



Analysis of a one dimensional biofilm model
by Lori Anne Pritchett

A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of
Philosophy in Mathematical Sciences
Montana State University
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Abstract:

Biofilm is a term used to describe the collection of organisms in an aqueous environment. A model which simulates a single species biofilm with one growth limiting substrate is derived. In this simple model, it is proved that the solution to the substrate equation is bounded. If diffusion is included in the biomass equations, then the biofilm volume fractions, thickness and velocity are also bounded. The model which does not include detachment suggests that a steady-state solution is possible if the inactivation rate is zero. It is also shown that a steady-state solution corresponding to the absence of active biomass is linearly unstable provided the bulk substrate satisfies an inequality involving the observed decay rate. Finally, this model is altered to include EPS. The production of EPS depends on the concentration level of a signaling chemical which is also included in the model. The numerical simulations of this new model indicate that a minimum production rate is needed for a significant amount of EPS to be produced.

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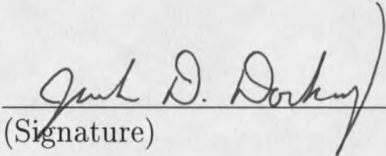
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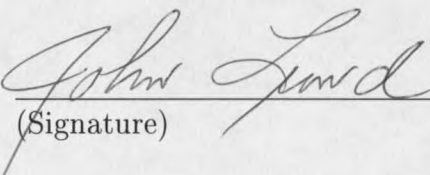
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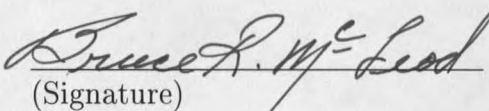
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I would like to dedicate this dissertation to my late grandparents, John Coleman and Ruby Pritchett, Glen and Edna Taylor and my late aunt, Colleen Baldy. I wish you could have lived to see the first doctor in the family.

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ABSTRACT

Biofilm is a term used to describe the collection of organisms in an aqueous environment. A model which simulates a single species biofilm with one growth limiting substrate is derived. In this simple model, it is proved that the solution to the substrate equation is bounded. If diffusion is included in the biomass equations, then the biofilm volume fractions, thickness and velocity are also bounded. The model which does not include detachment suggests that a steady-state solution is possible if the inactivation rate is zero. It is also shown that a steady-state solution corresponding to the absence of active biomass is linearly unstable provided the bulk substrate satisfies an inequality involving the observed decay rate. Finally, this model is altered to include EPS. The production of EPS depends on the concentration level of a signaling chemical which is also included in the model. The numerical simulations of this new model indicate that a minimum production rate is needed for a significant amount of EPS to be produced.

CHAPTER 1

BIOFILM MODELS

The term biofilm describes the collection of microorganisms that accumulate on surfaces in aqueous environments. Biofilms occur in a variety of places. Examples include: pipes in a waste-water treatment plant, medical implants and rocks in a stream bed. The presence of such build-up poses health risks and can effect a system's operation. Once a film forms on a surface, it is expensive to remove and it may return. Understanding the mechanisms that control the formation of biofilms could lead to better methods for prevention and removal.

Biofilms are complex systems. They contain both liquid and solid components. In each of these phases, several types of organisms and substrates are usually present. Studying the processes that take place inside a biofilm is difficult, since the thickness of most biofilms is on the order of 10 to 100 microns. With such a small scale, experiments are hard to design and perform. By using mathematical models, a particular process or environmental situation can be isolated and studied. The earliest models, developed in the late 1970's, were static models. The spatial distribution of the organisms and the thickness of the biofilm were fixed. The models described the substrate concentration inside a biofilm. The next generation of models allowed the thickness of the biofilm and the species distribution to evolve over time.

Wanner and Gujer [13] proposed one of the first dynamic models. The model is a set of partial differential equations derived from mass conservation principles. This model was one dimension in space and modeled variations in a direction perpendicular to the film's surface. Other transient models followed [6], and their development is similar to the approach taken by Wanner and Gujer. Although these models have been studied numerically, their solutions have not been studied mathematically. Furthermore, neither model includes the production of non-biomass substances. For example, most bacteria produce polymers that coat the cells in the biofilm. These polymers, called extracellular polymeric substances (EPS), allow the cells to attach to surfaces. It is believed that EPS contributes to other physical phenomenon inside a biofilm. Unfortunately the exact relationship between EPS and the observed physical changes is not well-understood. A mathematical model with EPS production would aid in the study of EPS formation in a biofilm. In this thesis, a general one dimensional biofilm model is derived and the solutions of this model are analyzed. This model is then adapted to include EPS production.

