dispersed flow models like CSTR and PFR are used although some diffusional resistance is encountered at the wall which is sometimes modeled with an effective liquid layer thickness across which all diffusional resistance effects are accounted for.

Simulation of fluid dynamics depends on the type of flow, whether it is laminar,

turbulent, or in the transition stage. If the fluid dynamics to be simulated is in the transitional or turbulent region it is necessary to include an additional model for the turbulence. The ability to solve the flow equations at a fine enough scale to resolve turbulent fluctuations requires massive computational resources and is not feasible for most practical applications (Calmet and Magnaudet, 1997). In view of this limitation turbulence models have been formulated and are being developed to allow simulations of turbulence to be performed. For the purposes of this modeling effort, it is assumed that the fluid flow is in the laminar region.

The concentration of dissolved substrates is assumed to be sufficiently small that it does not affect the viscosity or density of the bulk fluid. Another assumption is that biomass in the bulk does not affect the viscosity or density of the bulk fluid. This assumption may not be valid near the biofilm/bulk fluid interface where flow velocity is lowest and biomass concentration could be the highest. In this region, suspended biomass, which could be biofilm aggregates, may influence the local behavior of the bulk fluid by increasing the effective viscosity.

External mass transfer is often dealt with by use of a layer of effective thickness of fluid that is undisturbed for the purpose of including diffusional effects from bulk fluid to wall (Vogel, 1994). Note that this is not really undisturbed fluid but a region where diffusion is the dominant transport mechanism. This is an approximation to the real diffusive boundary layer which is used to account for the mass transfer resistance. Biofilm models with dispersed flow bulk fluid models have used an effective liquid layer thickness for diffusional resistance (Reichert et al., 1990; Reichert, 1994b). This dissertation improves on the prevailing mass transfer model component by solving mass transport in two dimensions around biofilm patches, thereby providing an analysis of mass transport in complicated geometries such as that shown in Figure 1. To solve problems such as that shown in Figure 1 with current models, would

be cumbersome. It would be necessary to model individual sections such as tubes of varying size and hence different residence times utilizing CSTR or PFR reactor models and allow for some external mass transfer to walls with biofilm.

The bulk fluid region provides the transport of liquid, dissolved constituents (chemical and biomass). Bulk fluid flow in the laminar flow region can be modeled with the Navier-Stokes equations to obtain the fluid velocity. A mass balance equation for the dissolved substrates, biomass species, and inert species is used to model their behavior.

Navier-Stokes Equations

The bulk fluid dynamics can be modeled by the Navier-Stokes equations for an isothermal incompressible Newtonian fluid with constant viscosity (Bird et al., 1960; Probstein, 1989). The continuity equation obtained from a mass balance on the fluid gives

$$\nabla \cdot \mathbf{u} = 0 \quad (2.1)$$

while the balance of momentum equations give

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{\nabla p}{\rho} + \nu \nabla^2 \mathbf{u} + \frac{\mathbf{f}}{\rho} \quad (2.2)$$

where $\mathbf{u} = \mathbf{u}(\mathbf{x}, t) = (u(\mathbf{x}, t), v(\mathbf{x}, t), w(\mathbf{x}, t))$ ($L t^{-1}$) is the bulk fluid velocity, $p = p(\mathbf{x}, t)$ ($M L^{-1} t^{-2}$) is the fluid pressure, ρ ($M L^{-3}$) is the fluid density, (assumed constant) ν ($L^2 t^{-1}$) is the fluid kinematic viscosity (assumed constant), $\mathbf{x} = (x, y, z)$ (L) are spatial coordinates, and $\mathbf{f}$ ($M L t^{-2}$) is sum of body forces acting on fluid (i.e., gravity forces etc.).

Recent formulations for swimming microorganisms use an immersed boundary condition to include the influence of swimming microorganisms on fluid dynamics (Dillon et al., 1995; Dillon et al., 1996; Fauci, 1993; Fauci and Peskin, 1988; Fauci,

1996). In these formulations individual tracking of microorganisms is used. Alternatively the effects of microbial suspensions could be lumped into variable viscosity which depends on the concentration of the microorganisms similar to way suspensions are dealt with. In this conceptual model, it is assumed that concentrations of microbial biomass are dilute and the biomass particles are small enough not to influence the local transport properties significantly.

The flow of liquid in the biofilm region could be modeled using higher viscosity in biofilm region. Stolzenbach (1989) looked at biofilm as a collection of momentum capturing particles for modeling flow in the biofilm. This resulted in a body force applied to the fluid by the biofilm proportional to fluid velocity in biofilm. A similar approach could have been applied in this study, but once flow is considered in the biofilm region, the modeling complexity becomes much greater.

Equation (2.2) could be modified to include a term similar to Darcy's law for porous media flow which would have a non zero permeability only in the biofilm and could be used to allow flow in the biofilm. These modifications could be performed on this model to more accurately model the behavior in biofilm once sufficient data becomes available to quantify flow in biofilms.

Species Balance Equation

The mass balance equation of dilute concentrations of dissolved species in the isothermal incompressible bulk fluid under laminar flow is given by the species balance equation (Bird et al., 1960; Probstein, 1989).

$$\frac{\partial c_i}{\partial t} = -\nabla \cdot \mathbf{J}_{T_i} + r_i \quad (2.3)$$

In equation (2.3) $c_i = c_i(\mathbf{x}, t)$ (M L^{-3}) is the substrate mass concentration, $r_i = r_i(\mathbf{x}, t, c_1, \dots, c_N)$ ($\text{M L}^{-3} \text{t}^{-1}$), is the production rate of species i which can be dependent on the other species in the bulk, and $\mathbf{J}_{T_i}$ ($\text{M L}^{-2} \text{t}^{-1}$), is the total mass flux of

species i and is given by

$$\mathbf{J}_{T_i} = \mathbf{u} \cdot \nabla c_i - D_i(\mathbf{x}) \nabla c_i. \quad (2.4)$$

The first term on the right hand side of equation (2.4) represents the convective flux due to bulk fluid flow and the second term represents the diffusive flux which is assumed to obey Fick's first law and $D_i(\mathbf{x})$ ($\text{L}^2 \text{ t}^{-1}$), is the diffusion coefficient for species i . If the flow is not resolved at the actual scale it occurs, D_i typically becomes larger than molecular diffusion and is called a dispersion coefficient. In some cases it becomes a function of the velocity field. For the unsteady state velocity case, the dispersion coefficient would then be implicitly a function of time.

Other types of flux related to thermal or pressure influences are assumed to be negligible for this modeling effort. It could be possible to add a chemotaxis flux term to equation (2.4) to include chemotaxis phenomena.

Insertion of (2.4) into (2.3) and recalling (2.1) gives a model equation for balance of dissolved species in the bulk fluid region

$$\frac{\partial c_i}{\partial t} + \mathbf{u} \cdot \nabla c_i = \nabla \cdot (D(\mathbf{x}) \nabla c_i) + r_i \quad (2.5)$$

The species balance equation (2.5) holds for all the dissolved species in the bulk. It is assumed that equation (2.5) also holds for particulate and inert species in the bulk.

In the case of inert or particulate species with no motility, $D_{X_i}(\mathbf{x})$ is a Brownian motion coefficient. In the case where particulate species possesses motility, it may represent motility speed. It may be better to use a chemotaxis expression for motile species where they are attracted or repelled by one or more of the dissolved species. For example, motile particulate species may be attracted by higher concentrations of a substrate and swim in the direction of increasing concentrations. Chemotaxis modeling could lead to other flux term for a particulate species to reflect the movement of motile species toward the increasing nutrient concentration.

In order that mass is conserved, the sum of the reaction terms must be equal to zero, i.e.:

$$\sum_{i=1}^N r_i = 0 \quad (2.6)$$

where N is the total number of species in the bulk fluid. The total number of species in the bulk fluid includes the number of dissolved constituents, N_D , the number of particulate species, N_X , the number of inert species, N_I , and the water phase.

$$N = N_D + N_X + N_I + 1 \quad (2.7)$$

In general it is not feasible to solve for all the dissolved constituents due to computing resource limitations and also the fact that not all of the coefficients for the reaction terms are known or even measurable. Some of these coefficients may need to be obtained in an indirect manner from other measurable parameters. A common assumption is that some constituents are not limiting and the species balance equation (2.5) is solved only for the relevant limiting species of interest. In some case the reaction rate may be influenced by other reactants or products which would require accounting for these other species to properly model the reaction rate.

As an example, the reaction of a microbial species with glucose as the primary substrate and oxygen as the electron acceptor would require the solution of (2.5) for substrate, oxygen, and biomass in the bulk. These three equations would be solved in conjunction with biofilm equations for the substrate, oxygen, and biomass in the biofilm. This could be fairly complicated if multiple microorganisms are modeled along with multiple states for a microorganism such as active and inactive. Other variations include cell death and lysis with a portion of cell lysis products yielding soluble nutrients for cell growth. Some reactions may be influenced by products which may influence the overall reaction rate. The microbial reaction kinetics may determine the number of constituents that must be modeled in a biofilm system.

Interfacial Processes

Interfacial processes occur at the biofilm/bulk fluid interface. The interface is defined as the surface location where a cell is attached to biofilm or substratum and no longer suspended in the bulk fluid. This is a mathematical interface definition which allows different regions to be defined and material balances written for each region with different assumptions. Some of the processes deemed important in biofilms (Characklis and Marshall, 1990) are described below. This general approach follows the process analysis approach (Characklis, 1990b; Characklis and Cooksey, 1983; Characklis, 1984; Characklis, 1990c).

Adsorption

Adsorption is the interphase accumulation or concentration of molecules or cells on a substratum or interface. In three dimensions, adsorption is a two dimensional process normal to the surface or interface. This process is influenced by the fluid flow in the region near the surface or interface (Escher and Characklis, 1990). Interest in the initial event leading to colonization of surfaces has been the subject of other researchers (Brannan and Caldwell, 1982; Malone and Caldwell, 1982; Caldwell et al., 1982; Kieft and Caldwell, 1982; Powell and Slater, 1983; Escher and Characklis, 1990; Mueller et al., 1992; Mueller, 1996).

Desorption

Desorption is the reverse of adsorption and refers to the movement of molecules or cells from the substratum back into the bulk liquid compartment. In one study it was noted that a significant number of cells contacting the surface do not become irreversibly attached; assuming so can introduce significant error (Powell and Slater, 1983).

Attachment

Attachment is defined as the capture and/or entrapment of cells in a biofilm. It refers to the interaction of bulk liquid compartment components with biofilm components as opposed to adsorption which occurs at the liquid/substratum interface.

Detachment

Detachment is the reverse of attachment and is the movement of cells from a biofilm into the bulk liquid compartment. Detachment is a loss of components from the biofilm as opposed to desorption which is the loss of components from the liquid/substratum interface. Detachment has been and continues to be a major factor in biofilm processes especially when it comes to modeling of biofilm processes.

Peyton (1992) looked at the kinetics of net detachment,

$$\text{net detachment} = \text{detachment} - \text{attachment}$$

to find a correlation with process variables to determine a good kinetic model for detachment. Research into the influence of substrate and shear stress on detachment kinetic have been investigated (Peyton and Characklis, 1993; Peyton, 1996) showing minimal shear stress dependence. This was over a relatively small variation in shear stress. Stewart (1993) discusses some models for biofilm detachment and an alternative model for biofilm detachment.

Detachment modeling has been treated in different ways by different researchers. Detachment is probably one of least understood physical processes associated with current models of biofilm dynamics. This creates difficulties when attempting to model the detachment process. Two types of detachment are often considered. The first type is termed *erosion*, and is a continuous process of the loss of single cells and small aggregates. The second type is a somewhat random event termed *sloughing*

where large particles of biomass detach from biofilm. In fluidized beds, another process for detachment is termed *abrasion* which can occur from collisions of substratum material (Brading, Jass and Lappin-Scott, 1995).

Much of the work on detachment is empirical in nature and not a whole lot is known on the detachment mechanism. Literature in this area reveals the use of biofilm thickness (Peyton and Characklis, 1992; Gujer and Wanner, 1990), biofilm thickness squared (Gujer and Wanner, 1990), shear stress (Rittmann, 1982; Wilderer et al., 1995; Bhamidimarri and See, 1992; Cao and Alaerts, 1995; Lau, 1995), constant value, and the average growth rate of the biofilm (Peyton, 1996; Peyton and Characklis, 1993; Peyton and Characklis, 1992) for correlations with net detachment. Rittmann (1989) used a detachment model proportional to the biofilm thickness. Peyton and Characklis (1992) also looked at first order detachment rate expression which was a function of biofilm thickness. They also suggested possible correlation with organic carbon utilization rate. G. E. Speitel and DiGiano (1987) suggested a detachment model incorporating a term based on Rittmann (1982) for shear with another term base on microbial growth rate. Shear and tensile forces are being investigated to find biofilm adhesion (Ohashi and Harada, 1996).

Another process that occurs at the interface is the transfer of energy from fluid to the biofilm. Recent work by Lewandowski and Stoodley (1995) who noticed biofilm streamers in a flowing system suggests that the pressure drop found with biofilm accumulation could be due to vortex shedding from biofilm clusters. This problem would require solution of equations governing motion of bulk fluid and also equations governing the motion and deformation of the viscoelastic biofilm. Previous work by Lewandowski et al. (1994) suggests biofilm models may need to be revised.

Biofilm Kinetics

An early discussion of biofilm kinetics was provided by Harremoës (1978). Karamanev and Nikolov (1991) reported on comparison of reaction rates in biofilm and suspended cells. Shreve and Vogel (1993) compared substrate utilization and growth kinetic between immobilized and suspended *Pseudomonas* cells. One conclusion was cellular kinetic parameters should be determined for the microorganism of interest in the setting in which it will be applied. The assumption that the kinetics for planktonic and biofilm cells are approximately the same has been used in modeling biofilm systems (Mirpuri et al., 1997).

Mathematical expressions for biofilm substrate utilization rate kinetics typically use a Monod kinetic expression (Monod, 1949). In the case of two substrates, a double Monod expression is often used (Jacob et al., 1996; Beg et al., 1997). There is some discussion as to relevance of this in the literature (e.g., see Bae and Rittmann (1996)). With K_s for oxygen typically small, a zero order approximation is often justified. Alternative formulations have been suggested in the literature (Haas, 1994). The biofilm kinetics model used for this work is an unstructured model (Nielsen and Villadsen, 1992).

Biofilm

The modeling of biofilm processes is an area of active research. The review article by Lazarova and Manem (1995) provides a updated review of biofilms and techniques to analyze biofilms in water and wastewater industries. These techniques included increased visualization and experimental techniques for measuring biofilm properties. The review article of Mattila-Sandholm and Wirtanen (1992) is also informative with regards to some biofilm processes and their relation to industrial settings. As more

becomes known about biofilms, some current modeling assumptions may need to be changed from the formulation used here.

The mathematical model used for the biofilm in this dissertation is based on the multi-species biofilm model given by Wanner and Gujer (1986). The derivation and development of this model can be found elsewhere (Gujer and Wanner, 1990). A more recent model that allows less restrictive assumptions is presented by Wanner and Reichert (1996) but some of assumptions that were relaxed involve processes for which little is known in the way of parameter values or reaction forms. For instance, items such as liquid phase production rate or solid diffusion in the biofilm solid matrix are not well characterized. In light of this, the older version of this model was retained for simplicity and implemented in this model. As additional research is performed and quantitative results for model parameters become available, it may prove useful to modify this part of the model to reflect the additional processes provided in Wanner and Reichert (1996).

In general this model uses mass balances along with the assumption that chemical species and microorganisms may be treated as a continuum (e.g., may be characterized by average values rather than shape and behavior of individual particles). This model is a one dimensional model in space with growth normal to the substratum. The concept of a Biofilm Volume Element (BVE) is used to describe a representative size of volume which contains biofilm and dissolved constituents. A typical size of a BVE is around $10\ \mu\text{m}$ (Wanner, 1989), normal to the substratum, tangential gradients are assumed to be negligible by comparison.

It would be advantageous to have a two dimensional model for the biofilm to match the bulk fluid dimension, but at this time the author does not know of a working multi-dimensional biofilm model. It has been suggested that the data necessary to formulate and validate a three dimensional model has not yet been reported in the

literature (Wanner, 1995). The model presented here could be extended to multi-dimensions but a formulation for deformation of the solid portion of the biofilm matrix would need to be used (Gujer and Wanner, 1990). A mathematical model for the deformation matrix could be complex as the polymer of the biofilm matrix has been reported to be viscoelastic in nature (Christensen and Characklis, 1990).

Mass Balances

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 (water) phase, ℓ , which fills a connected fraction of the biofilm volume and contains dissolved and suspended particulate materials. The suspended material consists of particles that can move in space independently of other suspended particles.
2. A series of solid phases, s , each composed of specific particulate material, such as a species of microorganisms, extracellular material, etc. These solids cannot move freely in space as they are attached to each other. Thus movement of one solid phase creates movement of other neighboring solid phases. Each type of attached solid constitutes a *solid phase*, which may contain other components (e.g., sorbed components, components stored within cells).

The transfer of suspended particles from the liquid phase to a solid phase (e.g., attachment) and from a solid phase to the liquid phase (e.g., detachment) must therefore be modeled as a transformation process, since educt and product do not belong to the same phase. This transformation process is different from transport processes within the phase. Due to the suspended particles and attached particles

Table 1. Simplifying Assumptions in Basic Biofilm Model. (Adapted from Gujer and Wanner (1990))

-
- A1 The biofilm is treated as a continuum: Components are not described by the structure and behavior of individual particles and molecules, but by averaging quantities such as concentrations and volume fractions.
 - A2 The biofilm consist of one liquid (water) phase and one or more solid phases.
 - A3 Each solid phase consists of the mass of one particulate component.
 - A4 The constituent particulate components are bound to each other and form a continuous solid matrix.
 - A5 The void spaces between the constituent particulate components are interconnected and occupied by the liquid phase.
 - A6 The liquid phase contains only dissolved components.
 - A7 Transport of the dissolved components in the liquid phase is by molecular diffusion.
 - A8 The dissolved components in the liquid phase are electrically neutral and behave ideally: Fick's first law of diffusion describes molecular diffusion.
 - A9 The ratio of diffusion coefficients in the biofilm and in pure water, $f = \frac{D_{fi}}{D_i}$, is constant.
 - A10 A solid phase contains no dissolved or suspended particulate components.
 - A11 The density of the constituent particulate components, ρ_s , is constant.
 - A12 Advective transport (displacement) of the solid phases is the result of volume changes of the constituent particulate components.
 - A13 Stoichiometry and kinetics of transformation processes do not depend on systems and compartments.
-

having different transport and transformation processes, different model equations (mass balance equations) need to be written for these two components.

Concentration is defined as the mass of a component within a unit volume. In homogeneous systems, where only one phase is present, the definition of unit volume is relatively easy. Heterogeneous systems where several phases may occur within any small finite control volume, the definition of unit volume becomes more complex.

The biofilm matrix contains k different phases with each occupying a fraction ϵ_k of the total biofilm volume. Using the index ℓ for the liquid phase and index s for the biofilm solid phases,

$$\sum_k \epsilon_k = \epsilon_\ell + \sum_s \epsilon_s = 1 \quad (2.8)$$

where ϵ_k = local volume fraction of the total biofilm volume occupied by phase k (-). In the biofilm model equations presented here, the following definitions for concentrations are used:

1. *Concentration C_{ki}* : The rates of transport and transformation processes are governed by the concentration of component i within one phase k . The concentration C_{ki} is the mass of component i contained in a unit volume of phase k . For the liquid phase, $C_{\ell i}$ is identical to the concentration of the component within the water squeezed from the biofilm matrix. This is the concentration that can be experimentally measured.

2. *Density ρ_k* : Each phase k consists of one major or bulk component such as water in the bulk or biomass in a specific solid phase. The concentration of this bulk component is its density. Since this bulk component plays a significant role for each phase, its concentration $C_{k,bulk}$ merits a special symbol, ρ_k . This density is not the bulk density which is $\epsilon_k \rho_k$. Bulk density is also referred to as dispersed density as it is mass over total volume. Note that particulate species are sometimes denoted by X_i in the literature and this is quite often the dispersed density and care must be

taken in applying literature values of biomass concentrations. In this case

$$X_i = \rho_{s_i} \epsilon_{s_i} \quad (2.9)$$

With the definitions given above mass balances on the dissolved and particulates species in the biofilm can be performed.

Dissolved Species With given assumptions (Table 1) the mass balance on dissolved species in the biofilm is given by

$$\frac{\partial \epsilon_\ell c_{\ell,i}}{\partial t} = -\nabla \cdot \mathbf{J}_{\ell,i} + r_{\ell,i} \quad (2.10)$$

where the flux $\mathbf{J}_{\ell,i}$ of species i is assumed to be give by Fick's first law as

$$\mathbf{J}_{\ell,i} = -D_{f\ell,i}(\mathbf{x}) \nabla c_{\ell,i} \quad (2.11)$$

where $D_{f\ell,i}$ is the diffusivity of dissolved substance i in the biofilm. Equation (2.10) is similar to (2.5) except that the fluid velocity in the biofilm, $\mathbf{u}_f$, is assumed to be zero or very small and providing negligible contribution to species balance in biofilm.

This assumption may not always be correct but under certain situations may not contribute significant error. In addition the volume fraction of liquid phase ϵ_ℓ needs to be used as a significant portion of the biofilm is not in liquid phase. In the bulk liquid phase it is assumed with dilute suspensions that the liquid volume fraction is approximately equal to one, (i.e., $\epsilon_\ell \approx 1$). If this assumption is not made, a balance on all species in bulk would be needed and overall balance on total suspension would be needed.

Solid Species With given assumptions (Table 1) the mass balance for solid species in the biofilm is given by

$$\rho_{s_k} \frac{\partial \epsilon_{s_k}}{\partial t} = -\nabla \cdot \mathbf{J}_{s_k} + r_{s_k} \quad (2.12)$$

where the solid flux, $\mathbf{J}_{s_k}$, is given by

$$\mathbf{J}_{s_k} = \nu_{s_k} \rho_{s_k} \epsilon_{s_k} \quad (2.13)$$

where $\nu_{s_k} = \nu_{s_k}(\mathbf{x}, t)$ is the velocity vector of species k of solid phase moving relative to the coordinate system. In the original model of biofilm processes, this was the only motion of solid species in the solid phase of the biofilm. In the expanded version of multispecies mathematical biofilm model, Wanner and Reichert (1996) allow the diffusion of particulate species in the biofilm. This formulation has an added flux term due to diffusion of solid species among other species in solid species in the biofilm matrix.

The physical significance of this diffusion-like term may not be clear but could be of importance for investigation. Parameter values for the diffusion coefficient of solid species in the biofilm matrix are not known but could be estimated by fitting the model to data as it becomes available. For simplicity this model follows the previous mathematical model for biofilm (Wanner and Gujer, 1986) that does not contain diffusion of particulates in the biofilm.

An expression is necessary to determine ν_{s_k} . It is assumed that the growth velocity at the substratum is zero (i.e., $\nu_{s_k}(L_f = 0, t) = 0$). Since equations (2.12) and (2.13) hold for all solid species in the biofilm, the sum of all solid species in the biofilm can be considered

$$\sum_{k=1}^{N_S} \frac{\partial \epsilon_{s_k}}{\partial t} = - \sum_{k=1}^{N_S} \nabla \cdot \nu_{s_k} \epsilon_{s_k} + \sum_{k=1}^{N_S} \frac{r_{s_k}}{\rho_{s_k}} \quad (2.14)$$

where N_S is the number of solid species in the biofilm. Equation (2.14) can be expanded and summation moved inside the derivatives along with the assumption that all solid species have same growth velocity, i.e.,

$$\nu_{s_k} = \nu_{s_i}, \quad i \neq k \quad (2.15)$$

to yield the equation

$$\frac{\partial}{\partial t} \left(\sum_{k=1}^{N_S} \epsilon_{s_k} \right) = - \left(\sum_{k=1}^{N_S} \epsilon_{s_k} \right) \nabla \cdot \boldsymbol{\nu}_{s_k} - \boldsymbol{\nu}_{s_k} \cdot \nabla \left(\sum_{k=1}^{N_S} \epsilon_{s_k} \right) + \sum_{k=1}^{N_S} \frac{r_{s_k}}{\rho_{s_k}} \quad (2.16)$$

The assumption that the velocity of solid phases (2.15) is implied from lack of a diffusional term in the flux of solid species (2.13) in the biofilm. This implies that all solid phase are subject to a common advection process. If any one attached particle moves, this causes displacement of its neighboring particles. Therefore, the advection velocity, $\boldsymbol{\nu}_{s_k}$ is identical for all solid phases and is the net result of the volume change of the bulk solid materials due to their production (e.g., biomass growth) and reduction (e.g., biomass death) or of a volume change of the liquid phase. From equation (2.8) an expression for the sum of the solid species in the biofilm can be obtained

$$\sum_{k=1}^{N_S} \epsilon_{s_k} = 1 - \epsilon_\ell$$

and insertion into equation (2.16) yields

$$\frac{\partial \epsilon_\ell}{\partial t} = -(1 - \epsilon_\ell) \nabla \cdot \boldsymbol{\nu}_{s_k} + \boldsymbol{\nu}_{s_k} \cdot \nabla \epsilon_\ell + \sum_{k=1}^{N_S} \frac{r_{s_k}}{\rho_{s_k}} \quad (2.17)$$

Equation (2.17) can be reduced further with the assumption of constant liquid volume fraction, ϵ_ℓ , in the biofilm liquid phase. This is the original assumption used by Wanner and Gujer (1986) and only recently allowed to change (Wanner and Reichert, 1996). While the liquid volume fraction has been reported to be other than constant (Zhang and Bishop, 1994a; Zhang and Bishop, 1994b; Zhang and Bishop, 1994c), modeling studies performed by Wanner and Reichert (1996) allowing the liquid volume fraction to change did not significantly change simulation results compared with the constant liquid volume assumption. For simplicity, in this dissertation the liquid volume fraction is assumed to be constant ($\epsilon_\ell = \text{constant}$). With this assumption, equation (2.17) can be rewritten as

$$\nabla \cdot \boldsymbol{\nu}_{s_k}(\mathbf{x}, t) = \frac{1}{1 - \epsilon_\ell} \sum_{k=1}^{N_S} \frac{r_{s_k}}{\rho_{s_k}} \quad (2.18)$$

Equation (2.18) was also obtained by (Szego et al., 1993a; Szego et al., 1993b; Szego, 1992) using integral (control volume) formulation for the mass balances.

Equation (2.18) gives a relationship for the divergence of ν_{s_k} but since ν_{s_k} is a vector, which in general three spatial dimensions, and one temporal dimension, additional equations are needed to determine the vectorial nature of ν_{s_k} . The vectorial nature of ν_{s_k} is related to mechanical properties of the biofilm of which mass balance and momentum balance of biofilm could yield additional equations for determination of ν_{s_k} . Gujer and Wanner (1990) note that most probably a new state variable must be introduced, such as the potential energy available for the deformation of the solid film matrix (π_s), which may depend on the viscoelastic nature of the biofilm. In addition, a function $\nu_s(\nabla\pi_s)$ must be defined, but presently no information is available for such a definition. The interface would include a balance on normal and tangential forces.

To get around the problem of obtaining the vectorial representation of the expanding biofilm, an assumption is made that the biofilm growth is predominantly normal to the substratum. This implies that

$$\nabla \cdot \nu_{s_k} \approx \frac{\partial}{\partial \eta}(\nu_{s_k} \cdot \eta) = \frac{\partial \nu_s}{\partial \eta} \quad (2.19)$$

where η is the unit normal to the substratum and convective expansion/contraction velocity ν_{s_k} is now assumed to be approximated by

$$\nu_{s_k} \approx \nu_{s_k} \cdot \eta \quad (2.20)$$

Applying (2.19) to equation (2.18) results in the following equation for spatial change of ν_{s_k} .

$$\frac{d\nu_{s_k}}{d\eta} = \frac{1}{1 - \epsilon_\ell} \sum_{k=1}^{N_S} \frac{r_{s_k}}{\rho_{s_k}} \quad (2.21)$$

with the boundary condition that $\nu_{s_k} = 0$ at the solid substratum ($\eta = 0$). With this

boundary condition equation (2.21) can be integrated with respect to η to obtain

$$\nu_{s_k}(\eta) = \frac{1}{1 - \epsilon_\ell} \int_0^\eta \sum_{k=1}^{N_s} \frac{r_{s_k}}{\rho_{s_k}} d\eta \quad (2.22)$$

Boundary Conditions

It is necessary to supply boundary conditions to solve the governing partial differential/integral equations formulated for the bulk fluid, biofilm, and interface regions. Description of boundary conditions will follow the format of boundary conditions for a equation for a location with no biofilm and for a location with biofilm. Locations with biofilm have boundary conditions for the biofilm substratum interface and the biofilm/bulk fluid interface. The biofilm/bulk fluid interphase boundary condition equations are treated as interface equations.

Navier-Stokes Equations

In order to solve (2.1)-(2.2) it is necessary to apply initial and boundary conditions for the problem to be well posed (Gresho, 1991a; Gresho, 1991b; Gresho, 1992). The initial boundary-value problem give by (2.1) and (2.2) is to find $\mathbf{u}(\mathbf{x}, t)$, $p(\mathbf{x}, t)$ in a bounded domain Ω with boundary Γ such that $\mathbf{u}(\mathbf{x}, t)$ is given on the boundary Γ by the equation

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{u}_\Gamma(\mathbf{x}, t) \quad (2.23)$$

and $\mathbf{u}$ is given at initial time $t = 0$ by

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}) \quad (2.24)$$

The boundary value $\mathbf{u}_\Gamma$ must satisfy the condition

$$\int_\Gamma \mathbf{u}_\Gamma \cdot \boldsymbol{\eta} ds = 0 \quad (2.25)$$

With the assumption of zero fluid flow in the biofilm, the velocity boundary condition at the biofilm/bulk fluid interface is $\mathbf{u}(\mathbf{x}, t) = \mathbf{0}$. This is not strictly true as movement of the biofilm/bulk fluid interface will add or subtract water from the biofilm region depending on whether the biofilm is expanding or contracting. If the velocity is not assumed to be zero at the boundary, a interface velocity condition will be needed between the bulk fluid and the biofilm surface. An additional boundary condition on the shear stress would also be needed. These boundary conditions would be provided from a balance of normal and tangential forces at the interface.

It is also necessary to specify the velocity condition at the inlet. This can be done by specifying the actual velocity $\mathbf{u}$ or specifying a profile such as a fully developed velocity profile. At the exit, it is convenient to use a no change in downstream direction boundary condition $\frac{\partial u}{\partial x} = 0$ if x is the direction downstream and $\frac{\partial v}{\partial y} = 0$ if y is the direction downstream. This does require a proper selection of domain used for simulation so that this assumption is reasonable. If the resulting computed solution appears to be influenced by the exit boundary condition, it is useful to extend the problem domain such that the exit boundary condition is more realistic. Boundary conditions at the exit of flowing systems is still an active area of research (Han and Bao, 1996; Chen et al., 1995; Christer and Johansson, 1993; Tezduyar and Liou, 1991; Sani and Gresho, 1994).

Species Balance Equations

It is necessary to apply boundary conditions to solve (2.5) for each dissolved constituent. Boundary conditions are needed at the inlet, outlet, walls without biofilm, and walls with biofilm. In the case of walls with biofilm, the boundary condition for the species balance equation comes from a differential algebraic equation at the

biofilm bulk fluid interface. Recall the total flux of a species i given by equation (2.4)

$$\mathbf{J}_{T_i} = \mathbf{u} \cdot \nabla c_i - D_i(\mathbf{x}) \nabla c_i \quad (2.4)$$

which provides convective and diffusive transport components.

Equation (2.4) can be applied to the inlet, outlet, and walls without biofilm on them. Boundary conditions in flowing systems in the one-dimensional version of equation (2.5) have been the subject of previous research (Danckwerts, 1953; Wehner and Wilhelm, 1956; Barry and Sposito, 1988; Novy et al., 1990; Novy et al., 1991).

Inlet Boundary Condition At the inlet it is common to specify an average concentration for a species i along with the velocity or flow rate. Thus, with the inlet velocity known, or effectively the average velocity, a reasonable boundary condition is

$$\mathbf{u}_0(\mathbf{x}) \bar{c}_{0i} = \mathbf{u}_0(\mathbf{x}) c_i(\mathbf{x}) - D_i \nabla c_i(\mathbf{x}) \quad (2.26)$$

where $\bar{c}_{0i}$ is the average inlet concentration. This formulation accounts for total flux entering the reactor. This becomes a Robin boundary condition or third type of boundary condition. This boundary condition is often used for one dimensional column modeling (Kim and Corapcioglu, 1997). This boundary condition describes a prescribed convective-diffusive flux (Padilla et al., 1997).

If the inlet located a distance from first location of biofilm (assuming sterile feed concentration), the gradient term in equation (2.26) is small and is often neglected. Inlet boundary conditions to reactors has been subject of research by others (Novy et al., 1990).

Outlet Boundary Condition The outlet boundary condition formulation is more difficult than the inlet boundary condition. In general, little is known about the exit boundary condition other than as little influence on solution upstream from

exit boundary as possible. To implement this boundary condition different formulations are possible.

One formulation is to use a no change in the direction normal to the exit such similar to the exit velocity boundary condition. This formulation is

$$\frac{\partial c}{\partial \eta} = 0 \quad (2.27)$$

where η is the direction normal to the exit. This boundary condition is also called a *reflection boundary condition* (Shamir and Harleman, 1967). This boundary condition seems to work adequately for higher flow rates but as flow velocity decreases it starts to resemble a no flux boundary condition. This boundary condition has been used for exit boundary condition on flow reactors (Kim and Corapcioglu, 1997).

As an alternative, the *transmission boundary condition* (Shamir and Harleman, 1967) allows more flow through a boundary as velocity decreases. This boundary condition guarantees a continuation of the slope of the concentration distribution through the boundary. This boundary condition is given by

$$\frac{\partial^2 c}{\partial \eta^2} = 0 \quad (2.28)$$

where η is the normal direction to the exit. This boundary condition was used by Simoes and Wang (1997).

The *free gradient* boundary condition developed by Widdowson et al. (1988) is similar to the *transmission boundary condition*. In the *free gradient* boundary condition the gradient defined by the n and $n - 1$ nodes is continuous and equal to the gradient defined by the $n + 1$ node (external to the problem domain) and n nodes. Mathematically this becomes

$$\left(\frac{\partial c}{\partial x} \right)_n = \left(\frac{\partial c}{\partial x} \right)_{n+1} \quad (2.29)$$

which can be implemented using backward differences and inserted in system of equations (Widdowson et al., 1988).

This boundary condition versus a zero flux boundary condition for the one-dimensional version of equation (2.5) with zero reaction, was more accurate when the solution approached the boundary of the finite domain (Widdowson et al., 1988). This boundary condition is very similar to (2.28) in implying zero curvature in the solution at the exit. Equation (2.28) yields accurate results and will be used for exit boundary condition for equation (2.5).

Impermeable Walls Without Biofilm Impermeable walls without biofilm and a non-reactive substratum require a no flux boundary condition. This conditions is expressed mathematically as

$$\mathbf{J}_i \cdot \boldsymbol{\eta}_{wall} = 0 \quad (2.30)$$

where $\boldsymbol{\eta}$ is the normal direction to a wall. With the no penetration boundary conditions on impermeable walls ($\mathbf{u} \cdot \boldsymbol{\eta} = 0$), results in

$$\frac{\partial c_i}{\partial \eta} = 0 \quad (2.31)$$

where η is the normal direction to the wall. In this modeling work, the substratum is considered to be non-reactive with the substrate.

Interface Equations

Interface equations link the biofilm region with the bulk fluid region. Since this interface is moving, a jump condition can arise across the interface for the dissolved and particulate species. The equations for the interface between the the biofilm and the bulk fluid are given by Gujer and Wanner (1990) in general form as:

$$\mathbf{n}_I \cdot \boldsymbol{\nu}_I (\epsilon_{k,f} C_{ki,f} - \epsilon_{k,b} C_{ki,b}) = (\mathbf{J}_{ki,f} - \mathbf{J}_{ki,b} + \mathbf{r}_{ki}'') \cdot \mathbf{n}_I \quad (2.32)$$

where $\boldsymbol{\nu}_I$ is the velocity of the biofilm/bulk fluid interface, (positive away from substratum), $\mathbf{n}_I$ is the unit normal to interface, i is the component index, f denotes

the biofilm region, b denotes the bulk liquid region, k is the phase index, (solid or liquid), r''_{ki} is the interfacial transfer rate, and $\mathbf{J}_{ki}$ is the flux of component i in form of phase k . With the assumption that the direction normal to the substratum is more important than directions tangential to substratum, equation (2.32) is reduced to the direction normal to substratum.

