Numerical simulation of biofilm accumulation in pipelines
by Sandor Szego

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Computer Science
Montana State University

Abstract:
Biofilms can be found in many natural and industrial systems. Their effects can be beneficial or damaging, therefore a need to control these complex ecological systems emerges. This thesis describes a computer model for biofilm accumulation in pipeline systems. First, from an initial conceptual model a mathematical model is derived using the conservation of mass principle. The resulting equations are non-linear, coupled, partial differential equations. A numerical method, using a finite volume approach, is developed to solve the system of equations in time and space. Since the geometry of the system changes due to biofilm accumulation, the grid must adjust itself to the changing geometry. A general three-point integration formula is used to advance the solution in time. Since the formula is nonlinear in the unknowns, Newton's Method is used to solve the discretized equations at every time step. Initial experiments and results are described to show the validity of the developed computer model. The behavior of the model is analyzed as selected numeric parameters are varied. The results are promising, though future work has to determine the predictive capacity of the model by comparing its output to real measurements.

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ABSTRACT

Biofilms can be found in many natural and industrial systems. Their effects can be beneficial or damaging, therefore a need to control these complex ecological systems emerges. This thesis describes a computer model for biofilm accumulation in pipeline systems. First, from an initial conceptual model a mathematical model is derived using the conservation of mass principle. The resulting equations are non-linear, coupled, partial differential equations. A numerical method, using a finite volume approach, is developed to solve the system of equations in time and space. Since the geometry of the system changes due to biofilm accumulation, the grid must adjust itself to the changing geometry. A general three-point integration formula is used to advance the solution in time. Since the formula is nonlinear in the unknowns, Newton's Method is used to solve the discretized equations at every time step. Initial experiments and results are described to show the validity of the developed computer model. The behavior of the model is analyzed as selected numeric parameters are varied. The results are promising, though future work has to determine the predictive capacity of the model by comparing its output to real measurements.

CHAPTER 1

INTRODUCTION

This thesis describes a computer model for biofilm processes in a pipeline. A *biofilm* is a layer of fixed biomass composed of microbial organisms and organic polymers of microbial origin attached to a solid surface (substratum). In the vernacular, a biofilm might be called slime or sludge. Simple — typically laboratory developed — biofilms consist of a single species, while naturally occurring biofilms can contain a number of different microorganisms. These species are subject to different interactions, such as symbiosis, competition for common substrates, etc. A very important characteristic of these complex ecological systems is that they can have a significant impact on the surrounding environment, e.g., by introducing corrosion on a metal surface. Biofilms occur in nature without human interaction, or can artificially be introduced to industrial or natural systems. Table 1 gives a few examples of systems where biofilms can and do exist, and also lists some of their effects. These examples show that some biofilms can serve beneficial purposes, while others can cause extensive damage in the natural or industrial environment. Understanding the processes and interactions occurring in these systems, and formulating conceptual and mathematical models enable us to control biofilm processes, and thus reduce their negative

and enhance their positive effects.

A detailed conceptual description of biofilms is required in order to be able to come up with a suitable mathematical model. It is important to distinguish between biofilms and biofilm systems. A biofilm system consists of five compartments [3]:

- Substratum. The solid surface where the microorganisms attach.
- Base film. Structured accumulation of cells.
- Surface film. Provides the transition between the base film and the bulk compartment.
- Bulk liquid. The flow regime of this compartment determines mass and heat transfer between the liquid and the film.
- Gas. Provides aeration or removal of gaseous reaction products.

The biofilm is the combination of the base film and the surface film. A very important characteristic of a biofilm is that a certain (typically large) portion of its volume consists of the continuous liquid medium (liquid phase). For example, in Characklis et al. [5] the data reported suggests that their *Pseudomonas Aeruginosa* biofilm was $\approx 90\%$ water.

Components of biofilm systems are cells, organic and inorganic products, substrates (growth limiting nutrients), and other nutrients. *Interactions* and *processes* between

Process	Effects
Biofilm in heat exchangers	Increased heat transfer resistance
Biofilm in porous media (soil)	Increased fluid resistance
Corrosion due to microbial processes	Reduced equipment lifetime
Biofilm in water distribution systems	Health risks
Biofilm on teeth and gums	Health risk (cavities)
Extraction of toxics from water	Reduced pollutant load

Table 1: Effects of biofilm processes in different systems

these components are transport (advection, diffusion), transfer (cell attachment and detachment, interfacial diffusion), and transformation (chemical reactions).

Geometric configuration is another very important characteristic of a given system. Two widely studied geometries are Continuous Flow Stirred Tank Reactors (CFSTR) and Plug Flow Reactors (PFR). CFSTRs are well mixed tanks where a continuous flow of reactants is present, and the well mixed bulk is constantly removed to sustain a constant bulk volume. Constituent concentrations in the bulk are constant throughout the CFSTR. PFRs are idealized models of pipelines, where the reactants enter the pipe at the inlet, and products leave the pipe at the outlet. Constituent concentrations can vary from inlet to outlet in the PFR.

Previous mathematical models for multispecies biofilms in CFSTR geometries [10], [4] have been based on the conservation of mass principle. Apart from geometry specific assumptions, many conceptual and mathematical formulations for CFSTR systems can be applied to PFR systems.

Models for biofilm processes can serve a variety of purposes. The purpose could

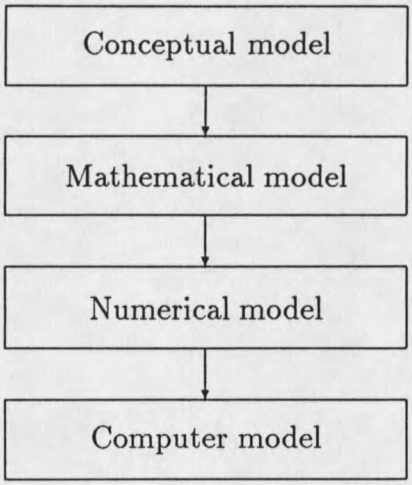

Figure 1: The modeling process

be to predict the concentrations of certain components, or thickness of the formed biofilm. Besides prediction, these models can be used to describe experimental results and to explain the modelers' conceptual understanding of the process . Simulation programs, such as BIOSIM [10], make use of a set of computational units. Each unit is essentially a CFSTR. Two units can be connected in series to simulate other geometries, such as a pipeline.