Chapter 2 contains the derivation of the model. The derivation is a slightly different approach than was used in [13] and [6]. Both [13] and [6] derived the model in only one spatial dimension. Although the final model in Chapter 2 is the same set of equations found in [13], these equations are the reduction of a three dimensional model to one dimension. This approach is used because a biofilm is a three dimensional

object. If a one dimensional model is used to study a biofilm it should be consistent with a three dimensional model.

Once this model is derived, Chapter 3 covers some of the qualitative properties. We will assume that a solution exists and is unique. With this assumption, we will show that the solution of the substrate equation is bounded. Under the assumption that biomass diffuses inside the biofilm, we prove that the solution related to the organism density is bounded. From this result, bounds on the biofilm thickness and velocity are proved. Another result found in this chapter is the behavior of the equation related to biomass density at the interface. It is proved that for all parameter values, the model tends to a steady-state value at the interface. This implies that the density of organisms at the film's surface approaches a fixed value.

With a small number of organisms present, a film quickly forms and then stabilizes at a thickness on the order of 100 microns. If the model duplicates this behavior, then the solutions would tend to a steady state solution. In Chapter 4, the existence and stability of steady state solutions is studied. The model without detachment included has two steady-state solutions. One is a trivial solution that corresponds to a biofilm with no active organisms present. This solution is linearly unstable if the organism growth rate at the interface is greater than the inactivation rate. The other solution exists if the inactivation rate is zero and if the organism growth rate at the interface is positive. The stability of this solution is analyzed numerically. The results are mixed, but most of the numerics indicate that the solution is stable.

Finally in Chapter 5, the model derived in Chapter 2 is altered to include EPS production. There is experimental evidence [3], [5], [8] that signaling chemicals control EPS production. Based on this information, the basic model is expanded to include EPS and chemical signaling. One description of a biofilm is a gel made up of EPS with cells embedded in the EPS. Using this description, the EPS is modeled like inactive biomass. However, the formation of EPS uses substrate when the signaling chemical reaches a threshold value. The numerical simulations of this new model indicate that there is a minimum rate at which the signaling chemical must be produced at before a significant amount of EPS is formed. Once this minimum has been exceeded the model predicts that most of the EPS occurs at the surface to which the film is attached and most of the organisms can be found near the interface. The model also appears to limit on steady-state solutions.

CHAPTER 2

DERIVATION OF THE MODEL

In this chapter, we will derive a one dimensional biofilm model. The derivation does not depend on specific transport, production or growth terms. A variety of functions for these quantities can be easily inserted into the model equations. Starting with a general three dimensional model, a one dimensional model is produced by assuming that only significant variations occur in a direction normal to the surface to which the film is attached. After establishing this one dimensional model, it is rescaled to a non-dimensional set of equations. It is this system that is studied in further detail in Chapter 3 and Chapter 4.

Physical System

We will assume that the biofilm is a single species biofilm with one growth limiting substrate present. The physical system is divided into two regions: the biofilm and the bulk liquid. The biofilm, attached to a surface called the substratum, consumes a substrate supplied in the bulk liquid. The fluid-biofilm interface, Γ , separates the two regions (See Figure 1).

To simplify the geometry of the problem, we will assume that the biofilm grows on a flat surface. Let $\mathbf{x} = (x, y, z)$. The yz plane corresponds to the substratum and x denotes the distance in the direction of the outward normal to this plane. We will

also assume that the model quantities are periodic in the yz plane. Therefore, the model will be derived inside a rectangular box with a square base with sides of length $2h$. The substratum is at the base of this box. The origin for the coordinate system is placed at the center of this square.