Dissolved components in the liquid phase exist on both sides of the biofilm/bulk fluid interface, and are not subject to an interfacial transfer process ($\epsilon_{\ell,b} = 1, r''_{\ell i} = 0$), so equation (2.32) yields:

$$\nu_I(\epsilon_{\ell,k}C_{\ell i,f} - C_{\ell i,b}) = \mathbf{J}_{\ell i,f} - \mathbf{J}_{\ell i,b} \quad (2.33)$$

For components in the solid phase, which occur in the biofilm only ($\epsilon_{s,b} = 0, \mathbf{J}_{si,b} = 0$) equation (2.32) yields:

$$\nu_I \epsilon_{s,f} C_{si,f} = \mathbf{J}_{si,f} + \mathbf{r}_{si}'' \quad (2.34)$$

Equation (2.34) may be applied to the solid material in the biofilm to predict the interface velocity, ν_I , at which the biofilm expands or shrinks. The interface velocity, ν_I is the result of two processes: (1) transport of bulk material towards the interface from growth processes, $\mathbf{J}_s$, and (2) production (e.g., attachment) or loss (e.g., detachment) of bulk material at the interface $\mathbf{r}_s''$.

An additional equation at the interface holds for dissolved components with the assumption that no electrically charged particles are considered and that no physiochemical interaction between different components are observed (Gujer and Wanner, 1990). This equation requires continuity of the concentration across the interface for dissolved constituents

$$C_{\ell i,b} = C_{\ell i,f} \quad (2.35)$$

and equation (2.33) becomes

$$\nu_I C_{\ell i,f}(\epsilon_{\ell,f} - 1) = \mathbf{J}_{\ell i,f} - \mathbf{J}_{\ell i,b}. \quad (2.36)$$

At steady state equation (2.36) reduces down to continuity of fluxes for dissolved species. In the case of unsteady state, the first term in equation (2.36) accounts for differences in water volume in bulk (all water) and biofilm (partially water).

Equation (2.22) evaluated at $\eta = L_f$ results in

$$\nu_{s_k}(L_f) = \frac{1}{1 - \epsilon_\ell} \int_0^{L_f(t)} \sum_{k=1}^{N_s} \frac{r_{s_k}}{\rho_{s_k}} d\eta \quad (2.37)$$

Equation (2.34) and equation (2.37) are combined to get an equation for the interface velocity. With a little algebra ν_I can be written as:

$$\nu_I = \nu_{s_k}(L_f) + \frac{1}{1 - \epsilon_\ell} \sum_{k=1}^{N_s} \frac{r''_{s_k}}{\rho_{s_k}} \quad (2.38)$$

L_f and ν_I are related by:

$$\frac{dL_f(t)}{dt} = \nu_I(t) \quad (2.39)$$

The net detachment expression, r''_s , can be formulated as

$$r''_s = (-aL_f^2 - bL_f - c - d\bar{\mu}_s - e\bar{\tau})\epsilon_s\rho_s \quad (2.40)$$

where a, b, c, d , and e are empirical coefficients for the detachment expression, $\bar{\tau}$ is the tangential shear stress on the biofilm surface, and $\bar{\mu}_s$ is the spatially averaged growth rate of biofilm defined as

$$\bar{\mu}_s = \frac{1}{L_f(t)} \int_0^{L_f(t)} r_s dz. \quad (2.41)$$

Detachment is treated as interfacial problem for this biofilm formulation. Gadani et al. (1993) include detachment as a first order decay term in the particulate growth reaction. This term as implemented in a hyperbolic tangent formulation allowing detachment to vary from zero at substratum to a maximum at the surface of the biofilm. Previously this had been just lumped into a first order decay term for biofilm biomass which included respiration and shear loss effects (Rittmann, 1982).

Biofilm Equations

It is necessary to supply boundary conditions to solve the mass balance equations for dissolved species (2.10) and solid species (2.12) in the biofilm. Since the substratum is considered to be nonreactive and impermeable, a no flux boundary condition like (2.30) hold for both dissolved species and particulate species in the biofilm. At the substratum

$$\mathbf{J} \cdot \boldsymbol{\eta})_{\text{substratum}} = 0 \quad (2.42)$$

holds for dissolved and particulate species.

For dissolved species equation (2.42) reduces down to (2.31) for the concentration in the biofilm. The flux of particulates (2.13) becomes

$$\nu_s)_{\text{substratum}} = 0. \quad (2.43)$$

This equation just states that the velocity of particulates at the substratum is zero and it is zero for all particulate components.

Nondimensionalisation of Model Equations

It is common to nondimensionalize mathematical equations arising from physical situations to allow interpretation of importance of terms in the equations.

$$\begin{aligned} t^* &= \frac{t}{\frac{L_\infty}{V_\infty}} & \mathbf{x}^* &= \frac{\mathbf{x}}{L_\infty} & \mathbf{u}^* &= \frac{\mathbf{u}}{V_\infty} & c_i^* &= \frac{c_i}{c_{\infty i}} & r_i^* &= \frac{r_i}{\frac{C_{\infty i} V_\infty}{L_\infty}} \\ p^* &= \frac{p - p_\infty}{\rho V_\infty^2} & \nu^* &= \frac{\nu}{\nu_\infty} & \mathbf{f}^* &= \frac{\mathbf{f}}{\frac{L_\infty}{V_\infty^2}} & D_i^* &= \frac{D_i}{D_{\infty i}} & \tau^* &= \frac{\tau}{\rho V_\infty^2} \end{aligned} \quad (2.44)$$

where the * superscript denotes a dimensionless quantity.

Navier Stokes Equations

Application of (2.44) to the Navier Stokes equations, (2.1)-(2.2) results in:

$$\nabla^* \cdot \mathbf{u}^* = 0 \quad (2.45)$$

$$\frac{\partial \mathbf{u}^*}{\partial t^*} + \mathbf{u}^* \cdot \nabla^* \mathbf{u}^* = -\nabla^* p^* + \frac{1}{Re_L} \nabla^{*2} \mathbf{u}^* + \mathbf{f}^* \quad (2.46)$$

where $Re_L = \frac{V_\infty L_\infty}{\nu_\infty}$ is the the Reynolds number used for nondimensionalisation.

Species Balance Equation

Applying (2.44) to (2.5) results in a nondimensional equation for species balance

$$\frac{\partial c_i^*}{\partial t^*} + \mathbf{u}^* \cdot \nabla^* c_i^* = \frac{1}{Re_L Sc_i} \nabla^{*2} D_i^* c_i^* + r_i^* \quad (2.47)$$

where $Sc_i = \frac{\nu_\infty}{D_{\infty i}}$ is the Schmidt number for species i . The Schmidt number reflects the ratio of viscous to diffusive properties which for most dissolved species of interest in water gives Schmidt numbers in the range $10^2 - 10^3$.

Biofilm Equations

Applying the nondimensional transformation (2.44) to the mass balance equation for dissolved species in biofilm (2.10) with mass flux given by (2.11) results in

$$\frac{\partial \epsilon_\ell C_{\ell,i}^*}{\partial t^*} = \frac{f_i}{Re_L Sc_i} \nabla^{*2} D_i^* C_{\ell,i}^* + r_{\ell,i}^* \quad (2.48)$$

where f_i is the ratio of diffusivity in the biofilm to diffusivity in the bulk for dissolved component i .

Discussion of the Mathematical Model

In this chapter the mathematical formulation of the model describing fluid dynamics, substrate transport and biofilm processes was presented in general and the simplification of the biofilm process model to one dimension was presented.

Modeling of fluid flow with equations (2.45) and (2.46) is performed routinely with addition of a turbulence model if problem size is such that computational resources are not available to allow a direct numerical simulation of turbulence. Most

engineering relevant flow situations are such that a turbulence model is necessary (Ferziger and Perić, 1996). In this simulation laminar flow is assumed to avoid the issue of turbulence modeling.

Modeling of substrate transport with (2.47) is common for dissolved substrates. The selection of a diffusion coefficient for particulate species in the bulk is a limitation and may represent Brownian motion. In practical use the diffusion coefficient may be very small and could require different numerical methods for solution. Modeling of biofilm with partial differential equations has been performed although some researchers suggest other techniques such as cellular automaton may provide more realistic microstructure (Wimpenny and Colasanti, 1997; Picioreanu et al., 1998b; Picioreanu et al., 1998a).

Solutions to equations (2.45) and (2.46) can be very complex depending on system geometry and flow rate conditions. Analytical solutions are available only for simple idealized cases. Due to the nonlinearity of the equations coupled with possibly complex geometry can lead to complex velocity variations. Rectangular geometry will be used for simulations in the remainder of this thesis. This choice simplified mesh generation for numerical solution but does introduce some approximations which may contribute some error to the solution.

The species balance equation (2.47) can contain complex behavior depending on flow (Reynolds number), transport conditions (Schmidt number) and reaction kinetics. In many situations the reactions at the surface will dominate the interior reactions as suspended concentrations are typically smaller in flow systems. For dissolved constituents in the bulk fluid, there is the physical requirement that concentrations cannot go negative.

While the equations for balance on particulate species in the bulk fluid would seem to allow for unbounded production of particulates, the link through the kinetics

to substrate concentrations should limit the production in the bulk. In theory, the biofilm could grow and plug off the flow area thus resulting in formation of a biobarrier. In this work, it is assumed that the biofilm thickness relative to flow geometry is small and plugging of flow area does not occur.

In the next chapter this mathematical model is solved numerically using finite differences. Examples are for single species biofilm with single substrate to demonstrate applicability of the model. Extension of this approach to multispecies and multisubstrates adds more complexity and solution time to the numerical model. It may be desirable to include other species not directly consumed but influential in the overall reaction rate. Tracking of pH for example can be important in some reaction and has been included in some simulations (Hjuler, 1996).

CHAPTER 3

SOLUTION OF MODEL EQUATIONS

This chapter contains the numerical solution techniques used to solve the mathematical model presented in the previous chapter in two spatial dimensions for the bulk fluid region and one spatial dimension for the biofilm. This allows for patches of biofilm on the walls of a two dimensional flow domain such as that shown in Figure 2. The solution method presented here is restricted for the steady-state solution of the model although it could be adapted for non steady-state. The superscript * is dropped from the nondimensional terms and equations presented in chapter 2 from here on out.

The Navier-Stokes equations (2.45) and (2.46) are rewritten in the stream function vorticity formulation. A numerical scheme for the solution of the stream function vorticity equations and boundary conditions is presented. With the velocity vector field known, the species balance equation and biofilm equations can be solved. An iteration between the species balance equations and biofilm equations allows easier numerical solution. The species balance equation is solved first with zero flux at boundary and then value of the concentration is determined at biofilm surface and the biofilm equations are solved for this concentration which results in a flux to the biofilm. This flux is then applied to the species balance equation and solved to yield a new value of the concentration at the biofilm surface. This iterative scheme continues until the change in concentrations is less than a specified tolerance for solution convergence.

For the purpose of illustration, a simple cavity depicted in Figure 4 will be used for demonstration of a typical domain with representative boundary conditions.

Sides of the cavity represented by dashed lines are inlet/outlet boundary locations which allow fluid flow in or out along with dissolved constituents in the fluid. Walls denoted with solid lines can have biofilm on them, but are assumed to be impermeable to fluid flow.

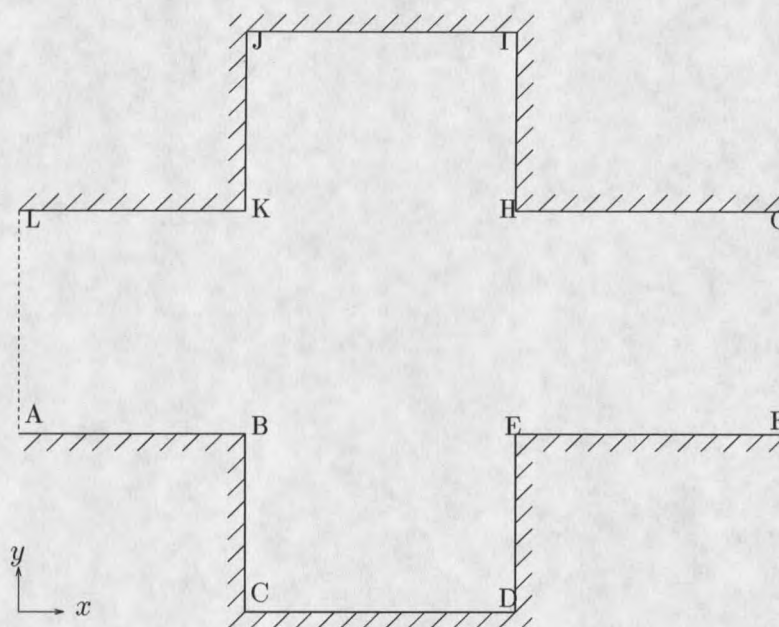


Figure 4. Example of two dimensional cavity for simulation.

Stream Function Vorticity Formulation

For ease of numerical solution it is convenient to solve the Navier-Stokes equation (2.45)–(2.46) in stream function/vorticity formulation. This approach is often used for two dimensional problems (Morrison and Napolitano, 1988; Napolitano, 1991; Huang and Seymour, 1995; Huang and Seymour, 1996; Huang and Wetton, 1996; Gerges and McCorquodale, 1997; Tokunaga and Yamauchi, 1997; Mancera and Hunt, 1997; Louaked et al., 1997; Murray and Carey, 1990) and has seen some use for three dimensional problems also (E and Liu, 1996; E and Liu, 1997). The stream function

vorticity formulation is obtained by defining the velocities to be derivatives of the stream function, ψ ,

$$u = \frac{\partial \psi}{\partial y} \quad (3.1)$$

$$v = -\frac{\partial \psi}{\partial x} \quad (3.2)$$

In general the vorticity, ω , is defined as the curl of the velocity field (Anderson et al., 1984)

$$\omega = \nabla \times \mathbf{u} \quad (3.3)$$

and taking the curl of (2.46) results in equations for the vorticity. For the two dimensional case, there is just one nonzero component of the vorticity which will be denoted by ω , where

$$\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \quad (3.4)$$

In the two dimensional case, the one vorticity transport equation is

$$\frac{\partial \omega}{\partial t} + \mathbf{u} \cdot \nabla \omega = \frac{1}{Re_{L_\infty}} \nabla^2 \omega \quad (3.5)$$

The stream function ψ is only defined by equations (3.1) and (3.2) to within an arbitrary constant in terms of the velocity. With the definitions (3.1) and (3.2), the continuity equation (2.45) is automatically satisfied. Lines of constant ψ form streamlines with the average velocity being the difference in the stream function values divided by the distance between the stream functions (Milne-Thomson, 1968; Shames, 1982). In this formulation, flux is taken as positive from left to right.

Substitution of (3.1) and (3.2) into (3.4) results in a Poisson equation for the stream function

$$\nabla^2 \psi = -\omega \quad (3.6)$$

Equations (3.5) and (3.6) are a set of coupled equations that with boundary conditions can be solved to get the values of stream function and vorticity. If the

stream function is known, (3.5) becomes a linear equation for the vorticity. When the vorticity is known, equation (3.6) is just a Poisson equation for the stream function. This linearity allows iteration between the two and has been a solution option used in the past although some arguments are made for simultaneous solution of equations (3.5) and (3.6) (Gresho, 1991a; Gresho, 1991b; Gresho, 1992).

With the change of variables it is necessary to write the boundary conditions for (2.45)–(2.46) in stream function vorticity formulation also. This requires rewriting the no slip, no penetration boundary conditions for the solid walls and biofilm walls along with the inlet and outlet boundaries in terms of the stream function and vorticity.

Boundary Conditions

Boundary conditions are needed to solved equations (3.6) and (3.5). Boundary conditions for the Navier-Stokes equations need to be rewritten to apply to the stream function vorticity formulation. Recalling the three type of boundaries shown in Figure 4 it becomes necessary to formulate equations for inlet/outlet and walls with or without biofilm. Permeable boundaries denoted by dashed lines represent locations of inflow or outflow. Solid lines denote impermeable walls which do not allow flow tangentially or normal to them. The impermeable walls may have biofilm located on them and treatment of this differs slightly from the impermeable wall without biofilm.

Solid Walls Boundary conditions are needed on the solid walls for the domain shown in Figure 4. On these walls, the conditions of no slip and no penetration are enforced. This development of boundary conditions for the stream function vorticity formulation follows the approach used by Peyret and Taylor (1983).

In general dotting the velocity into the normal and tangential unit vectors provides the normal and tangential velocity components which are related to the normal and tangential derivatives of the stream functions. These relationships are

given by

$$\left(\frac{\partial\psi}{\partial\tau}\right)_{\Gamma} = \mathbf{V}_{\Gamma} \cdot \boldsymbol{\eta} \quad (3.7)$$

and

$$\left(\frac{\partial\psi}{\partial\eta}\right)_{\Gamma} = -\mathbf{V}_{\Gamma} \cdot \boldsymbol{\tau} \quad (3.8)$$

where $\boldsymbol{\eta}$ and $\boldsymbol{\tau}$ are, respectively, the outward normal and tangential unit vectors to Γ .

Equation (3.7) can be integrated along Γ to obtain the general form of the boundary condition on Γ

$$\psi = f(x, y) \quad (3.9)$$

and (3.8) can be written as

$$\frac{\partial\psi}{\partial\eta} = g(x, y) \quad (3.10)$$

where $f(x, y)$ must satisfy the total flux condition

$$\int_{\Gamma} \nabla f \cdot \boldsymbol{\tau} ds = 0 \quad (3.11)$$

Note that these boundary conditions are on ψ but boundary conditions are also need for the vorticity ω to solve equation (3.5). Equation (3.9) can will be applied directly in the solution for ψ while (3.10) will be implemented in the formulation of a boundary condition for the vorticity ω . Boundary conditions for ω must be obtained from the information known about the stream function ψ .

Solid Walls Without Biofilm The standard formulation for a solid wall are the no slip and no penetration boundary conditions. With the rectangular domain shown in Figure 4, the boundary conditions become applied at horizontal and vertical walls.

Consider the part $y = 0$ on the boundary Γ . From (3.9) and (3.10), the boundary conditions are

$$\psi(x, 0) = f_0(x) \quad (3.12)$$

$$\frac{\partial \psi}{\partial y}(x, 0) = -g_0(x) \quad (3.13)$$

Impermeable walls with no biofilm have boundary conditions of no slip and no penetration which implies the tangential and normal components of the velocity are zero at the wall. This implies that the value of ψ along a wall is constant. Using a horizontal wall for an example gives

$$\psi(x) = f_0(x) = \text{constant} \quad (3.14)$$

and

$$\frac{\partial \psi}{\partial y} = -g_0(x) \quad (3.15)$$

Boundary conditions for the vorticity, ω , in the stream function vorticity formulation are subject to debate as for formulation and implementation (Gresho, 1991a; Gresho, 1992; Gresho, 1991b).

Solid Walls With Biofilm For impermeable walls with biofilm, the current treatment is to assume that there is no liquid flow inside the biofilm region or that effect of liquid flow is negligible (Wanner and Gujer, 1986; Gujer and Wanner, 1990). While this assumption may not be totally correct, it is typically used and probably will continue to be used until an alternative formulation describing the velocity in the biofilm region is developed. With this assumption, equations (3.14) and (3.15) hold at the biofilm bulk fluid interface.

Consider a horizontal wall with biofilm located at a portion. The boundary conditions (3.14) and (3.15) can be modified slightly. Equation (3.14) now becomes

$$\psi(x, L_f) = f_0(x, L_f) = \text{constant} \quad (3.16)$$

and equation (3.15) becomes

$$\frac{\partial \psi}{\partial y} = -g_0(x, L_f) \quad (3.17)$$

Equations (3.14) and (3.15) can be viewed as special cases of (3.16) and (3.17) with $L_f = 0$.

If the interface is moving rapidly relative to the local flow velocity, equation (3.14) will need to be rewritten to reflect that the normal velocity component at the biofilm bulk fluid interface is non zero. Note that this may be a small component of momentum and mass of water in balance equations and will depend on how much of the biofilm is water at the interface. The effect of mass flux of water added or removed from the biofilm region on the mass of water in the bulk region due to expansion or contraction of biofilm thickness was omitted in the multispecies biofilm model by Wanner and Gujer (1986). This water flux is included in the formulation of the mixed culture biofilm model (Wanner and Reichert, 1996).

Research into liquid flows in biofilm region and influence on mass transport properties has recently become an active area of research (de Beer, Stoodley, Roe and Lewandowski, 1994; de Beer and Stoodley, 1995; de Beer, Stoodley and Lewandowski, 1994; Lewandowski et al., 1993; Lewandowski and Stoodley, 1995; Lewandowski et al., 1995; Lewandowski et al., 1994; Bishop et al., 1995). As a better quantification of flow in biofilm region becomes available, it may be possible to formulate an expression such as Darcy's Law for the biofilm region. If this is the case, another term is added to the right hand side of (2.2) which would then include a permeability coefficient which would be a function of the biofilm volume fraction, cluster size, etc. This formulation would alter the vorticity equation but the stream function vorticity method could still be used. In this case, the no slip no penetration boundary condition would hold at the substratum assuming an impermeable substratum.

Inlet For this simulation the inlet velocity profile is assumed to be known and be fully developed parabolic velocity profile in the x direction with variation only with y (see Shames (1982)). With this assumption, the inlet velocity profile is given

in terms of the average velocity u_{ave} and the y coordinates of points A and L, y_l and y_u respectively (see Appendix A) as

$$u(y) = -\frac{6u_{ave}}{(y_u - y_l)^2} [y^2 - y(y_u + y_l) + y_u y_l] \quad (3.18)$$

With the inlet velocity profile (3.18) known, a boundary condition needs to be written in terms of stream function vorticity formulation to be applied as boundary conditions for equations (3.6) and (3.5). Since the inlet velocity is given by (3.18) it can be integrated with respect to y (recall equation (3.1)) to obtain an equation for stream function, ψ , at the inlet. Note that the constant of integration is chosen such that $\psi = 0$ on the lower wall of inlet. This results in an equation for ψ at the inlet (see Appendix A)

$$\psi(y) = -\frac{6\psi(y_u)}{(y_u - y_l)^3} \left[\frac{y^3 - y_l^3}{3} - \frac{(y^2 - y_l^2)(y_u + y_l)}{2} + (y - y_l)y_u y_l \right]. \quad (3.19)$$

where $\psi(y_u)$ is the value of ψ on the upper wall.

To get vorticity boundary conditions at the inlet, the inlet velocity profile (3.18) is differentiated with respect to y and substituted into (3.4) along with assumption that

$$\frac{\partial v}{\partial x} = 0. \quad (3.20)$$

Equation (3.20) implies that the inlet is far enough away from a cavity or corner so as not to be influenced by it. This also implied that the inlet is far enough away from the first biofilm patch so as not to be influenced by it. This approach gives the inlet vorticity boundary condition (see Appendix A)

$$\omega(y) = -\frac{12\psi(y_u)}{(y_u - y_l)^3} \left[\frac{y_u + y_l}{2} - y \right]. \quad (3.21)$$

An alternative approach would be to supply velocity values at the inlet which could be numerically integrated to obtain the stream function values and differentiated to obtain the vorticity values. Note that the $\partial v / \partial x$ would need to be specified also to calculate the inlet vorticity.

Outlet Boundary conditions at the outlet of a flowing system are difficult to formulated and are an ongoing area of research (Christer and Johansson, 1993; Heywood et al., 1996; Tezduyar and Liou, 1991). A common approach is to assume that at the exit the flow has reestablished into uniform flow. This may require extending the domain slightly beyond area of interest to assure that this is met. An analysis of the solution obtained should allow estimation of whether this was enough or the imposition of uniform flow affected the solution.

Making the assumption of uniform flow at the exit boundary conditions on the stream function and vorticity can be obtained. For the outlet boundary condition, a boundary condition for the stream function, ψ is (Fletcher, 1988b)

$$\frac{\partial^2 \psi}{\partial x^2} = 0 \quad (3.22)$$

which is implemented as

$$\frac{\partial^2 \psi}{\partial y^2} = -\omega \quad (3.23)$$

from equation (3.6). For the vorticity boundary condition

$$\frac{\partial \omega}{\partial x} = 0 \quad (3.24)$$

can be used (Fletcher, 1988b). These exit boundary conditions assume that there is essentially no change in stream lines down the flow direction. This requires proper selection of the outlet location so that this is physically realistic for the problem of interest.

Note that proper form of boundary conditions on the stream function and vorticity at the outflow are necessary (Tezduyar and Liou, 1991) for accurate simulation of fluid flow. The problem of outlet boundary conditions will arise again for the species balance equations (Patankar, 1980).

Perturbation Scheme

Biofilm thickness, L_f , is assumed constant in this model formulation but it can vary along a wall. The geometry shown in Figure 4 is rectangular in nature. Application of finite differences to this geometry where biofilm can vary along a horizontal surface can be simplified by using a perturbation scheme to apply boundary conditions at another location. A typical example of this is shown in Figure 5 where a $f(x)$ (such as $L_f(x)$) varies above the wall. Treating the wall as the original domain for placement of nodes to solve the bulk fluid equations simplifies solution procedure.

To simplify the numerical solution a perturbation scheme is introduced which allows the interface boundary conditions for the bulk fluid to be applied at the original domain so the original discretization can still be used for solution of the bulk fluid equations. In this manner the equations for the bulk fluid do not need to be reformulated for the change in domain due to biofilm presence.

Consider a horizontal wall at y_0 and a curve above it $y = f(x)$ that is the boundary. However, the boundary conditions (B.C.'s) need to be applied at y_0 to retain the original finite difference mesh (see Figure 5).

A Taylor series expansion of the variable in question, say $u(x, y)$ for example, can be written:

$$u(x, f(x)) = u(x, y_0) + \frac{\partial u(x, y_0)}{\partial y}(f(x) - y_0) + \sum_{k=2}^{\infty} \frac{\partial^k u(x, y_0)}{\partial y^k} \frac{(f(x) - y_0)^k}{k!} \quad (3.25)$$

Here it is assumed that $f(x) - y_0$ is small so that the higher order terms, $k \geq 3$, can be neglected. Assume the boundary condition $u(x, f(x))$ is known and equation (3.25) can be written as:

$$u(x, y_0) + \frac{\partial u(x, y_0)}{\partial y}(f(x) - y_0) + \frac{\partial^2 u(x, y_0)}{\partial y^2} \frac{(f(x) - y_0)^2}{2!} = u(x, f(x)) = g(x) \quad (3.26)$$

which is a boundary condition of the third type.

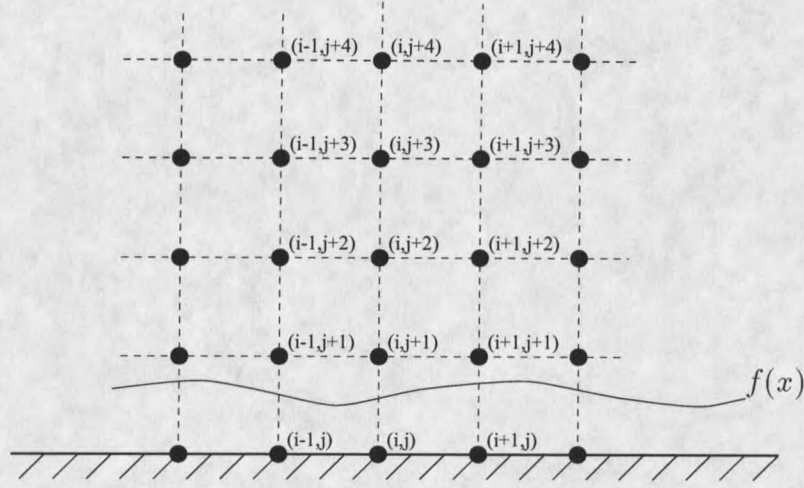


Figure 5. Horizontal wall with perturbation of boundary.

For the discretized version of (3.26) the result is using forward differences for the derivatives is:

$$u_{i,j} + \frac{3u_{i,j} - 4u_{i,j+1} + u_{i,j+2}}{2h} L_f(x_i) + \frac{u_{i,j} - 2u_{i,j+1} + u_{i,j+2}}{2h^2} L_f^2(x_i) = g(x_i) \quad (3.27)$$

where $u_{i,j} = u(x_i, y_j)$ and

$$L_f(x_i) = f(x_i) - y_j \quad (3.28)$$

the biofilm thickness denotes the perturbation quantity.

Equation (3.27) is general form for perturbation and for each problem to be solved takes a specialized form. Appendix B contains some perturbation expressions for Dirichlet or Neumann boundary conditions.

Numerical Discretization

The equations for fluid dynamics are nonlinear and few analytical solutions are known for more than simple one dimensional problems. This also holds for the species balance and biofilm equations which obtain nonlinearity in their reaction term which typically couples multiple species together. In addition the interface equations may

have nonlinear formulations. Expressions for the reactions in the species balance and biofilm equations tend to be complicated and nonlinear which makes analytical solution difficult even in one spatial dimension. Multiple spatial dimensions essentially requires numerical techniques for solution of the governing partial differential equations of the mathematical model. The finite difference method is used to solve the mathematical model described in Chapter 2 of this thesis.

In general the approach utilizes second order finite differences to minimize error introduction with first order methods noting that some journals have a policy of not accepting numerical work performed with first order finite differences (Freitas, 1993). This policy has invoked some discussion (e.g., see (Leonard, 1995)) which is probably appropriate.

Grid Generation

To use finite differences to solve the mathematical equations it is necessary to put a grid over the problem to allow finite difference formulation. The general approach used here in formulating the grid and database containing the node information is described in more detail by Peralta and Chen (1995). This method of generating a grid and retaining the nodal information is useful and allows easier generation of nodal information for connected rectangular domains. A overview and summary of some of the information provide by Peralta and Chen (1995) will be covered here.

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 by Peralta and Chen (1995). 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.

It is necessary to solve equations (3.6) and (3.5) numerically for problems of practical interest. In this development a uniform mesh in both x and y is used with $\Delta x = \Delta y = h$ as the mesh spacing is applied to cavity shown in Figure 4 to yield the cavity with mesh shown in Figure 6. The nodal points are then found from $x_i = (i - 1)h$ for $1 \leq i \leq I$ and $y_j = (j - 1)h$ for $1 \leq j \leq J$. The global ordering of the nodes starts with the interior nodes proceeding from bottom to top and left to right. Once the interior nodes are computed, the boundary nodes are numbered also from bottom to top and left to right.

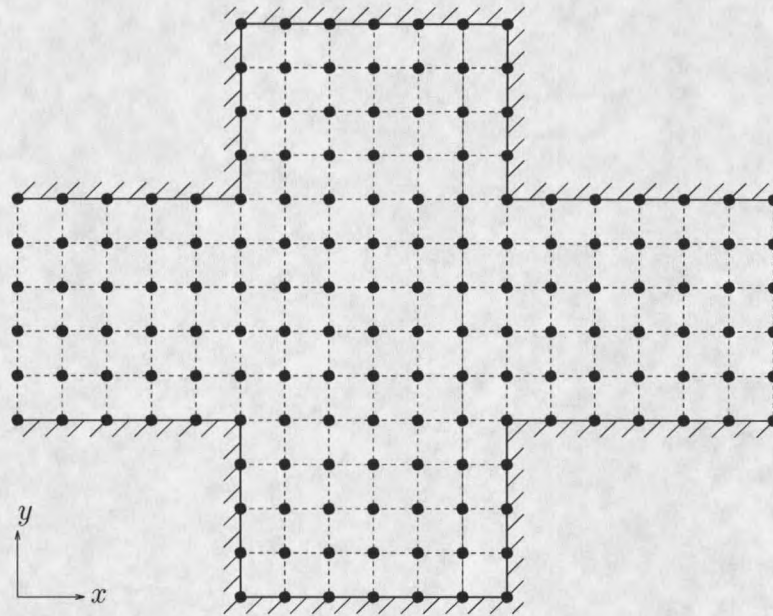


Figure 6. Example cavity with uniform finite difference mesh.

A typical node on the interior of the domain has eight neighbors as shown in Figure 7 that can be used in finite difference formulations. The information that is needed is the nodes located adjacent to node (i, j) . In general the most commonly used nodes are nodes $(i + 1, j)$, $(i - 1, j)$, $(i, j + 1)$, $(i, j - 1)$, and (i, j) . These nodes allow formulation of second order finite difference schemes.

Using the approach of Peralta and Chen (1995) the finite difference expressions

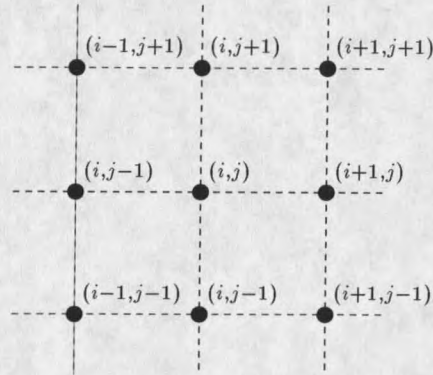


Figure 7. Interior node with neighbors.

are written for the interior nodes only. When an equation is written for a node near the boundary it may contain the boundary node as an unknown. If the boundary condition is a Dirichlet boundary condition then the value is known and it can be substituted in the finite difference expression. However, if the boundary has Neumann or Robin boundary condition, it is necessary to formulate a finite difference expression for the derivative term in terms of interior nodes normal to boundary. This equation is then added to finite difference expression.

Figure 8 shows a node (i, j) on a horizontal wall with its neighbors. The four nodes $(i, j + 1)$, $(i, j + 2)$, $(i, j + 3)$, and $(i, j + 4)$ are stored as neighbor nodes to implement the normal boundary condition as required. Nodes $(i + 1, j)$ and $(i - 1, j)$ are also stored in database in case they are needed. These nodes may be necessary if the tangential derivative is desired along a wall.

It is not necessary to use a uniform mesh, a nonuniform mesh may be more efficient where sharp gradients in the solution are anticipated. A finer mesh where the solution changes most rapidly and coarser where it shows the least variation would allow a more efficient solution of problem with better accuracy. Finite difference formulations can be derived for graded meshes to represent partial derivative terms

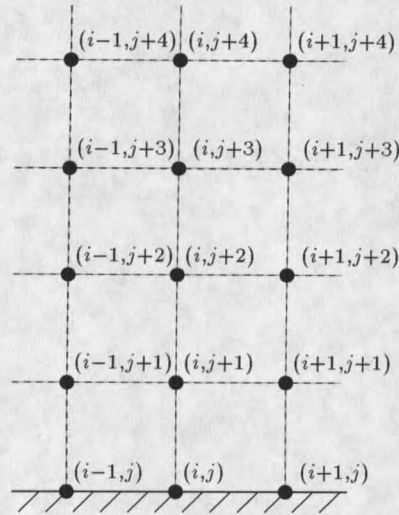


Figure 8. Boundary node with neighbors.

(Ferziger and Perić, 1996). A uniform mesh allows easier convergence analysis. Higher order expressions are available (Boresi and Chong, 1991) which use additional nodes farther away from center node. Some recent formulations use an expression which is compact yet is fourth order (Spotz and Carey, 1995; Saldanha and Ananthakrishnaiah, 1995; Liao and Zhu, 1996). Some expressions are even available for non-uniform grids (Li and Baldacchino, 1995).

Stream Function Vorticity

The equations for the flow (3.5) and (3.6) are discretized using finite differences. Both centered differences and upwind differences were implemented. Since the interest is in low Reynolds numbers for this application, centered differences perform very well and can be used for $Re < 1000$ (Peralta and Chen, 1995). The equations and boundary conditions are described by computing the coefficients of the node point and neighbors used in the finite difference expression. For the Navier Stokes equations, two systems of equations result. The first is from the continuity equation for the stream function,

and the second is from the vorticity transport equation.

If second order centered finite differences are used with a uniform mesh with mesh spacing h , equation (3.6) for a interior node becomes

$$\frac{\psi_{i+1,j}(t) + \psi_{i-1,j}(t) + \psi_{i,j+1}(t) + \psi_{i,j-1}(t) - 4\psi_{i,j}(t)}{h^2} + \omega_{i,j}(t) = 0 \quad (3.29)$$

and equation (3.5) becomes

$$\begin{aligned} & \frac{\partial \omega_{i,j}(t)}{\partial t} + \frac{\psi_{i,j+1}(t) - \psi_{i,j-1}(t)}{2h} \frac{\omega_{i+1,j}(t) - \omega_{i-1,j}(t)}{2h} \\ & + \frac{\psi_{i-1,j}(t) - \psi_{i+1,j}(t)}{2h} \frac{\omega_{i,j+1}(t) - \omega_{i,j-1}(t)}{2h} \\ & - \frac{1}{Re_{L\infty}} \frac{\omega_{i+1,j}(t) + \omega_{i-1,j}(t) + \omega_{i,j+1}(t) + \omega_{i,j-1}(t) - 4\omega_{i,j}(t)}{h^2} = 0 \end{aligned} \quad (3.30)$$

where $\psi_{i,j}(t) = \psi(ih, jh, t)$ and $\omega_{i,j}(t) = \omega(ih, jh, t)$.