Previous work on pipelines focused on determining the growth of biofilm on pipewalls and its effect on heat resistance [2]. That model assumes a uniform film consisting of a single species only. It is also assumed that only a single reaction is present in the system and its rate can be expressed using Monod kinetics (to be discussed later).

The goal of this thesis is to describe a computer model for biofilm accumulation in pipelines. The organization follows the basic steps of modeling shown in Figure 1.

In Chapter 2 I give a detailed overview and mathematical formulation of biofilm processes in pipelines. Chapter 3 contains the governing equations that are based on the conservation of mass principle. Chapter 4 explains the numerical methods applied to solve the coupled, non-linear, partial differential equations resulting from the governing equations. Finally, Chapter 5 presents computer simulation runs of different systems.

CHAPTER 2

BIOFILM PROCESSES IN PIPELINES

Many industrial and natural biofilm system geometries can efficiently be modeled by the plug flow reactor. Examples, among many others, include natural streams, heat exchangers, oil pipes, water distribution and waste water systems. A common characteristic of these systems is that there exists a significant advective motion of the liquid medium (bulk compartment) that carries all reactants and products to downstream locations. In fact, this and the existence of radial concentration gradients in the bulk compartment are the only differences between biofilm systems in PFRs and in CFSTRs.

Components

The systems of our concern typically contain the following components: substrates (and nutrients), cells, particles, abiotic components, products, and biocides. For modeling purposes, these components can be divided into two classes:

- Soluble components, and

- Particulate components[1].

In the bulk compartment both classes of components can be described by their concentrations (units: ML^{-3}). The liquid phase in the biofilm compartment could contain all the above components, but the following simplifying assumption is made: *The liquid phase in the film compartment does not contain any particulate components.* There are many ways the concentration (or the mass) of particulates in the film can be defined: (1) X' biofilm particulate mass per unit substratum area (units: ML^{-2}); (2) X biofilm particulate mass per unit biofilm volume (units: ML^{-3}); (3) X'' biofilm particulate mass per unit reactor volume (units: ML^{-3}). Most laboratory measurement methods determine the mass of the particulates in the film using one of the above units. However, it is easy to convert between these units using the relationship $X(\mathbf{x},t) = X'(\mathbf{x},t)/L_F(\mathbf{x},t)$, where $L_F(\mathbf{x},t)$ is the thickness of the film at location $\mathbf{x} = [x,y,z]^T$ and time t. Note that $L_F(\mathbf{x},t)$ is defined as the distance between the surface of the substratum and the surface of the film-liquid interface at point $\mathbf{x}$. Since $\mathbf{x}$ has to lie on the surface of the substratum, it has to satisfy

$$g(\mathbf{x}) = 0, \tag{1}$$

where $g(\cdot)$ defines the surface of the substratum.

In our approach we make use of the second measure, which can be written as

$$X_i = \varepsilon_i(\mathbf{x},t)\varrho_i(\mathbf{x},t), \tag{2}$$

[1]cells and certain products (extracellular polymers)

where X_i is the "concentration" of the *ith* particulate component in the film, ε_i is the fraction of biofilm volume occupied by the *ith* component (void fraction), and ϱ_i is the specific gravity or density of the same component. In general both ε and ϱ can be functions of time t and spatial position $\mathbf{x}$. If we assume that the density of a particulate component is constant (regardless of its position in the film), then (2) becomes

$$X_i(\mathbf{x}, t) = \varepsilon_i(\mathbf{x}, t)\varrho_i. \tag{3}$$

In other words, *if the density (specific gravity) of particulate component i is a known constant*, then by determining $\varepsilon_i(\mathbf{x}, t)$ the concentration of particulate i in the film can be calculated.

The unknown material concentrations can be described as a vector:

$$\mathbf{Q} = \begin{pmatrix} \mathbf{Q_s} \\ \hline \\ \mathbf{Q_p} \end{pmatrix} \tag{4}$$

where the elements of $\mathbf{Q}$ are as follows.

In the bulk,

$$\mathbf{Q_s} = [Q_{si}] = \varepsilon_l C_i,\ i = 1, 2, .., N_{sub} \text{ and} \tag{5}$$

$$\mathbf{Q_p} = [Q_{pi}] = \varepsilon_l C_i,\ i = 1, 2, .., N_{part}, \tag{6}$$

where $\varepsilon_l = 1$ and C_i is the concentration of component i.

In the film,

$$\mathbf{Q_s} = [Q_{si}] = \varepsilon_l C_i,\ i = 1, 2, .., N_{sub} \text{ and} \tag{7}$$

$$\mathbf{Q_p} = [Q_{pi}] = \varepsilon_i \varrho_i,\ i = 1, 2, .., N_{part} - 1, \tag{8}$$

where ε_l is the liquid volume fraction of the biofilm. Note that $\sum_{i=1}^{N_{part}} \varepsilon_i + \varepsilon_l = 1$, thus only $N_{part} - 1$ particulate void fractions (ε_i) are free parameters.

Reactions

The components described in the previous section interact with each other via biochemical reactions. These reactions can be described by their stoichiometric and kinetic coefficients. The stoichiometric equations describe the material balance of a certain reaction, while the kinetic equations determine the rate of the reaction.