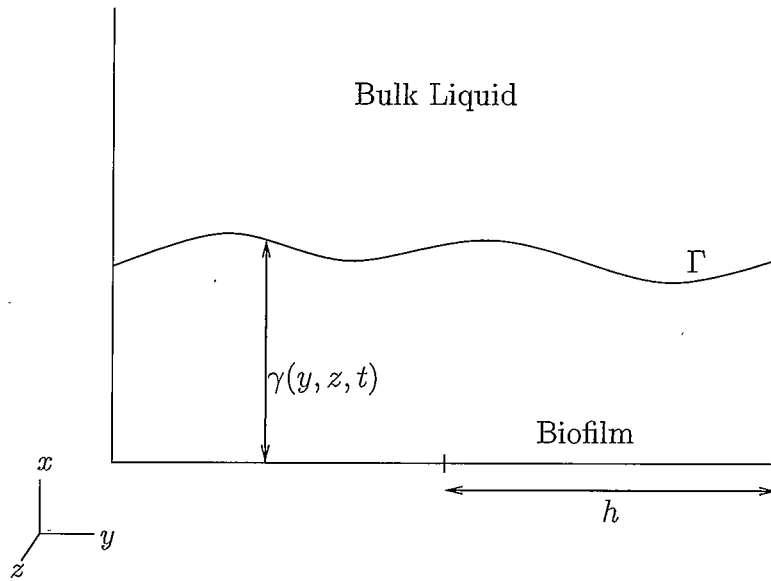


Figure 1. Biofilm and Bulk Liquid.

The composition of the biofilm is microorganisms and substrate. The organisms are called biomass. Although one species is present, it is divided into two subpopulations. Active biomass which consumes substrate and the inactive biomass which is inert material and does not consume substrate. The model consists of equations derived from mass balance principles that describe the substrate concentration, active and inactive biomass profiles inside the biofilm. This system of equations is coupled

with an equation that describes the evolution of the fluid-biofilm interface. We begin with the equations inside the biofilm.

Model Equations Inside the Biofilm

Active Biomass

Let $\rho(\mathbf{x}, t)$ be the active biomass density at \mathbf{x} and time t . Consider an arbitrary control volume, Ω , found inside the biofilm compartment. The total mass of active cells in Ω is

$$\int_{\Omega} \rho(\mathbf{x}, t) d\sigma.$$

This quantity changes as new cells are created and as active biomass passes through the surface of Ω . Thus,

$$\frac{d}{dt} \int_{\Omega} \rho(\mathbf{x}, t) d\sigma = - \int_{\partial\Omega} \mathbf{J}_{\rho}(\mathbf{x}, t) \cdot \mathbf{n} d\tau + \int_{\Omega} F_{\rho}(\mathbf{x}, t) d\sigma$$

where $\partial\Omega$ is the boundary of Ω , \mathbf{J}_{ρ} is the flux of active biomass, \mathbf{n} is the outward direction normal to $\partial\Omega$ and F_{ρ} is the net production rate of active biomass.

Provided that the boundary of Ω is smooth and \mathbf{J}_{ρ} is C^1 , the divergence theorem states

$$\int_{\partial\Omega} \mathbf{J}_{\rho} \cdot \mathbf{n} d\tau = \int_{\Omega} \nabla \cdot \mathbf{J}_{\rho} d\sigma.$$

Therefore, the mass balance equation can be written as

$$\frac{d}{dt} \int_{\Omega} \rho d\sigma = \int_{\Omega} F_{\rho} - \nabla \cdot \mathbf{J}_{\rho} d\sigma.$$

If ρ is a C^1 function in \mathbf{x} and t , then

$$\frac{d}{dt} \int_{\Omega} \rho(\mathbf{x}, t) d\sigma = \int_{\Omega} \frac{\partial \rho}{\partial t}(\mathbf{x}, t) d\sigma.$$

Since Ω is an arbitrary volume, this results in the partial differential equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J}_{\rho} = F_{\rho}.$$

Cells inside a biofilm are not mobile. Their movement can only occur as the surrounding material expands. Thus, the flux of biomass is a convection process. If $\mathbf{v}(\mathbf{x}, t)$ is the biomass velocity at \mathbf{x} , then

$$\mathbf{J}_{\rho} = \mathbf{v}\rho.$$

Hence, the active biomass equation in the biofilm is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{v}\rho) = F_{\rho}. \quad (2.1)$$