Applying equation (3.30) to the interior nodes and substituting values or expressions for equations for boundary nodes results in the formulation

$$\frac{\partial \omega_h}{\partial t} + A_h(\psi) \omega_h = \mathbf{b} \quad (3.31)$$

for the determination of the vorticity ω_h at the interior nodes. Note that A_h is a function of ψ as a result of the convective terms in equation (3.30). Application of equation (3.29) for the interior nodes results in the matrix formulation for ψ_h of

$$B_h \psi_h + \omega_h = \mathbf{c} \quad (3.32)$$

where substitution of boundary values and/or equations for boundary nodes in terms of interior nodes results in $\mathbf{c}$. Equations (3.31) and (3.32) are coupled set of equations in terms of ψ_h and ω_h . To reduce memory requirements, only the non zero entries in the matrices of equations (3.31) and (3.32) are stored using the compressed row storage (CRS) format (Barrett et al., 1994; Saad, 1994, pp. 64). Two different methods were implemented for calculating the steady solutions to equations (3.32) and (3.31) (Chen et al., 1994).

In the first one, the time derivative in equation (3.31) is set equal to zero, and the resulting elliptic system is solved. The discretized continuity equation for ψ depends on ω , and the coefficients of the vorticity equation depend on the stream function. If the vorticity is known, (3.32) is a linear system for ψ . This equation can be solved using successive over relaxation (SOR) iteration (Young, 1971; Hageman and Young, 1981). The acceleration parameter λ was determined empirically. $\lambda = 1.6$ worked well. Also, if the values of the stream function are known, equation (3.31) 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):

- I. Give an initial guess for the vorticity and solve (3.32) for ψ_h .
- II. Obtain the boundary conditions for the vorticity by applying the equivalent of (3.29) with one-sided derivatives at the boundary. Relax the boundary values for ω .
- III. Solve (3.30) using the values of ψ obtained from I) and the boundary conditions obtained from II).
- IV. Relax the vorticity.
- V. Use the new vorticity to solve (3.32) 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

$$\omega^{(i)} = (1 - \lambda_\omega)\omega^{(i-1)} + \lambda_\omega\hat{\omega}^{(i)} \quad (3.33)$$

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

(1983) recommend using a different parameter to relax the boundary values of ω . In practice this will speed up the convergence.

The second method to calculate the steady-state velocities consisted of giving an initial value for the stream function and vorticity and follow the solution in time until a steady-state solution is obtained. This uses a difference term for the time derivative in equation (3.31) and determination of what time the spatial derivatives and convective terms in (3.31) are evaluated. If the convective terms are evaluated at time n , the equation (3.31) is linear in the vorticity. Using implicit evaluation of the spatial derivatives on the vorticity in (3.31) results in the formulation for ω_h^{n+1}

$$(I + \Delta t A_h^n) \omega_h^{n+1} = \omega_h^n + \Delta t \mathbf{b} \quad (3.34)$$

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 denoted by ψ_h^0 and ω_h^0 respectively. These values were either for no flow or the values for a different Reynolds number already calculated. The vorticity equation (3.34) is advanced one time step using the stream function values at the previous step. This way it is not necessary to solve a nonlinear system. The vorticity at the new time is calculated by solving the continuity equation, which implies using SOR.

$$B_h \psi_h^{n+1} = -\omega_h^{n+1} + \mathbf{c} \quad (3.35)$$

The time stepping is continued until the solution at two consecutive times varies less than a specified tolerance ϵ . Different solutions convergence tolerances were used for solution of the numerical equations. The iteration procedure described above is similar to iteration procedures used by other researchers (Huang and Seymour, 1996).

Species Balance Equation

Once the steady-state solution to the stream function vorticity problem is known, the steady state velocity $\mathbf{u}_{ss}(\mathbf{x})$ can be computed. With the steady-state velocity known, the species balance equation (2.47) can be solved for a dissolved species subject to their boundary condition.

Using second order centered finite differences with a uniform mesh, equation (2.47) becomes

$$\begin{aligned}
 & u_{i,j} \frac{C_{i+1,j} - C_{i-1,j}}{2h} + v_{i,j} \frac{C_{i,j+1} - C_{i,j-1}}{2h} \\
 & - \frac{D_{i+1,j} - D_{i-1,j}}{2h} \frac{C_{i+1,j} - C_{i-1,j}}{2h} - \frac{D_{i,j+1} - D_{i,j-1}}{2h} \frac{C_{i,j+1} - C_{i,j-1}}{2h} \\
 & - D_{i,j} \frac{C_{i+1,j} + C_{i-1,j} + C_{i,j+1} + C_{i,j-1} - 4C_{i,j}}{h^2} - r_{i,j} = 0
 \end{aligned} \tag{3.36}$$

where $D_{i,j} = D(x_i, y_j)$, $C_{i,j} = C(x_i, y_j)$ and

$$r_{i,j} = r(x_i, y_j, C_1, C_2, \dots, C_{N-1}, C_N) \tag{3.37}$$

The equation solver that is used to solve the discretized equation for species balance (3.36) is designed for linear equations. While a nonlinear solver could be applied it is easier to follow the general formulation of Peralta and Chen (1995) which assumes linear equation form. The reaction term in the bulk from suspended cells is typically smaller than the consumption due to the biofilm on the walls.

In order to accommodate a nonlinear reaction term, $r_{i,j}(C)$, the reaction term is linearized by taking the first order term of the Taylor expansion of reaction term around the concentration a previous solution to equation (3.36) at $C_{i,j}^{k-1}$,

$$r_{i,j}(C_{i,j}^k) \approx r_{i,j}(C_{i,j}^{k-1}) + \frac{\partial r(C_{i,j}^{k-1})}{\partial C} (C_{i,j}^k - C_{i,j}^{k-1}) \tag{3.38}$$

It is assumed that the first partial derivative of the reaction term in equation (3.36) is available in analytical form. If this is not the case, the first partial derivative would

need to be approximated numerically. Equation (3.36) is solved for C^k iteratively using linearized reaction term (3.38) until specified stopping tolerance ϵ_c .

$$\|C^k - C^{k-1}\| \leq \epsilon_c \quad (3.39)$$

While equations (3.36) and (3.38) are written for a single constituent there are usually multiple dissolved constituent and biomass species in the bulk which would require iteration between equations (3.36) and (3.38) for all the species in bulk. Alternatively, the linearized equations could be solved for all the species and then iterated to update the bulk reaction term. Note that unless the reactor is really long or flow really slow, the residence time in reactor is short enough that the consumption of substrate in bulk relative to the flux to the biofilm is rather small.

Biofilm Equation

Solution of the species balance equation (3.36) yields a concentration solution near boundary of biofilm which allows the calculation of substrate concentration C_{L_f} at the biofilm surface. For a horizontal wall the substrate concentration is calculated from the solution at the nodes of solution to global bulk mesh with the perturbation scheme using second order terms

$$C_{L_f} \approx C_{i,j} + \frac{\partial C_{i,j}}{\partial y} L_f + \frac{\partial^2 C_{i,j}}{\partial y^2} \frac{L_f^2}{2} \quad (3.40)$$

A similar expression is used for vertical walls with the expansion about the x direction.

It is necessary to approximate the partial derivatives in (3.40) to obtain the interface concentration, C_{L_f} . Using second order finite differences gives the numerical approximation for the interface concentration C_{L_f} , of a dissolved constituent, C ,

$$C_{L_f} \approx C_{i,j} + \frac{-3C_{i,j} + 4C_{i,j+1} - C_{i,j+2}}{2h} L_f + \frac{C_{i,j} - 2C_{i,j+1} + C_{i,j+2}}{h^2} \frac{L_f^2}{2} \quad (3.41)$$

Higher order finite difference expressions could be used in (3.40) for more accurate representation of partial derivatives.

For particulate species in bulk, it was assumed that there was net detachment so the flux of particles is away from boundaries and interface concentration of biomass species is not calculated this way. For a particulate species, assuming net detachment, there would be an applied flux resulting from excess growth applied as boundary condition in solution of particulate mass balance in bulk fluid region.

A case of single substrate and monopopulation will be used to for the numerical formulation. The extension to multiple substrates is straight forward. The spatial dimension normal to the surface will be denoted by z . Let the single substrate be denoted by C . Equations (2.10) and (2.11) can be combined to get an equation for balance on C

$$\frac{\partial C}{\partial t} = \frac{Df}{\epsilon_\ell} \frac{\partial^2 C}{\partial z^2} + \frac{r}{\epsilon_\ell} \quad (3.42)$$

Equations (2.39) and (2.38) can be combined to yield an equation for the change in biofilm thickness

$$\frac{dL_f}{dt} = \frac{1}{\rho_s \epsilon_s} \int_0^{L_f(t)} r_s dz + \frac{r_s''}{\rho_s \epsilon_s} \quad (3.43)$$

To handle the moving boundary problem of the biofilm bulk fluid interface Gujer and Wanner (1990) use a coordinated transformation that eliminates the moving boundary for the biofilm region. This transformation is given by:

$$\zeta(t) = \frac{z}{L_f(t)} \quad (3.44)$$

Use of this transformation eliminates the problem of adapting the mesh when domain changes or dropping/adding mesh elements as needed.

Any function $f_1(t, z)$ may be expressed in ζ -coordinates as $f_2(t, \zeta)$ according to the following transformation rules:

$$f_1(t, z) = f_2(t, \zeta) \quad (3.45)$$

$$\frac{\partial f_1(t, z)}{\partial z} = \frac{1}{L_f(t)} \frac{\partial f_2(t, \zeta)}{\partial \zeta} \quad (3.46)$$

$$\frac{\partial f_1(t, z)}{\partial t} = \frac{\partial f_2(t, \zeta)}{\partial t} + \frac{\partial \zeta}{\partial t} \frac{\partial f_2(t, \zeta)}{\partial \zeta} = \frac{\partial f_2(t, \zeta)}{\partial t} - \frac{\zeta \nu_I}{L_f(t)} \frac{\partial f_2(t, \zeta)}{\partial \zeta} \quad (3.47)$$

With this transformation, equation (3.42) becomes:

$$\frac{\partial C}{\partial t} = \frac{D_i f}{\epsilon_\ell L_f^2(t)} \frac{\partial^2 C}{\partial \zeta^2} + \frac{\zeta \nu_I}{L_f(t)} \frac{\partial C}{\partial \zeta} + \frac{r}{\epsilon_\ell} \quad (3.48)$$

and equation (3.43) becomes:

$$\frac{dL_f}{dt} = \frac{L_f(t)}{\rho_s \epsilon_s} \int_0^1 r_s d\zeta + \frac{r_s''}{\rho_s \epsilon_s} \quad (3.49)$$

Equations (3.48) and (3.49) are the two differential equations that must be solved for a monopopulation biofilm with a single substrate. Equations (3.48) and (3.49) are integral-differential equations. These equations contain nonlinear terms due to the transformation, the reactions r and r_s are quite often nonlinear and complicate the equation behavior. The Monod kinetic model (Monod, 1949) is a good example of this with the kinetics expression for a single substrate given by

$$\mu(C) = \mu_{\max} \frac{C}{K_C + C} \quad (3.50)$$

where $\mu_{\max}$ is the maximum specific growth rate and K_C is the saturation constant corresponding to the concentration at half the maximum specific consumption rate (Bailey and Ollis, 1986). In the case of two substrates a double Monod kinetic expression of the form

$$\mu(C_1, C_2) = \mu_{\max} \frac{C_1}{K_{C_1} + C_1} \frac{C_2}{K_{C_2} + C_2} \quad (3.51)$$

can be used.

Due to the complexity of equations (3.48) and (3.49), they are solved with a numerical scheme. Spatial derivatives in equation (3.48) are approximated by the use of second order central finite difference expressions. With the second term on the right hand side of equation (3.48) being a convective like term it might be advantageous

to use upwind differencing if the interface velocity ν_I is very large. In the steady-state case this term is zero. For small growth rates central differences are adequate and upwinding expressions or alternative techniques are not needed. The integral in equation (3.49) is approximated by trapezoidal integration. To implement the numerical scheme the biofilm is divided up into N_f grid points with the substratum denoted by point 1 and the biofilm surface denoted by point N_f shown in Figure 9.

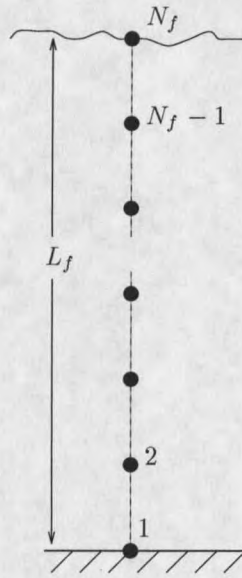


Figure 9. Numerical grid for biofilm equations.

This choice of discretization scheme gives $\Delta\zeta = \frac{1}{N_f-1}$ and $\zeta_j = \Delta\zeta(j-1) = \frac{j-1}{N_f-1}$ for $1 \leq j \leq N_f$. With this discretization equation (3.48) becomes:

$$\frac{\partial C_j}{\partial t} \approx \frac{D_{if}}{\epsilon_\ell L_f^2(t)} \frac{C_{j+1} - 2C_j + C_{j-1}}{\Delta\zeta^2} + \frac{\zeta_j \nu_I(t)}{L_f(t)} \frac{C_{j+1} - C_{j-1}}{2\Delta\zeta} + \frac{r(C_j)}{\epsilon_\ell} \quad (3.52)$$

where $C_j = C(\zeta_j, t)$. Note that equation (3.52) holds only on the interior nodes of the biofilm ($2 \leq j \leq N_f - 1$) as the boundary conditions at the substratum and the biofilm surface are need to write a similar expression for nodes 1 and N_f . In this thesis an iteration scheme will be used between solution of biofilm equations and

species balance equations which allows the surface concentration C_{N_f} to be constant solution iteration. At the substratum the no flux boundary condition will allow an equation similar to equation (3.52) to be written for node 1.

This process of discretizing the spatial derivatives forms a set of coupled ordinary differential equations to be solved for concentrations at the nodes in the biofilm. This solution method is sometimes called the *method of lines* (Fletcher, 1988a). For this simulation the equations for biofilm are solved with a ODE solver running to an approximate steady-state solution with the resulting substrate flux applied to substrate balance equation in bulk as a boundary condition.

The substrate flux is then calculated using the numerical approximation

$$J = -D_f \frac{\partial C}{\partial z} = -\frac{D_f}{L_f} \frac{\partial C}{\partial \zeta} \approx \frac{D_f}{L_f} \frac{3C_{N_f} - 4C_{N_f-1} + C_{N_f-2}}{4\Delta\zeta} \quad (3.53)$$

Using composite trapezoidal integration (Kincaid and Cheney, 1991, pg. 445) for the integral in (3.49) results in the following numerical approximation to (3.54)

$$\frac{dL_f}{dt} \approx \frac{L_f(t)}{\rho_s \epsilon_s} \frac{\Delta\zeta}{2} \left[r_s(C_1) + 2 \sum_{i=2}^{N_f-1} r_s(C_i) + r_s(C_{N_f}) \right] + \frac{r_s''}{\rho_s \epsilon_s} \quad (3.54)$$

where $r_s(C_j) = r_s(C(\zeta_j, t))$.

Recalling the net detachment expression being considered (equation (2.40)),

$$r_s'' = (-aL_f^2 - bL_f - c - d\bar{\mu}_s - e\bar{\tau}) \rho_s \epsilon_s \quad (2.40)$$

L_f is directly available while $\bar{\mu}_s$ and $\bar{\tau}$ need to be calculated. Applying (3.44) to $\bar{\mu}_s$ and using composite trapezoidal integration, $\bar{\mu}_s$ is approximated by

$$\bar{\mu}_s \approx \frac{\Delta\zeta}{2} \left[r_s(C_1) + 2 \sum_{i=2}^{N_f-1} r_s(C_i) + r_s(C_{N_f}) \right] \quad (3.55)$$

and $\bar{\tau}$ is the average shear stress at this location.

Boundary Conditions

It is also necessary to discretize the boundary conditions to solve the model equations. The boundary conditions will be implemented in numerical form using the perturbation scheme described to allow retention of mesh on rectangular grid.

Stream Function Vorticity-Walls Different numerical formulation of the boundary conditions been used for solution of the stream function vorticity formulation (See (Gresho, 1991a; Gresho, 1991b; Gresho, 1992) for review of some.). A typical numerical implementation of boundary conditions follows from which the implementation using perturbation condition will have as a special case.

A typical numerical boundary formulation is the approach by Peyret and Taylor (1983). By forcing equation (3.6) to hold on the boundary Γ of the domain

$$\omega(x, 0) = -\frac{\partial^2 \psi(x, 0)}{\partial x^2} - \frac{\partial^2 \psi(x, 0)}{\partial y^2} \quad (3.56)$$

From (3.12),

$$\frac{\partial^2 \psi(x, 0)}{\partial x^2} = f_0''(x) \quad (3.57)$$

but $\partial^2 \psi(x, 0)/\partial y^2$ is not known and an expression for it must be determined. To determine an expression for $\partial^2 \psi(x, 0)/\partial y^2$, Taylor expansions can be used (Peyret and Taylor, 1983) with mesh spacing h to obtain the second-order-accurate formula

$$\frac{\partial^2 \psi(x, 0)}{\partial y^2} \approx -\frac{\psi(x, 2h) - 8\psi(x, h) + 7\psi(x, 0)}{2h^2} - \frac{3}{h} \frac{\partial \psi(x, 0)}{\partial y} \quad (3.58)$$

Substituting the boundary conditions (3.12) and (3.13) into equation (3.58) and using (3.57), the equation for the vorticity on the wall, (3.56), becomes

$$\omega(x, 0) \approx -f_0''(x) + \frac{1}{2h^2} [\psi(x, 2h) - 8\psi(x, h) + 7f_0(x)] - \frac{3}{h} g_0(x) \quad (3.59)$$

Typically $f_0''(x)$ is constant on a wall but with perturbation scheme the value at the wall is not constant so an approximation for $f_0''(x)$ is needed. Since the vorticity

ω is being calculated and the stream function ψ is already known, the values of ψ can be used to approximate $f_0''(x)$ with a second order finite difference approximation. This results in the numerical equation for the vorticity at the boundary

$$\begin{aligned} \omega(x, 0) \approx & - \frac{\psi(x+h, 0) - 2\psi(x, 0) + \psi(x-h, 0)}{h^2} \\ & + \frac{\psi(x, 2h) - 8\psi(x, h) + 7\psi(x, 0)}{2h^2} - \frac{3}{h}g_0(x) \end{aligned} \quad (3.60)$$

Boundary conditions for other walls are similar but for example x and y become interchanged in above equations. For nodes that are interior corners which have two different normal directions depending on which direction the approach is made from are dealt with differently. To use this formulation it is necessary to deal with each different direction when the vorticity is needed and average the two values to get the value at the node. This allows convergence of the problem. Walls with biofilm will have conditions holding at the biofilm bulk fluid interface with assumption of negligible fluid flow in biofilm region.

Now consider the presence of biofilm on the solid walls and the use of perturbation condition. For the stream function equation (3.16) provides the same boundary condition as (3.14) if $L_f = 0$. Taking a Taylor expansion around $\psi(x, 0)$ in vertical direction for a horizontal wall gives

$$\psi(x, L_f) = \psi(x, 0) + \frac{\partial\psi}{\partial y}L_f + \frac{\partial^2\psi}{\partial y^2}\frac{L_f^2}{2} + \frac{\partial^3\psi}{\partial y^3}\frac{L_f^3}{6} + \frac{\partial^4\psi}{\partial y^4}\frac{L_f^4}{24} + O(L_f^5). \quad (3.61)$$

By substituting finite difference expressions in equation (3.61) yields an equation which can be solved for $\psi(x, 0)$ in terms of neighbor nodes, L_f , and $\psi(x, L_f)$. Some examples of this are given in Appendix B. If $L_f = 0$ in equation (3.61) then the boundary condition becomes $\psi(x, 0) = \text{constant}$ as expected.

Implementation of the boundary condition given in equation (3.17) is the next challenge. Taking a Taylor expansion for $\partial\psi(x, L_f)/\partial y$ around $(x, 0)$ gives

$$\frac{\partial\psi}{\partial y}(x, L_f) = \frac{\partial\psi}{\partial y}(x, 0) + \frac{\partial^2\psi}{\partial y^2}\bigg|_0 L_f + \frac{\partial^3\psi}{\partial y^3}\bigg|_0 \frac{L_f^2}{2}$$

$$+ \frac{\partial^4 \psi}{\partial y^4} \Big|_0 \frac{L_f^3}{6} + \frac{\partial^5 \psi}{\partial y^5} \Big|_0 \frac{L_f^4}{24} + O(L_f^5). \quad (3.62)$$

A numerical formulation for equation (3.62) can be obtained by substitution of finite difference expressions for the partial derivatives after selecting desired order of approximation in terms of L_f . A typical example of this for a $O(L_f^4)$ expression is shown in Appendix B.

In this case more is known about the behavior of ψ at (x, L_f) as shown in equation (3.17) where for no penetration

$$\frac{\partial \psi}{\partial y}(x, L_f) = 0. \quad (3.63)$$

Substituting (3.63) into equation (3.62) gives

$$\frac{\partial \psi}{\partial y}(x, 0) = - \frac{\partial^2 \psi}{\partial y^2} \Big|_0 L_f - \frac{\partial^3 \psi}{\partial y^3} \Big|_0 \frac{L_f^2}{2} - \frac{\partial^4 \psi}{\partial y^4} \Big|_0 \frac{L_f^3}{6} - \frac{\partial^5 \psi}{\partial y^5} \Big|_0 \frac{L_f^4}{24} + O(L_f^5) \quad (3.64)$$

for $\partial \psi / \partial y(x, 0)$. Substituting equation (3.64) into equation (3.61) gives

$$\psi(x, L_f) = \psi(x, 0) - \frac{\partial^2 \psi}{\partial y^2} \Big|_0 \frac{L_f^2}{2} - \frac{\partial^3 \psi}{\partial y^3} \Big|_0 \frac{L_f^3}{3} - \frac{\partial^4 \psi}{\partial y^4} \Big|_0 \frac{L_f^4}{8} + O(L_f^5). \quad (3.65)$$

Finite difference expressions can be substituted in (3.65) for the partial derivatives to yield a numerical equation. Using fourth order expression for the partial derivatives and neglecting terms of $O(L_f^3)$ and greater gives

$$\begin{aligned} \psi_0 = & \frac{24 h^3}{24 h^3 - 35 h L_f^2 + 20 L_f^3} \psi_b - \frac{104 h L_f^2 - 72 L_f^3}{24 h^3 - 35 h L_f^2 + 20 L_f^3} \psi_1 \\ & - \frac{-114 h L_f^2 + 96 L_f^3}{24 h^3 - 35 h L_f^2 + 20 L_f^3} \psi_2 - \frac{56 h L_f^2 - 56 L_f^3}{24 h^3 - 35 h L_f^2 + 20 L_f^3} \psi_3 \\ & - \frac{-11 h L_f^2 + 12 L_f^3}{24 h^3 - 35 h L_f^2 + 20 L_f^3} \psi_4 \end{aligned} \quad (3.66)$$

The other modifications can be added to the vorticity equation (3.60) by substituting an expression for $g_0(x)$. Equation (3.65) provides an expression for $g_0(x)$ which when truncating terms of $O(L_f^3)$ and greater gives

$$g_0(x) = \frac{\partial^2 \psi}{\partial y^2} L_f + \frac{\partial^3 \psi}{\partial y^3} \frac{L_f^2}{2}. \quad (3.67)$$

Substituting finite difference expressions in (3.67) for the partial derivatives and substituting in equation (3.60) gives

$$\begin{aligned}\omega(x, 0) \approx & - \frac{\psi(x+h, 0) - 2\psi(x, 0) + \psi(x-h, 0)}{h^2} \\ & + \frac{\psi(x, 2h) - 8\psi(x, h) + 7\psi(x, 0)}{2h^2} \\ & - \left(\frac{35\psi_0 - 104\psi_1 + 114\psi_2 - 56\psi_3 + 11\psi_4}{12h^2} \right) \frac{3L_f}{h} \\ & - \left(\frac{-10\psi_0 + 36\psi_1 - 48\psi_2 + 28\psi_3 - 6\psi_4}{4h^3} \right) \frac{3L_f^2}{2h}\end{aligned}\quad (3.68)$$

Stream Function Vorticity-Inlet Numerical implementation of the inlet boundary conditions just requires evaluation of equations (3.19) and (3.21) with the separation distance of upper and lower boundary of inlet. This will yield values of ψ and ω that can be substituted into equations developed for interior nodes which use inlet nodes in their formulation.

Stream Function Vorticity-Outlet At the outlet, the boundary condition for ψ (equation (3.22)) is a derivative condition, and is implemented using a backward difference expression as

$$0 = \frac{\partial^2 \psi}{\partial x^2} \approx \frac{\psi_{-2} + 2\psi_{-1} + \psi_0}{h^2} \quad (3.69)$$

where $\psi_0 = \psi(x_i, y_j)$, $\psi_{-1} = \psi(x_{i-1}, y_j)$, and $\psi_{-2} = \psi(x_{i-2}, y_j)$. This equation can be solved for and expression for ψ_0 and substituted into equations for interior nodes which use ψ_0 .

For the vorticity a second order numerical implementation of equation (3.24) is

$$0 = \frac{\partial \omega}{\partial x} \approx \frac{\omega_{-2} + 2\omega_{-1} + \omega_0}{h^2} \quad (3.70)$$

where $\omega_0 = \omega(x_i, y_j)$, $\omega_{-1} = \omega(x_{i-1}, y_j)$, and $\omega_{-2} = \omega(x_{i-2}, y_j)$. This equation can be solved for ψ_0 in terms of ω_{-1} and ω_{-2} and substituted into equations for interior

nodes which use ω_0 . These equations are used to numerically apply the boundary conditions which results in solution for ψ and ω .

Species Balance Boundary Conditions

The species balance equations need boundary conditions applied at the inlet, outlet, walls with no biofilm, and walls with biofilm. The walls with biofilm will be discussed in the interface boundary conditions. There are 2 main types of boundary implementations for the species balance equation. The first boundary condition is for inlet and outlet boundaries.

Recalling the general expression for total flux of species i given by equation (2.4) for the bulk fluid region

$$\mathbf{J}_{T_i} = \mathbf{u} \cdot \nabla c_i - D_i(\mathbf{x}) \nabla c_i. \quad (2.4)$$

contains both convective and diffusive terms. At these boundaries there is fluid movement in and out of the domain.

Inlet Boundary Condition At the inlet the concentration is assumed to be uniform for this simulation (i.e., $C(y) = C_0$, see (2.26)). For this two dimensional simulation this assumption gives the following boundary condition formulation at the inlet for the concentration

$$u(y)C_0 = u(y)C(y) - D \frac{\partial C}{\partial x} \quad (3.71)$$

A numerical implementation is given by using a second order forward finite difference expression for the partial derivative in equation (3.71). The numerical formulation then becomes

$$u_{i,j}C_0 = u_{i,j}C_{i,j} - D_{i,j} \frac{3C_{i,j} - 4C_{i+1,j} + C_{i+2,j}}{2h} \quad (3.72)$$

which is solved for $C_{i,j}$ and substituted into equations referencing $C_{i,j}$.

Outlet Boundary Condition At the outlet the boundary condition is more difficult to formulate as outlet concentration is unknown. The domain for solution of velocity was chosen with assumption velocity field was fully developed. A similar assumption can be used for the species balance equation in that a no change with downstream direction can be used. Usually this is not a bad assumption especially for high flow rates as influence of exit boundary condition on upstream concentration solution is expected to be less. As the flow rate decreases influence of exit boundary condition has more influence as diffusion becomes a more important physical process (Patankar, 1980). This can make selection of the boundary condition difficult. Proper formulation is needed to get an accurate and solvable numerical scheme.

Assuming a horizontal exit with flow left to right and using the *transmission boundary condition* (Shamir and Harleman, 1967) gives

$$\frac{\partial^2 C}{\partial x^2} = 0 \quad (3.73)$$

Using a second order backward finite difference expression for the partial derivative in (3.73) results in

$$C_{i,j} = 2 C_{i-1,j} - C_{i-2,j} \quad (3.74)$$

which is substituted into equations formed for interior nodes which require boundary node information.

Walls For this simulation, the concentrations at the solid walls are assumed to be unknown and must be computed based on wall flux information. In the case of walls with biofilm, iterations between solution of concentration in bulk and biofilm equations are performed until solution converges to specified tolerance. Walls without biofilm are assumed to be nonreactive with dissolved species so a no flux boundary condition (see equation (2.31)) is used there.

A general formulation for the impermeable wall boundary condition can be written as

$$\alpha = -D \frac{\partial C}{\partial y} \bigg|_{wall} \approx D_{i,j} \frac{3C_{i,j} - 4C_{i,j+1} + C_{i,j+2}}{2h} \quad (3.75)$$

where α is the wall flux (Assumed to be known.) and $C_{i,j}$ is boundary node of interest on impermeable wall.. For nonzero diffusivity, $D_{i,j} > 0$, equation (3.75) can be solved for expression for $C_{i,j}$

$$C_{i,j} = \frac{2h}{D_{i,j}} \alpha + \frac{4}{3} C_{i,j+1} - \frac{1}{3} C_{i,j+2} . \quad (3.76)$$

For walls with biofilm, the perturbation scheme in Appendix B for a Neumann boundary condition is applied.

Biofilm

The dissolved species in the biofilm equation process equations have a no flux boundary condition at the substratum ($L_f = 0$). A general boundary condition used at the substratum ($\zeta = 0$), is that there is no flux of dissolved or particulate components into the substratum given by

$$\frac{\partial C}{\partial z} = 0 . \quad (3.77)$$

To implement (3.77) an imaginary node or *ghost node* (Shamir and Harleman, 1967) is used and denoted by index 0. This node is below node 1 in the biofilm film which is located at the biofilm/substratum interface. Using a second order centered finite difference expression for the flux at the substratum gives

$$0 = -D \frac{\partial C}{\partial z} \approx -D_1 \frac{C_2 - C_0}{2h} \quad (3.78)$$

which requires $C_2 = C_0$. With $C_2 = C_0$ an equation at node 1 similar to (3.48) can be formulated. With this boundary condition, the equation for node 1 is:

$$\frac{\partial C_1}{\partial t} \approx \frac{D_i f}{\epsilon_\ell L_f^2(t)} \frac{2C_2 - 2C_1}{\Delta \zeta^2} + \frac{r(C_1)}{\epsilon_\ell} \quad (3.79)$$

The boundary condition for the solid biofilm constituents is a zero convective velocity at the substratum. The boundary condition at the surface of the biofilm is given by the interface equations.

Interface Equations

The interface equations are algebraic/differential equations which must be considered. Note that interface velocity ν_I is involved in interface equations. For the case of fixed biofilm, the interface velocity is zero and the flux from bulk is equal into biofilm for dissolved components (see equation (2.33)).

For the steady-state case being considered here the interface velocity ν_I is zero so interface conditions (equations (2.33)–(2.34))simplify considerably. With the adoption of an iterative scheme between the biofilm and species balance equations, the interface equations are not directly solved.

Solution Algorithm

The numerical equations described above are solved in a sequential and iterative manner. The stream function vorticity equations are solved for steady state value given initial biofilm thickness. Species balance equations in bulk are solved next subject to no flux boundary condition the first time and then the biofilm equations are solved with bulk species balances solution providing the concentration at the biofilm surface.

The biofilm equations are solved using a ordinary differential equation solver, LSODE (Hindmarsh, 1983), to give a flux value to be applied to the substrate balance equation in bulk liquid.

- I. Solve equations (3.29) and (3.30) until steady state solution reached.
- II. Solve (3.36) and (3.48) in iterative manner until convergence is reached.

Discussion of Numerical Solution

The mathematical model formulated in Chapter 2 was solved using the Finite Difference method. The Navier-Stokes equations were solved in the stream function/vorticity format. Numerical validation tests for the stream function/vorticity equations are contained in Appendix C. In the range of Reynolds numbers tested this second order scheme performed well. Results of the numerical validation tests demonstrate the convergence rate of the Finite Difference method used. Convergence tests for the species balance equation are also included in Appendix C. The central difference scheme used exhibited some oscillations near sharp gradients as expected. With higher flow convergence of the species balance equation slowed down.

There appears to be an upper limit on the Peclet number ($Pe = Re Sc$) for which the numerical solution behavior is reasonable. In the range $5000 < Re Sc < 10,000$ the numerical solution starts to exhibit some oscillations due to the central difference scheme. Refinement of the mesh improves the solution but the oscillations are still observed at higher Pe numbers. It may be necessary to use an upwinding scheme to advance above this limit.

The coupled iteration between the biofilm equations and the species balance equations the choice of the boundary relaxation factor had a strong influence on the convergence behavior and rate. At higher flow rates the concentration variation over the length of reactor would not significantly affect the flux of substrate consumed by the biofilm. As the consumption relative to substrate loading rate increased, additional solution time was need to complete the iterations between the species balance equation and the biofilm equations.

In the initial stages of iterations between the species balance equation and

biofilm equations a lower tolerance on the linear equation solver was often useful. As the solution was closer to convergence the tolerance on the solver was lowered for more accurate solutions. This approach resulted in decreased overall solution time and is often recommended for inner iteration (Ferziger and Perić, 1996).

The perturbation scheme appears to have a limit on the perturbation size which should be less than the mesh size used. Use of the perturbation scheme allowed retention of the original mesh.

CHAPTER 4

MODEL EVALUATION

To evaluate the model described in the previous chapters of this thesis, dissolved oxygen data from an experiment performed using an artificial biofilm patch in an open channel reactor was used. This chapter starts with a brief description of the experimental approach. Reactor geometry and flow characteristics, artificial biofilm patch creation and placement, and the measuring of dissolved oxygen concentration with a microprobe are discussed. Kinetic parameters for the biofilm were estimated from the experimental data. With estimates of the kinetic parameters a model simulation along with experimental measurement of the velocity in the channel allowed a computer simulation of the experiment to be performed. A discussion of the model results compared to the experimental data follows.

Experimental Methods

The experimental data used in this model evaluation was obtained by Abrahamson (1995). The experimental approach consisted of an open channel reactor with a patch of artificial biofilm contained at one location downstream from the inlet region. Dissolved oxygen measurements were taken with a microsensor in the bulk near the biofilm patch and into the biofilm patch. A detailed discussion of the experimental protocol using dissolved oxygen probes and the construction of the artificial biofilm is given by Abrahamson et al. (1996). Microsensors have been used to obtain dissolved oxygen profiles in biofilms (Lewandowski, 1994; Lewandowski et al., 1994; Revsbech, 1989a; Revsbech, 1989b; de Beer, Stoodley, Roe and Lewandowski, 1994;

Zhang et al., 1994; Zhang et al., 1995; van Loosdrecht et al., 1994; Fu and Bishop, 1995), trickling filters (Kuenen et al., 1986; Whalen et al., 1969; Chen and Bungay, 1981) and microbial mats (Jørgensen and Des Marais, 1990; Jørgensen and Revsbech, 1985; Revsbech et al., 1986).

Kinetic parameters (i.e., $V_{\max}$, K_s , D_f) were estimated from dissolved oxygen profiles by the procedure described by Lewandowski et al. (1991). Lewandowski (1994) extended the earlier (Lewandowski et al., 1991) to include an empirical model for the diffusive boundary layer. Simulation with these parameters allows evaluation of qualitative and quantitative capabilities of the model.

Reactor Setup

An open channel reactor with a glass slide located in the bottom of the channel was used in the experiment. The channel was 2 cm wide and had an entrance path length of 18 cm to the point of measurement. The artificial biofilm was attached to the glass bottom of the flume. The film covered the entire 2 cm width and had a approximate length along the flow path of 1.6 cm as shown in Figure 10. Bulk fluid was gravity fed to the reactor at a steady-state rate resulting in a uniform flow depth of 1.5 cm. Biofilm patch thickness was estimated to be around 300 μm . Actual thickness may have varied a little around this value with a possible shape shown in Figure 11. This profile was sketched based on further data analysis (Abrahamson, 1995) after the modeling simulations had been performed.

Artificial Biofilm Construction

An artificial biofilm was constructed which consisted of a homogeneous distribution of viable bacteria encapsulated inside an alginate matrix. The alginate was produced by *Pseudomonas aeruginosa* 8830, a stable mucoid variant capable of producing copious amounts of polymer (Darzins and Chakrabarty, 1984). Several spread plates of this

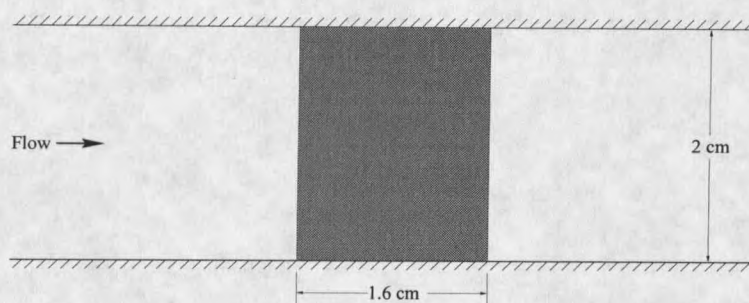


Figure 10. Plan view of reactor with artificial biofilm.