The Stoichiometry Matrix

In biofilm systems many biochemical reactions can occur at the same time, such as "growth" reactions for each microorganism and reactions among chemicals (oxidization, reduction). Many components can and do participate in every reaction, thus the stoichiometric equation for the ith reaction has the following form:

$$\alpha_{i,1} P_1 + ... + \alpha_{i,k} P_k \rightarrow \alpha_{i,k+1} P_{k+1} + ... + \alpha_{i,l} P_l. \tag{9}$$

Components on the left hand side of the arrow are consumed and components on the right hand side are produced. If the left hand side coefficients are negated, then the conservation of mass principle leads to

$$\alpha_{i,1} M_{P_1} + ... + \alpha_{i,k} M_{P_k} + \alpha_{i,k+1} M_{P_{k+1}} + ... + \alpha_{i,l} M_{P_l} = 0, \tag{10}$$

where M_{P_i} is the molar weight of component P_i. If the above equation is written for all reactions, then the following matrix equation can be obtained:

$$\boldsymbol{\alpha}\mathbf{M} = 0 \tag{11}$$

where $\boldsymbol{\alpha}$ is the stoichiometry matrix, and $\mathbf{M}$ is the molar weight vector of the components present in the reactions. The dimensions of $\boldsymbol{\alpha}$ are $N_{rxn} \times (N_{sub} + N_{part})$, where N_{rxn} is the number of reactions present in the system, and $\mathbf{M}$ is a column vector of $(N_{sub} + N_{part})$ entries.

Reaction Kinetics

The net rate of production of all components can be expressed in terms of the stoichiometry matrix and the reaction rate vector:

$$\mathbf{W} = \boldsymbol{\alpha}^T \mathbf{r}, \tag{12}$$

where

$$\mathbf{r} = [r_1, r_2, ..., r_{N_{rxn}}]^T, \tag{13}$$

and r_i is the reaction rate of reaction i.

The rate of a given reaction depends on the participating components:

$$r_i = \prod_{j=1}^{N_{part}+N_{sub}} R_{i,j}(C_j) \tag{14}$$

where $R_{i,j}$ is the reaction kinetic expression of component j in reaction i, and C_j is the concentration of component j (soluble or particulate). The model utilizes four

types of reaction kinetics, each having a single numerical parameter ($K_{i,j}$), as follows.

- Zero order

$$R_{i,j} = K_{i,j} \tag{15}$$

- First order

$$R_{i,j} = K_{i,j} C_j \tag{16}$$

- Monod

$$R_{i,j} = \frac{C_j}{K_{i,j} + C_j} \tag{17}$$

- Inhibition

$$R_{i,j} = \frac{1}{K_{i,j} + C_j} \tag{18}$$

If component k does not participate in reaction i, then its reaction kinetic expression is zero order with $K_{i,k} = 1$. A typical reaction rate equation for a single particulate, single substrate reaction is

$$r = \mu_{max} C_{part} \frac{C_{sub}}{K_{sub} + C_{sub}}, \tag{19}$$

where μ_{max} is the maximum growth rate of the cell, and K_{sub} is the so called half saturation coefficient of the substrate in that reaction.

Detachment and Attachment

Biofilm accumulation on solid surfaces is the net result of many physical and chemical processes, including

- Adsorption. Cells attach to the substratum surface. This can be reversible or irreversible.
- Desorption. Absorbed cells can leave the substratum, and enter the bulk compartment.
- Attachment. Cells in the bulk compartment attach to an already existent biofilm.
- Detachment. A single cell or a group of cells leave the biofilm.

In our model we assume the existence of an initial layer of biofilm, thus adsorption and desorption are not included in the model.

Attachment and adsorption are very similar processes, with the exception that in attachment cells are captured by the film, while in adsorption the capturing medium is the substratum.

Detachment can be either erosion or sloughing. Erosion refers to a continuous loss of a small amount of biofilm, while sloughing means rapid, massive loss of biomass.

The model utilizes a net detachment expression,

$$net\ detachment = detachment - attachment.$$

This expression describes the net flux of particulate mass leaving the biofilm surface. It is also important to note that this process is assumed to be present at the interface only, which might not be a correct assumption. In biofilm research the important parameters that determine the magnitude of detachment/attachment is an open research topic. The model assumes the interfacial flux of particulate mass is a quadratic function of the biofilm thickness,

$$R_{det} = a_2 L_f^2 + a_1 L_f + a_0. \tag{20}$$

Positive flux means detachment, while negative flux means attachment.

Advection and Diffusion

In a pipeline system advection moves components in the flow direction, and the growth of the biofilm imposes an advective motion on the particles in the film.

The streamwise flow can be turbulent or laminar, which determines the velocity profiles in the pipe, as well as the diffusion coefficients.

Diffusion occurs both in the radial and axial direction. The axial diffusion is typically orders of magnitude smaller than the advection in the same direction, thus

it can be omitted. Diffusion in the radial direction is a very important phenomenon. It transfers soluble and particulate components to and from the center of the pipe and into the film. The rate of diffusion is determined by the flow regime. In laminar flow the diffusion coefficient of a given component in the pipe is equal to the molecular diffusion of the component, while in turbulent flow conditions the diffusion coefficient varies from the eddy diffusion to the molecular one as particles move from the center of the pipe towards the wall of the pipe. An empirical formula for determining the eddy diffusivity is given in [1].

CHAPTER 3

GOVERNING EQUATIONS

The governing equations for both the bulk liquid and biofilm compartments are based on the conservation of mass principle,

$$accumulation\,rate + transport = production.$$

Using the notation introduced in the previous sections,

$$\frac{\partial}{\partial t}\int\int\int_V \mathbf{Q}\,dV + \oint_S (\mathbf{S} - \mathbf{S}_v)\,\mathbf{n}\,dS = \int\int\int_V \mathbf{W}\,dV, \tag{21}$$

where $\mathbf{S}$ represents the inviscid (convective) and $\mathbf{S}_v$ represents the viscous fluxes, $\mathbf{W}$ is the vector of source terms (reactions), V is any arbitrary volume in the system, S is the surrounding surface of volume element V, and $\mathbf{n}$ is the normal of the infinitesimal surface dS. In the bulk compartment $\mathbf{Q}$ is the vector of concentrations of all components (N_{sub} substrates and N_{part} particulates). In the film compartment,

$$\mathbf{Q} = \begin{pmatrix} \varepsilon_l C_1 \\ \vdots \\ \varepsilon_l C_{N_{sub}} \\ \varepsilon_1 \varrho_{1+N_{sub}} \\ \vdots \\ \varepsilon_{N_{part}} \varrho_{N_{part}-1+N_{sub}} \end{pmatrix}. \tag{22}$$