Inactive Biomass

Let $\bar{\rho}(\mathbf{x}, t)$ be the inactive biomass density at \mathbf{x} and time t . The total mass of inactive material found in a control volume Ω is

$$\int_{\Omega} \bar{\rho}(\mathbf{x}, t) d\sigma.$$

Change in the total mass occurs from material transport and production of inactive biomass. Thus, the mass balance equation is

$$\frac{d}{dt} \int_{\Omega} \bar{\rho}(\mathbf{x}, t) d\sigma = - \int_{\partial\Omega} \mathbf{J}_{\bar{\rho}}(\mathbf{x}, t) \cdot \mathbf{n} d\tau + \int_{\Omega} F_{\bar{\rho}}(\mathbf{x}, t) d\sigma$$

where the flux of inactive material is $\mathbf{J}_{\bar{\rho}}$ and the production rate of inactive material is $F_{\bar{\rho}}$. Following the same reasoning as above, this integral equation is equivalent to

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot \mathbf{J}_{\bar{\rho}} = F_{\bar{\rho}}.$$

We assume that the transport of inactive biomass is the same as active biomass.

Hence, the flux of inactive biomass is

$$\mathbf{J}_{\bar{\rho}} = \mathbf{v}\bar{\rho}.$$

With this equation, the inactive biomass equation inside the biofilm is

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\mathbf{v}\bar{\rho}) = F_{\bar{\rho}}. \quad (2.2)$$

Substrate

If $S(\mathbf{x}, t)$ is the substrate concentration at \mathbf{x} and time t , then the total amount of substrate found in Ω is

$$\int_{\Omega} S(\mathbf{x}, t) d\sigma.$$

Like the biomass, this quantity changes as substrate moves through Ω and as active biomass consumes substrate. This change in substrate can be expressed as

$$\frac{d}{dt} \int_{\Omega} S(\mathbf{x}, t) d\sigma = - \int_{\partial\Omega} \mathbf{n} \cdot \mathbf{J}_S(\mathbf{x}, t) d\tau - \int_{\Omega} F_S(\mathbf{x}, t) d\sigma$$

where \mathbf{J}_S is the flux of substrate. The quantity F_S represents the rate of substrate usage inside the biofilm. F_S is assumed to be positive and the minus sign on the last

integral indicates that substrate is consumed and not produced inside the biofilm. Again, the divergence theorem and the assumption that Ω is an arbitrary volume leads to

$$\frac{\partial S}{\partial t} + \nabla \cdot \mathbf{J}_S = -F_S.$$

The transport of substrate is modeled by Fick's law; which states

$$\mathbf{J}_S = -D\nabla S$$

where the constant D is the diffusion coefficient for substrate. Thus, the equation for substrate is

$$\frac{\partial S}{\partial t} = D\nabla^2 S - F_S. \quad (2.3)$$

Velocity

In both biomass equations, the velocity field is not specified. To determine the velocity, we will make the following assumptions. Material inside a biofilm convects as new biomass is produced. Hence, the divergence of the velocity is proportional to the rate of biomass production. Thus,

$$\nabla \cdot \mathbf{v} = k(F_\rho + F_{\bar{\rho}}) \quad (2.4)$$

where k is the constant of proportionality. Since the velocity contains three components, this equation is not enough to determine \mathbf{v} . Therefore, we will also assume that the velocity field is irrotational. Under this assumption,

$$\mathbf{v}(\mathbf{x}, t) = \nabla\phi(\mathbf{x}, t) \quad (2.5)$$

where ϕ is a velocity potential. Combining equations (2.4) and (2.5) leads to

$$\nabla^2 \phi = k (F_\rho + F_{\bar{\rho}}). \quad (2.6)$$

By using equation (2.6), equation (2.5) can be used to solve for \mathbf{v} . Using equation (2.5), the biomass equations can now be written as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \nabla \phi) = F_\rho \quad (2.7)$$

and

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \nabla \phi) = F_{\bar{\rho}}. \quad (2.8)$$

Fluid-Biofilm Interface

If u is some physical quantity, then the material derivative of u is given by

$$\frac{Du}{Dt} = \frac{\partial u}{\partial t} + \mathbf{w} \cdot \nabla u$$

where \mathbf{w} is the velocity. The material derivative is the change of u an observer would see while traveling along the vector field \mathbf{w} .

We will assume that the surface which separates the bulk liquid from the biofilm has no diffusional layer and that this surface can be described by the equation

$$u(x, y, z, t) \equiv x - \gamma(y, z, t) = 0. \quad (2.9)$$

We will also assume that biomass on this surface will remain on this surface as the biofilm grows. Thus, the material derivative of u is zero on the interface.