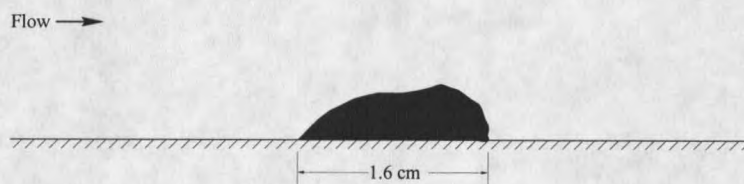


Figure 11. Sketch of artificial biofilm profile.

organism were made on yeast, tryptone, and glucose (YTG) agar plates and incubated at room temperature for several days after which a uniform layer of alginate covered the entire plate. The conglomerate of alginate and bacteria, which is too viscous to be directly filtered, was transferred to a test tube and diluted with ultrapure water (10:1). This slurry was mixed using a homogenizer and centrifuged at 20,000 rpm for 20 minutes. The supernatant was transferred to another test tube and the pellet of bacteria was discarded. The homogenizer/centrifugation step was repeated to remove any remaining bacteria from the supernatant. Finally the supernatant was filtered through a 0.2 μm filter into a sterile test tube. Excess water was removed from the diluted alginate with a rotary evaporator until the alginate formed a gel which had the same consistency as the originally produced by the bacteria on the agar plates.

The sterile alginate served as the matrix material of the artificial biofilm entrapping bacterial cells. The final step in the artificial biofilm construction was to

add a known number of *Pseudomonas aeruginosa* 8830 bacteria to the alginate. The bacteria were grown to steady-state in a chemostat and centrifuged to pellet the cells. This pellet which contained 4×10^{10} cells was then suspended in 0.5 ml of sterile alginate by stirring, resulting in a biofilm cell density of $8 \times 10^{10} \frac{\text{cells}}{\text{ml}}$ alginate. The homogeneous suspension of cells was then fixed to the bottom of the open channel reactor.

Experimental Procedure

A Clark type oxygen microelectrode, as described by Jørgenson and Revsbech (1988), was constructed and used to determine the dissolved oxygen concentration profiles through the biofilm. The probe consisted of an outer casing which housed both a single cathode and a Ag/AgCl reference electrode. The circuit was completed with a 0.5 M KCl electrolyte filling the solution. The inner components of the probe were separated from the bulk aqueous environment by a silicon rubber membrane which permitted the passage of dissolved oxygen. The single cathode was cathodically polarized (-0.8 V) against the Ag/AgCl reference electrode. When oxygen diffused to the cathode tip, it was reduced resulting in a flow of electrons. This current was proportional to the concentration of dissolved oxygen present at a localized region in the biofilm.

The electrode was calibrated in water by aeration and subsequent purging with pure nitrogen before measurements began. This determined the current associated with saturated and zero oxygen concentrations. The calibration curve was then used to determine the dissolved oxygen concentrations from the recorded data. The microelectrode mounted to a motor driven micropositioner was moved vertically through the biofilm in 20 μm increments. After each step, the current in the system was measured and recorded by the computer, resulting in a profile of oxygen concentration versus distance.

At a point, the probe samples 22 readings and rejects the high and low values. From the resulting 20 values, the mean and standard deviation are computed. If the standard deviation is below the set acceptable levels (5%), the mean value is accepted and the probe moves onto the next sample site. If the standard deviation is too large, the sampling process is repeated at this site until the standard deviation is less than 5%. Near the estimated substratum a few readings were taken in $10\text{ }\mu\text{m}$ intervals. The microprobe did not reach the substratum since mechanical interference could have damaged the probe resulting in an aborted experiment.

Since the microprobe did not reach the substratum, the estimate of the distance from the last measured value and the substratum is unknown. This distance is assumed to be small. A typical procedure is to start measuring in the bulk fluid region away from the mass transfer boundary layer and probe in the direction toward the substratum. Using this procedure the starting point is denoted as zero and distances are relative to this starting point. Measurements of dissolved oxygen are taken by microprobe at points increasingly closer to the substratum. As the microprobe proceeds toward the substratum, its progress is monitored by a microscope and the point estimated to be the biofilm surface is noted. When the microprobe is estimated to be at the substratum this value is then recorded and the difference between this value and the value at the surface yields an estimated value of the biofilm thickness.

Experimental Results

The dissolved oxygen microsensor was used to sample the dissolved oxygen concentration at three different sites in the artificial biofilm and the bulk region adjacent to the biofilm sampling site. Dissolved oxygen measurements started in the bulk fluid region and proceeded toward the substratum stopping slightly before impacting the substratum and damaging the microsensor probe. Figure 12 shows the profile view

of the sampling location for dissolved oxygen (DO) measurements in the artificial biofilm patch.

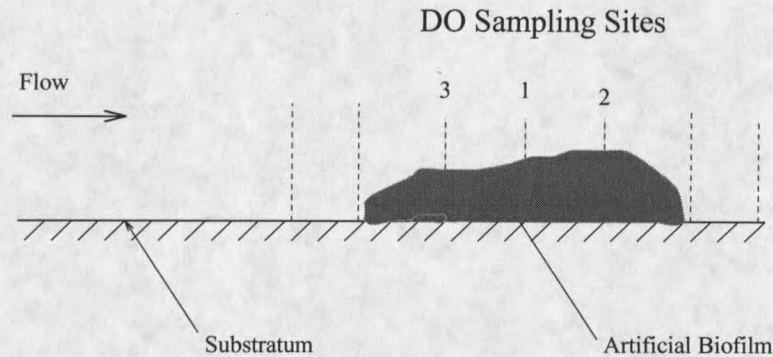


Figure 12. Dissolved oxygen sampling sites.

Experimental data for the dissolved oxygen values sampled at the three points in the artificial biofilm patch are shown in Figure 13. These three profiles show some variation in the substratum concentration and effective diffusive boundary thickness.

Kinetic Parameter Estimation

Kinetic parameters were estimated from the dissolved oxygen concentration measurements obtained from 3 different locations in the artificial biofilm patch. It was assumed that the kinetic parameters were uniform throughout. Depending on the effectiveness of the mixing of cells and alginate there could be spatial variation in the kinetics parameters. Additional variation in the height of the artificial biofilm patch could have resulted from the application of the alginate/cell mixture to the bottom of the reactor. The method used to estimate biofilm kinetic parameters from dissolved oxygen data has been reported (Lewandowski et al., 1991; Lewandowski, 1994; Lewandowski et al., 1994).

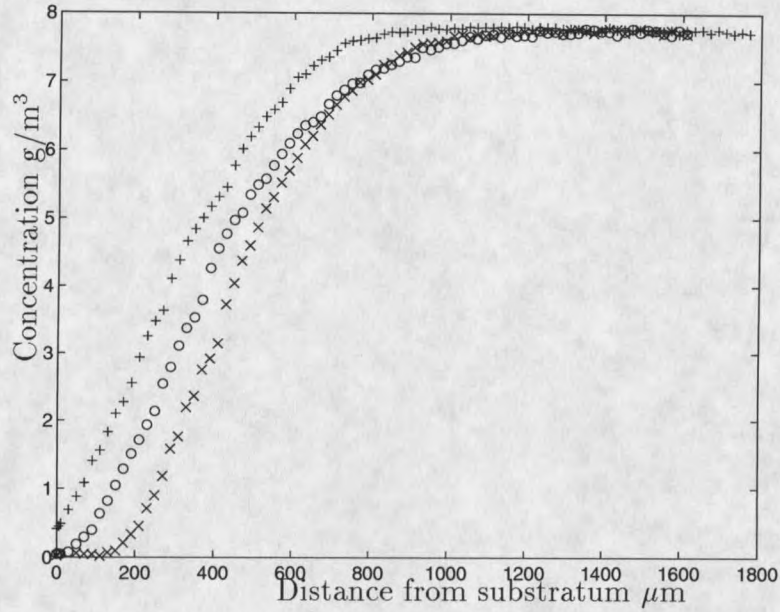


Figure 13. Plot of experimental dissolved oxygen data take at sites # 1 (o), # 2 ($\times$), and # 3 (+).

Combining equation (2.10) and (2.11) at steady state with the reaction term given by single Monod expression for a single species biofilm gives

$$0 = D_f \frac{d^2 C}{dx^2} - V_{\max} \frac{C}{K_s + C}, \quad 0 < x < L_f \quad (4.1)$$

In (4.1) $V_{\max}$ is a combination of variables $\mu_{\max}$, ρ_s , ϵ_s , and $Y_{x/s}$ defined by

$$V_{\max} = \frac{\mu_{\max} \rho_s \epsilon_s}{Y_{x/s}}. \quad (4.2)$$

Here $V_{\max}$ and K_s can be thought of as the usual Michaelis-Menten kinetic terms. Note that in (4.1) it is the ratio of $V_{\max}$ to D_f that significantly influences the behavior if K_s is small.

Model Simulation

In order to approximate experimental conditions in the channel reactor with the

model developed in this dissertation, it was assumed that the reactor geometry could be approximated by a rectangular conduit with depth twice the 1.5 cm flow depth in the channel. The two dimensional simulation was carried out along the center line of the reactor. A analytical velocity solution for laminar flow in a rectangular conduit (White, 1991) was used to estimate the centerline velocity profile from the measured flow rate.

Based on an average velocity of 0.055 cm/s, the estimated $Re_{L\infty}$ value was 19. The artificial biofilm was approximated in the model by a rectangular biofilm approximately 1.6 cm in length and 300 μm in height. Initial estimates of kinetic parameters were $K_O = 0.1 \text{ mgL}^{-1}$, $V_{\text{max}} = 0.231 \text{ mgL}^{-1}\text{s}^{-1}$, $f = 0.9$, and $Sc = 390$, $\nu = 0.897 \times 10^{-2} \text{ cm}^2\text{s}^{-1}$, and $D_O = 23 \times 10^{-6} \text{ cm}^2\text{s}^{-1}$.

Figure 14 contains a plot of the simulated and measured dissolved oxygen profiles for point # 1 on the artificial biofilm patch. The qualitative behavior is reasonable, however there is a significant offset between profiles. Simulated and measured profiles at the other two locations showed similar results. Thus using the a priori parameters the model appears to simulate the overall profile shape but accuracy decreases with depth into the biofilm.

In an effort to determine whether the model could simulate the measured profiles, the parameters with the strongest influence were varied. Parameters with the strongest influence are the Reynolds number (Re), Schmidt number (Sc), and the specific uptake rate (V_{max}). Location # 1 was used during the parameter modification procedure to measure the qualitative agreement with the measured profiles. The three parameters Re , Sc , and V_{max} were calibrated to the 83 data points at location # 1, yielding $Re_{L\infty} = 40$, $Sc_O = 255$, and $V_{\text{max}} = 0.174 \text{ mgL}^{-1}\text{s}^{-1}$. A plot of the calibrated profile and the measured profile for location # 1 is shown in Figure 15.

Figure 15 shows strong agreement between observed and simulated profiles.

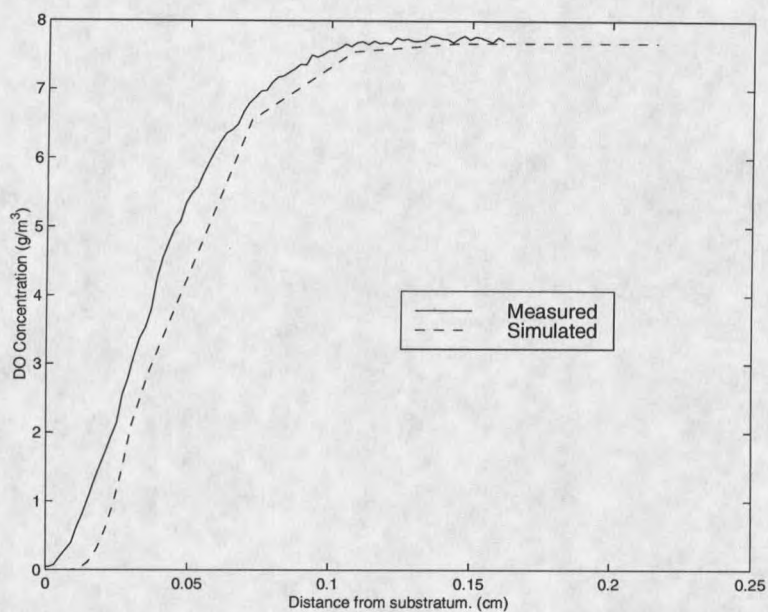


Figure 14. Comparison of measured (-) and simulated (- -) dissolved oxygen profiles at point # 1 for original parameters.

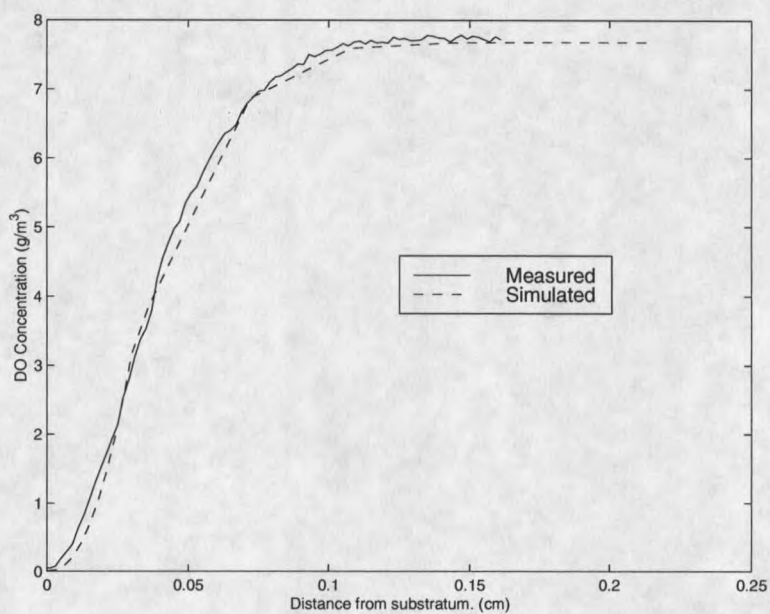


Figure 15. Comparison of measured (-) and simulated (- -) dissolved oxygen profiles at point # 1 for modified parameters.

The simulated dissolved oxygen profile was smoothed by cubic interpolation. The resulting profile shown in Figure 16 shows more curvature than evident in the piecewise linear plot of Figure 15.

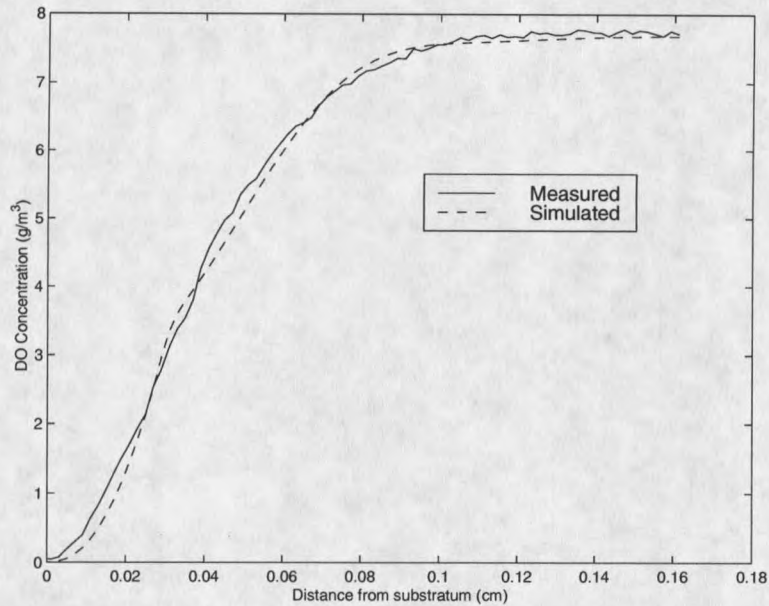


Figure 16. Comparison of measured (-) and simulated (- -) dissolved oxygen profiles at point # 1 for modified parameters. Cubic interpolation of simulated values used to get values at measured sites.

Next the profiles at sites # 2 and # 3 were simulated using $Re_{L\infty} = 40$, $Sc_O = 255$, and $V_{\max} = 0.174 \text{ mgL}^{-1}\text{s}^{-1}$. Figure 17 shows the comparison for location # 3 with the modified parameters. The measured dissolved oxygen profile at this point does not follow the impermeable nonreactive substratum boundary condition. This probably occurred because the left most data point was near, but not on, the substratum although it is plotted as being the substratum value.

A comparison of observed vs. simulated profiles for all three locations is shown in Figure 18. This sketch shows the general qualitative ability of the model with the calibrated parameters. Exact dimensions of the biofilm patch were not known so this

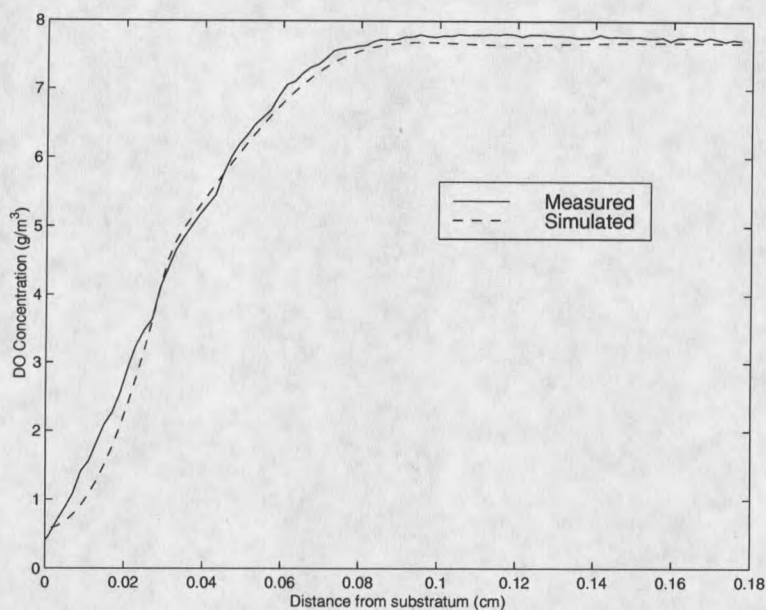


Figure 17. Comparison of measured (-) and simulated (- -) dissolved oxygen profiles at point # 3 for modified parameters. Cubic interpolation of simulated values used to get values at measured sites.

is estimated based on dissolved oxygen profiles.

Discussion

The computer model presented in this dissertation was applied to an experimental biofilm system. This biofilm system consisted of an artificial biofilm patch located in an open channel reactor. Dissolved oxygen measurements were taken with a oxygen microsensor. The biofilm was an artificial biofilm patch constructed to be homogeneous.

The major assumptions regarding the biofilm model imposed on the biofilm patch were (Abrahamson, 1995): 1) cell density was uniform throughout the biofilm in space and time, 2) oxygen was the only limiting nutrient, 3) transport through the biofilm follows Fick's second law, 4) molecular diffusivity of oxygen was constant in

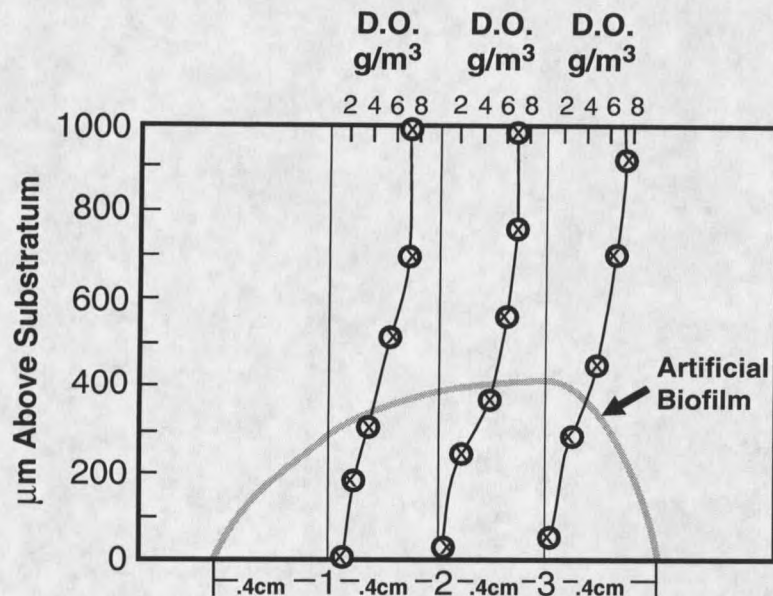


Figure 18. Comparison of simulated (x) and measured ($-$) profiles (Cunningham et al., 1995).

the biofilm, 5) the system was considered to be at steady state, and 6) oxygen uptake followed Monod kinetics.

Additional assumptions were made in modeling the flow and transport around the biofilm patch. The open channel reactor was approximated as two dimensional flow neglecting edge effects. The substrate behavior was also assumed to follow approximate two dimensional behavior at the center line. These assumptions allowed the model developed in this dissertation to compute the flow and transport around the artificial biofilm patch. The calculations assumed a uniform biofilm thickness of $300\ \mu\text{m}$.

Estimates of the physical flow and transport properties (viscosity and diffusivity) were not measured but taken from standard properties table and published data. Estimates of biofilm kinetics parameters were by the method suggested by Lewandowski et al. (1991).

The model simulations were in qualitative agreement with the observed dissolved oxygen profiles, but quantitatively there was a difference. After calibrating three key parameters to one profile, the model simulations closely matched the data for all three observed profiles (Figures 16 and 17). The model can simulate the qualitative dissolved oxygen behavior.

Further analysis of the kinetic parameters from the biofilm patch suggest the calibrated parameter values were appropriate (Abrahamson, 1995). The kinetic parameters were estimated using the so-called output least squares (OLS) approach (Appendix D). The OLS estimate of $V_{\max}$ is similar to the calibrated value used in the simulations of Figures 16 and 17. Decreasing $V_{\max}$ can influence the dissolved oxygen profile shape near the biofilm surface. An increase in oxygen flux to the biofilm requires a steeper gradient in the dissolved oxygen profile at the biofilm bulk fluid interface. With the assumption of no flow in the biofilm patch the slope should be approximately linear until bulk fluid velocity becomes more influential in the bulk oxygen transport.

The Reynolds number influences the sharpness of the profile and the extent to which the bulk concentration nears the biofilm surface. However, as the Reynolds number is increased, the effective Peclet number increases (recall $Pe = Re Sc$ in (2.47)). This effective increase in the Prandtl number increases the slope of the dissolved oxygen profile near the biofilm surface. Thus calibration decreased the Schmidt number to maintain the approximate slope observed in the measured dissolved oxygen profiles.

Small variations in the surface structure could cause small local deviations in the velocity. These deviations could be normal to the biofilm surface. This behavior has been observed near a thin biofilm under laminar flow (Brading, Boyle and Lappin-Scott, 1995). In their experiment small latex beads were used for particle velocimetry

to investigate fluid flow near the biofilm. They studied a thin biofilm for which the effective velocity profile went to zero at the biofilm surface. However, there was erratic behavior over a small distance of around $6\text{ }\mu\text{m}$. Beyond this distance the flow maintained the expected laminar velocity profile. Slight eddies in the flow near the interface could influence the vertical mass transport to rates greater diffusion alone.

Small variations in the measured dissolved oxygen profiles were observed. These might just be electro-chemical noise. There is also the possibility that the microprobe influences the concentration boundary layer (Glud et al., 1994), but this affect is probably small and it was neglected here.

There is some uncertainty about the length of the biofilm patch. The length was assumed to be 1.6 cm (Cunningham et al., 1995) for the simulations. However, in a subsequent publication, Abrahamson (1995) listed the length of the patch as 1.0 cm. Decreasing the length with a slight increase in the thickness above 300-cm would likely improve the model evaluation.

It can be concluded that the model presented in this dissertation can simulate the flow and transport effects locally near a biofilm surface. Further experiments and applications of the model could determine the effect of whether the model calibration parameters can predict a valid range for simulations. Additional dissolved oxygen measurements in a artificial biofilm patch would be valuable for model evaluation.

CHAPTER 5

APPLICATION TO BIOFILM SYSTEMS

In this chapter the MMP (microscale microbial process) model developed in this dissertation is applied to some relevant biofilm systems. The first application involves a comparison to AQUASIM (Reichert, 1994a) a simulation model used for biofilms systems. This provides a benchmark check on the behavior of the results of the MMP model. The MMP model is then applied to systems with heterogeneous biomass distributions on the upper and lower walls of a two-dimensional tube. The model calculated the amount of dissolved oxygen (limiting substrate) removed for each of several patterns of biomass distribution along the tube. The results show the effect of biofilm heterogeneity on dissolved oxygen utilization.

Comparison With AQUASIM

The AQUASIM model (Reichert, 1994a; Reichert et al., 1995; Reichert, 1995; Reichert, 1994b) is based on the mixed culture biofilm model (Wanner and Reichert, 1996). The AQUASIM model does not solve the species balance equation (2.5) as performed here but instead uses compartments (Reichert, 1994b, pp. 42). These compartments are typically considered well mixed CSTR's connected in series to model the bulk fluid flow. It was possible to use both AQUASIM and the MMP model to simulate the effluent concentration of dissolved oxygen for flow through a tube having a uniformly thick biofilm attached to both walls.

The benchmark problem considered was a conduit 0.6 cm in depth and length of 3.6 cm. For the AQUASIM simulation a width of 0.6 cm was used. Effective liquid

layer film thickness (L_L) used in the AQUASIM simulation was 0.007 cm. Other parameters common to both models included: inlet oxygen concentration of 7.68 g/m^3 , substrate diffusivity of $1.99 \times 10^{-4} \text{ m}^2/\text{d}$, half saturation concentration 0.0115 g/m^3 , maximum specific growth rate $0.1/\text{d}$, bacterial density $3 \times 10^5 \text{ g/m}^3$, yield coefficient 0.4, liquid volume fraction 0.8, biofilm thickness $110 \mu\text{m}$, and average velocity 58 m/d .

Effluent dissolved oxygen concentrations for the two models are shown in Table 2. This results shows that there is a close agreement between AQUASIM and MMP models.

Table 2. Comparison of effluent concentrations between MMP and AQUASIM models for benchmark problem.

	Effluent Concentration
MMP	7.30 g m^{-3}
AQUASIM	7.34 g m^{-3}

Biofilm Distribution Heterogeneity Simulations

There is interest in the effect of patchy biofilm patterns on the removal of a substrate from the fluid. AQUASIM cannot simulate patchy biofilm configurations but the model developed in this dissertation can. The model output of interest is the substrate utilization fraction, which is the difference between the inflow and outflow mass rates normalized by the inflow mass rate. In these simulations dissolved oxygen is assumed to be the limiting substrate.

Distributed Versus Uniform Biomass Simulations

To simulate patchiness, the MMP model was configured with discrete patches of one-dimensional biofilm (uniform thickness) distributed over a series of elevated substratum section or 'ribs'. Two configurations used this approach while the third had

a uniformly thick biofilm on upper and lower walls without ribs. Identical amounts of biofilm were used for each configuration.

Tube width was 0.6 cm with length 4.8 cm. For the case without ribs, a biofilm with a uniform thickness of $111.5\ \mu\text{m}$ and length of 3.6 cm was used. This distribution will be referred to as the flat case. For the next two cases ribs 0.06 cm in height and 0.036 cm in length were used (Figure 19).

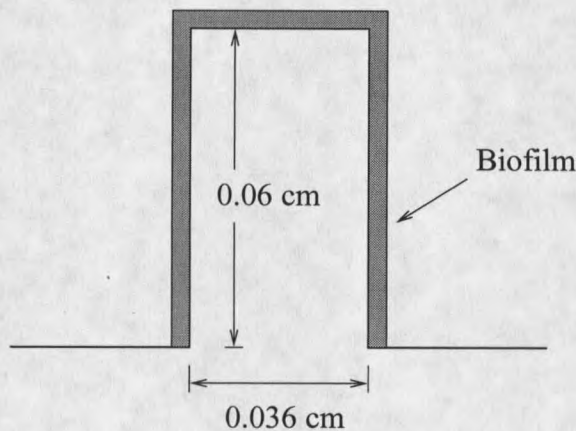


Figure 19. Sketch of a 'rib' geometry for maximum and minimum spacing simulations of distributed biomass.

In the second case, there were 38 ribs per side spaced 0.072 cm (Figure 20) apart with a $67\ \mu\text{m}$ thick biofilm. This case will be referred to as the minimum case. The third distribution used 22 ribs per side spaced 0.132 cm (Figure 21) apart and biofilm thickness of $110\ \mu\text{m}$. This is referred to as the maximum case.

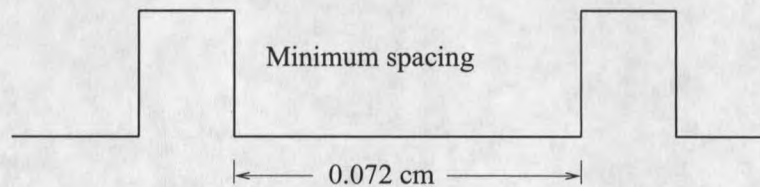


Figure 20. Sketch of 'rib' spacing for minimum spacing case.

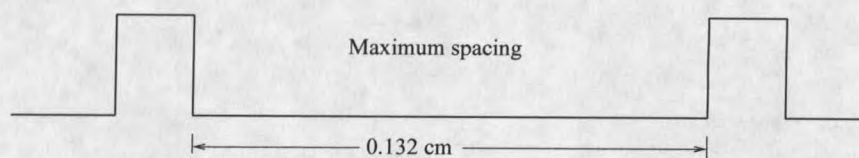


Figure 21. Sketch of 'rib' spacing for maximum spacing case.

Each of these three cases was simulated at Reynolds numbers of: 0.1, 0.4, 1.0, 4.0, and 8.0. Other model parameters are the same as those used in the comparison of MMP to AQUASIM. The results of these simulations in terms of the dissolved oxygen utilization fraction are shown in Table 3 for the different Reynolds numbers.

Table 3. Dissolved oxygen utilization fractions obtained with varying flow rates for the maximum spacing, minimum spacing, and flat biomass distributions.

Re	0.1	0.4	1.0	4	8
Maximum	0.8644	0.3701	0.1712	0.0429	0.02151
Minimum	0.832	0.355	0.1622	0.04097	0.02043
Flat	0.8390	0.3815	0.1793	0.0449	0.0225

A graphical comparison of the results contained in Table 3 is shown in Figure 22. A log-log plot was chosen because it approximately linearized the relationship. Also shown in Figure 22 are utilization fractions for the simulations discussed in the increased biomass heterogeneity section.

Each of these three biomass distributions (maximum, minimum, and flat) approach an asymptotic slope of -1 around $Re = 1$. This is expected as the biomass has become fully penetrated by the dissolved oxygen around $Re = 1$. After the biomass is fully penetrated at values above the small K_s value used here, further increases in the flow rate will not increase oxygen flux to the biomass.

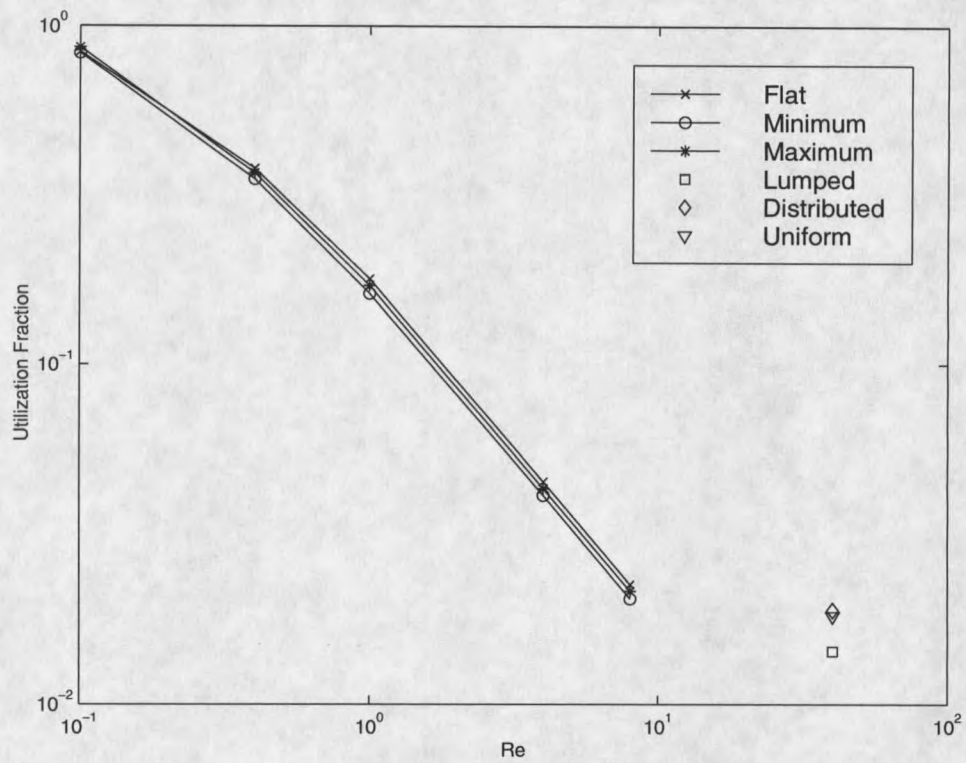


Figure 22. Utilization fractions as a function of the function of the Reynolds number for the flat (x), minimum spacing (o), maximum spacing ($*$), lumped ($\square$), distributed ($\diamond$), and uniform (∇) cases.

Visualization of Velocity and Dissolved Oxygen Data

Velocity vector plots of velocity normalized to centerline velocity around two patches at 2.55 cm along the flow path for the maximum spacing configuration at Reynolds numbers 0.1, 0.4 and 4.0 are shown in Figures 23, 24, and 25 respectively.

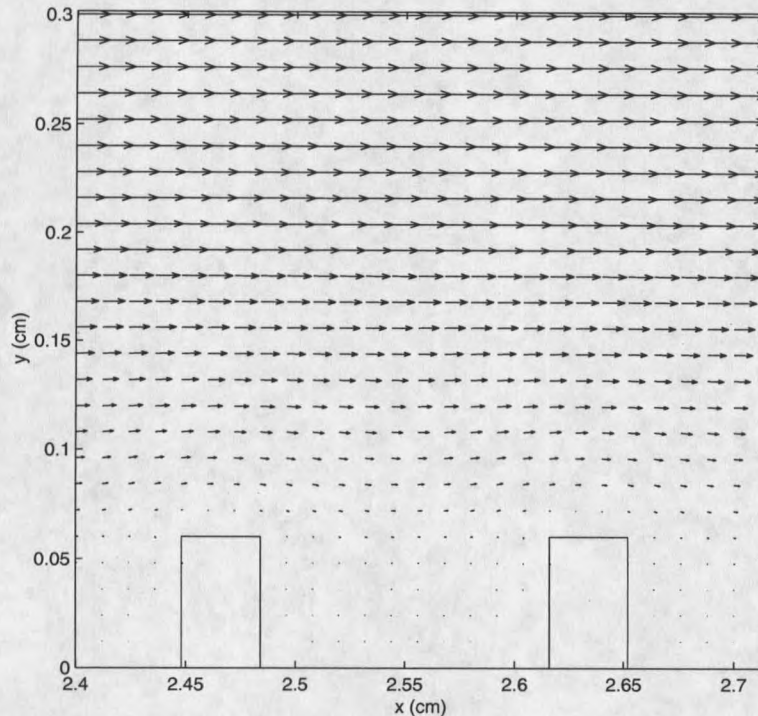


Figure 23. Velocity vector plot around two patches for the maximum spacing at $Re = 0.1$. The centerline velocity is 2.13 m/d.

Over this range of flow rates the general structure of the velocity field did not change significantly in shape. Velocity is influenced slightly near the top of the ribs. Velocity penetration between the two ribs is minimal and can be considered skimming flow (Jumars and Nowell, 1984).

Velocity variations around the minimum spacing patches was less dependent on the Reynolds number than in the maximum case. The velocity vector plot at $Re = 4.0$ for the minimum spacing around 2.55 cm along the flow patch is shown in

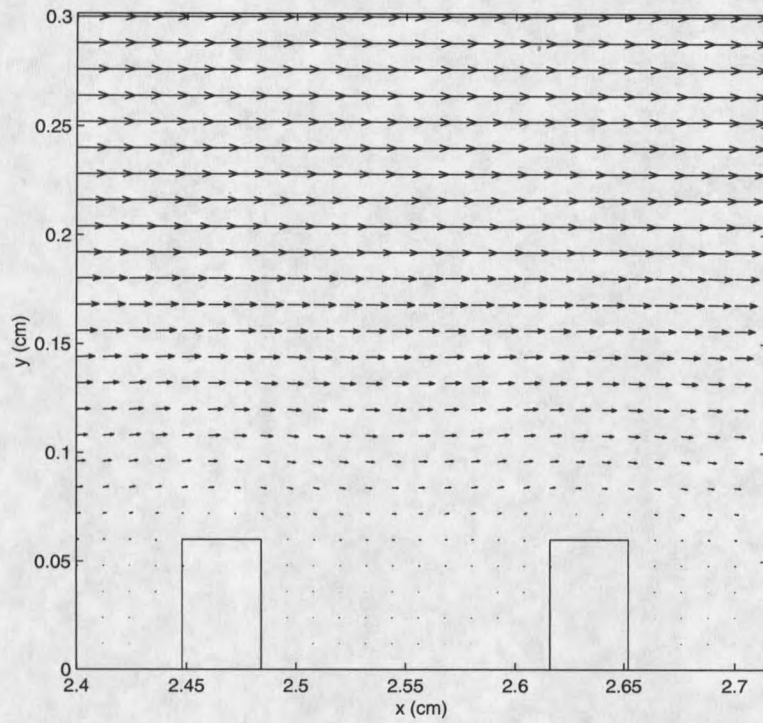


Figure 24. Velocity vector plot around two patches for the maximum spacing at $Re = 0.4$. The centerline velocity is 8.52 m/d.