The reason for including only $N_{part} - 1$ particulate components in $\mathbf{Q}$ is due to the constraint

$$\sum_{i=1}^{N_{part}} \varepsilon_i + \varepsilon_l = 1. \tag{23}$$

The size of all vectors in the biofilm compartment is $N_{sub} + N_{part} - 1$. Now the form of $\mathbf{S}$ and $\mathbf{S}_v$ has to be determined. The vector of inviscid fluxes in the bulk compartment is the following:

$$\mathbf{S} = \begin{pmatrix} \varepsilon_l C_i (\mathbf{u} - \mathbf{u_v}) \\ \vdots \\ \varepsilon_l C_{N_{sub}} (\mathbf{u} - \mathbf{u_v}) \\ \varepsilon_l C_{N_{sub}+1} (\mathbf{u} - \mathbf{u_v}) \\ \vdots \\ \varepsilon_l C_{N_{sub}+N_{part}} (\mathbf{u} - \mathbf{u_v}) \end{pmatrix} \tag{24}$$

where C_i is the concentration of substrates and particulates, $\mathbf{u}$ is the imposed velocity profile, and $\mathbf{u_v}$ is the velocity with which the control surface S is moving. Thus $\mathbf{u} - \mathbf{u_v}$ is the velocity of the liquid relative to the coordinate system. The direction of the flow is in the axial (x) direction. The shape of the imposed velocity profile depends on the flow regime. In laminar flow a parabolic profile is assumed:

$$u(y) = u_{max} \frac{y - y_B}{R - y_B} (2 - \frac{y - y_B}{R - y_B}), \tag{25}$$

where R is the radius of the pipe, y_B is the thickness of the biofilm, y is the coordinate in the radial direction, $u(y)$ is the magnitude of the velocity, and u_{max} is calculated from the flowrate using

$$u_{max} = 2\frac{q}{A}, \tag{26}$$

where q is the flowrate and A is the area of the cross-section. In the case of turbulent flow, the velocity profile is given by

$$u(y) = u_{max}(\frac{y - y_B}{R - y_B})^{\frac{1}{n}}, \tag{27}$$

where

$$u_{max} = \frac{q}{A}\frac{(n+1)(n+2)}{2n^2} \text{ and}$$
$$n = n(Re) \approx 7. \tag{28}$$

The vector of viscous fluxes in the bulk compartment, in accordance with Fick's law is

$$\mathbf{S}_v = \begin{pmatrix} D_1 \nabla C_1 \\ \vdots \\ D_{N_{sub}} \nabla C_{N_{sub}} \\ D_{N_{sub}+1} \nabla C_{N_{sub}+1} \\ \vdots \\ D_{N_{sub}+N_{part}} \nabla C_{N_{sub}+N_{part}} \end{pmatrix}, \tag{29}$$

where D_i is the diffusion coefficient of component i. The coefficient D_i is the function of the flow regime (laminar or turbulent) and the spatial coordinates; i.e.

$$D_i = D_i(Re, x, y, z), \tag{30}$$

where Re is the Reynolds number. For laminar flow conditions D_i is equal to the molecular diffusion of component i, while under turbulent conditions D_i varies from a large turbulent diffusion coefficient in the bulk to molecular diffusion in the boundary

layer. The inviscid and viscous fluxes in the film compartment are different from those in the bulk,

$$\mathbf{S} = \begin{pmatrix} -\varepsilon_l C_1 \mathbf{u_v} \\ \vdots \\ -\varepsilon_l C_{N_{sub}} \mathbf{u_v} \\ \varepsilon_1 \varrho_1 (\mathbf{u_s} - \mathbf{u_v}) \\ \vdots \\ \varepsilon_{N_{part}-1} \varrho_{N_{part}-1} (\mathbf{u_s} - \mathbf{u_v}) \end{pmatrix} \text{ and}$$

$$\mathbf{S}_v = \begin{pmatrix} D_{F1} \nabla C_1 \\ \vdots \\ D_{FN_{sub}} \nabla C_{N_{sub}} \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \tag{31}$$

where $\mathbf{u}_s$ is the solid velocity of the particulates. The vectors $\mathbf{S}$ and $\mathbf{S}_v$ reflect the assumptions that (a) soluble components do not get displaced as the solid phases move and (b) particulate components do not diffuse inside the film compartment. Since the diffusional resistance inside the film is typically greater than that in the bulk, different diffusion coefficients are used (D_{Fi}). These coefficients are calculated from the molecular ones using an appropriate constant D_{bb} and the formula

$$D_{Fi} = D_{bb} D_i. \tag{32}$$

In the above vectors the value of $\mathbf{u_s}$ is unknown. This can be determined if we write the governing equations for the N_{part} particulates, divide them by ϱ_i and sum them

using a *fixed volume* ($u_v = 0$)

$$\oint_S \mathbf{u}_s \mathbf{n}\, dS = \frac{1}{1-\varepsilon_l} \int\int\int_V \left(\sum_{i=1}^{N_{part}} \frac{W_{N_{sub}+i}}{\varrho_i}\, dV \right), \tag{33}$$

or in differential form (using Gauss' theorem)

$$\nabla \mathbf{u_s} = \frac{1}{1-\varepsilon_l} \sum_{i=1}^{N_{part}} \frac{W_{N_{sub}+i}}{\varrho_i}. \tag{34}$$

To determine the magnitude and direction of $\mathbf{u_s}$ these equations are not sufficient. However, the biofilm growth is assumed to be one dimensional, perpendicular to the pipe wall. Thus, the previous equation can be simplified as

$$\frac{du_s}{dy} = \frac{1}{1-\varepsilon_l} \sum_{i=1}^{N_{part}} \frac{W_{N_{sub}+i}}{\varrho_i}. \tag{35}$$

This equation can be solved with the initial condition $u_s = 0$ at the solid wall.