Let $\mathbf{v} = (v_1, v_2, v_3)$ be the limit of the velocity from inside the biofilm at the point $(\gamma(y, z, t), y, z)$. The material derivative of (2.9) evaluated on the interface is

$$\begin{aligned} \frac{D}{Dt} (x - \gamma(y, z, t)) &= -\frac{\partial \gamma}{\partial t} + \mathbf{v} \cdot \nabla (x - \gamma) \\ &= -\frac{\partial \gamma}{\partial t} + v_1 \left(1 - \frac{\partial \gamma}{\partial x}\right) + v_2 \left(-\frac{\partial \gamma}{\partial y}\right) + v_3 \left(-\frac{\partial \gamma}{\partial z}\right). \end{aligned}$$

Since the material derivative is zero and $\mathbf{v} = \nabla \phi$, this can be written as

$$\frac{\partial \gamma}{\partial t} + \frac{\partial \phi}{\partial y} \frac{\partial \gamma}{\partial y} + \frac{\partial \phi}{\partial z} \frac{\partial \gamma}{\partial z} = \frac{\partial \phi}{\partial x}. \quad (2.10)$$

Boundary Conditions

Biomass

Since biomass does not interact or pass through the substratum a no-flux condition is placed along this surface. If \mathbf{n} is the outward normal of the substratum surface, then for points on the substratum

$$\mathbf{n} \cdot (\mathbf{v}\rho) = 0, \quad \mathbf{n} \cdot (\mathbf{v}\bar{\rho}) = 0.$$

With the simple geometry placed on this problem, these boundary conditions are equivalent to

$$v_1(0, y, z, t)\rho(0, y, z, t) = 0, \quad v_1(0, y, z, t)\bar{\rho}(0, y, z, t) = 0$$

where v_1 is the x component of \mathbf{v} . Along the sides of the box, where $y = \pm h$ and $z = \pm h$, periodic boundary conditions are placed on ρ and $\bar{\rho}$. This choice is made to avoid mathematical complications that can arise with solid boundaries and is based on the assumption that ρ and $\bar{\rho}$ are periodic functions in the yz plane.

Substrate

Substrate does not interact or pass through the substratum. So a no-flux condition is appropriate. Using the geometry of the problem, the boundary condition is

$$\frac{\partial S}{\partial x}(0, y, z, t) = 0.$$

In the bulk liquid, substrate is fed in at a constant rate. If the fluid is well-stirred, the concentration is constant along Γ . If S_{bulk} is the concentration of the substrate in the bulk liquid, then

$$S(\gamma(y, z, t), y, z, t) = S_{bulk}.$$

Periodic boundary conditions are placed on S and $\mathbf{n} \cdot \nabla S$, where \mathbf{n} is the outward normal direction along the sides of the box.

Velocity Potential

We will assume that the biofilm velocity at the substratum is zero. In terms of the velocity potential, this boundary condition is stated as

$$\mathbf{n} \cdot \nabla \phi(0, y, z) = 0$$

where \mathbf{n} is the outward normal of the substratum. This simplifies to the condition

$$\frac{\partial \phi}{\partial x}(0, y, z, t) = 0.$$

Along the sides, periodic boundary conditions are placed on ϕ . At the interface, \mathbf{v} is perpendicular to the surface; thus ϕ is constant on the interface. Since ϕ is a

potential, an arbitrary value for ϕ can be assigned on γ . Therefore, we set

$$\phi(\gamma(y, z, t), y, z, t) = 0.$$

Production Terms

In this section, we will specify the net biomass production and substrate usage functions. We will not assume specific kinetic terms. Instead the general form and mathematical properties of these functions is addressed.

Active Biomass

Active biomass is produced as it consumes substrate. It decreases as it converts to inactive biomass. We will assume that both the active biomass production and the conversion to inactive biomass occurs at rates proportional to the active biomass density. Under these assumptions,

$$F_\rho = R(S)\rho - K_i\rho \tag{2.11}$$

where K_i is the inactivation rate and R is the net production rate from substrate utilization. We assume that R has the following properties: $R \in C^1$ for $S \geq 0$, $R'(S) > 0$ and $R(0) < 0$. The last property allows a loss of biomass for low substrate concentrations. A Monod kinetic term is a common function used to model cellular reproduction in a biofilm [2]. A function with a Monod kinetic term which satisfies these properties is

$$R(S) = \frac{\hat{\mu}S}{K + S} - K_d \tag{2.12}$$

where $\hat{\mu}$ is a maximum growth rate and K is the Monod constant. The parameter K_d represents the organism decay rate.