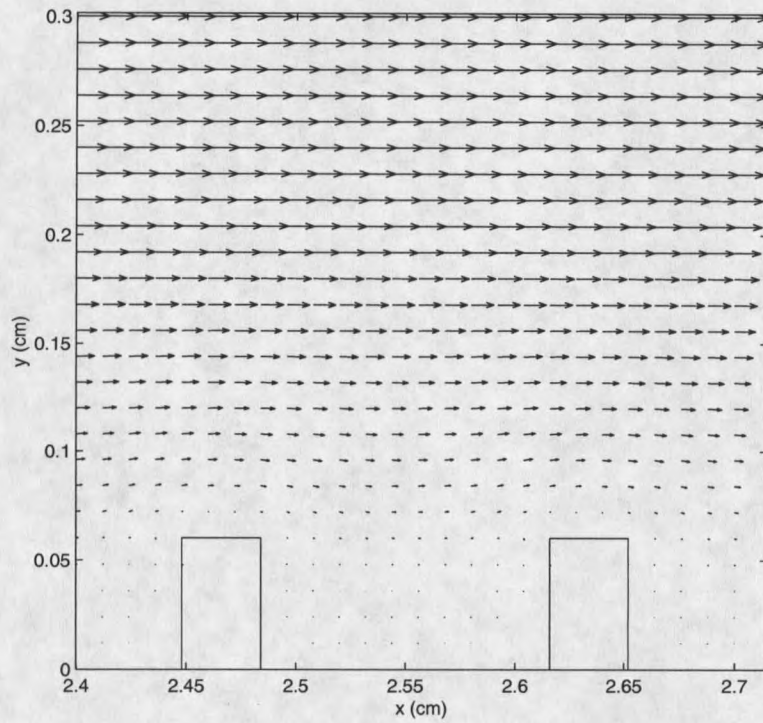


Figure 25. Velocity vector plot around two patches for the maximum spacing at $Re = 4.0$. The centerline velocity is 85.2 m/d

Figure 26. Variations with flow rate changed the magnitude of the velocity but had minimal influence on the velocity vector field. The flow is observed to skim across the top of the ribs with very small velocity between the ribs.

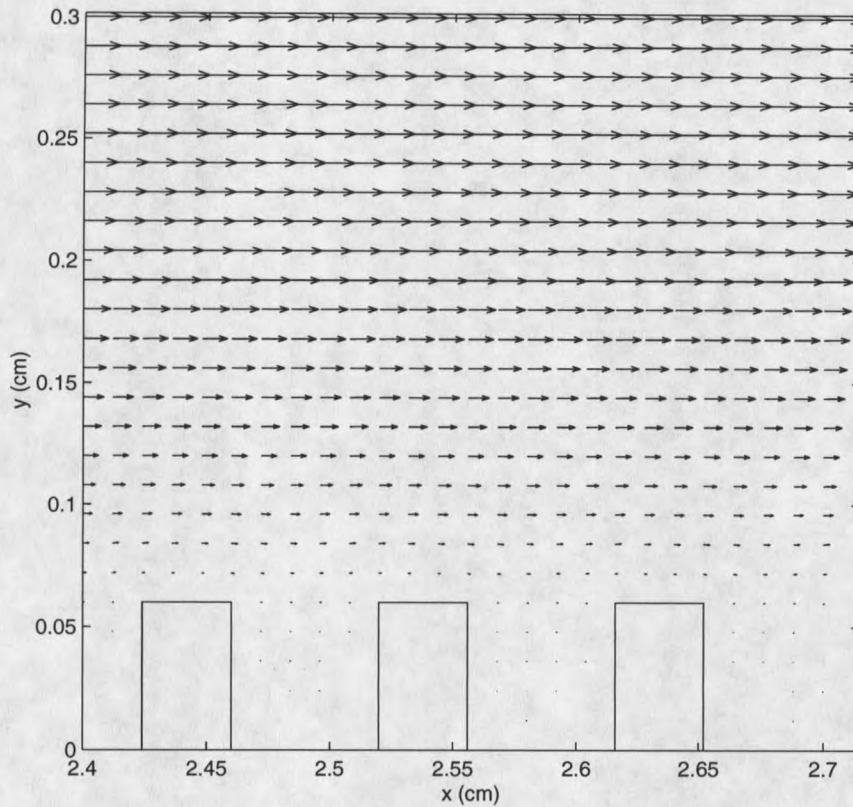


Figure 26. Velocity vector plot around two patches for the minimum spacing at $Re = 4.0$. The centerline velocity is 85.2 m/d.

Dissolved oxygen concentration contours around two patches of the maximum spacing configuration near the midpoint of the tube at Reynolds number of 0.1 and 0.4 are shown in Figure 27 and 28. At these flow rates there was some transport limitation to the biofilm located on the ribs. Figure 27 shows areas where the dissolved oxygen concentration is less than 0.1 g/m^3 and can be considered anaerobic.

Increasing the flow rate to $Re = 0.4$ resulted in increased dissolved oxygen concentration on the top of the rib enough that this section of biofilm was fully

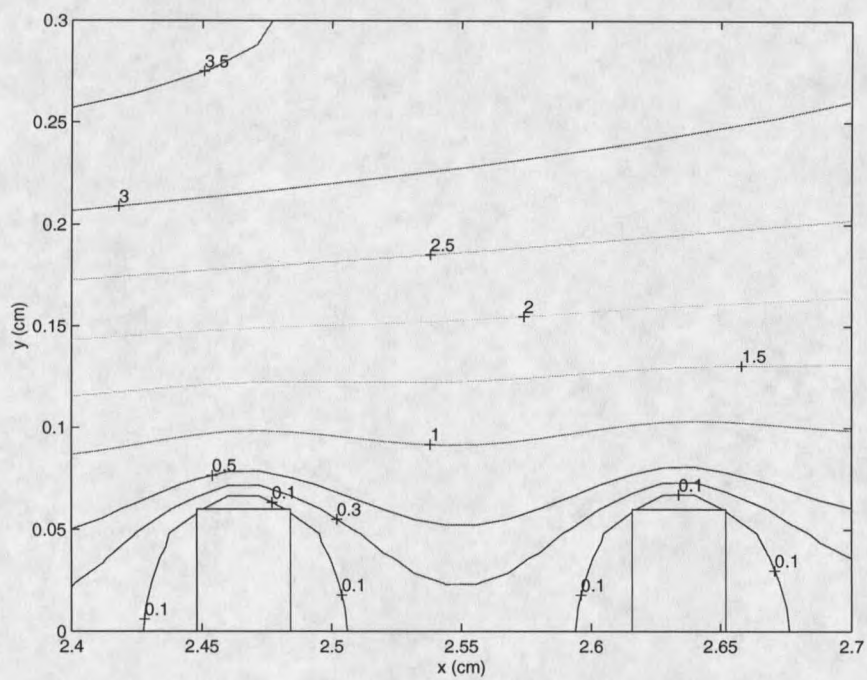


Figure 27. Dissolved oxygen contour plot around two patches for the maximum spacing at $Re = 0.1$.

penetrated. However, there is still a zone near the the bottom of the rib at the substratum where anaerobic conditions exist as shown in Figure 28. The anaerobic area in the corners has decreased but is still present.

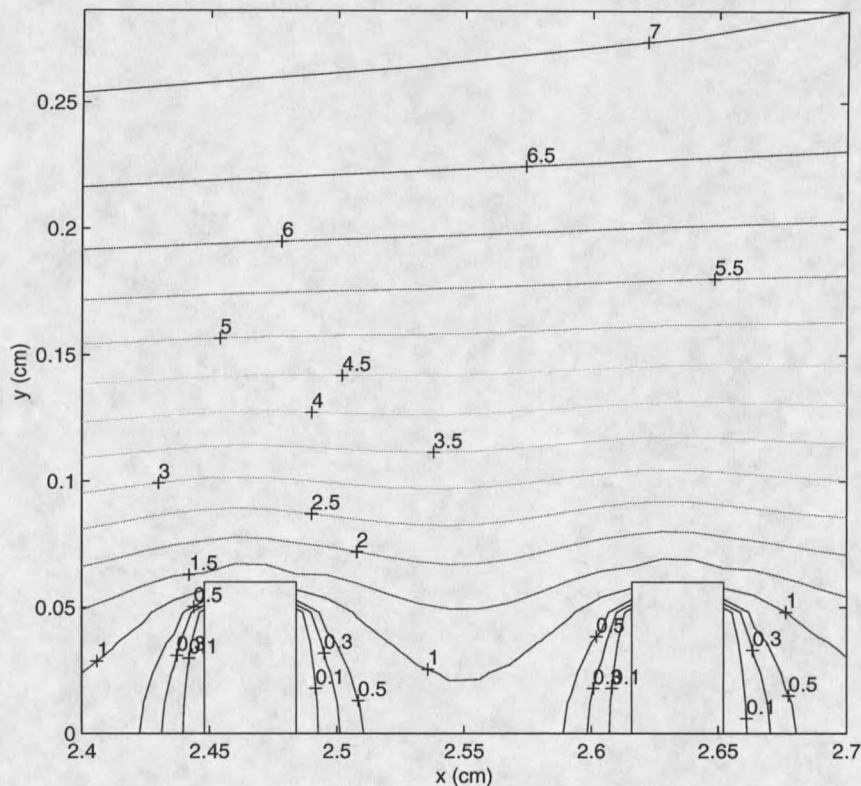


Figure 28. Dissolved oxygen concentration (g/m^3) around two patches for the maximum spacing at $Re = 0.4$.

As the flow rate is increased sufficiently the anaerobic zones cease to exist. There is still some variation of the dissolved oxygen concentration around the ribs as shown in Figure 29 for the minimum spacing at $Re = 4.0$. The region between the two patches which exhibits little velocity flow (Figure 26) shows the importance of diffusive transport in this region.

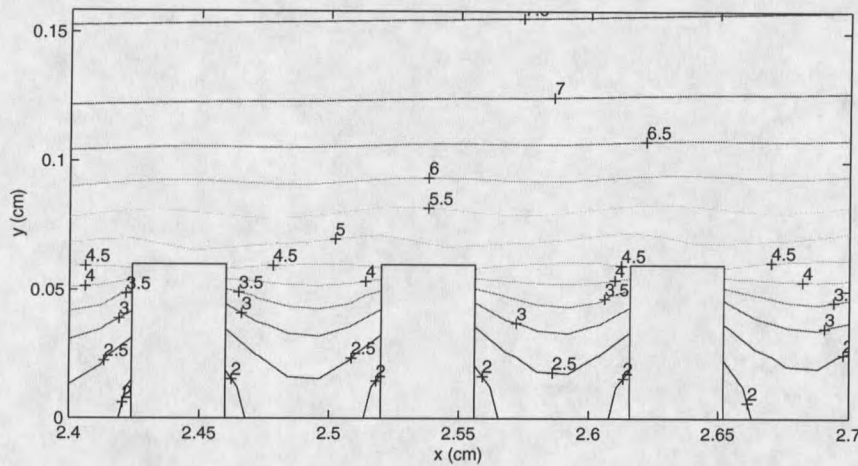


Figure 29. Dissolved oxygen concentration (g/m^3) around two patches for the minimum spacing at $Re = 4.0$.

Increased Biomass Heterogeneity

These simulations show how biofilm heterogeneity in the form of biofilm patchiness influences the substrate utilization. A tube 2 cm in width and 16 cm in length with three different distributions of biofilm was simulated: 1) a lumped $200\ \mu\text{m}$ thick biofilm of length 8 cm, 2) ten patches with thickness of $200\ \mu\text{m}$ and length 0.8 cm with 0.8 cm distance between patches, and 3) a $125\ \mu\text{m}$ thick and 12.8 cm long uniform biofilm. In each case the distribution on upper and lower wall was symmetric. Parameters used in the AQUASIM/MMP comparison were used for these simulations at a Reynolds number of 40. Results of the simulation in terms of utilization fraction are listed in Table 4 and plotted in Figure 22. These simulations with different biomass distributions show a difference in the dissolved oxygen utilization fraction with the lumped being significantly different from the distributed and uniform distribution.

Table 4. Dissolved oxygen utilization fractions obtained in lumped, distributed, and uniform biofilm simulations.

Distribution	ConversionFraction
Lumped – 200 μm	0.0143
Distributed – 200 μm	0.0189
Uniform – 125 μm	0.0182

Discussion

The MMP model was applied to simulation of some relevant biofilm systems. The first simulation was a comparison with the AQUASIM model in a uniform biofilm configuration. A high level of agreement was observed.

Rough surfaces have been known to cause changes in velocity profiles. Depending on size and spacing of roughness elements different types of flow patterns develop. I consider three regimes: a) Independent flow, b) Interactive flow, and c) Skimming flow (Morris, 1955; Davis and Barmuta, 1989; Carling, 1992; Young, 1992).

The simulations performed with the biofilms located on ribs illustrate some of these effects. In the flat case the standard parabolic profile is observed outside the uniform film. However this is not the case for the maximum and minimum spacing scenarios. Figure 26 shows that there is very little velocity between the two ribs for the minimum spacing. In effect the velocity is skimming over the surface with very little penetration between the two ribs. In the maximum spacing case there was slightly more velocity influence but it was still a very minor influence on dissolved oxygen transport. Velocity near the substratum and sides of the ribs is very small. As a consequence of this small local velocity the mass transport in these areas is dominated by diffusive transport.

Figures 27 and 28 show variation in the dissolved oxygen concentrations between the two ribs. Diffusion is a strong transport mechanism in the corners next to

the ribs as shown by the anoxic zones while the bulk and top of the rib are aerobic. Convection in these corners and lower regions between the two ribs is negligible as shown in the velocity vector profiles in Figures 23 and 24. Even after the biofilm has become fully penetrated the diffusive transport is the dominant transport mechanism between the ribs as shown in Figure 29.

As the Reynolds number was increased from 0.1 to 0.4 the concentration contours near the rib surface with biofilm begin to follow the biofilm surface. (de Beer et al., 1997) observed that around clusters in a heterogeneous biofilm the diffusive boundary layer followed the biofilm shape as the flow rate was increased. At sufficiently high flow rates the diffusive boundary layer followed the biofilm surface. The clusters observed were $150 - 200 \mu\text{m}$ thick separated by interstitial voids. Void fraction (of the substratum area) was approximately 50%. Length of the cluster was approximately $375 \mu\text{m}$. These clusters are of different shape than the ribs with biofilm used here but similar behavior is observed. There are qualitative similarities of mass transport between the simulations here and their experimental observations.

The comparison of three different biomass distributions – the lumped, distributed and uniform provided some interesting results. The distributed case had approximately the same utilization as the uniform thinner biofilm. This may be attributable to the mixing that occurs between successive patches for the distributed case. The thinner uniform biofilm has less initial substrate flux due to its smaller thickness. Higher flux for the lumped biofilm creates a diffusive boundary layer that is larger than the thinner uniform film for the same distance from the start of the biofilm. Less dissolved oxygen conversion in the lumped case is attributed to the concentration boundary layer developing so that the mass transfer limitation is greater than the other two cases.

Overall area available for mass transfer interaction with the biofilm is larger for the distributed and uniform thin cases. In the distributed scenario, the dissolved oxygen has a chance to undergo diffusion and mixing processes to attain a higher available surface concentration at the start of the next patch. The Reynolds number was fixed for these cases but they should eventually have the same dissolved oxygen conversion fraction as the flow rate is increased.

Conclusions from these simulations are:

- Local behavior can be analyzed (anaerobic zones).
- Heterogeneity can influence dissolved oxygen consumption.

CHAPTER 6

CONCLUSIONS

- A mathematical model coupling laminar fluid flow, substrate transport, and biofilm reaction was formulated. Fluid flow and substrate transport are modeled in two dimensions and are coupled with a one dimensional biofilm model.
- The mathematical model was solved using second order finite differences. Convergence of the velocity solution in the range of interest ($Re < 100$) was reasonable. Solution of the advection-diffusion-reaction equation was limited to values of the Peclet number ($Pe = Re Sc$) less than 10,000.
- Model simulations were compared with dissolved oxygen measurements taken in an artificial biofilm patch. Model simulations were in agreement with the qualitative behavior of the experimental data. Calibration of the model produced a strong agreement with the measured dissolved oxygen profiles.
- Applied to biofilm systems this model allows simulation of local behavior. Fluid flow and dissolved oxygen transport interactions with biofilms can be modeled for anaerobic regions.
- Model simulations predict variations in dissolved oxygen consumption with different biomass distributions.

CHAPTER 7

FUTURE WORK

This research has shown that the coupled processes of fluid dynamics, substrate transport and biofilm reaction can be modeled at a microscale. Future versions of the approach used here may need to alter the biofilm model equations to account for additional effects such as fluid flow and heterogeneous structure. A addition that would be useful would be accounting for two dimensional effects in the biofilm. In some cases, it might be necessary to model the biofilm region in three dimensions along with the fluid flow.

This work has shown that sharp gradients in substrate concentration can occur near biofilms under laminar flow at low flow rates. At higher flow rates, there will be a decrease in the diffusive boundary layer which would require a finer mesh. Use of the finite element method might be advantageous to capture these phenomenon. A finite element approach also be used for the biofilm region.

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APPENDICES

APPENDIX A

Uniform Inlet Boundary Conditions

This appendix contains the derivation of boundary conditions at the entrance of a steady-state two dimensional fully developed laminar flow inlet. The approach take here follows the approach of Malvern (1969).

Velocity

Consider laminar flow between two parallel plates as shown in Figure 30 with parallel flow in the x direction with $v = w = 0$ everywhere.

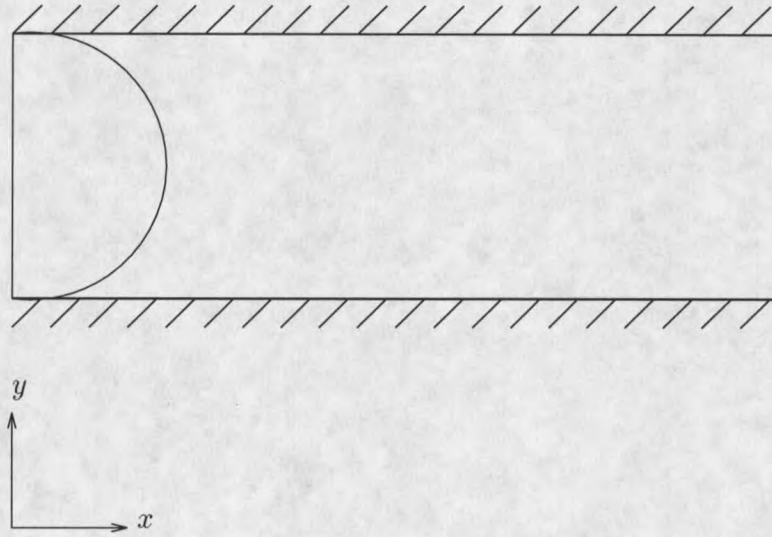


Figure 30. Infinite parallel walls for two dimensional flow.

Then the continuity equation (2.1) implies

$$\frac{\partial u}{\partial x} = 0 \quad (\text{A.1})$$

and hence u is independent of x . With $v = w = 0$ and u independent of x , the Navier-Stokes equations (2.2) reduce to

$$-\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \frac{\partial^2 u}{\partial y^2} = 0 \quad (\text{A.2})$$

$$-\frac{1}{\rho} \frac{\partial p}{\partial y} - g = 0 \quad (\text{A.3})$$

where g is gravitational constant from the body forces in (2.2). If gravity force in negligible or y direction does not coincide with direction of gravity, equation (A.3) shows that the pressure, p , is not a function of y . Considering gravity gives

$$p(x, y) = -\gamma y + f_1(x) \quad (\text{A.4})$$

where γ is the specific weight and $f_1(x)$ is arbitrary function of x , equal to the (generally unknown) pressure distribution on the lower wall. Note that at high Reynolds numbers laminar flow in long pipes has been observed to be influenced by Coriolis force due the Earth's rotation (Draad and Nieuwstadt, 1998).

Equation (A.2) now takes the form

$$\mu \frac{\partial^2 u}{\partial y^2} = f_1'(x) \quad (\text{A.5})$$

which can be integrated to general form

$$\mu u(x, y) = \frac{y^2}{2} f_1'(x) + y f_2(x) + f_3(x) \quad (\text{A.6})$$

where $f_2(x)$ and $f_3(x)$ are arbitrary functions of x .

Equation (A.1) gave $\partial u / \partial y \equiv 0$, hence

$$0 = \mu \frac{\partial u}{\partial x} = \frac{y^2}{2} f_1''(x) + y f_2'(x) + f_3'(x) \quad (\text{A.7})$$

for all x and y , which implies that

$$f_1''(x) = 0 \quad (\text{A.8})$$

$$f_2'(x) = 0 \quad (\text{A.9})$$

$$f_3'(x) = 0 \quad (\text{A.10})$$

This yields

$$f_1(x) = C_1 x + C_3 \quad (\text{A.11})$$

$$f_2(x) = C_2 \quad (\text{A.12})$$

$$f_3(x) = C_4 \quad (\text{A.13})$$

where C_1, C_2, C_3 , and C_4 are constants. Then equation (A.5) becomes

$$\mu u(y) = \frac{y^2}{2} C_1 + y C_2 + C_4. \quad (\text{A.14})$$

Since the lower wall is stationary, the boundary condition for a viscous fluid requires $u \equiv 0$ at $y = y_l$, which gives

$$0 = \frac{y_l^2}{2} C_1 + y_l C_2 + C_4. \quad (\text{A.15})$$

The upper wall is also stationary, which requires $u \equiv 0$ at $y = y_u$, hence

$$0 = \frac{y_u^2}{2} C_1 + y_u C_2 + C_4. \quad (\text{A.16})$$

From equations (A.4) and (A.11)

$$C_1 = \frac{\partial p}{\partial x} \quad (\text{A.17})$$

Equations (A.14) and (A.15) can be solved simultaneously to get expressions for C_2 and C_4 in terms of C_1

$$C_2 = -\frac{C_1}{2}(y_u + y_l) \quad (\text{A.18})$$

$$C_4 = C_1 y_u y_l. \quad (\text{A.19})$$

Substitution of (A.18) and (A.19) into (A.14) results in expression for $u(y)$

$$u(y) = \frac{C_1}{2\mu} [y^2 - y(y_u + y_l) + y_u y_l]. \quad (\text{A.20})$$

It is necessary to know the pressure gradient (A.17) to fully determine the velocity profile (A.20). Alternatively, if the average velocity, u_{ave} , in the channel is known, C_1 is can be eliminated in terms of the average channel velocity.

The total flow rate in the channel is equal the average flow rate times the channel thickness. The total flow rate is the integral over the depth of the velocity.

$$u_{ave}(y_u - y_l) = \int_{y_l}^{y_u} u(y) dy \quad (\text{A.21})$$

$$= \int_{y_l}^{y_u} \frac{C_1}{2\mu} [y^2 - y(y_u + y_l) + y_u y_l] dy \quad (\text{A.22})$$

$$= \frac{C_1}{2\mu} \left[\frac{(y_u - y_l)(y_u^2 + y_u y_l + y_l^2)}{3} - \frac{(y_u - y_l)(y_u + y_l)^2}{2} + (y_u - y_l)y_u y_l \right] \quad (\text{A.23})$$

Solving equation (A.23) for u_{ave} gives

$$u_{ave} = -\frac{C_1}{12\mu}(y_u - y_l)^2 \quad (\text{A.24})$$

which when solved for C_1 results in

$$C_1 = -\frac{12\mu}{(y_u - y_l)^2} u_{ave}. \quad (\text{A.25})$$

Substitution of (A.25) into (A.20) results in velocity profile in terms of average velocity

$$u(y) = -\frac{6u_{ave}}{(y_u - y_l)^2} [y^2 - y(y_u + y_l) + y_u y_l] \quad (3.18)$$

Note that equation () was derived from dimensional equations. Application of the nondimensional values (2.44) results in same equation as () only with variables being nondimensional variables (I.e., denoted by superscript *). The following development of the boundary conditions will use nondimensional version of (). A plot of the velocity normalized by the average velocity, u_{ave} , is shown in Figure 31.

The equation for the pressure in the channel (A.4) can be rewritten using (A.11) and (A.25) to get

$$p(x, y) = -\gamma y - \frac{12\mu u_{ave}}{(y_u - y_l)^2} x + C_3 \quad (\text{A.26})$$

which is the general equation for the pressure. At the inlet, ($x = 0$, the boundary condition can be expressed as

$$p(0, y) = p_0(y) = -\gamma y + C_3. \quad (\text{A.27})$$

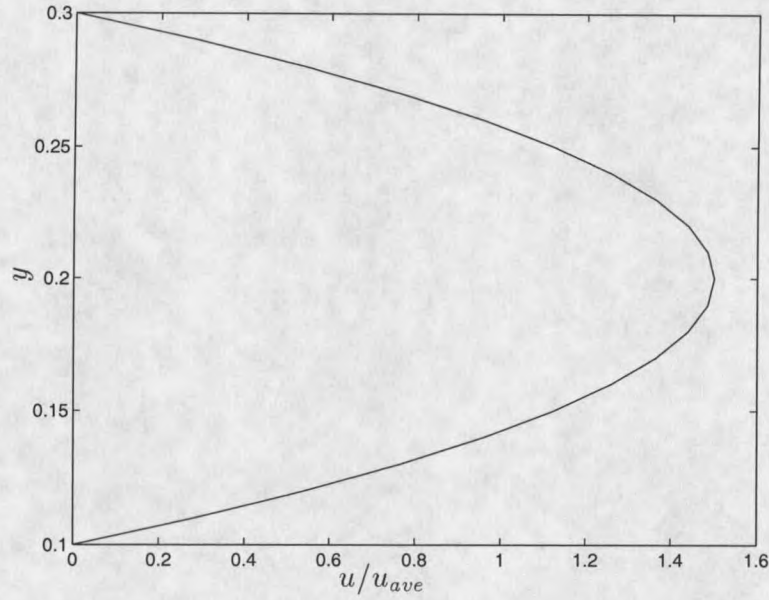


Figure 31. Normalized velocity profile at inlet.

If $\bar{p}_0$ denotes the pressure at the top of the channel, then equation (A.27) can be written as

$$p(x, y) = \bar{p}_0 + \gamma(y_u - y) - \frac{12\mu u_{ave}}{(y_u - y_l)^2} x \quad (\text{A.28})$$

in terms of average velocity, u_{ave} , pressure at top wall, $\bar{p}_0$, and the fluid viscosity, μ .

Recalling the nondimensionalisation equations (2.44), equation (A.28) becomes

$$p^*(x^*, y^*) = \bar{p}_0^* + \frac{y_u^* - y^*}{Fr} - \frac{12}{Re_L} \frac{u_{ave}^*}{(y_u^* - y_l^*)^2} x^*$$

where $Fr = V_\infty^2 / gL_\infty$ is the nondimensional Froude number.

Stream function/Vorticity

A boundary condition on the stream function at the inlet is necessary for solution of the stream function-vorticity formulation form of the fluid dynamics equations (3.6)

and (3.5). Recalling the definition of u in terms of the stream function (3.1)

$$u = \frac{\partial \psi}{\partial y} \quad (3.1)$$

can be integrated with respect to y to obtain

$$\psi(x, y) = \int u(y) dy + f_4(x). \quad (A.29)$$

Recalling the definition of v in terms of the stream function (3.2) along with fully developed flow in x direction of channel $v \equiv 0$, implies

$$f_4'(x) = 0. \quad (A.30)$$

This gives

$$f_4(x) = C_5$$

where C_5 is a constant. In particular equation (A.29) can be written in a alternative form

$$\psi(y) = \psi(y_l) + \int_{y_l}^y u(y) dy. \quad (A.31)$$

Note that the average velocity in terms of the stream function is

$$u_{ave} = \frac{\psi(y_u) - \psi(y_l)}{y_u - y_l} \quad (A.32)$$

$$= \int_{y_l}^{y_u} u(y) dy. \quad (A.33)$$

Equation (A.32) that the difference in stream function values for two stream lines divided by normal distance between them gives the average velocity between the two stream lines.

Substituting equations () and (A.32) into (A.31) and integrating choosing $\psi(y_l) = 0$ results in

$$\psi(y) = -\frac{6\psi(y_u)}{(y_u - y_l)^3} \left[\frac{y^3 - y_l^3}{3} - \frac{(y^2 - y_l^2)(y_u + y_l)}{2} + (y - y_l)y_u y_l \right]. \quad (3.19)$$

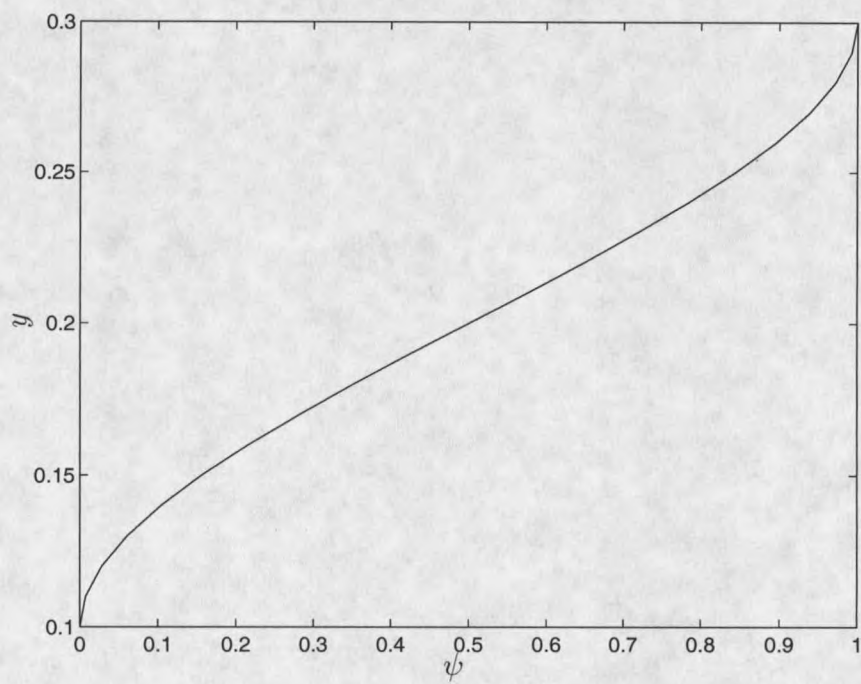


Figure 32. Sample plot of the stream function, ψ , at inlet.

A plot of the stream function at the inlet for $y_u = 0.3$, $y_l = 0.1$, and $\psi(y_u) = 1.0$ is shown in Figure 32.

The vorticity is given by (3.4) as

$$\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \quad (3.4)$$

As assumed in the development $v \equiv 0$ so

$$\omega(y) = -\frac{\partial^2 u}{\partial y^2} \quad (\text{A.34})$$

and equation () can be differentiated twice with respect to y to obtain the equation for the vorticity at the inlet

$$\omega(y) = -\frac{12\psi(y_u)}{(y_u - y_l)^3} \left[\frac{y_u + y_l}{2} - y \right]. \quad (3.21)$$

A plot of the vorticity is shown in Figure 33 for values of $y_u = 0.3$, $y_l = 0.1$, and $\psi(y_u) = 1.0$.

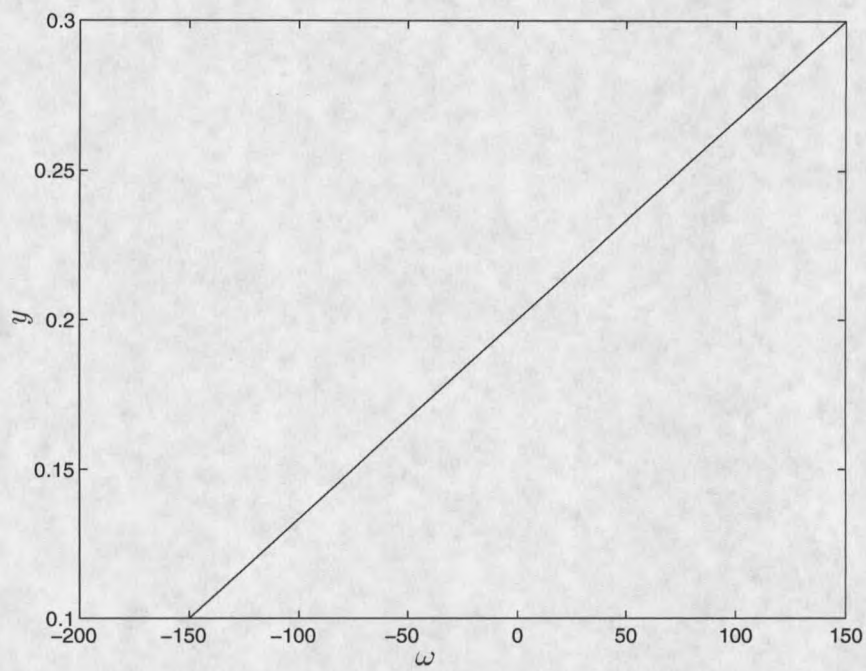


Figure 33. Sample plot of the vorticity, ω , at inlet.

APPENDIX B
Perturbation Scheme

In this appendix, a general perturbation scheme is developed and applied to different boundary conditions which arise in solution of the model equations described in Chapter 4. Three different boundary condition types (Dirichlet, Neumann, and Robin) lead to three possible cases for implementation of perturbation expression.

In general boundary conditions for a function $u(x, y, t)$ can be expressed in the form

$$\alpha(x, y, t)u(x, y, t) + \beta(x, y, t)\frac{\partial u}{\partial n}(x, y, t) = \gamma(x, y, t), \quad (x, y, t) \in \partial\Omega \quad (\text{B.1})$$

where α , β , and γ are known functions, $\partial\Omega$ is the boundary of the space time domain Ω , and $\partial u/\partial n$ denotes the derivative normal to a boundary in either space or time (Allen et al., 1988). *Dirichlet* conditions are boundary conditions wherein u is specified, that is, $\beta = 0$. *Neumann* conditions describe the case when the normal derivative of the function is specified, that is, when $\alpha = 0$. When $\alpha \neq 0$ and $\beta \neq 0$, one has specified a *Robin* boundary condition. Dirichlet, Neumann and Robin boundary conditions are also known by the aliases Type 1, Type 2, and Type 3 boundary conditions, respectively. Whenever $\gamma = 0$, the boundary condition is said to be *homogeneous*.

The boundary condition for stream function ψ on the wall are Dirichlet (3.12) and Neumann (3.13) while the boundary conditions on the concentration and biomass equations are of the Neumann type.

General Perturbation Scheme

Consider a horizontal wall at say y_0 and a curve above it $y = f(x)$ that is the boundary but the boundary conditions (B.C.'s) need to be applied at y_0 to retain the original mesh (see Figure 34).

To apply the boundary condition which is known at $(x, f(x))$ on the original finite difference mesh, a perturbation scheme is used to transfer the boundary condition to (x, y_0) which is horizontal wall boundary. In general the perturbation

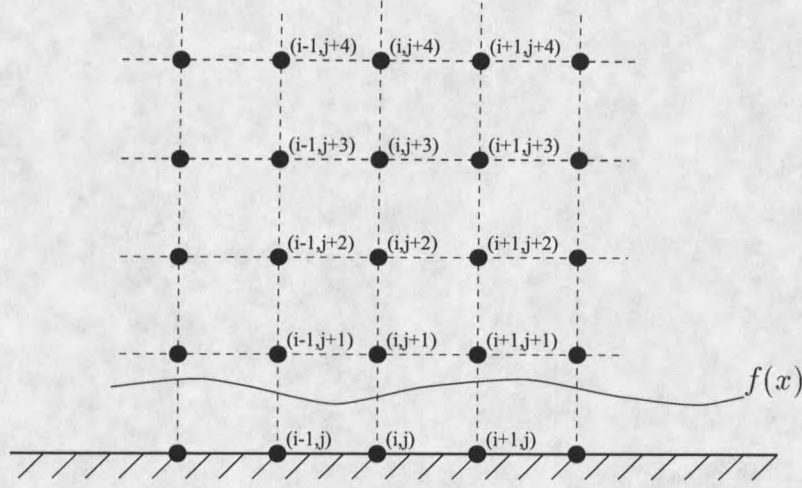


Figure 34. Horizontal wall with perturbation of boundary.

expression for a Dirichlet boundary condition can be implemented by considering a Taylor series expansion of the variable in question, say $u(x, y)$ for example:

$$u(x, f(x)) = u(x, y_0) + \frac{\partial u}{\partial y}(x, y_0)[f(x) - y_0] + \sum_{k=2}^{\infty} \frac{\partial^k u}{\partial y^k}(x, y_0) \frac{[f(x) - y_0]^k}{k!} \quad (\text{B.2})$$

Here it is assumed that $f(x) - y_0$ is small so that the higher order terms, $k \geq 3$, can be neglected. Assume that the boundary condition $u(x, f(x))$ is known and (B.2) can be written as: which resembles a Robin boundary condition for $u(x, y_0)$ except

$$u(x, y_0) + \frac{\partial u}{\partial y}(x, y_0)[f(x) - y_0] + \frac{\partial^2 u}{\partial y^2}(x, y_0) \frac{[f(x) - y_0]^2}{2!} = u(x, f(x)) = g_0(x) \quad (\text{B.3})$$

that second order derivative term is contained in (B.3). In general, perturbation scheme of order greater than 0 will yield a Robin like boundary condition.