To solve the governing equations described above, appropriate boundary conditions are needed. At the solid wall the fluxes are zero, since we assume that no corrosion exists. Due to the axisymmetry of the problem, at the centerline the boundary condition is

$$\left. \frac{\partial \mathbf{Q}}{\partial n} \right|_{axis} = 0. \tag{36}$$

The inlet conditions are specified, while the outlet conditions are extrapolated from the interior solutions.

The last problem to consider is the treatment of the bulk liquid-biofilm interface. This interface moves in time as the film grows/shrinks. Using the control surface

ideas mentioned earlier, describing the interface behavior is fairly straightforward. Two coinciding volume elements, one in the bulk and one in the film compartment, can be separated by the interface at all times. This means that the volumes will move and deform in time to follow the interface movement. Characklis et al. [4] derives the interface boundary condition,

$$[(\mathbf{S} - \mathbf{S}_v) \cdot \mathbf{n_I}]_B - [(\mathbf{S} - \mathbf{S}_v) \cdot \mathbf{n_I}]_F = (\mathbf{R}_F \cdot \mathbf{n_I}), \tag{37}$$

where R_F denotes the surface production of components, n_I is the normal to the interface, and indices B and F mean bulk and film, respectively. There are three special cases: (a) soluble components, (b) particulates in the bulk at the interface, and (c) particulates in the film. Since there is no surface production of substrates at the interface, and the advective velocity is also 0, the following boundary condition holds for substrates,

$$-\mathbf{u_v} \cdot \mathbf{n_I}(\varepsilon_l C_i)_B - [D_i \nabla C_i \cdot \mathbf{n_I}]_B = -\mathbf{u_v} \cdot \mathbf{n_I}(\varepsilon_l C_i)_F - [D_i \nabla C_i \cdot \mathbf{n_I}]_F. \tag{38}$$

The expression for the particulate components in the bulk compartment (no film contributions) is

$$(\mathbf{u} - \mathbf{u_v}) \cdot \mathbf{n_I}(\varepsilon_l C_i)_B - [D_i \nabla C_i \cdot \mathbf{n_I}]_B = [(\mathbf{R}_i)_F \cdot \mathbf{n_I}]. \tag{39}$$

The boundary condition for the particulates in the film has a similar form (no bulk contributions and no diffusion in the film),

$$-(\mathbf{u}_s - \mathbf{u_v}) \cdot \mathbf{n_I}(\varepsilon_i \varrho_i)_F = [(\mathbf{R}_i)_F \cdot \mathbf{n_I}]. \tag{40}$$

This boundary condition applies to all but one particulate component. The last equation can be used to determine $\mathbf{u_v}$ at the interface $(\mathbf{u_v})_I$. After some algebra,

$$(\mathbf{u_v})_I = \mathbf{u}_s + \frac{1}{1-\varepsilon_l} \sum_{i=1}^{N_{part}} \frac{(\mathbf{R}_i)_F}{\varrho_i}. \tag{41}$$

This final result gives us an expression for the change in biofilm thickness L_F, since

$$\frac{dL_F}{dt} = (u_v)_I, \tag{42}$$

where $(u_v)_I$ is the magnitude of the interface velocity.

This system of equations is well-posed, and using a numerical technique to be described in the following section, allows the investigation of important biofilm processes.

CHAPTER 4

NUMERICAL TECHNIQUE

The general form of the governing equations and the boundary conditions are discretized and advanced in time using the finite volume approach. The physical space is divided into a (large) number of control volumes (see Fig. 2, and the volume averaged values of $\mathbf{Q}$ are determined in each control volume. Since the problem at hand is axisymmetric, and a structured grid is used, a general indexing scheme can be utilized. Two indices will suffice to describe axisymmetric domains, where the first index (i) spans the "columns" of the domain, and the second index (j) spans the "rows". "Rows" are approximately aligned with the direction of the flow (axial direction), and "columns" go from the centerline to the pipe wall (radial direction). The discretized version of the governing equation for volume (i, j) is

$$\begin{aligned}\frac{\partial(\mathbf{Q}_{ij}V_{ij})}{\partial t} + \Big[&(\mathbf{S}-\mathbf{S}_v)_{i+1/2,j}\cdot\mathbf{n}_{i+1/2,j}S_{i+1/2,j} - \\ &(\mathbf{S}-\mathbf{S}_v)_{i-1/2,j}\cdot\mathbf{n}_{i-1/2,j}S_{i-1/2,j} + \\ &(\mathbf{S}-\mathbf{S}_v)_{i,j+1/2}\cdot\mathbf{n}_{i,j+1/2}S_{i,j+1/2} - \\ &(\mathbf{S}-\mathbf{S}_v)_{i,j-1/2}\cdot\mathbf{n}_{i,j-1/2}S_{i,j-1/2}\Big] = \mathbf{W}_{ij}V_{ij},\end{aligned} \tag{43}$$