Inactive Biomass

Inactive biomass does not consume substrate. Once biomass has become inert it can not become active. We also assume that inactive biomass does not decay. Therefore, the net production of inactive biomass is

$$F_{\bar{p}} = K_i \rho. \quad (2.13)$$

Substrate

Substrate consumption is proportional to the active biomass density. Thus,

$$F_S = \frac{1}{Y} G(S) \rho \quad (2.14)$$

where Y is a yield coefficient and G is a function with the following properties: $G \in C^1$ for $S \geq 0$, $G'(S) > 0$ and $G(0) = 0$. Again, a Monod equation is the typical choice to model substrate usage [2]. Notice, that

$$G(S) = \frac{\hat{\mu} S}{K + S} \quad (2.15)$$

satisfies the properties given above. As before, $\hat{\mu}$ represents a maximum growth rate and K is the Monod constant.

One Dimensional Model

In summary, the model equations are

$$\frac{\partial S}{\partial t} = D\nabla^2 S - \frac{1}{Y}G(S)\rho, \quad (2.16a)$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \nabla \phi) = R(S)\rho - K_i \rho, \quad (2.16b)$$

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \nabla \phi) = K_i \rho, \quad (2.16c)$$

$$\nabla^2 \phi = kR(S)\rho, \quad (2.16d)$$

$$\mathbf{v} = \nabla \phi \quad (2.16e)$$

inside the biofilm with the equation

$$\frac{\partial \gamma}{\partial t} + \frac{\partial \phi}{\partial y} \frac{\partial \gamma}{\partial y} + \frac{\partial \phi}{\partial z} \frac{\partial \gamma}{\partial z} = \frac{\partial \phi}{\partial x} \quad (2.17)$$

for the interface and boundary conditions

$$\frac{\partial S}{\partial x}(0, y, z, t) = 0, \quad (2.18a)$$

$$v_1(0, y, z, t)\rho(0, y, z, t) = 0, \quad v_1(0, y, z, t)\bar{\rho}(0, y, z, t) = 0, \quad (2.18b)$$

$$\frac{\partial \phi}{\partial x}(0, y, z, t) = 0, \quad (2.18c)$$

$$S(\gamma(y, z, t), y, z, t) = S_{bulk}, \quad (2.18d)$$

$$\phi(\gamma(y, z, t), y, z, t) = 0. \quad (2.18e)$$

Table 1 and 2 list the variables and parameters in the model. The last column in each table displays the units. The symbol m_s is substrate mass units, m_ρ and $m_{\bar{\rho}}$ are mass units of active and inactive biomass, l and t are units of length and time.

Symbol	Description	Units
S	Substrate concentration	$m_s l^{-3}$
ρ	Active biomass density	$m_\rho l^{-3}$
$\bar{\rho}$	Inactive biomass density	$m_{\bar{\rho}} l^{-3}$
\mathbf{v}	Velocity	$l t^{-1}$
ϕ	Velocity potential	t^{-1}
γ	Interface height	l

Table 1. Model variables.

Symbol	Description	Units
S_{bulk}	Bulk liquid substrate concentration	$m_s l^{-3}$
D	Diffusion constant	$l^2 t^{-1}$
Y	Yield coefficient	$m_\rho m_s^{-1}$
K_i	Inactivation rate	t^{-1}
k	Constant of proportionality	$m_\rho^{-1} l^3$
R	Active biomass growth rate (substrate related)	t^{-1}
G	Substrate utilization rate	t^{-1}
$\hat{\mu}$	Maximum growth rate	t^{-1}
K	Monod constant	$m_s l^{-3}$
K_d	Decay rate	t^{-1}

Table 2. Model parameters and functions.