For a Neumann boundary condition along a horizontal wall, (B.2) can be used by replacing $u(x, y)$ with $u_y(x, y)$ to get

$$u_y(x, f(x)) = u_y(x, y_0) + \frac{\partial^2 u}{\partial y^2}(x, y_0)[f(x) - y_0] + \sum_{k=2}^{\infty} \frac{\partial^{k+1} u}{\partial y^{k+1}}(x, y_0) \frac{[f(x) - y_0]^k}{k!} \quad (\text{B.4})$$

Truncating (B.4) after the 2^{nd} expansion term, gives an equation for the perturbation

of Neumann boundary condition

$$u_y(x, y_0) + \frac{\partial^2 u}{\partial y^2}(x, y_0)[f(x) - y_0] + \frac{\partial^3 u}{\partial y^3}(x, y_0) \frac{[f(x) - y_0]^2}{2!} = u(x, f(x)) = g_1(x) \quad (\text{B.5})$$

which is a Robin boundary condition for $u_y(x, y_0)$.

For a horizontal wall with the mesh below it (see Figure 35), a perturbation scheme is given by

$$u(x, y_0) + \frac{\partial u}{\partial y}(x, y_0)[y_0 - f(x)] + \frac{\partial^2 u}{\partial y^2}(x, y_0) \frac{[y_0 - f(x)]^2}{2!} = u(x, f(x)) = g_0(x) \quad (\text{B.6})$$

for a Dirichlet boundary condition and

$$u_y(x, y_0) + \frac{\partial^2 u}{\partial y^2}(x, y_0)[y_0 - f(x)] + \frac{\partial^3 u}{\partial y^3}(x, y_0) \frac{[y_0 - f(x)]^2}{2!} = u(x, f(x)) = g_1(x) \quad (\text{B.7})$$

for a Neumann boundary condition.

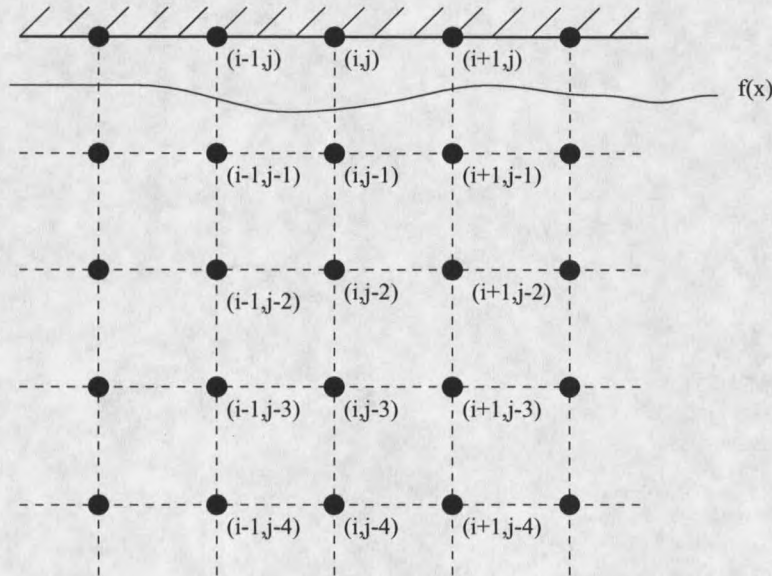


Figure 35. Top wall with perturbation below wall.

For a vertical wall, the perturbation expression will be with respect to x direction. For a wall with nodes to right (see Figure 36), this becomes

$$u(x_0, y) + \frac{\partial u}{\partial x}(x_0, y)[f(y) - x_0] + \frac{\partial^2 u}{\partial x^2}(x_0, y) \frac{[f(y) - x_0]^2}{2!} = u(f(y), y) = g_0(y) \quad (\text{B.8})$$

for Dirichlet boundary condition and

$$u_y(x_0, y) + \frac{\partial^2 u}{\partial x^2}(x_0, y)[f(y) - x_0] + \frac{\partial^3 u}{\partial x^3}(x_0, y) \frac{[f(y) - x_0]^2}{2!} = u(f(y), y) = g_1(y) \quad (\text{B.9})$$

for a Neumann boundary condition.

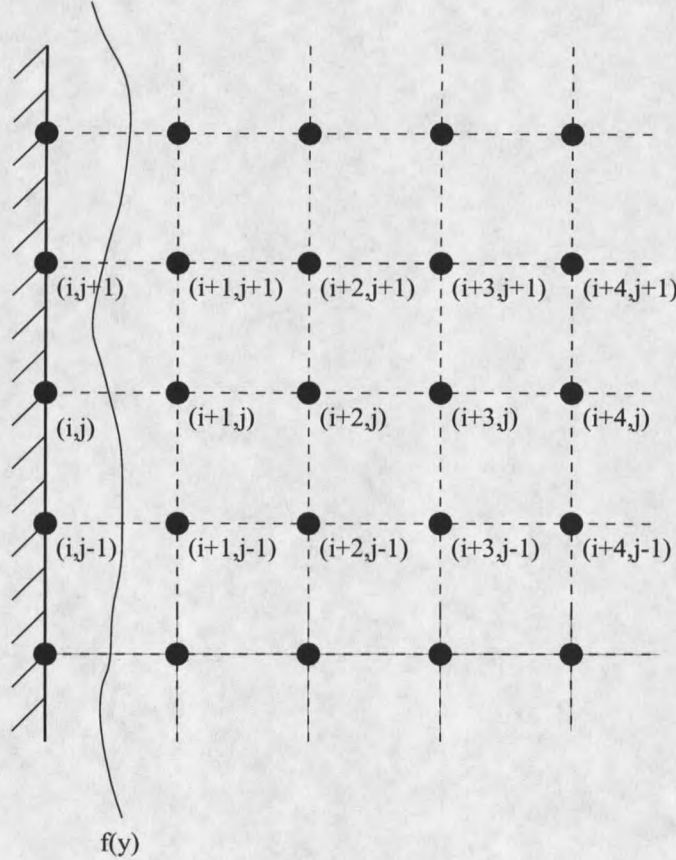


Figure 36. Vertical wall with perturbation to right.

For a vertical wall with nodes on left side, the perturbation expression for a Dirichlet boundary condition becomes

$$u(x_0, y) + \frac{\partial u}{\partial x}(x_0, y)[x_0 - f(y)] + \frac{\partial^2 u}{\partial x^2}(x_0, y) \frac{[x_0 - f(y)]^2}{2!} = u(f(y), y) = g_0(y) \quad (\text{B.10})$$

and for Neumann boundary condition

$$u_y(x_0, y) + \frac{\partial^2 u}{\partial x^2}(x_0, y)[x_0 - f(y)] + \frac{\partial^3 u}{\partial x^3}(x_0, y) \frac{[x_0 - f(y)]^2}{2!} = u(f(y), y) = g_1(y) \quad (\text{B.11})$$

Interior corners have two directions for which a perturbation can be used. A general perturbation expression could be obtained from a Taylor expansion about both directions but the approach taken here is to use a perturbation for each direction of interior normal and use expressions found previously for horizontal and vertical walls.

Numerical Formulation

The derivative terms in equations (B.3) and (B.5) are evaluated numerically using finite difference expression. Boresi and Chong (1991) provide one-sided forward difference expressions which can be used to provide discrete versions of (B.3) and (B.5). The question of which difference expressions to use is answered by the solution method for mathematical problem which was chosen in Chapter 4. In Chapter 4 the discretised equations for interior nodes are written and expressions for boundary nodes are used to replace the unknown boundary value in the equations for interior nodes.

It would appear that second order finite difference expressions could be used for $\partial u / \partial y$ and $\partial^2 u / \partial y^2$ to result in a discretised version of (B.3). Second order finite difference expressions involving the two nodes (x_i, y_{j+1}) and (x_i, y_{j+2}) normal to the boundary node (x_i, y_j) could be used to obtain an expression for $u(x_i, y_j)$ from (B.3).

Equation (B.5) contains the third order term $\partial^3 u / \partial y^3$ which requires more nodes normal to boundary to achieve a finite difference representation. Fourth order finite difference expressions are available (Boresi and Chong, 1991) containing the four nodes (x_i, y_{j+1}) , (x_i, y_{j+2}) , (x_i, y_{j+3}) , and (x_i, y_{j+4}) normal to the boundary node (x_i, y_j) . These also provide a more accurate approximation of the derivative terms than second order approximations. This can come at a price of greater solution difficulty.

$$\left. \frac{\partial u}{\partial y} \right)_{(x_i, y_j)} \approx \frac{-50u_{i,j} + 96u_{i,j+1} - 72u_{i,j+2} + 32u_{i,j+3} - 6u_{i,j+4}}{24h} \quad (\text{B.12})$$

$$\left. \frac{\partial^2 u}{\partial y^2} \right|_{(x_i, y_j)} \approx \frac{35u_{i,j} - 104u_{i,j+1} + 114u_{i,j+2} - 56u_{i,j+3} + 11u_{i,j+4}}{12h^2} \quad (\text{B.13})$$

where $u_{i,j} = u(x_i, y_j)$, $u_{i,j+1} = u(x_i, y_{j+1})$ etc. Note that (B.12) and (B.13) assume uniform mesh size which restricts the mesh size near wall to be uniform for at least four mesh spaces from wall.

Use of a fourth order accurate finite difference expression may seem to be a waste of computer storage and does not increase the accuracy of the interior solution which is only second order accurate (see Chapter 4). However, an advantage of using the fourth order finite difference expressions is when solving the discretised equation for the value $u_{i,j}$ to be replaced in equation formed for interior node.

Letting $L_f(x_i) = f(x_i) - y_j$ and substituting (B.12) and (B.13) into (B.3) and solving for $u_{i,j} = u(x_i, y_j)$ yields

$$\begin{aligned} u_{i,j} = & -\frac{L_f(96h - 104L_f)}{24h^2 - 50hL_f + 35L_f^2}u_{i,j+1} - \frac{L_f(-72h + 114L_f)}{24h^2 - 50hL_f + 35L_f^2}u_{i,j+2} \\ & -\frac{L_f(32h - 56L_f)}{24h^2 - 50hL_f + 35L_f^2}u_{i,j+3} - \frac{L_f(-6h + 11L_f)}{24h^2 - 50hL_f + 35L_f^2}u_{i,j+4} \\ & + \frac{24h^2}{24h^2 - 50hL_f + 35L_f^2}u(x_i, f(x_i)) \end{aligned} \quad (\text{B.14})$$

The denominator of the coefficients in (B.14) has complex zeros of value $(0.7143 \pm 0.4189i)h$ which means that denominator does not go to zero.

For the discretised version of (B.3) the result is using forward difference for the derivative is:

$$u(x_i, y_j) + \frac{u(x_i, y_{j+1}) - u(x_i, y_j)}{\Delta y}(f(x_i) - y_j) = g(x_i) \quad (\text{B.15})$$

For the Neumann boundary condition (B.5), it is necessary to have $\partial^3 u / \partial y^3$ for which a fourth order finite difference expression is (Boresi and Chong, 1991)

$$\left. \frac{\partial^3 u}{\partial y^3} \right|_{(x_i, y_j)} \approx \frac{-10u_{i,j} + 36u_{i,j+1} - 48u_{i,j+2} + 28u_{i,j+3} - 6u_{i,j+4}}{4h^3} \quad (\text{B.16})$$

Applying (B.12), (B.13) and (B.16) to equation (B.5) and solving for $u_{i,j}$ results in

$$\begin{aligned}
 u_{i,j} = & -\frac{96h^2 - 208hL_f + 108L_f^2}{-50h^2 + 70hL_f - 30L_f^2}u_{i,j+1} - \frac{-72h^2 + 228hL_f - 144L_f^2}{-50h^2 + 70hL_f - 30L_f^2}u_{i,j+2} \\
 & -\frac{32h^2 - 112hL_f + 84L_f^2}{-50h^2 + 70hL_f - 30L_f^2}u_{i,j+3} - \frac{-6h^2 + 22hL_f - 18L_f^2}{-50h^2 + 70hL_f - 30L_f^2}u_{i,j+4} \\
 & + \frac{24h^3}{-50h^2 + 70hL_f - 30L_f^2}u_y(x_i, f(x_i))
 \end{aligned} \tag{B.17}$$

as an discretised expression for (B.5). The roots in the denominators of the coefficients in equation (B.17) are complex with values $(1.1667 \pm 0.5528i)h$ so the denominator does not have any real zeros.

Equations (B.6) and (B.7) require the use of backward difference formulas for approximation of the derivatives in them. Fourth order finite difference expressions are available (Boresi and Chong, 1991) for $\partial u / \partial y$, in terms of four nodes (x_i, y_{j-1}) , (x_i, y_{j-2}) , (x_i, y_{j-3}) , and (x_i, y_{j-4}) backward of node (x_i, y_j) $\partial^2 u / \partial y^2$, and $\partial^3 u / \partial y^3$.

$$\left. \frac{\partial u}{\partial y} \right|_{(x_i, y_j)} \approx -\frac{-50u_{i,j} + 96u_{i,j-1} - 72u_{i,j-2} + 32u_{i,j-3} - 6u_{i,j-4}}{24h} \tag{B.18}$$

$$\left. \frac{\partial^2 u}{\partial y^2} \right|_{(x_i, y_j)} \approx \frac{35u_{i,j} - 104u_{i,j-1} + 114u_{i,j-2} - 56u_{i,j-3} + 11u_{i,j-4}}{12h^2} \tag{B.19}$$

$$\left. \frac{\partial^3 u}{\partial y^3} \right|_{(x_i, y_j)} \approx -\frac{-10u_{i,j} + 36u_{i,j-1} - 48u_{i,j-2} + 28u_{i,j-3} - 6u_{i,j-4}}{4h^3} \tag{B.20}$$

Insertion of (B.18) and (B.19) for $\partial u / \partial y$ and $\partial^2 u / \partial y^2$ respectively into equation (B.6) and letting $L_f(x) = y_0 - f(x)$ and solving for $u_{i,j}$ results in

$$\begin{aligned}
 u_{i,j} = & -\frac{L_f(96h - 104L_f)}{24h^2 - 50hL_f + 35L_f^2}u_{i,j-1} - \frac{L_f(-72h + 114L_f)}{24h^2 - 50hL_f + 35L_f^2}u_{i,j-2} \\
 & -\frac{L_f(32h - 56L_f)}{24h^2 - 50hL_f + 35L_f^2}u_{i,j-3} - \frac{L_f(-6h + 11L_f)}{24h^2 - 50hL_f + 35L_f^2}u_{i,j-4} \\
 & + \frac{24h^2}{24h^2 - 50hL_f + 35L_f^2}u(x_i, f(x_i))
 \end{aligned} \tag{B.21}$$

for the perturbation of a top wall with Dirichlet boundary condition.

Inserting (B.18), (B.19), and (B.19) for $\partial u/\partial y$, $\partial^2 u/\partial y^2$, and $\partial^3 u/\partial y^3$ respectively into equation (B.7) and solving for $u_{i,j}$ results in

$$\begin{aligned}
 u_{i,j} = & -\frac{96h^2 - 208hL_f + 108L_f^2}{-50h^2 + 70hL_f - 30L_f^2} u_{i,j-1} - \frac{-72h^2 + 228hL_f - 144L_f^2}{-50h^2 + 70hL_f - 30L_f^2} u_{i,j-2} \\
 & -\frac{32h^2 - 112hL_f + 84L_f^2}{-50h^2 + 70hL_f - 30L_f^2} u_{i,j-3} - \frac{-6h^2 + 22hL_f - 18L_f^2}{-50h^2 + 70hL_f - 30L_f^2} u_{i,j-4} \\
 & + \frac{24h^3}{-50h^2 + 70hL_f - 30L_f^2} u_y(x_i, f(x_i))
 \end{aligned} \quad (B.22)$$

for perturbation of a top wall with Neumann boundary condition.

For numerical solution of (B.8) and (B.9) expressions for $\partial u/\partial x$ and $\partial^2 \partial x^2$ are available (Boresi and Chong, 1991) and are similar to (B.12) and (B.13) with x replacing y and j constant and i varying. Use of these finite difference formula in equation (B.8) and $L_f(y_j) = f(y_j) - x_i$ results in

$$\begin{aligned}
 u_{i,j} = & -\frac{L_f(96h - 104L_f)}{24h^2 - 50hL_f + 35L_f^2} u_{i+1,j} - \frac{L_f(-72h + 114L_f)}{24h^2 - 50hL_f + 35L_f^2} u_{i+2,j} \\
 & -\frac{L_f(32h - 56L_f)}{24h^2 - 50hL_f + 35L_f^2} u_{i+3,j} - \frac{L_f(-6h + 11L_f)}{24h^2 - 50hL_f + 35L_f^2} u_{i+4,j} \\
 & + \frac{24h^2}{24h^2 - 50hL_f + 35L_f^2} u(f(y_j), y_j)
 \end{aligned} \quad (B.23)$$

for the Dirichlet boundary condition.

For the Neumann boundary condition the result is

$$\begin{aligned}
 u_{i,j} = & -\frac{96h^2 - 208hL_f + 108L_f^2}{-50h^2 + 70hL_f - 30L_f^2} u_{i+1,j} - \frac{-72h^2 + 228hL_f - 144L_f^2}{-50h^2 + 70hL_f - 30L_f^2} u_{i+2,j} \\
 & -\frac{32h^2 - 112hL_f + 84L_f^2}{-50h^2 + 70hL_f - 30L_f^2} u_{i+3,j} - \frac{-6h^2 + 22hL_f - 18L_f^2}{-50h^2 + 70hL_f - 30L_f^2} u_{i+4,j} \\
 & + \frac{24h^3}{-50h^2 + 70hL_f - 30L_f^2} u_y(f(y_j), y_j)
 \end{aligned} \quad (B.24)$$

for a wall with nodes to right.

Expressions for vertical walls with nodes to left with $L_f(y_j) = x_i - f(y_j)$ become

$$u_{i,j} = -\frac{L_f(96h - 104L_f)}{24h^2 - 50hL_f + 35L_f^2} u_{i-1,j} - \frac{L_f(-72h + 114L_f)}{24h^2 - 50hL_f + 35L_f^2} u_{i-2,j}$$

$$\begin{aligned}
& -\frac{L_f(32h - 56L_f)}{24h^2 - 50hL_f + 35L_f^2}u_{i-3,j} - \frac{L_f(-6h + 11L_f)}{24h^2 - 50hL_f + 35L_f^2}u_{i-4,j} \\
& + \frac{24h^2}{24h^2 - 50hL_f + 35L_f^2}u(f(y_j), y_j)
\end{aligned} \tag{B.25}$$

for the Dirichlet boundary condition.

For the Neumann boundary condition the result is

$$\begin{aligned}
u_{i,j} = & -\frac{96h^2 - 208hL_f + 108L_f^2}{-50h^2 + 70hL_f - 30L_f^2}u_{i-1,j} - \frac{-72h^2 + 228hL_f - 144L_f^2}{-50h^2 + 70hL_f - 30L_f^2}u_{i-2,j} \\
& -\frac{32h^2 - 112hL_f + 84L_f^2}{-50h^2 + 70hL_f - 30L_f^2}u_{i-3,j} - \frac{-6h^2 + 22hL_f - 18L_f^2}{-50h^2 + 70hL_f - 30L_f^2}u_{i-4,j} \\
& + \frac{24h^3}{-50h^2 + 70hL_f - 30L_f^2}u_y(f(y_j), y_j)
\end{aligned} \tag{B.26}$$

for a wall with nodes to left.

APPENDIX C
Numerical Validation Tests

This appendix contains the results of some numerical validation tests performed to check the numerical solution.

Consider the sequence of mesh spacings $\{\frac{1}{5}, \frac{1}{8}, \frac{1}{10}, \frac{1}{16}, \frac{1}{20}, \frac{1}{25}, \frac{1}{32}, \frac{1}{40}, \frac{1}{50}, \frac{1}{64}, \frac{1}{80}\}$ which can be used to generate convergence information. If desired the sequence could be continued on until desired error is obtained. The sequence given above is enough to demonstrate the convergence rate of the method. Given significant computing resources, the sequence could be extended if desired. To measure the error the following mathematical norms may be used.

Let $u \in \mathfrak{R}^M$, where $u = (u_1, u_2, \dots, u_{M-1}, u_M)$, $u_j \in \mathfrak{R}$. It is useful to define some mathematical norms to get a measure of difference of solutions. The ℓ_∞ norm, or *inf* norm, is defined as:

$$\|u\|_\infty = \max_{1 \leq j \leq M} |u_j| \quad (\text{C.1})$$

the ℓ_1 norm is defined as:

$$\|u\|_1 = \sum_{j=1}^M |u_j| \quad (\text{C.2})$$

and the ℓ_2 norm is defined as:

$$\|u\|_2 = \left(\sum_{j=1}^M |u_j|^2 \right)^{1/2} \quad (\text{C.3})$$

The root mean squared (RMS) norm is defined as:

$$\|u\|_{\text{RMS}} = \left(\frac{1}{M} \sum_{j=1}^M |u_j|^2 \right)^{1/2} \quad (\text{C.4})$$

The use of these norms will allow information about the convergence of the numerical solution to the analytical solution when one is known. Even if an analytical solution is not known, these norms can provide information on how refinements in mesh size change the numerical solution.

Velocity

For a straight tube with fully developed velocity profile, analytical solutions are available for example the profile for laminar flow between two parallel plates.

The order of convergence can be given by from estimate

$$O_{error} = \frac{\log(e_{N_1}/e_{N_2})}{\log(h_{N_1}/h_{N_2})} \quad (C.5)$$

where e_N the error with mesh spacing h_N .

The analytical velocity solution for fully developed uniform flow between two parallel plates is available (Bird et al., 1960; Shames, 1982; Malvern, 1969) to compare with numerical solution. Availability of the analytical solution allows direct comparison with numerical solution to determine convergence of numerical solution as mesh size h is reduced for a uniform mesh. Since second order expressions for derivative terms were used in numerical discretization, it is anticipated that the order of convergence will be $O(h^2)$. While the velocity components are derivatives of the stream function it would seem that the order of velocity convergence would be less than order of stream function. However, the vorticity is solved using second order formulation and the vorticity is derivatives of the velocity components. This combination provides second order convergence of the velocity components.

The convergence of the numerical solution to the analytical solution will depend on the mesh size and the Reynolds number for the flow rate between the parallel plates. Three different Reynolds numbers are analyzed to determine effect of Reynolds number on solution convergence. Tables 5-7 contain convergence data for Reynolds numbers of 0.1, 1.0, and 10.0 respectively.

The accuracy of the solutions shows little dependence on the Reynolds number for $0.1 \leq Re_{L_\infty} \leq 10$.

A plot of the convergence curves for the three different Reynolds numbers is shown in Figure 37. Best fit lines can be obtained for the three convergence curves shown in Figure 37 in terms of the Reynolds number and mesh size h by fitting a curve of form

$$\|u_h - u_e\| = C Re^a h^b \quad (C.6)$$

Table 5. Tube velocity solution error for $Re_{L\infty} = 0.1$.

h	$\ \mathbf{u}_h - \mathbf{u}_e\ _\infty$
0.20000000	0.16000000
0.12500000	0.06260000
0.10000000	0.04000000
0.06250000	0.01562500
0.05000000	0.01000000
0.04000000	0.00640000
0.03125000	0.00390625
0.02500000	0.00250000
0.02000000	0.00160000
0.01250000	0.00062500

Table 6. Tube velocity solution error for $Re_{L\infty} = 1.0$.

h	$\ \mathbf{u}_h - \mathbf{u}_e\ _\infty$
0.20000000	0.16000000
0.12500000	0.06250000
0.10000000	0.04000000
0.06250000	0.01562500
0.05000000	0.01000000
0.04000000	0.00640000
0.03125000	0.00390625
0.02500000	0.00250000
0.02000000	0.00160000
0.01250000	0.00062500

Table 7. Tube velocity solution error for $Re_{L_\infty} = 10.0$.

h	$\ \mathbf{u}_h - \mathbf{u}_e\ _\infty$
0.20000000	0.16000000
0.12500000	0.06250000
0.10000000	0.04000000
0.06250000	0.01562500
0.05000000	0.01000000
0.04000000	0.00640000
0.03125000	0.00390625
0.02500000	0.00250000
0.02000000	0.00160000
0.01250000	0.00062500

to obtain parameters a and b for best fit.

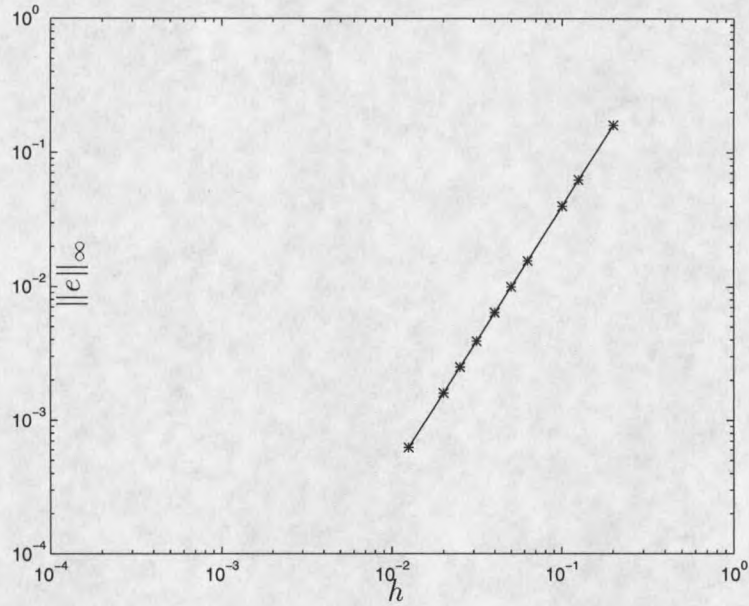


Figure 37. Plot of velocity solution error for parallel plates.

From the data contained in Tables 5–7, the method shows $b \approx 2$. These values of parameters indicate second order convergence in mesh size h . Over the range of Reynolds numbers evaluated at, there was very little influence of the Reynolds number

on accuracy of the solution.

Concentration

It is also necessary to evaluation solution to concentration solutions for the model. The problem of heat/mass transfer in a circular conduit is generally referred to as the Graetz problem (Mikhailov and Özisik, 1984; Shah and London, 1978; Shah and Bhatti, 1987). For problems of constant cross sectional area other than circular conduit, these problems are referred to as Graetz type problems. This problem is generally solved for fully hydrodynamic developed flow in a pipe or between two parallel plates. Much work on solving this problem has been undertaken in the area of heat transfer in a fluid flowing in laminar range. Using the analogy of equations for heat and mass transfer, analytical solutions for heat transfer can be used for validation of numerical solution of the species balance problem.

Solution for the Graetz Graetz problem is usually with Dirichlet or Neumann wall boundary conditions. Since the iterative procedure used to solve the concentration equations in bulk is coupled with biofilm equations for concentration through flux boundary conditions applied to the concentration equation, the solution to the extended Graetz problem with Neumann boundary condition provides a test for numerical errors formulation errors. The Graetz solution neglects axial conduction which leads to an over estimation of the temperature field in the entrances vicinity (Yin and Bau, 1996). Use of the Graetz solution provides a check on the behavior of the numerical solution but exact analytical versus numerical comparison is not appropriate.

The problem solution will have two distinct regions. With a uniform inlet substrate concentration, there will be a developing concentration profile which will eventually obtain a shape which is maintained down the axial direction with decreasing maximum concentration.

The numerical solution was lower on the boundaries than the Graetz solution near the entrance as expected (Yin and Bau, 1996). Further along the flow path, the numerical solution for the wall was slightly larger than the Graetz solution which is characteristic (Yin and Bau, 1996).

Biofilm

The numerical solution of the biofilm equations also need to be validated. One approach is to use a sequence of meshes in the biofilm to obtain error estimates. Note that a single mesh for the bulk will be used and changes in biofilm solution will be analyzed. Different parts of biofilm solution can be looked at. The interface flux can be looked at for all mesh values to see changes and values of flux at h and $h/2$ can be compared to see convergence rates for flux. Substrate concentration can also be evaluated using mesh refinement from h to $h/2$. If one assumes a fixed value of the substrate concentration at the biofilm surface, the biofilm equations can be tested as a stand alone test. Accuracy of the biofilm solution is expected to depend on number of points in the biofilm and film thickness. It is useful to look at accuracy of biofilm equations as function of surface concentration and biofilm thickness. A analytical solution is not available for Monod kinetics, but for thin biofilms or high surface substrate concentration, the biofilm can be fully penetrated which allows approximate analytical solution.

Figure 38 contains a plot of the maximum error as a function of the mesh size used. This biofilm was $300\text{ }\mu\text{m}$ thick with $V_{\text{max}}/D_f = 3000\text{ mg/L/cm}^2$ and $K_s = 0.1\text{ mg/L}$. The finest mesh ($h = 3\text{ }\mu\text{m}$), was used as the true solution for comparison. This figure shows the convergence rate is approximately second order.

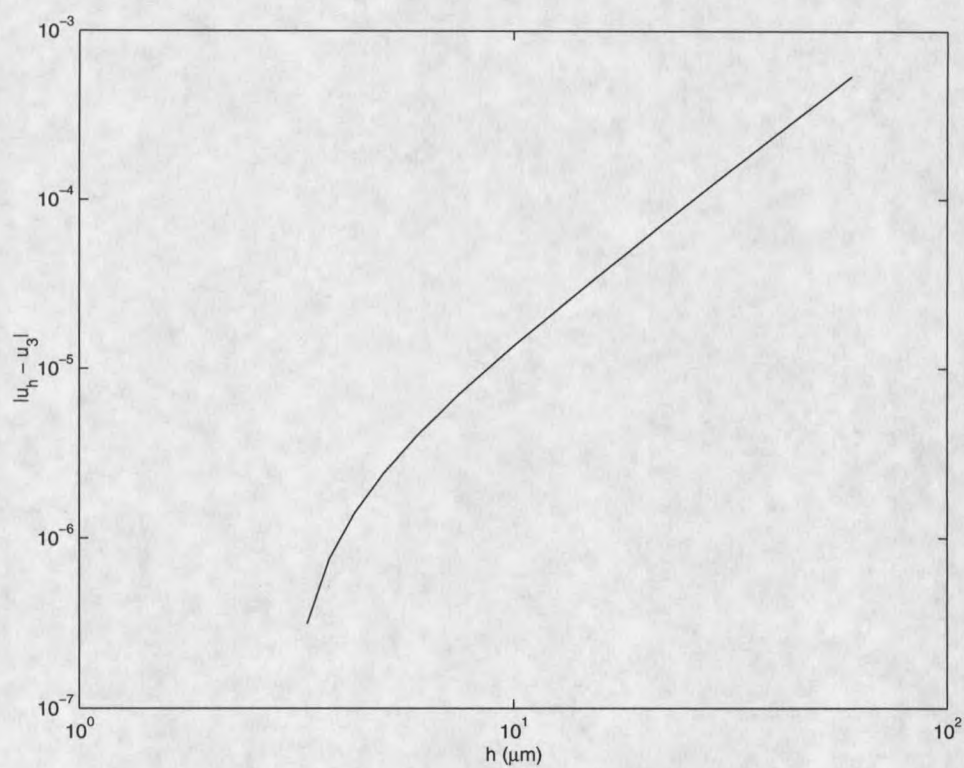


Figure 38. Plot of biofilm equation solution error as a function of mesh size (h).

Perturbation Scheme

The influence of the perturbation scheme on the velocity and concentration solutions needs to be examined. Examination of this will allow assessment of need for use of perturbation expression. For a straight tube with biofilm in significant stretch of tube of constant thickness, the velocity profile should be fully developed parabolic flow which allows assessment of accuracy of perturbation scheme.

The case when $L_f = 0$ should produce comparable results to other methods for the solution of the Navier-Stokes equations for fluid velocity. The numerical tests for the velocity solution in a tube used the perturbation formulation with $L_f = 0$. The results that were found were in close agreement with the analytical solution.

For non zero L_f values, a few results are shown here which demonstrate the ability of the perturbation scheme to predict the velocity around biofilm patches. A contour plot of the u velocity component with patches of biofilm located on the wall of a tube is shown in Figure 39. In this simulations the nondimensional biofilm thickness is 0.003 cm and the zero contour line reflects the position of the biofilm rather well.

The perturbation scheme was implemented under assumption of small changes which such as shown in Figure 40. Biofilm thickness varies in a sinusoidal manner along the channel length. In this example, the change in L_f is small along the flow length and the u velocity component follows the biofilm surface. Figure 40 is not to scale so the variation of the biofilm surface over the length of the biofilm is exaggerated. This example does show that for a smooth transition in the biofilm thickness, the perturbation scheme provides a smooth transition in the velocity solution to match the biofilm surface.

The perturbation scheme used in this dissertation allows a non zero velocity on the boundary of the original mesh in order to obtain a zero velocity at the biofilm/fluid interface. The velocity on the boundary is not used in the numerical solution of the

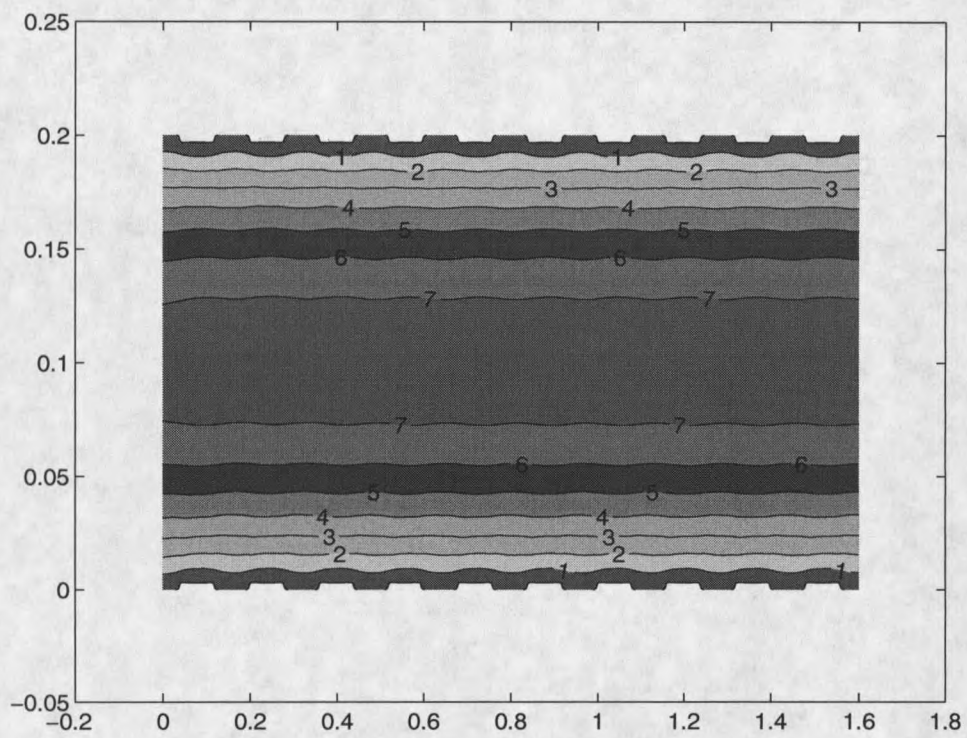


Figure 39. U Velocity contours for a patchy biofilm using perturbation scheme with biofilm thickness of $300\mu\text{m}$.