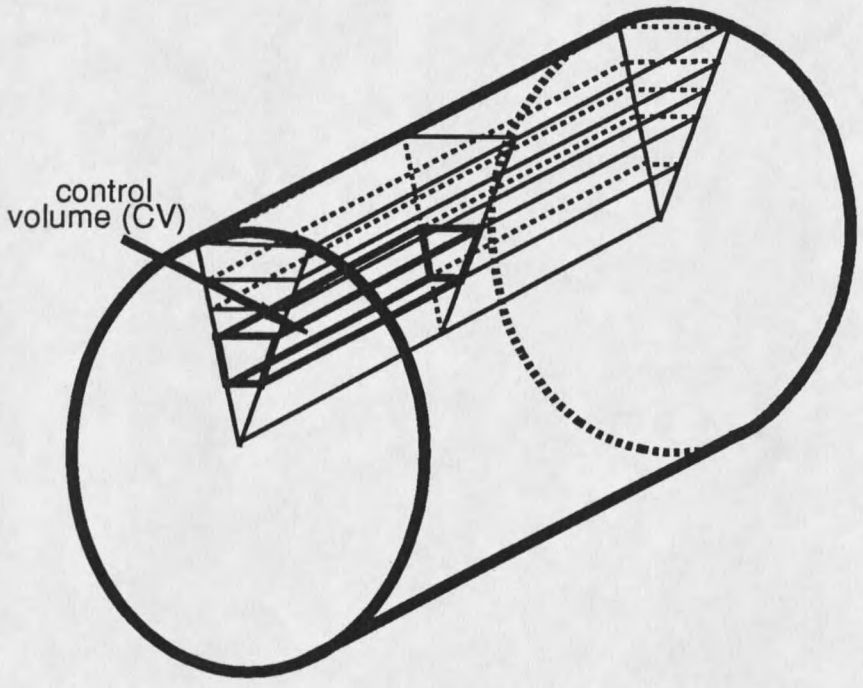

Figure 2: The discretized spatial domain.

where $\mathbf{Q}_{ij}$ and $\mathbf{W}_{ij}$ are the volume averaged values of $\mathbf{Q}$ and $\mathbf{W}$,

$$\mathbf{Q_{ij}} = \frac{1}{V_{ij}} \int\int\int_{V_{ij}} \mathbf{Q} dV, \tag{44}$$

$$\mathbf{W_{ij}} = \frac{1}{V_{ij}} \int\int\int_{V_{ij}} \mathbf{W} dV. \tag{45}$$

Similarly, $\mathbf{n}_{i\pm1/2,j}$ and $\mathbf{n}_{i,j\pm1/2}$ are the surface normals of the four surfaces enclosing volume element V_{ij}, and the surface averaged fluxes for the four surfaces are

$$(\mathbf{S} - \mathbf{S}_v)_{i\pm1/2,j} = \frac{1}{S_{i\pm1/2,j}} \oint_{S_{i\pm1/2,j}} (\mathbf{S} - \mathbf{S}_v) dS, \tag{46}$$

$$(\mathbf{S} - \mathbf{S}_v)_{i,j\pm1/2} = \frac{1}{S_{i,j\pm1/2}} \oint_{S_{i,j\pm1/2}} (\mathbf{S} - \mathbf{S}_v) dS. \tag{47}$$

To simplify the notation, the flux and source terms are grouped into a residual, and

thus (43) has the form:

$$\frac{\partial(\mathbf{Q}_{ij}V_{ij})}{\partial t} + \mathbf{R}_{ij} = 0, \tag{48}$$

where

$$\begin{aligned}\mathbf{R}_{ij} = \Big[&(\mathbf{S}-\mathbf{S}_v)_{i+1/2,j}\cdot\mathbf{n}_{i+1/2,j}S_{i+1/2,j} - \\ &(\mathbf{S}-\mathbf{S}_v)_{i-1/2,j}\cdot\mathbf{n}_{i-1/2,j}S_{i-1/2,j} + \\ &(\mathbf{S}-\mathbf{S}_v)_{i,j+1/2}\cdot\mathbf{n}_{i,j+1/2}S_{i,j+1/2} - \\ &(\mathbf{S}-\mathbf{S}_v)_{i,j-1/2}\cdot\mathbf{n}_{i,j-1/2}S_{i,j-1/2}\Big] - \mathbf{W}_{ij}V_{ij}.\end{aligned} \tag{49}$$

Equation (48) is advanced in time using a general three point integration formula [8]:

$$\frac{(1+\psi)\Delta(\mathbf{Q}V)^n_{ij} - \psi\Delta(\mathbf{Q}V)^{n-1}_{ij}}{\Delta t^n} = (\theta-1)\mathbf{R}^n_{ij} - \theta\mathbf{R}^{n+1}_{ij}, \tag{50}$$

where $\Delta(\cdot)$ is the forward difference operator, defined as

$$\Delta(\cdot) = (\cdot)^{n+1} - (\cdot)^n \tag{51}$$

and ψ, θ are parameters that determine the integration scheme to be used. For example, $\psi = \theta = 0$ corresponds to the classical forward Euler integration formula, $\psi = 0$ and $\theta = 1$ results in the backward Euler scheme. For $\theta = 0$ the integration can be performed without any difficulty, since the unknowns $\mathbf{Q}^{n+1}$ are present on the left hand side only. For $\theta \neq 0$ both the left and the right hand side contain the unknowns $\mathbf{Q}^{n+1}$, and thus the equation becomes nonlinear. In this paper we choose Newton's

Method to linearize the equations and find the solution using a number of iterative steps. In order to apply Newton's Method, the equation has to have the form of $f(x) = 0$. This form for (50) is

$$L(\mathbf{Q}^{n+1}) = \frac{(1+\psi)\Delta(\mathbf{Q}V)_{ij}^{n} - \psi\Delta(\mathbf{Q}V)_{ij}^{n-1}}{\Delta t^n} - \left[(\theta-1)\mathbf{R}_{ij}^{n} - \theta\mathbf{R}_{ij}^{n+1}\right] = 0. \qquad (52)$$