Provided that the change of the model quantities in the yz plane is small, this model can be reduced to one spatial variable. Under this assumption, the equations inside the biofilm reduce to

$$\frac{\partial S}{\partial t} = D \frac{\partial^2 S}{\partial x^2} - \frac{1}{Y} G(S) \rho, \quad (2.19a)$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} \left(\rho \frac{\partial \phi}{\partial x} \right) = R(S) \rho - K_i \rho, \quad (2.19b)$$

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x} \left(\bar{\rho} \frac{\partial \phi}{\partial x} \right) = K_i \rho, \quad (2.19c)$$

$$\frac{\partial^2 \phi}{\partial x^2} = k R(S) \rho, \quad (2.19d)$$

$$v = \frac{\partial \phi}{\partial x} \quad (2.19e)$$

and the interface equation is

$$\frac{d\gamma}{dt} = \frac{\partial \phi}{\partial x} (\gamma(t), t). \quad (2.20)$$

With one spatial variable, we can solve for the velocity. By integrating equation (2.19d) and using the boundary condition (2.18c), the velocity is given by

$$v(x, t) = k \int_0^x R(S(\xi, t)) \rho(\xi, t) d\xi. \quad (2.21)$$

To determine the constant k , we will assume that the biomass density is constant.

Under this assumption, the densities ρ and $\bar{\rho}$ can be written as

$$\rho(x, t) = \rho_0 f(x, t),$$

$$\bar{\rho}(x, t) = \rho_0 \bar{f}(x, t)$$

where f is the volume fraction of active biomass, \bar{f} is the volume fraction of inactive biomass and ρ_0 is the intrinsic density of the cells. Substituting these equations into

equations (2.19b) and (2.19c) yields

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x}(vf) = R(S)f - K_i f, \quad (2.22a)$$

$$\frac{\partial \bar{f}}{\partial t} + \frac{\partial}{\partial x}(v\bar{f}) = K_i \bar{f}. \quad (2.22b)$$

We will assume that f and \bar{f} satisfy

$$f + \bar{f} = 1 - \epsilon_l$$

where ϵ_l is the liquid volume fraction. If ϵ_l is constant, this equation allows us to solve for the constant k . By adding equations (2.22a) and (2.22b), we have

$$(1 - \epsilon_l) \frac{\partial v}{\partial x} = R(S)f.$$

Comparing this to equation (2.21) leads to

$$kR(S)\rho_0 f(x, t) = \frac{1}{1 - \epsilon_l} R(S)f(x, t).$$

Therefore, k satisfies the equation

$$k = \frac{1}{\rho_0(1 - \epsilon_l)}$$

and the velocity equation is

$$v(x, t) = \frac{1}{1 - \epsilon_l} \int_0^x R(S(\xi, t))f(\xi, t) d\xi. \quad (2.23)$$

In one dimension, γ represents the thickness of the biofilm. To simplify the notation, let $L = \gamma$. Since $v = \frac{\partial \phi}{\partial x}$, equation (2.20) leads to the differential equation

$$\frac{dL}{dt} = \frac{1}{1 - \epsilon_l} \int_0^{L(t)} R(S(\xi, t))f(\xi, t) d\xi \quad (2.24)$$

which describes how the thickness of the biofilm changes.

Dimensionless Model

Let $\hat{x} = \frac{x}{\hat{l}}$ where \hat{l} denotes the characteristic length scale of a biofilm which is typically on the order of 100 microns [2]. The time variable is re-scaled as

$$\hat{t} = t\hat{\mu}$$

and the model variables are re-scaled to

$$\hat{S} = \frac{S}{K}, \quad \hat{f} = \frac{f}{1 - \epsilon_l}, \quad \hat{v} = \frac{v}{\hat{l}\hat{\mu}}, \quad \hat{L} = \frac{L}{\hat{l}}.$$

With this choice, we define the dimensionless parameters

$$\epsilon = \frac{\hat{l}^2 K}{D}, \quad \alpha = \frac{K_i}{\hat{\mu}}.$$

The functions G and R are also re-scaled to

$$\hat{G}(\hat{S}) = \frac{1}{\hat{\mu}} G(K\hat{S}) \tag{2.25a}$$

and

$$\hat{R}(\hat{S}) = \frac{1}{\hat{\mu}} R(K\hat{S}). \tag{2.25b}$$

If G and R are defined by equations (2.15) and (2.12), then

$$\hat{G}(\hat{S}) = \frac{\hat{S}}{1 + \hat{S}}$$

and

$$\hat{R}(\hat{S}) = \frac{\hat{S}}{1 + \hat{S}} - \frac{K_d}{\hat{\mu}}.$$

This motivates the definition of the following parameters

$$\frac{1}{\varphi^2} = (1 - \epsilon_l) \frac{\hat{\mu}^2 \rho_0}{YKD}, \quad \beta = \frac{K_d}{\hat{\mu}}.$$