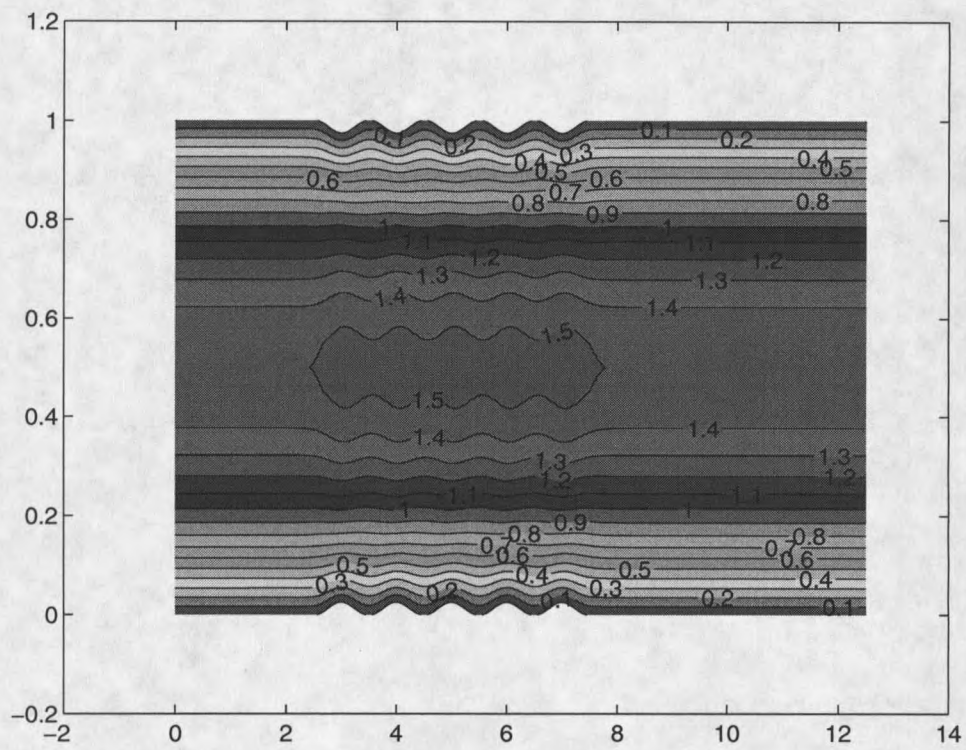


Figure 40. U velocity contours around a wavy biofilm.

species balance equation so this is not a severe problem. Large changes from one node to the next, did exhibit the vorticity increase similar to an interior corner.

Perturbation of the concentration equation does allow a slight flux to be applied at the boundary even when the biofilm flux is zero. The amount of this flux depends on the magnitude of the derivatives in the perturbation expansion. In practice, as the perturbation parameter approaches the mesh size, the error in flux can be around 20%. In the cases tested, the error was typically around 10 – 15% for perturbations that were equal to or greater than half the mesh size. This error depends on the local concentration solution and is not easily generalized.

APPENDIX D

Experimental Data and Kinetic Parameter Estimation

This appendix contains a description of dissolved oxygen (DO) profiles measurements taken from the bulk fluid into the biofilm with microsensor for the experimental setup is discussed in Chapter 4. A detailed description of the experimental setup, microsensor construction, and experimental procedure can be found elsewhere (Abrahamson, 1995).

Experimental Data

Dissolved oxygen (DO) profiles taken in the artificial biofilm patch can be used to obtain estimates of the local *in situ* biofilm kinetics parameters. Figure 41 shows the profile view of the sampling location for dissolved oxygen (DO) measurements. Thickness of the artificial biofilm at the sampling locations was estimated from inflections in the DO profiles and from estimates made while doing the sampling (Abrahamson, 1995).

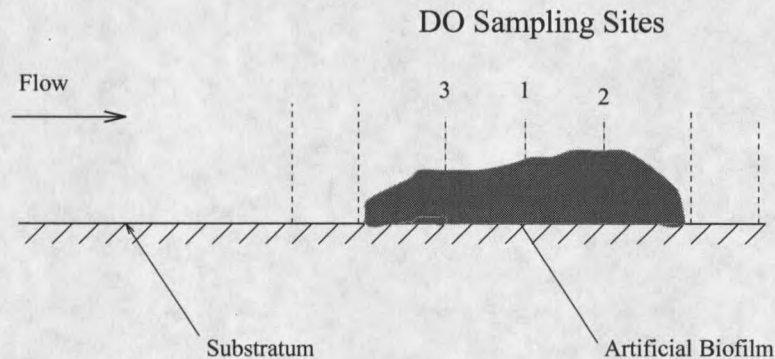


Figure 41. Dissolved oxygen sampling sites.

A plan view of the artificial biofilm patch is shown in Figure 42. Initially the artificial biofilm patch was planned to be of uniform height ($\approx 300\mu\text{m}$ in the channel). From the measured dissolved oxygen profiles, and observations while performing the experiment, the artificial biofilm patch may not have been uniformly thick. Since the surface the of the artificial biofilm patch was not completely mapped out to generate

map of the biofilm height, it was assumed to be constant across the cross section of the reactor corresponding to the measured sites.

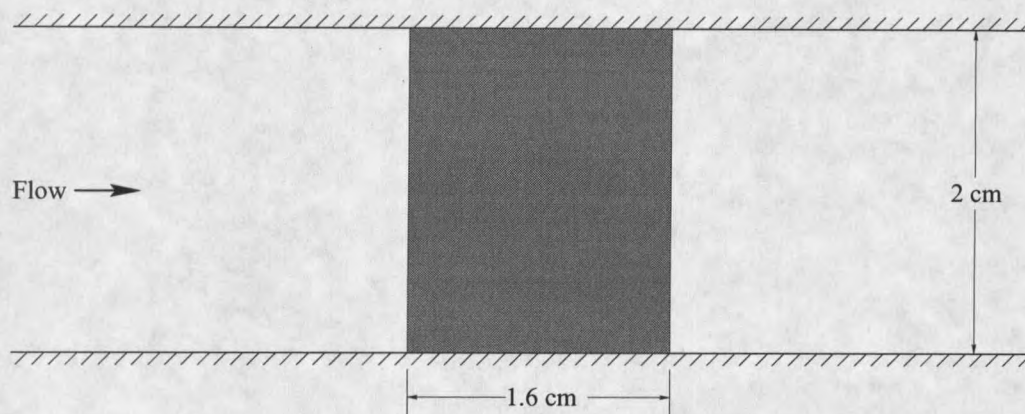


Figure 42. Plan view of open channel reactor with artificial biofilm patch used in the experiment.

The dissolved oxygen measurements taken at sites # 1, # 2, and # 3 were taken from the bulk down toward the artificial biofilm and near the vicinity of the substratum. The profiles are shown in Figures 43–45. Substratum location was estimated by last DO sampling point when it appeared that microprobe was in danger of physically contacting the substratum and damaging the probe.

Dissolved oxygen measurements shown in the figures have the nearest data point to substratum listed as the 0 value. In reality, this is not the true substratum location, but the actual value should be close to this location. This is characteristic of all the measured dissolved oxygen profiles. If during the experiment the probe is observed approaching the substratum and the experimenter slows the approach rate it is possible to come close to the substratum.

There is some variability evident in Figures 43–45. Some variability is expected in the dissolved oxygen measurements, although a uniform region is expected for part of the bulk fluid region until the diffusive boundary layer starts. Part of the

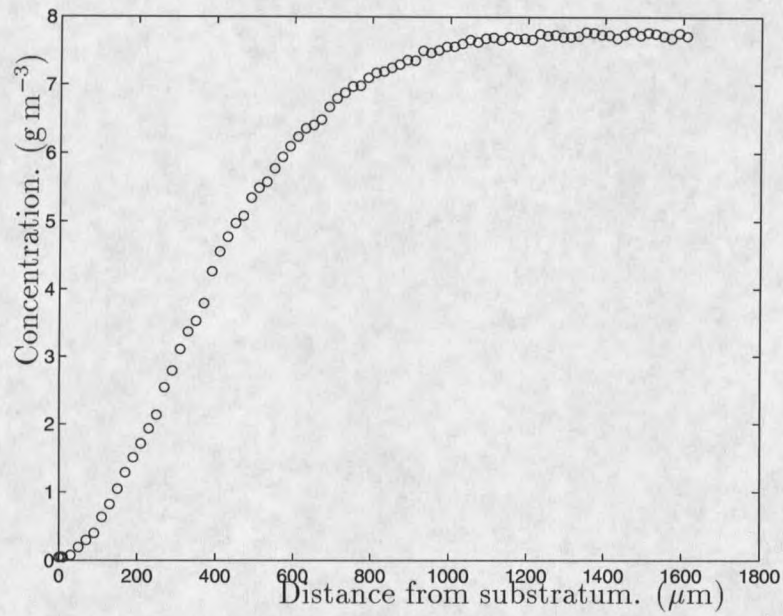


Figure 43. Experimental dissolved oxygen measurements at site # 1.

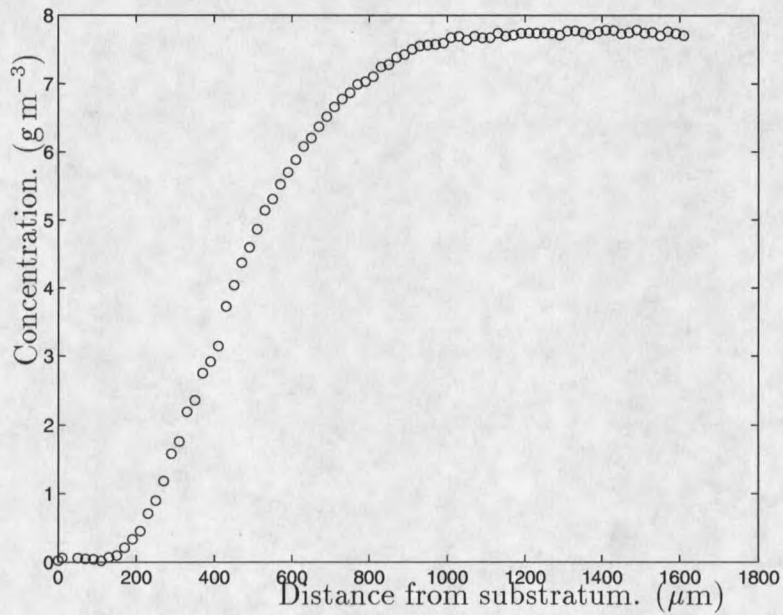


Figure 44. Experimental dissolved oxygen measurements at site # 2.

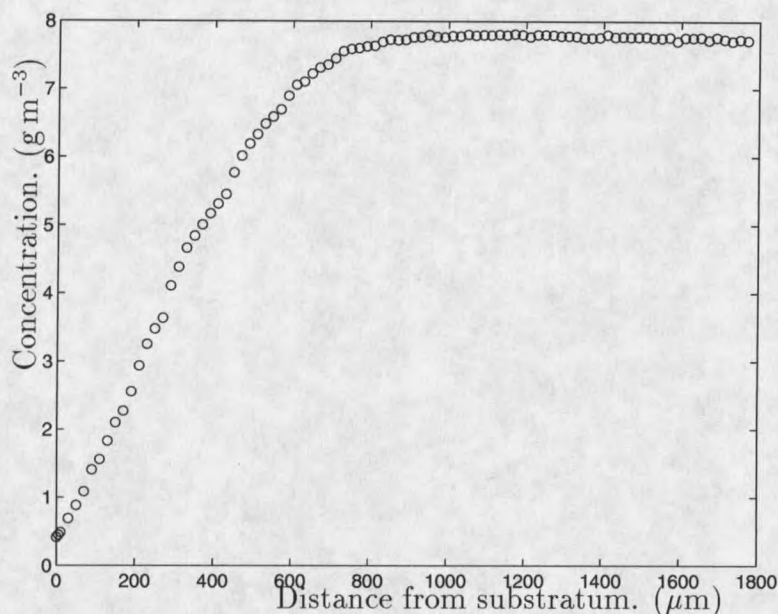


Figure 45. Experimental dissolved oxygen measurements at site # 3.

dissolved oxygen profiles in the bulk fluid region appear uniform around some mean value. Using the last 20 points in the bulk fluid region, the mean and standard deviation values were calculated for these three profiles. Values of these parameters are tabulated in Table 8.

Table 8. Calculated means and variances of dissolved oxygen measurements in the bulk fluid region.

Site #	$\bar{c}$ (mg L ⁻¹)	σ_c (mg L ⁻¹)	C. V.
1	7.737	0.02857	0.003693
2	7.746	0.02539	0.003278
3	7.755	0.02406	0.003103

The consumption of oxygen by the biofilm leads to development of a concentration boundary layer sometimes called the diffusive boundary layer (DBL) (Jørgensen and Revsbech, 1985; Jørgensen and Des Marais, 1990). An experiment with a higher

velocity showed a decrease in the effective diffusive boundary thickness as estimated from the dissolved oxygen profiles (Abrahamson, 1995). This behavior is consistent with other observations in biofilm systems (de Beer et al., 1997) and microbial mats (Jørgensen and Revsbech, 1985; Jørgensen and Des Marais, 1990).

The unknown distance from the substratum to the last measured DO value taken is expected to be small. Visual observation of microprobe movement via a light microscope enabled monitoring of the progress and termination when the microprobe appeared to be close to the substratum. In general the microprobe movement would be terminated if it appeared that the next step would put the probe in contact with the substratum. As a result of this termination of movement, there is some error associated with the exact location of the substratum relative to the measured dissolved oxygen profiles.

This unknown value of offset to the spatial locations of the DO profiles could influence the analysis of the data when estimating kinetic parameters. Influence of this unknown substratum location will probably be more significant when biofilm is fully penetrated by the dissolved oxygen. This is anticipated when applying the standard "no flux" boundary condition at the substratum when modeling the biofilm using a reaction diffusion equation. This unknown offset distance from last DO reading to the substratum may vary between profiles. A more sophisticated experimental setup might be able to quantify this offset and keep it approximately uniform among profiles sampled at different locations.

Kinetic Parameter Estimation

Lewandowski et al. (1991) fit a 3rd order polynomial to the DO concentration profile and differentiate it to obtain the kinetic parameters (K_s , $V_{\max}$, D_f) in (4.1). This method does not work perfectly well for all the profiles as Abrahamson (1995) was able

to obtain kinetic parameter estimates for only one site sampled. Another disadvantage is that in general a curve fit to the DO data does not belong to the family of solutions to the model differential equation.

The method of parameter estimation proposed here uses the output least squares (OLS) method (Banks and Kunish, 1989). This results in solution of the differential equation containing for different values of the kinetic parameter values. Using the experimental data residuals are generated and the sum squared residual is formed. Minimization of the sum squared error was used to generate estimate the kinetic parameters $V_{\max}/D_f$ and K_s .

Prior to just running the kinetic parameter estimation procedure described here, some simulation tests were performed on synthetic data with known error. Initially, cases were run with zero error to determine the validity of the basic method. Error in this method can arise from numerical solution of the differential equation (4.1) and from the least squares routine used to obtain estimates of kinetic parameters.

Dissolved oxygen profiles taken from the well mixed region of the bulk water into the biofilm region tend to follow the typical profile shown in Figure 46. This typical profiles shows the biofilm region where equation (4.1) is assumed to hold. In the region outside of the biofilm, the dissolved oxygen profile is influenced by the fluid velocity above the biofilm and the diffusivity of oxygen. Jørgenson and Revsbech (1988) provided an example of measured dissolved oxygen profiles near a microbial mat as influenced by the fluid velocity over a range of fluid velocities. Influence of bulk fluid velocity on the diffusive boundary layer in biofilm systems has been reported (de Beer, Stoodley, Roe and Lewandowski, 1994; Lewandowski et al., 1994; de Beer et al., 1997; de Beer, Stoodley and Lewandowski, 1994).

As the fluid velocity is increased the dissolved oxygen profile outside the microbial mat becomes steeper with the effective concentration boundary layer thick-

ness decreasing and biofilm surface concentration increasing. The diffusive boundary thickness increases with distance from the start of a reaction with biofilm located on the surface. Once this diffusive boundary layer is fully developed it can be approximately constant for a uniform surface with uniform surface flux. In general, the effective thickness correlations will be listed in terms of Reynolds and Schmidt numbers (Cussler, 1984; Weber and DiGiano, 1996).

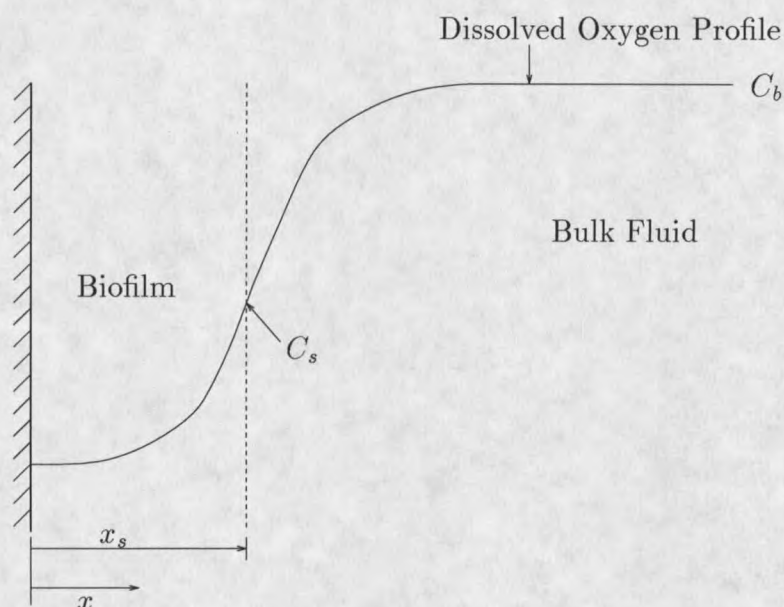


Figure 46. Sketch of typical dissolved oxygen profile.

One problem that may arise is when the curve that is a best fit does not match the behavior or assumptions of the model that is trying to be used. This arises when the curve is not part of the allowable solutions to the model equations. Given that the diffusion reaction equation with Monod kinetic model does not have an analytical solution, curves generated from standard curve fit programs are not solutions to the differential equation.

An alternative technique to determine the parameters $V_{\max}$, K_s , and D_f in

equation (4.1) is to write equation (4.1) as

$$0 = \frac{d^2 C}{dx^2} - \frac{V_{\max}}{D_f} \frac{C}{K_s + C} \quad (\text{D.7})$$

which has two parameters $\frac{V_{\max}}{D_f}$ and K_s which control the solution behavior. For the steady-state case it is the ration of $\frac{V_{\max}}{D_f}$ which controls the behavior. Let $C(x, \frac{V_{\max}}{D_f}, K_s)$ denote the solution to equation (D.7) subject to appropriate boundary conditions. This approach is to find the values of $\frac{V_{\max}}{D_f}$ and K_s corresponding to the function from this family which best fits the experimental data in the least squares sense.

Let (x_i, C_i) , $i = 1 \dots n$, be n experimental observations taken within the biofilm each consisting of a distance from the substratum, x_i , and a substrate concentration measurement, C_i . The objective then becomes to minimize the function

$$J(\frac{V_{\max}}{D_f}, K_s) = \sum_{i=1}^n \left[C(\frac{V_{\max}}{D_f}, K_s; x_i) - C_i \right]^2 \quad (\text{D.8})$$

over U_{ad} which is an admissible set of parameters. The allowable parameter space for the the values of $\frac{V_{\max}}{D_f}$ and K_s are the positive reals. In reality the parameters are bounded below by 0 and a upper bound of ∞ . In most problems of this nature the actual allowable space could be defined much smaller by imposing a finite upper bound on the parameters with zero as lower bound. Order of magnitude estimates could be found from the literature which could be multiplied by a large number to establish upper bounds.

This method is a finite dimensional version of the Output Least Squares (OLS) method outlined by Banks and Kunish (1989) which has been applied to various parameter estimation problems involving both ordinary and partial differential equations.

The OLS method for parameter estimation can be described as follows. Define

the parameter map, Φ , by

$$\Phi\left(\frac{V_{\max}}{D_f}, K_s\right) = \begin{bmatrix} C\left(\frac{V_{\max}}{D_f}, K_s, x_1\right) \\ C\left(\frac{V_{\max}}{D_f}, K_s, x_2\right) \\ \vdots \\ C\left(\frac{V_{\max}}{D_f}, K_s, x_n\right) \end{bmatrix} \quad (\text{D.9})$$

This is simply the projection of the solution $C(\frac{V_{\max}}{D_f}, K_s)$ into n-dimensional Euclidean space created by evaluating the solution at the points $x_i, i = 1, \dots, n$.

Let $Q = \Phi(U_{\text{ad}})$ be the image of U_{ad} under the parameter to observation map Φ . Assuming a system parameter value $(\frac{V_{\max}}{D_f}, K_s)$ and a state observation C_{ob} is obtained by a process Γ which may also includes error ε . Due to the error C_{ob} will normally not be contained in Q . C_{ob} is then projected onto Q and Φ inverted to obtain the parameter estimates $((\frac{\widehat{V_{\max}}}{D_f}), \widehat{K_s})$. This process is illustrated graphically in Figure 47. The error ε in the data may be in the form of micro-sensor electro-mechanical noise and/or modeling error.

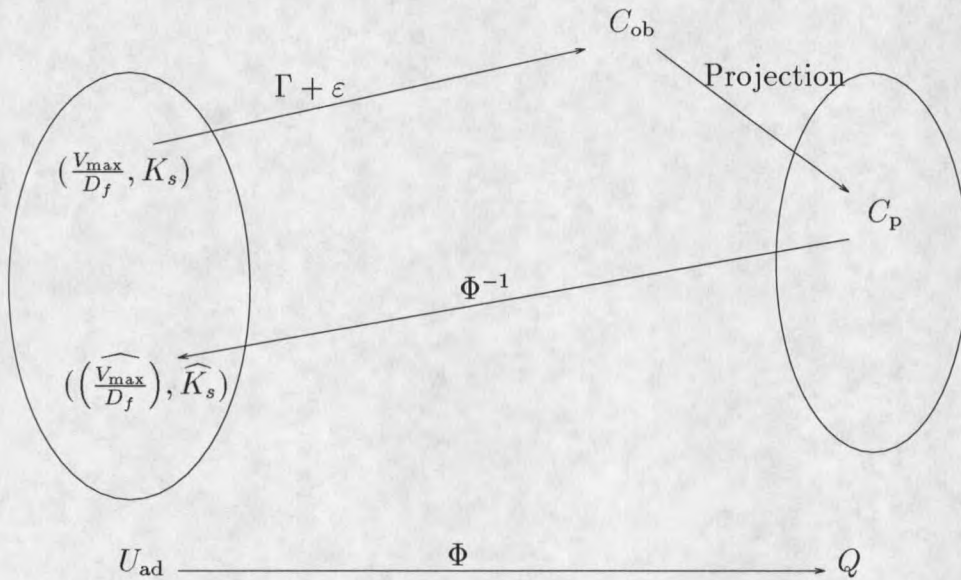


Figure 47. Schematic depiction of the Output Least Squares method.

Another source of error could be influence of the microprobe on the fluid flow

(Glud et al., 1994). This source of error would be expected to be influenced by the flow rate. In this work this is assumed to be negligible inside the artificial biofilm patch due to lack of convective flow but this may be more important in heterogeneous biofilms. Influence of the probe on fluid flow outside the biofilm could have an effect on the data taken outside the artificial biofilm patch.

The behavior of Φ is critical in the ability to accurately estimate the kinetic parameters. Under the assumption that solutions to equation (D.7) depend continuously on the values of the parameters $(\frac{V_{\max}}{D_f}, K_s)$, the parameter solution map is continuous and therefore J is a continuous function of $(\frac{V_{\max}}{D_f}, K_s)$. Assuming that U_{ad} is compact gives the existence of minimizing parameter values in U_{ad} . An example of such an admissible set would be a closed rectangle. This is a reasonable assumption as the lower bound for $\frac{V_{\max}}{D_f}$ and K_s can be taken as 0 while the upper bound could be estimated from literature values for K_s for oxygen and particular organism. Values of $\frac{V_{\max}}{D_f}$ could be estimated from the literature and multiplied by a large number to set an upper bound. The uniqueness of a minimizing parameter depends on the uniqueness of the projection of C_{ob} onto Q and the ability to invert Φ in a neighborhood of the projection C_p .

Implementation of the method requires construction of the parameter map to output map Φ . Since the model differential equation, (D.7), cannot be solved in closed form, this requires use of a nonlinear second order boundary value problem solver. Once the parameter to output map Φ is constructed, the minimization of the function J can be performed using a standard minimization or nonlinear least squares algorithm. The particular choice of both the boundary value solver and the minimization algorithm should be tailored to the individual problem.

Differential Equation Solution

Equation (D.7) holds for any distance inside the biofilm so theoretically the parameter space could be searched using some or all of the sampling points inside the biofilm. This would be useful if the exact location of the interface is not known.

Consider a collection of n sample points in the biofilm, (x_i, C_i) for $i = 1 \dots n$, with $x_1 < x_2 < \dots < x_n$. Let L_f denote the biofilm thickness such that $x_n = L \leq L_f$. Boundary conditions for equation (D.7) are a no flux boundary condition at the substratum

$$\frac{dC(0)}{dx} = 0 \quad (\text{D.10})$$

and a known concentration at L ($L \leq L_f$) is described by

$$C(L) = C_n . \quad (\text{D.11})$$

In practice the value of C_n may contain error so it is also a parameter that can be estimated in the least squares parameter estimation. If the biofilm thickness location is not known exactly it can be estimated from the inflection point in the dissolved oxygen profile.

The value of $C(L)$ is treated as a constant in the numerical solution of equation (D.7). While performing the parameter estimation via the least squares routine, this parameter is allowed to vary. It is expected that the variation of this parameter is smaller than that of the two kinetic parameters desired. With this change the parameter map Φ is also a function of C_n which is implicitly part of the function J . Thus ultimately three parameters are to be estimated by the least squares routine. Error associated with C_n is expected to be small, assuming reasonable measurement error associated with the microsensor.

Equation (D.7) was solved numerically using second order centered finite difference expression for the second order derivative term and a second order centered

finite difference expression for the first order no flux boundary condition (D.10) at the substratum. This boundary condition is sometimes referred to as a *reflection boundary condition* and was implemented using a ghost node (Shamir and Harleman, 1967). For the boundary condition at the surface of the biofilm or the portion of the biofilm chosen for the estimation of parameters, the concentration was also a parameter to be estimated in least squares formulation. Newton's method was used to solve the resulting system of nonlinear equations. Initially the value was set to be the value of the last measured data point C_n . This value was then modified by the least squares optimization function to obtain a best fit.

For the numerical discretization of (D.7), let x_k , $k = 1, \dots, m$ represent a uniform discretization of $[0, L_f]$ such that $x_2 - x_1 = x_3 - x_2 = \dots = x_{k+1} - x_k = \dots = x_m - x_{m-1} = h$ with $0 = x_1 < x_2 < \dots < x_{m-1} < x_m = L \leq L_f$. Letting $C_k = C(x_k)$, $k = 1, \dots, m$ for this discretization results in the nonlinear system of equations to be solved

$$\begin{bmatrix} -2 & 2 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 1 & -2 & 1 \\ 0 & \cdots & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} C_1 \\ \vdots \\ C_k \\ \vdots \\ C_{m-1} \end{bmatrix} - h^2 \frac{V_{\max}}{D_f} \begin{bmatrix} \frac{C_1}{K_s + C_1} \\ \vdots \\ \frac{C_k}{K_s + C_k} \\ \vdots \\ \frac{C_{m-1}}{K_s + C_{m-1}} \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ \vdots \\ 0 \\ -C_m \end{bmatrix} \quad (\text{D.12})$$

The resulting nonlinear system of equations (D.12) was solved using Newton's method (Dennis and Schnable, 1983; Ascher et al., 1988). Newton's method or some alternative technique for nonlinear equations is necessary due the the nonlinear reaction term in (D.12). In solving the nonlinear system of equations, the reaction term to zero if the concentration was negative in order to maintain the correct sign of the reaction and the denominator did not become zero. The next guess was modified to be zero if it was less than zero. This step improved the convergence rate of Newton's method in some cases.

Initial parameter estimates were based on a small nonzero K_s value and a value of $\frac{V_{\max}}{D_f}$ obtained from a zero order kinetics estimate. The solution to (D.7) was obtained on a fine grid spacing ($m = 101$) for an initial guess of $\frac{V_{\max}}{D_f}$ and K_s . Alternatively, small nonzero estimates of parameters obtained from the literature could be used. The size of the grid should be selected to ensure resolution of the nonlinear term in (D.12). Analysis of the solution of the diffusion reaction differential equation should be performed to verify the differential equation solution.

Once the numerical solution to equation (D.12) was obtained it was interpolated to the sampled points using the `interp1` function in MATLAB ©(Mat, 1997a) with the cubic spline option. With the interpolated value at the the sampled points the sum squared error function (D.8) was formed.

Equation (D.8) was solved using the `leastsq` routine in the Optimization Toolbox (Mat, 1997b). This routine is a gradient based method of determining the optimal parameters. The minimizing parameter values were obtained using the Levenberg-Marquart algorithm (Dennis and Schnable, 1983). Other options using gradient based searching are available if desired. An alternative to gradient based methods is the simplex method (Nelder and Mead, 1965). This method is used by the `fmins` routine in MATLAB ©(Mat, 1997a).

This offset distance may have an influence on the estimation of kinetic parameters when the biofilm is fully penetrated. This is anticipated due to applying (D.10) at the last point when this point was not the true location of the substratum. If the last sample point is significantly away from the substratum, the required curvature in concentration profile may not be established enough to approach the boundary condition given by (D.10). A possible alternative solution procedure would be to apply a different boundary condition such as

$$C(x_0) = C_1 \quad (\text{D.13})$$

at the last sampled point. If a reliable estimate of the distance between the last sample point and the substratum was known, the original boundary condition (D.10) should be used.

Use of (D.13) would add an additional parameter, $\widehat{C}_1$, to be estimated. Application of this method could be influenced by noise in the data. For sufficiently small sampling intervals, the data would be expected to be uniformly distributed around the true value and a minor influence of end point would be expected. However, if the last point sampled happened to be an outlier, it may significantly influence the model concentration profile such that a strong deviation from the no flux boundary condition.

Another alternative would be to add a fourth parameter denoting the unknown distance from last measured point to the substratum, say δ , and estimate this distance from the parameter estimation routine used. These approaches are somewhat sensitive to the error in the sampled data. If the error is small, either approach may be expected to adequately estimate the kinetic parameters.

Simulation Case 1

For this simulation, a smaller value for K_s is used to more accurately reflect the fact that reported values of K_s for oxygen tend to be small. The biofilm film thickness for this case was 0.0400 cm with a surface concentration $C_s = 2.0 \text{ mg L}^{-1}$ and kinetic parameters $V_{\max}/D_f = 3000 \text{ mg L}^{-1} \text{ cm}^{-2}$ and $K_s = 0.1 \text{ mg L}^{-1}$. The differential equation was solved using $h = 0.0004 \text{ cm}$. Values of the resulting oxygen concentration were taken in 0.002 cm intervals resulting in 21 data points. These data points were then used for estimating the parameter values in three different cases using some or all of the sample data. Three different cases using different numbers of the data points were considered.

Case 1A uses all 21 data points and the estimated kinetic parameters are shown in Table 9. Values of the kinetic parameters show good agreement with the true values with relative error in the kinetic parameter estimates being less than 0.0004%. For Case 1B, just the first 11 points from the substratum are used as data for estimating the parameters. Estimates of the kinetic parameters are in Table 9. Values of the kinetic parameters show good agreement with true values with relative error of the kinetic parameters being less than 0.04%. Case 1C used the first 16 points from the substratum are used as the data for parameter estimation. Estimates of the kinetic parameters are in Table 9. Values of the kinetic parameters show good agreement with true values with the relative error being less than 0.07%.

Table 9. Kinetic parameter estimates obtained by least squares for cases 1A-1C.

Case #	$\frac{V_{max}}{D_f}$ (mg L ⁻¹ cm ⁻²)	Percent Error	K_s (mg L ⁻¹)	Percent Error
1A	3000.002724	9.8e-5	0.100000386	3.86e-4
1B	3000.253988	8.47e-3	0.1000327057	3.27e-2
1C	3000.497868	1.66e-2	0.1000648291	6.48e-2

Simulation Study 2

In this simulation study, the effect on the estimates of the parameters with a error in the estimation of the substratum is modeled. In this case the the substratum is actually 0.0005 cm farther away than the data would seem to indicate. This simulation mimics the case where the probe stops a small distance from the substratum. Kinetic parameters used for this simulation were $V_{max}/D_f = 3000.0$ mg L⁻¹ cm² and $K_s = 0.1$ mg L⁻¹ with a biofilm thickness of 0.0400 cm. The concentration at the interface was 2.0 mg L⁻¹. Three different cases were run using different number of data points from true solutions. True values were sampled in 0.002 cm intervals, with the

substratum value being discarded leaving 20 sample points. These sampled points had 0.0005cm subtracted from position locations to simulate the effect of underestimating distance from the substratum. Three different cases were considered using different number of the sampled data points.

In this case 2A, all twenty of the available data points were used as experimental data for kinetic parameter estimation. Results of the parameter estimation are shown in Table 10 with best fit curve shown in Figure 48. Relative error in the estimates are 2.64% for $V_{\max}/D_f$ and 19.4% for K_s respectively.

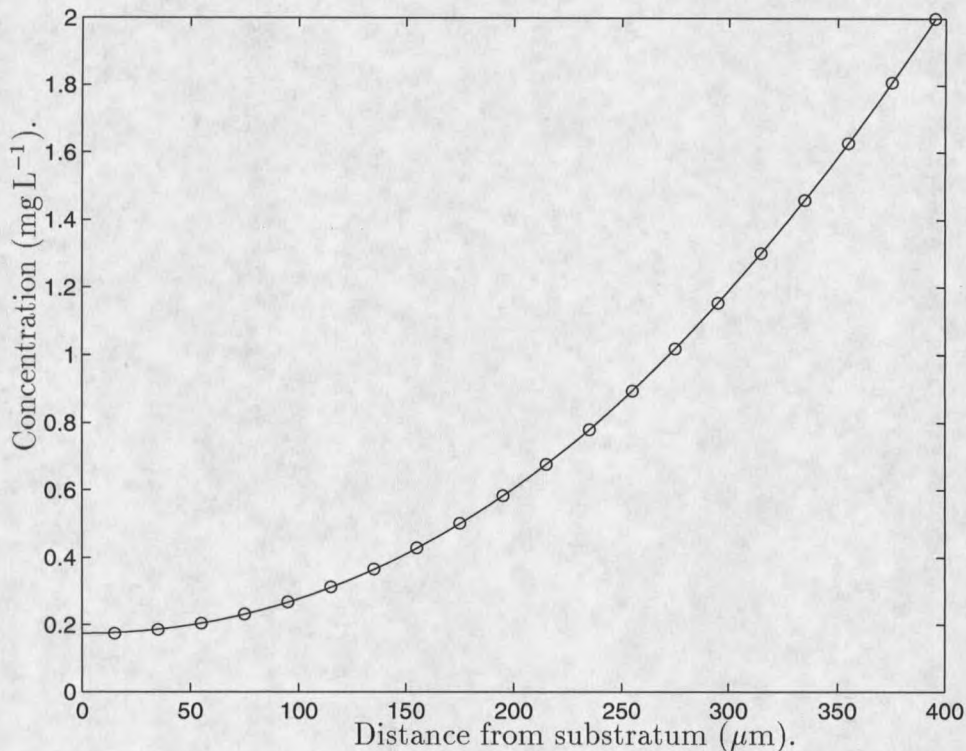


Figure 48. Plot of best fit solution (—) and experimental data (o) for case 2A.

The solution surface demonstrates the defined by the SSE defines the region where search is to be performed. By baring the parameters K_s and $V_{\max}/D_f$ around the true values a solution surface can be generated for the SSE as a function of K_s and

Table 10. Kinetic parameter estimates obtained by least squares for cases 2A–2C.

Case #	$\frac{V_{max}}{D_f}$ (mg L ⁻¹ cm ⁻²)	Percent Error	K_s (mg L ⁻¹)	Percent Error
2A	2920.76207	2.64	0.08062273637	19.4
2B	2666.61983	11.4	0.05216920103	47.8
2C	2863.94473	4.54	0.07355139309	26.5

V_{max}/D_f . A contour plot of this function is shown in Figure 49 with the parameter estimates $(K_s, V_{max}/D_f)$, denoted by $\times$. It is evident from the solution contour plot that there is a sort of "trough" with a fairly flat area with the minimum located there. It would appear the the minimum found in Case 2A is correct for the solution surface. Tighter convergence criteria on the least squares algorithm might improve the guess slightly but there influence of the offset at the substratum is evident in location of minimum differing from the true value.

Contour plots and also surface plots of the parameter estimation response surface are sometimes used to show the influence of the parameters (Riefler et al., 1998). For the surface shown here, the concentration at the biofilm bulk fluid interface was kept constants. Additional solution surfaces could be generated by holding one of the parameters constant and varying the other two. These might indicate influence of the other parameters.

In this case 2B, just the first 11 points of the available 20 data points were used as experimental data for parameter estimation. Results of the parameter estimation are shown in Table 10. The best fit curve is shown if Figure 50. Relative error of the kinetic parameters estimates is worse than in Case 2A with relative errors of 11.4% for V_{max}/D_f and 47.8% for K_s . This test case seems to imply that use of all points in the biofilm is beneficial to accurate parameters estimates.