The linear scheme is then

$$L'(\mathbf{Q}^P)\Delta\mathbf{Q}^P = -L(\mathbf{Q}^P), \qquad (53)$$

where P is the iteration index. Thus $\mathbf{Q}^{P=0} = \mathbf{Q}^n$, and $\mathbf{Q}^{P\to\infty} = \mathbf{Q}^{n+1}$. The expression of L is complicated by the fact that the volume elements change in time. The model utilizes the *Geometric Conservation Law* [6],[11]:

$$L(\mathbf{Q}^P) = \frac{V_{ij}^{P+1}(\mathbf{Q}_{ij}^{P} - \mathbf{Q}_{ij}^{n})}{\Delta t^n} - \frac{\psi}{1+\psi}\frac{V_{ij}^{n-1}\Delta(\mathbf{Q}_{ij}^{n-1})}{\Delta t^n} + \frac{\mathbf{Q}_{ij}^{n}}{1+\psi}\left[(\theta-1)\hat{\mathbf{R}}_{ij}^{n} - \theta\hat{\mathbf{R}}_{ij}^{P}\right] - \frac{1}{1+\psi}\left[(\theta-1)\mathbf{R}_{ij}^{n} - \theta\mathbf{R}_{ij}^{P}\right], \qquad (54)$$

where $\hat{\mathbf{R}}_{ij}$ is the "geometric residual"

$$\hat{\mathbf{R}}_{ij} = -\Big[\mathbf{u}_v \cdot \mathbf{n}_{i+1/2,j}S_{i+1/2,j} - \mathbf{u}_v \cdot \mathbf{n}_{i-1/2,j}S_{i-1/2,j} + \mathbf{u}_v \cdot \mathbf{n}_{i,j+1/2}S_{i,j+1/2} - \mathbf{u}_v \cdot \mathbf{n}_{i,j-1/2}S_{i,j-1/2}\Big]. \qquad (55)$$

To determine the first derivative of $L(\mathbf{Q})$ we make the simplifying assumption that the geometric residual does not depend on the vector of unknowns $\mathbf{Q}^P$. This significantly reduces the complexity. Although the assumption is not true, the dependence is very

slight. Using this assumption,

$$L'(\mathbf{Q}^P) = \frac{V_{ij}^{P+1}}{\Delta t^n}\mathbf{I}_{ij} + \frac{\theta}{1+\psi}\frac{\partial \mathbf{R}_{ij}^P}{\partial \mathbf{Q}}, \tag{56}$$

where

$$\begin{aligned}\frac{\partial \mathbf{R}_{ij}}{\partial \mathbf{Q}} = \big[&(\mathbf{D}-\mathbf{D}_v)_{i+1/2,j}\cdot \mathbf{n}_{i+1/2,j}S_{i+1/2,j} - \\ &(\mathbf{D}-\mathbf{D}_v)_{i-1/2,j}\cdot \mathbf{n}_{i-1/2,j}S_{i-1/2,j} + \\ &(\mathbf{D}-\mathbf{D}_v)_{i,j+1/2}\cdot \mathbf{n}_{i,j+1/2}S_{i,j+1/2} - \\ &(\mathbf{D}-\mathbf{D}_v)_{i,j-1/2}\cdot \mathbf{n}_{i,j-1/2}S_{i,j-1/2}\big] - \frac{\partial \mathbf{W}_{ij}}{\partial \mathbf{Q}}V_{ij}.\end{aligned} \tag{57}$$

In the above equations $\mathbf{I}$ is the identity matrix, and $\mathbf{D}$ and $\mathbf{D}_v$ are the inviscid and viscous Jacobians, respectively. The indices of the Jacobians denote that the matrices multiply vectors $\Delta\mathbf{Q}$ at the same locations, e.g. $\mathbf{D}_{i+1/2,j}$ multiplies $\Delta\mathbf{Q}_{i+1/2,j}$.

Our next task is to determine the surface averaged values of $\Delta\mathbf{Q}$. This can be done by extrapolating the volume averaged values to the surfaces. Two extrapolations exist, one from the "right" (positive) and one from the "left" (negative) [12]; that is,

$$\mathbf{Q}_{l\mp 1/2}^{\pm} = \mathbf{Q}_l \mp \frac{\phi}{4}[(1\pm\kappa)(\mathbf{Q}_l - \mathbf{Q}_{l-1}) + (1\mp\kappa)(\mathbf{Q}_{l+1}-\mathbf{Q}_l)], \tag{58}$$

where l is a generic index for i or j, depending on the direction of the interpolation. Values of ϕ and κ determine the order and type of the interpolation formula. If $\phi = 0$ is selected, then the resulting extrapolation formula is first-order upwind,

$$\mathbf{Q}_{l\mp 1/2}^{\pm} = \mathbf{Q}_l. \tag{59}$$

Other parameter choices result in second-order upwind, second order central differences and third-order upwind-biased extrapolation [7]. For simplicity first-order upwind extrapolations are used in this paper.

Using the left and right extrapolation values, the inviscid fluxes (using general index l) are given by

$$\mathbf{S}^{\pm}_{l+1/2} \cdot \mathbf{n}_{l+1/2} = \frac{\tilde{\mathbf{u}}^{\mp}_{l+1/2} \pm |\tilde{\mathbf{u}}^{\mp}_{l+1/2}|}{2} \mathbf{Q}^{\mp}_{l+1/2}, \tag{60}$$

where $\tilde{\mathbf{u}}$ is component of the relative velocity normal to the surface $l + 1/2$

$$\tilde{\mathbf{u}}_{l+1/2} = (\mathbf{u} - \mathbf{u}_v)_{l+1/2} \cdot \mathbf{n}_{l+1/2}. \tag{61}$$

To determine $\mathbf{u}$ at the surfaces, the same extrapolation formulas can be used as described in eq. 58. Note that in the biofilm, $\mathbf{u}_s$ and $\mathbf{u}_v$ are known at the surfaces, so the trivial extrapolation $(\cdot)^{+}_{l+1/2} = (\cdot)^{-}_{l+1/2} = (\cdot)_{l+1/2}$ can be used. A similar expression can be derived for the inviscid Jacobians, yielding

$$\tilde{\mathbf{D}}_{l+1/2} \Delta \mathbf{Q}_{l+1/2} = \tilde{\mathbf{D}}^{+}_{l+1/2} \Delta \mathbf{Q}_{l} + \tilde{\mathbf{D}}^{-}_{l+1/2} \Delta \mathbf{Q}_{l+1}, \tag{62}$$

where the first-order extrapolation formula for $\Delta \mathbf{Q}_{l+1/2}$ has been utilized, and the generalized Jacobian matrix $\tilde{\mathbf{D}} = \mathbf{D} \cdot \mathbf{n}$ has been introduced.