For these cases with the Michaelis-Menten kinetics model, it reflects the need

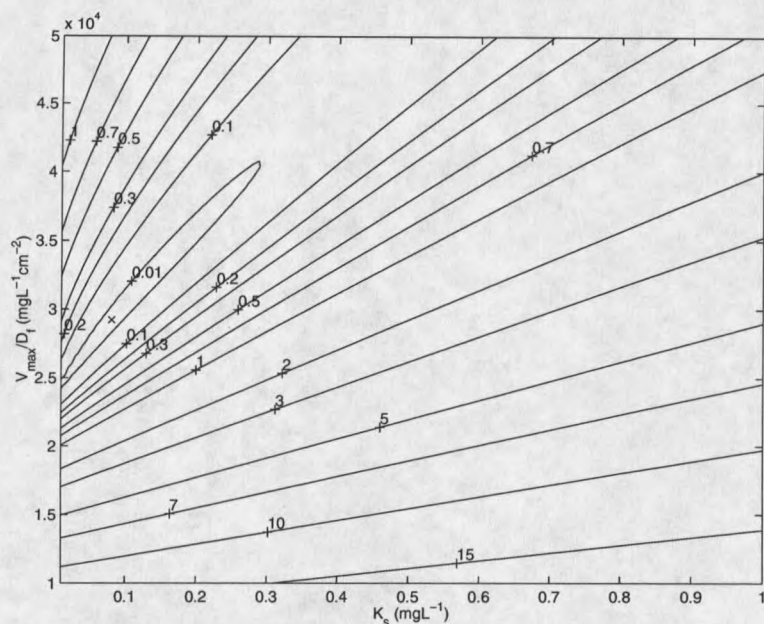


Figure 49. Contour plot of the SSE function around the best estimate pair $(K_s, V_{\max}/D_f)$ denoted by $\times$ for Case 2.

to have data representing the reaction as it varies from first order behavior to zero order. The offset distance (usually unknown) will influence the kinetic parameter estimates.

In this case 2C, just the first 16 points of the available 20 data points were used as experimental data for parameter estimation. Results of the parameter estimation are shown in Table 10 with best fit curve shown in Figure 51. The parameter estimate values obtained show a closer agreement than the parameters obtained in Case 2B. The relative errors were 4.54% for $V_{\max}/D_f$ and 26.5% for K_s .

Simulation Study 3

This study compares parameter estimates from a synthetic data set with and without added error to approximated experimental error. Different types of error can be analyzed by applying error to exact synthetic data and attempting to find best fit

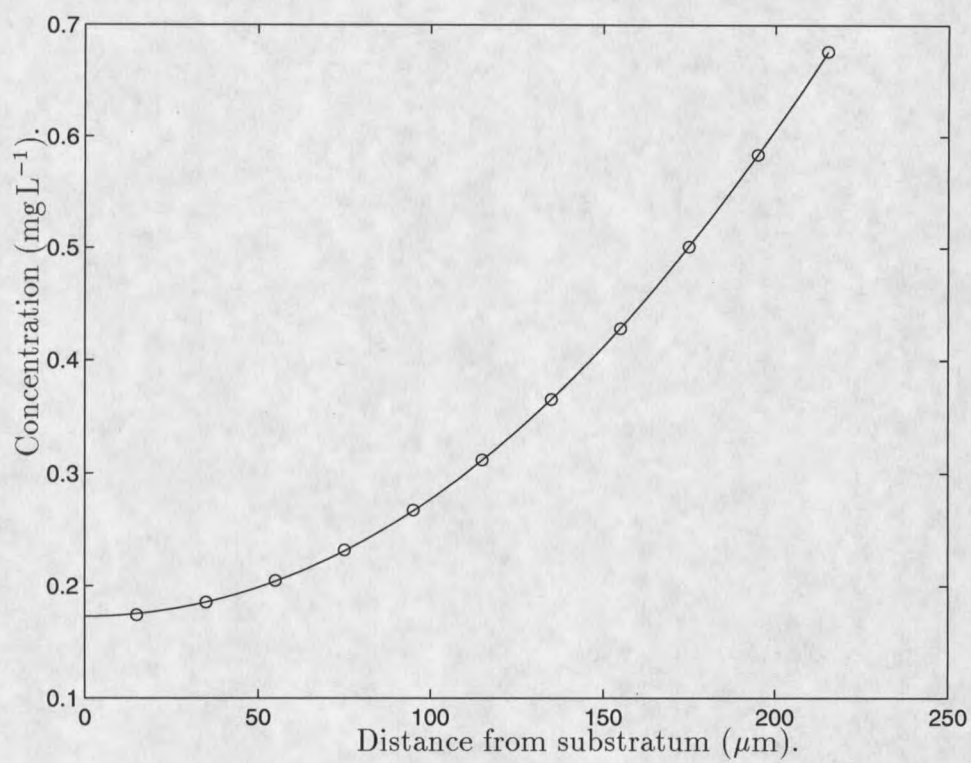


Figure 50. Plot of best fit solution (—) and experimental data (o) for case 2B.

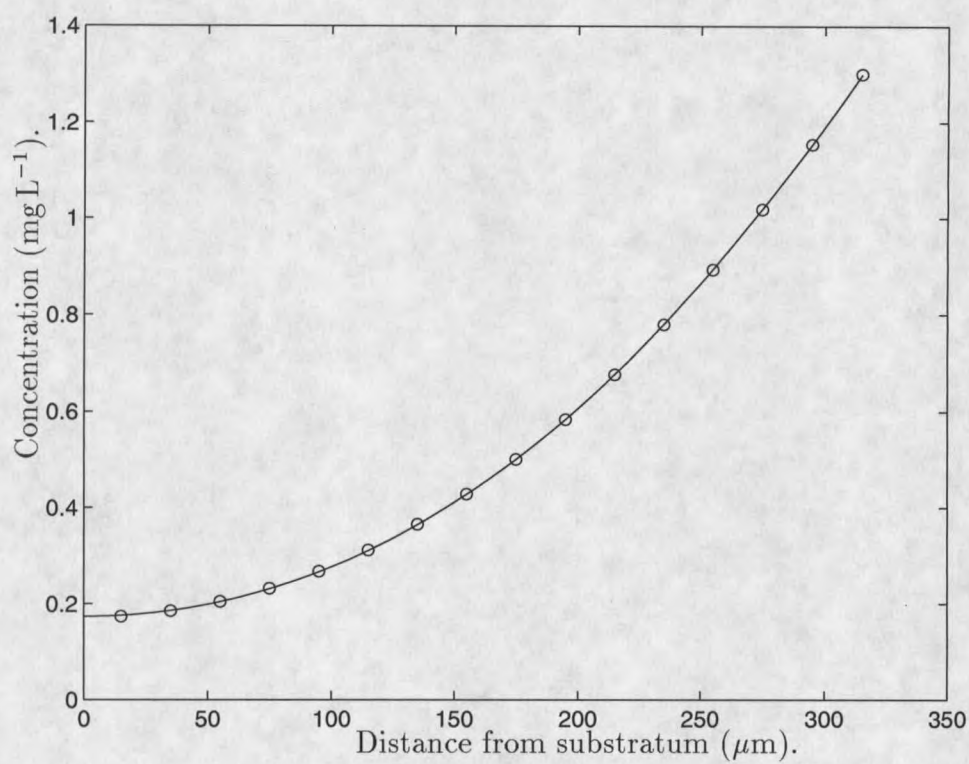


Figure 51. Plot of best fit solution (—) and experimental data (o) for case 2C.

parameters.

The synthetic data was generated using kinetic parameters of $V_{\max}/D_f = 8000 \text{ mg L}^{-1} \text{ cm}^{-2}$ and $K_s = 0.1 \text{ mg L}^{-1}$ for a biofilm $400 \mu\text{m}$ thick with an interface concentration of $C_s = 3.0 \text{ mg L}^{-1}$. This profile was sampled in $20 \mu\text{m}$ intervals to obtain synthetic sample data.

For case 3A, the data is taken as sampled with out addition of synthetic error to demonstrate ability to resolve the parameters in an ideal situation. Using the `leastsq` routine resulted in parameter estimates of $K_s = 0.1 \text{ mg L}^{-1}$ and $V_{\max}/D_f = 8000 \text{ mg L}^{-1} \text{ cm}^2$ and $C_s = 3.0 \text{ mg L}^{-1}$. A plot of the sample data (o) and the profile generated with the best fit parameters (-) is shown in Figure 52.

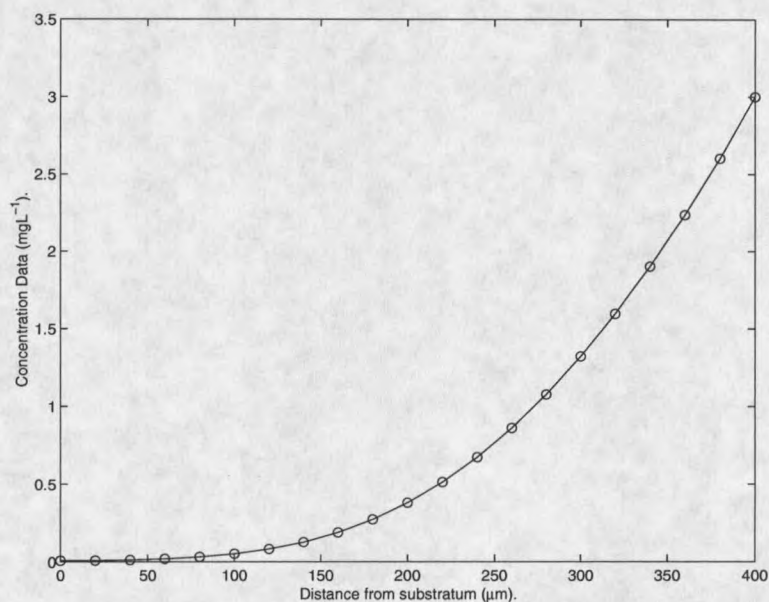


Figure 52. Plot of sample data (o) and line of best fit using parameter estimates obtained for Case 3A.

For case 3B, the influence of potential error in the values of the concentration measurements is performed by adding values from a random normal distribution and scaled such that standard deviation approaches reasonable measurement error. The

random error was obtained by using the **randn** function in MATLAB (Mat, 1997a). The **randn** function produces normally (ideally) distributed error with standard error of unity. To closer the magnitude of error that might be found in microsensor data, the random error was scaled by 0.01.

With this scaling, mean of this random error became -0.003879, the standard deviation was 0.007984, and a skewness value of 0.6496. This error was added to the true synthetic data. A plot of the error at sample locations is shown in Figure 53.

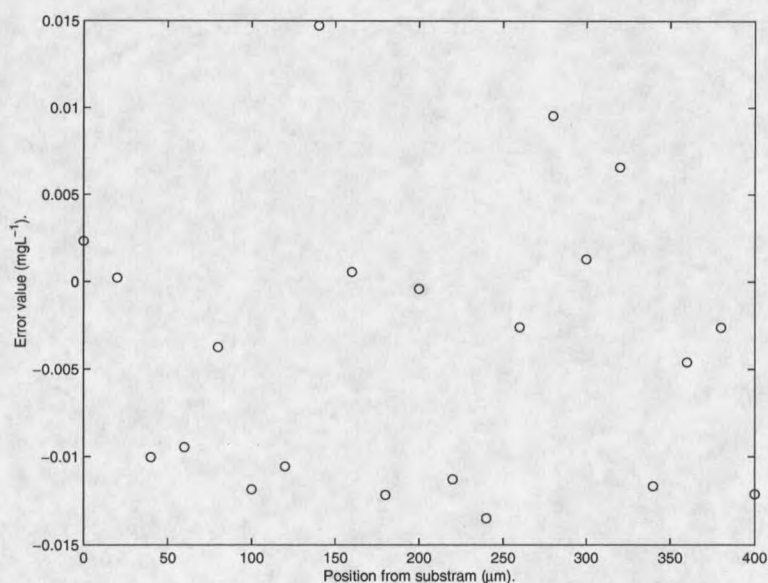


Figure 53. Plot of the random error (o) versus sampling location for case 3B.

Using this data with error results in parameters estimates of $K_s = 0.08345 \text{ mg L}^{-1}$, $C_s = 2.990 \text{ mg L}^{-1}$, and $V_{\max}/D_f = 7770 \text{ mg L}^{-1} \text{ cm}^2$. A plot of the profile based on these parameters (-) and the sample data points (o) is shown in Figure 54.

Analysis of Experimental Data

With the results of the simulation studies completed, and idea of the behavior of the least squares solution is available for use in analysis of the experimental dissolved

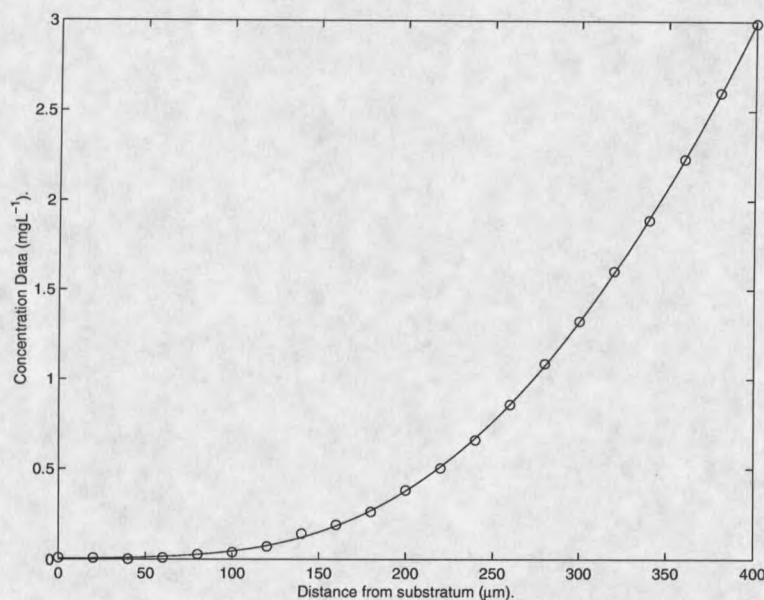


Figure 54. Profile generated from best fit parameters (-) and sample data (o) for Case 3B.

oxygen data. A behavior of the least squares fitting of data with errors is important as the experimental data does appear to have some error associated with it. There are three dissolved oxygen profiles taken in the artificial biofilm patch at three different locations. Estimated thickness of the biofilm at each location is provided by Abrahamson (1995) from analysis of DO profile and observations from light microscope while performing the experimental analysis.

Estimates of the kinetic parameters can be obtained using some or all of the data estimated to be in the biofilm region. An offset value should be applied at the substratum to account for the fact the the microsensor did not actually contact the substratum. By taking three different values for estimated thickness and offset at the substratum, a range of values can constructed for the kinetic parameters. This can provide a reasonable estimate of kinetics prior to model simulation and any modification of these values to fit the experimentally observed dissolved oxygen

profiles can be analyzed for influence on the model.

An alternative to the method described above is to apply another boundary condition such that the boundary condition is no longer a now flux condition but a value that is to be estimated also. This is probably more important in the case of full penetration where the curvature of the solution to the differential equation is not evident. It is assumed that this is to do lack of measurements close to the substratum. In the case of partial penetration the actual substratum location is not as important for analysis of kinetic parameters as no flux condition is satisfied when substrate concentration goes to zero inside the biofilm. For the experimental data shown here, it will probably be a problem primarily for site # 1.

The three different profiles are analyzed for estimates of kinetic parameters. For each profile, a different offset value and number of points are considered.

Site # 1 Site # 1 was located at the approximate center of artificial biofilm patch. This was a patch where the DO concentration goes to approximately zero at the last measurement. Since this concentration is approximately zero the no flux boundary condition at the substratum should be acceptable. At this point the estimated thickness was 380 μm .

Table 11. Kinetic parameter estimates obtained by least squares for site # 1.

# points	$\frac{V_{\max}}{D_f}$ ($\text{mg L}^{-1} \text{cm}^{-2}$)	K_s (mg L^{-1})
14	6194	9.873e-09
16	6035	1.072e-05
17	5711	4.871e-07
19	5454	2.389e-06

Site # 2 Site # 2 was located approximately $\frac{3}{4}$ of the distance from the upstream location of the artificial biofilm patch. Kinetic parameters were estimated using different values of number of points from substratum with results shown in Table 12. At this location the estimated thickness was 420 μm (Abrahamson, 1995).

Table 12. Kinetic parameter estimates obtained by least squares for site # 2.

# points	$\frac{V_{\max}}{D_f}$ ($\text{mg L}^{-1} \text{cm}^{-2}$)	K_s (mg L^{-1})
16	17208	2.295e-01
18	9204	2.274e-02
20	7140	3.892e-08
21	6460	2.019e-07
22	5837	2.392e-08

Site # 3 Site # 3 was located approximately $\frac{1}{4}$ of the distance from the upstream edge of the artificial biofilm patch. The experimental data is shown in Figure 45. At this location the artificial biofilm patch is fully penetrated with dissolved oxygen. For this profile the boundary condition at the substratum is more critical. From the evidence of the experimental data the application of the no flux boundary condition at the substratum needs to be examined. It is probably more appropriate to apply the undetermined value to be fit during parameter estimation procedure. This method is somewhat sensitive to the last data point taken, but unless this point is an outlier, the method works reasonably well. Abrahamson (1995) estimated the thickness at 280 μm .

The values shown in Tables 11–13 can be combined into a single value to represent average values for the total artificial biofilm patch. Abrahamson (1995) reported a value of $V_{\max}/D_f$ of 5263 mg/L/cm^2 for site # 2, This value is close to the common value of approximately 6000 mg/L/cm^2 computed by the parameter

Table 13. Kinetic parameter estimates obtained by least squares for site #3 with offset = 50 μm .

# points	$\frac{V_{\max}}{D_f}$ ($\text{mg L}^{-1} \text{cm}^{-2}$)	K_s (mg L^{-1})
16	6269.637858	1.07220350e-05

estimation method used here.

Small values of K_s were often obtained by this parameter estimation method. This could have been a result of noise in the data around the points in the dissolved oxygen profiles where K_s has the most influence. Small values of K_s are reported for dissolved oxygen. With the values of $V_{\max}/D_f$ observed here, the influence of small K_s values on the dissolved oxygen profiles is very small. As a result, small noise in the data would be expected to make obtaining accurate values of K_s difficult.

Parameter estimates are influence by the number of points selected for parameter estimation. This implies the approximate thickness of the biofilm should be known accurately to enable accurate kinetic parameter estimates.

APPENDIX E

Capillary Model Simulations

This appendix contains some results of simulations with the MMP model applied to capillary tubes with expansion. Capillary models can be used to approximate porous media (Dullien, 1991; Kaviany, 1995). Considering just a tube with an expansion and contraction allows demonstration of the application of the MMP model to capillary models. Simulations could be extended to form series of tubes with expansions.

Two cavities with different expansion lengths were simulated. Each cavity has an initial width of 0.16 cm and then undergoes an expansion to 0.32 cm. The first case, denoted as expansion # 1, the expansion is 0.32 cm. In the second case, denoted as expansion # 2, it is 0.16 cm long. After each expansion the width returns to 0.16 cm. A uniform biofilm of thickness 50 μm thick is located on the walls starting 0.24 cm from the inlet and ending 0.24 cm from the exit for each cavity.

Kinetic and transport parameters are the same as those obtained in the evaluation/calibration in Chapter 4 with the exception of the Reynolds number. Three different Reynolds numbers were used; 0.1, 1.0, and 10.0 with inlet dissolved oxygen concentration of 7.68 g/m³.

Dissolved oxygen concentration contours for expansion # 1 are shown in Figure 55, 57, and 59 for Reynolds numbers 0.1, 1.0, and 10.0 respectively.

Velocity vector plots for the lower part of the capillary tube with expansion # 1 are shown in Figures 56, 58, and 60 for Reynolds numbers 0.1, 1.0, and 10.0 respectively.

These figures show variations in the dissolved oxygen depending on the Reynolds number. As the Reynolds number is increased from 0.1 to 10.0, the dissolved oxygen concentration behavior changes. At $Re = 0.1$, the diffusive nature of the expansion is visible. As the Reynolds number increases, there are still regions where lower dissolved oxygen concentration values are observed in the corners of the expansion.

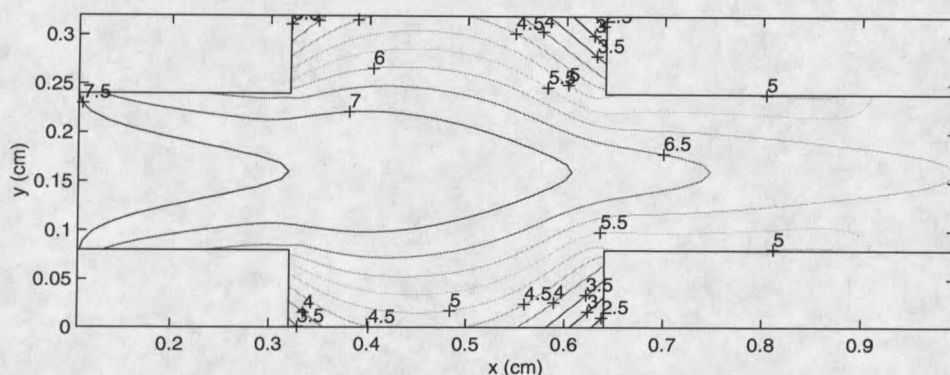


Figure 55. Dissolved oxygen concentration contours for cavity expansion # 1 at $Re = 0.1$.

The reason for these lower dissolved oxygen concentration values is evident from the plots of the velocity in the expansion region.

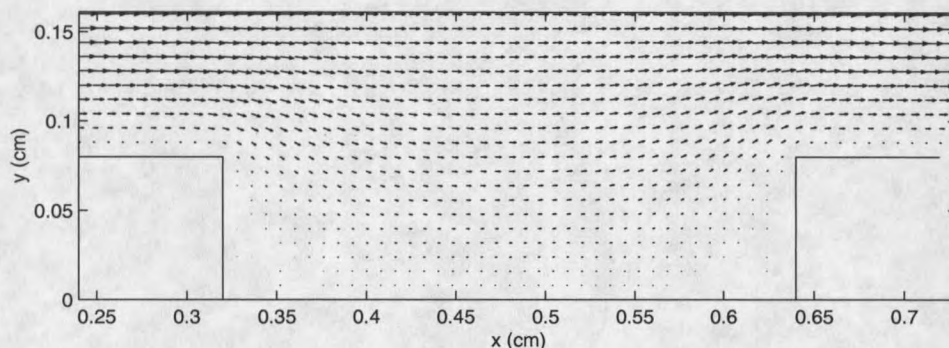


Figure 56. Velocity vector plot for cavity expansion # 1 at $Re = 0.1$.

There is very little velocity in the corners of expansion # 1 at any of the Reynolds number. As the Reynolds number is increases, the corner immediately after the expansion shows less influence of velocity than the corner at the contraction. This results in the dissolved oxygen behavior observed in Figure 59. This figure shows how the dissolved oxygen contour follows the velocity vector pattern. The strong coupling of fluid dynamics with mass transport is very evident in this expansion.

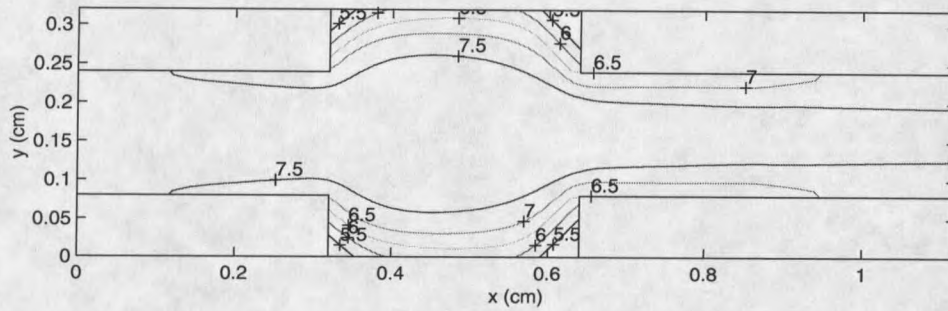


Figure 57. Dissolved oxygen concentration contours for cavity expansion # 1 at $Re = 1.0$.

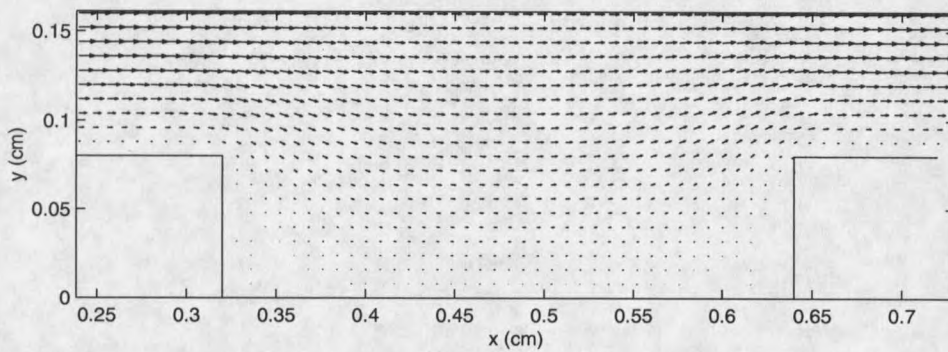


Figure 58. Velocity vector plot for cavity expansion # 1 at $Re = 1.0$.

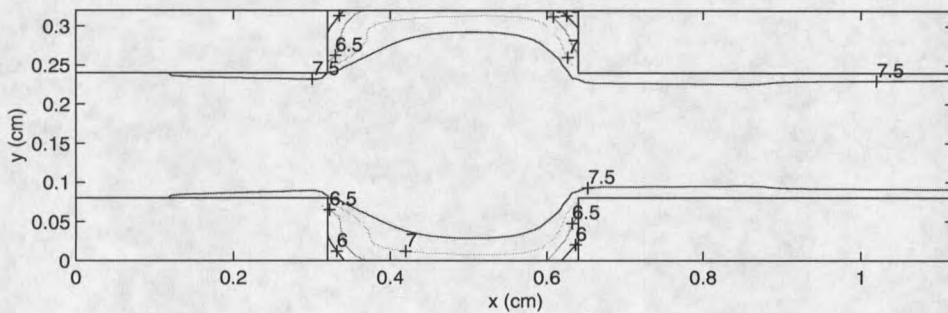


Figure 59. Dissolved oxygen concentration contours for cavity expansion # 1 at $Re = 10.0$.

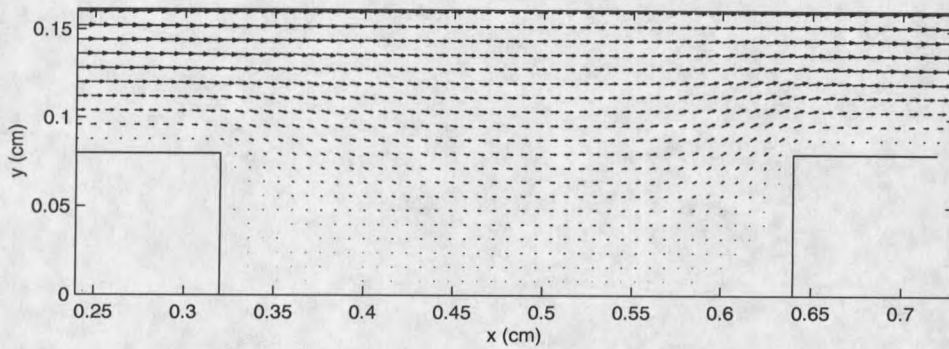


Figure 60. Velocity vector plot for cavity expansion # 1 at $Re = 10.0$.

Contours of the dissolved oxygen concentration simulation results for cavity expansion # 2 are shown in Figures 55, 57, and 59 for Reynolds numbers 0.1, 1.0, and 10.0 respectively.

Velocity vector plots for the lower part of the capillary tube with expansion # 2 are shown in Figures 62, 64, and 66 for Reynolds numbers 0.1, 1.0, and 10.0 respectively.

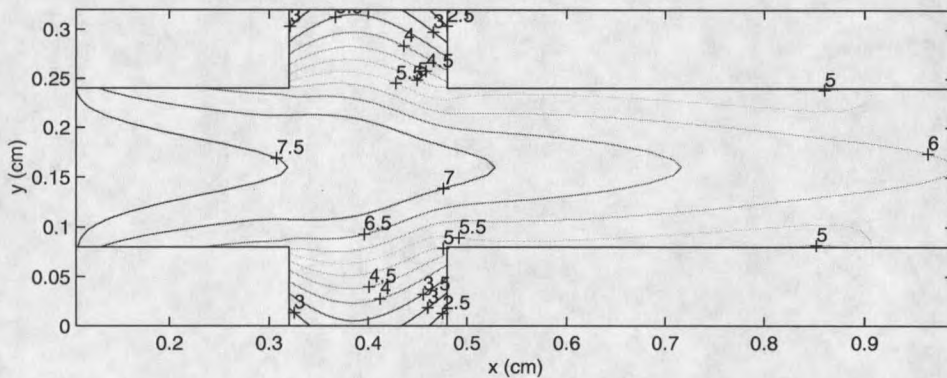


Figure 61. Dissolved oxygen concentration contours for cavity expansion # 2 at $Re = 0.1$.

As shown in the velocity vector plots for expansion # 2, there is less velocity penetration into the expansion. The major difference in the velocity plots can be

observed by comparing the midpoints of the expansion. For expansion # 2, the velocity is very small near the midpoint of the expansion (Figure 66) in contrast to that of expansion # 1 (Figure 60).

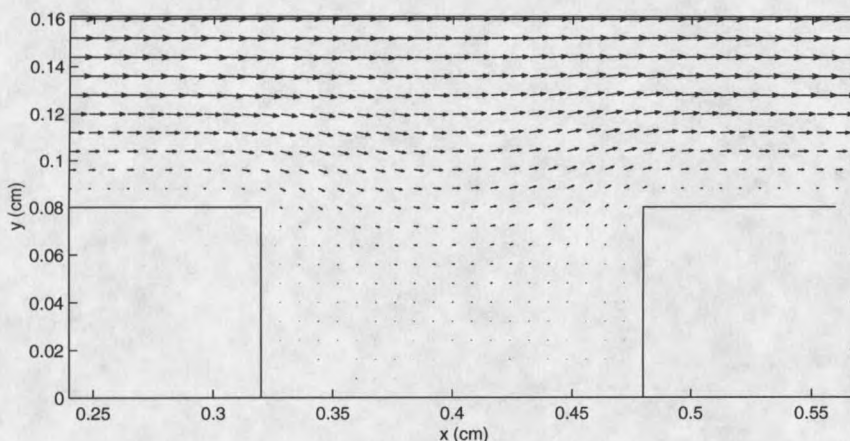


Figure 62. Velocity vector plot for cavity expansion # 2 at $Re = 0.1$.

This lack of significant velocity in expansion # 2 is reflected in the dissolved oxygen concentration contours. The diffusive nature of dissolved oxygen transport is very evident in the dissolved oxygen concentration plots. In contrast to expansion # 1, the horizontal wall of the expansion exhibits this diffusive transport effect. Dissolved oxygen transport limitations in the corners results in lower dissolved oxygen observed.

These simulations with uniform thickness biofilms show the degree of variability that could be observed in capillary models which include biofilm. Sharp corners may not be observed in an experimental system which would affect the solution behavior. Rounded corners would change the velocity pattern behavior in the expansion region. These simulations show a strong effect of velocity on local mass transfer to the biofilm surface. It would be reasonable to infer that the degree of sharpness of the corners can significantly influence the biofilm behavior observed in biofilm systems.

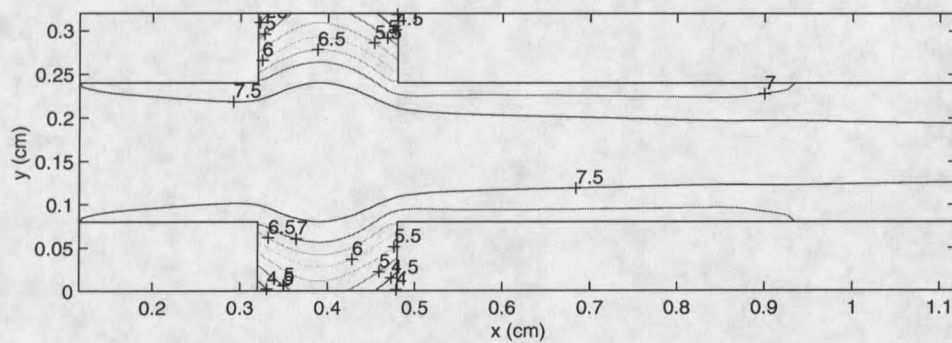


Figure 63. Dissolved oxygen concentration contours for cavity expansion # 2 at $Re = 1.0$.

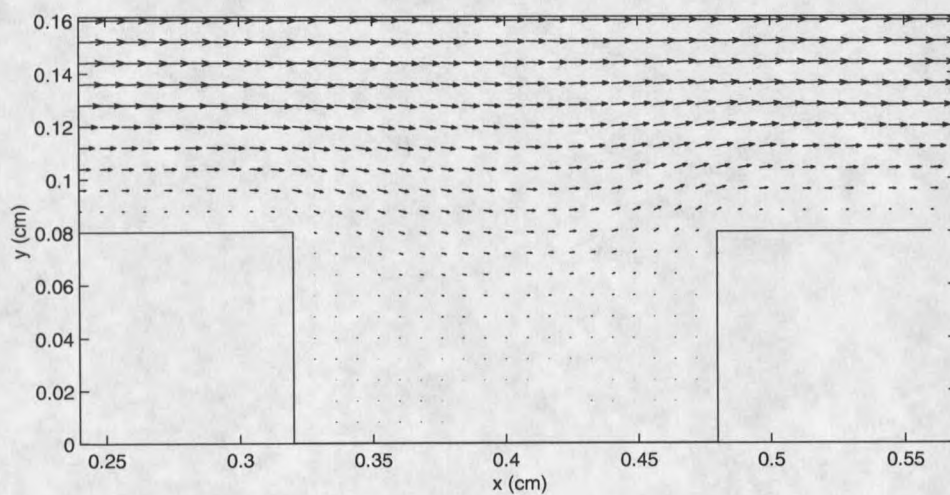


Figure 64. Velocity vector plot for cavity expansion # 2 at $Re = 1.0$.

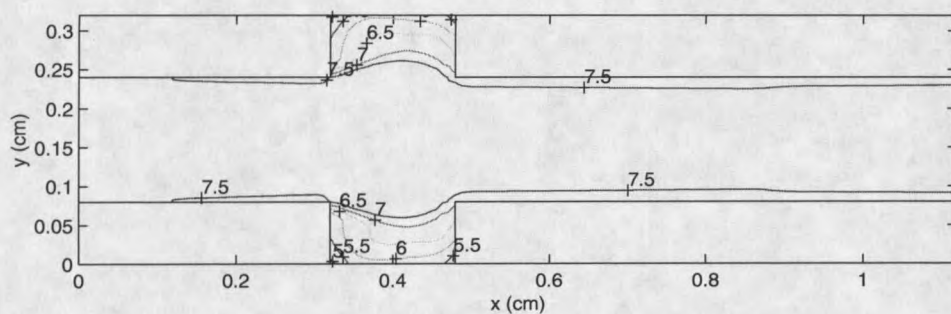


Figure 65. Dissolved oxygen concentration contours for cavity expansion # 2 at $Re = 10.0$.

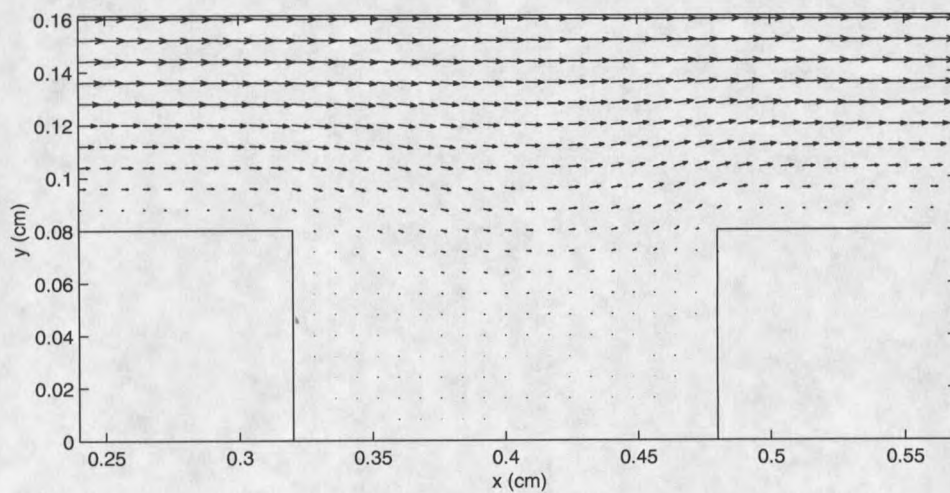


Figure 66. Velocity vector plot for cavity expansion # 2 at $Re = 10.0$.

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