The viscous fluxes can be determined from the directional derivative of the concentration, thus for component k it has the form

$$(\tilde{\mathbf{S}}_v)_k = (D_k)_{l+1/2} \mathbf{n}_{l+1/2} \cdot \nabla C_k = (D_k)_{l+1/2} \frac{dC_k}{dn_{l+1/2}}. \tag{63}$$

Diffusion coefficient $(D_k)_{l+1/2}$ is determined as the average of the diffusion coefficients of the volumes that share the surface under consideration. The above equation can be simplified, if we assume that the axial diffusion is insignificant,

$$(D_k)_{l+1/2}\frac{dC_k}{dn_{j+1/2}} = (D_k)_{j+1/2}|\nabla\eta|_{j+1/2}\frac{\partial C_k}{\partial\eta}_{j+1/2}, \tag{64}$$

where η represents the generalized curvilinear coordinate in the j direction. The components of the above equation can easily be determined from known concentrations and volume elements from the relationships

$$\left(\frac{\partial C_k}{\partial\eta}\right)_{j+1/2} = (C_k)_{j+1} - (C_k)_j \text{and}$$
$$|\nabla\eta|_{j+1/2} = \frac{S_{j+1/2}}{0.5(V_j + V_{j+1})}. \tag{65}$$

In words, $|\nabla\eta|$ is determined as the ratio of the surface of interest and the volumes sharing that surface. Similarly to the inviscid Jacobians, the viscous Jacobians can be written as the sum of "positive" and "negative" contributions,

$$(\tilde{\mathbf{D}}_v)_{j+1/2}\Delta\mathbf{Q}_{j+1/2} = (\tilde{\mathbf{D}}_v)^+_{j+1/2}\Delta\mathbf{Q}_j + (\tilde{\mathbf{D}}_v)^-_{j+1/2}\Delta\mathbf{Q}_{j+1}, \tag{66}$$

where

$$(\tilde{\mathbf{D}}_v)^\pm_{j\pm1/2} = \mp D_{j\pm1/2}|\nabla\eta|_{j\pm1/2}\left(\frac{1}{\varepsilon_l}\right)_j \mathbf{I}. \tag{67}$$

The source term and its Jacobian remain to be specified. The form of the source term is given in equation (12). The Jacobian can be calculated in a straightforward manner using (12) and (14) - (18).

Substituting the expressions for fluxes, source terms and their Jacobians into (53) results in a set of coupled linear equations for $\Delta\mathbf{Q}^P$. These equations written for $\Delta\mathbf{Q}^P$ in volume (i,j) will have contributions from itself, and also from volumes $(i+1,j)$, $(i-1,j)$, $(i,j-1)$, $(i,j+1)$. However, after a closer inspection of the contribution of $(i+1,j)$ we can conclude that it is zero for positive flow velocities. Thus we can perform a marching algorithm, meaning that we solve the equations for volumes in the ith column, and then repeat the procedure for the next column. The next column is $i+1$ for positive flow fields (which is typically the case), and $i-1$ for negative flows. Further simplification of the equations results from the marching algorithm. The contribution of $(i-1,j)$ is zero, since the previous column already converged, thus $\Delta\mathbf{Q}_{i-1,j} = 0$. As a result, at every column a block-tridiagonal system of equations has to be solved. The block-size is $N_{sub} + N_{part}$ in the bulk, and $N_{sub} + N_{part} - 1$ in the film. Recursive techniques, such as the block Thomas algorithm ([8]) can be used effectively to solve this system of equations.

The two remaining quantities that have to be determined are $\mathbf{u}_s$ and $\mathbf{u}_v$. If we assume that the streamwise direction is perpendicular to the normal of the solid wall, a discretized version of (33) is

$$[u_s(\mathbf{e}_{u_s}\cdot\mathbf{n})S]_{i,j+1/2} - [u_s(\mathbf{e}_{u_s}\cdot\mathbf{n})S]_{i,j-1/2} = \frac{1}{1-\varepsilon_l}\left(\sum_{k=1}^{N_{part}}\frac{W_{Nsub+k}}{\varrho_k}\right), \qquad (68)$$

where $\mathbf{e}_{u_s}$ is the unit vector of $\mathbf{u}_s$. This equation can be solved for u_s starting from the wall, where it is 0, and incrementally determine its value for each surface $S_{i,j+1/2}$

to the interface. After determining the value of u_s at the interface, $(\mathbf{u}_v)_I$ can be determined using the value of $\mathbf{R}_F$.

At this point all values are known at time n, so the next step is to determine the movement of the grid. The grid is allowed to move in the j direction (normal to the wall) only. Knowing the interface velocity $(\mathbf{u}_v)_I$, the velocities of the surfaces $S_{i,j+1/2}$ in the full domain can be determined. The velocity $\mathbf{u}_v$ linearly varies from the full value at the interface to zero at the wall and at the centerline. The velocity determined this way gives the velocity of the centroids of the surfaces, thus a further computational step is needed to determine the vertex velocities. The actual displacement of the vertices is determined by multiplying the vertex velocity with the time step. A very simple way of calculating the vertex velocities is

$$\mathbf{u}_{i+1,j+1/2} = \mathbf{u}_{i,j+1/2} + 2(\mathbf{u}_{i,j+1/2} - (\mathbf{u}_v)_{i+1/2,j+1/2}), \text{ and}$$

$$\mathbf{u}_{0,j+1/2} = (\mathbf{u}_v)_{1/2,j+1/2}, \tag{69}$$

where $\mathbf{u}_{i,j+1/2}$ is the vertex velocity of the "left" end of surface $S_{i+1/2,j+1/2}$, $\mathbf{u}_{i+1,j+1/2}$ is the vertex velocity of the "right" end of the same surface, and $(\mathbf{u}_v)_{i+1/2,j+1/2}$ is the known centroid velocity of the same surface. The velocity of the very first vertex has to be determined using the second part of the equation, or some other additional information. The disadvantage of the above method of determining the velocity of the first vertex is that this way a "jagged" grid can be produced, if the growth of the film is uneven (Figure 3).