The bulk substrate concentration is re-scaled as

$$S_b = \frac{S_{bulk}}{K}.$$

Dropping the hats, the dimensionless model becomes

$$\epsilon \frac{\partial S}{\partial t} = \frac{\partial^2 S}{\partial x^2} - \frac{1}{\varphi^2} \frac{S}{1 + S} f, \quad (2.26a)$$

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x} (vf) = \frac{S}{1 + S} f - \beta f - \alpha f, \quad (2.26b)$$

$$\frac{dL}{dt} = v(L(t), t), \quad (2.26c)$$

$$v(x, t) = \int_0^x \left(\frac{S(\xi, t)}{1 + S(\xi, t)} - \beta \right) f(\xi, t) d\xi \quad (2.26d)$$

with the boundary conditions

$$\frac{\partial S}{\partial x}(0, t) = 0, \quad (2.27a)$$

$$S(L(t), t) = S_b, \quad (2.27b)$$

$$v(0, t)f(0, t) = 0. \quad (2.27c)$$

Values for the model parameters are found in a variety of sources [13], [6],[12].

Typical values are found in Table 3 and how this translates to the size of the parameters in the dimensionless model are found in Table 4.

Symbol	Description	Order of Magnitude	Units
S_{bulk}	Bulk liquid substrate concentration	Varies	g cm^{-3}
D	Diffusion constant	10^{-5}	$\text{cm}^2 \text{s}^{-1}$
Y	Yield coefficient	10^{-1}	g of biomass/g of substrate
K_i	Inactivation rate	10^{-6}	s^{-1}
ρ_0	Intrinsic biomass density	10^{-3}	g cm^{-3}
$\hat{\mu}$	Maximum growth rate	10^{-5}	s^{-1}
K	Monod constant	$10^{-8} - 10^{-6}$	g cm^{-3}
K_d	Decay rate	10^{-6}	s^{-1}
ϵ_l	Liquid volume fraction	10^{-1}	-

Table 3. Typical values for the model parameters.

Symbol	Definition	Order of Magnitude
ϵ	$\frac{\hat{l}^2 \hat{\mu}}{D}$	10^{-4}
α	$\frac{K_i}{\hat{\mu}}$	10^{-1}
$\frac{1}{\varphi^2}$	$(1 - \epsilon_l) \frac{\hat{l}^2 \hat{\mu} \rho_0}{Y K D}$	$10^{-1} - 10^1$
β	$\frac{K_d}{\hat{\mu}}$	10^{-1}
S_b	$\frac{S_{bulk}}{K}$	$10^{-1} - 10$

Table 4. Dimensionless Parameters.

CHAPTER 3

SOLUTION PROPERTIES

Basic questions about the solution to the model equations include existence and uniqueness, bounds on solutions and limiting behavior. The vector function $\mathbf{u}(x, t) = [S(x, t), f(x, t), v(x, t), L(t)]^T$ is a solution to the system provided each component satisfies the appropriate equation and satisfies the given initial conditions. Furthermore, each function is C^1 in the t variable, C^2 in the x component for S and C^1 in the x component for f and v . Due to the mixed nature of the equations in the model, the existence and uniqueness of solutions is difficult to establish. Therefore, we will assume that solutions exist and are unique for $0 \leq t \leq T_1$ for some time T_1 . In this chapter, two results are presented. Under the assumption that solutions exist and are unique, bounds for S , f , v and L are proved. The last section describes the limiting behavior of the f solution at the boundary $x = L(t)$.

A Maximum Principle for Parabolic Equations

What follows are several well-known results for parabolic equations. Their proofs are omitted, but can be found in [10]. These theorems lead to a maximum principle and a comparison theorem for certain types of non-linear parabolic equations.

Consider a bounded domain, E , in the xt plane where E is bounded below by $t = 0$ and above by $t = T_1$. Let the closure of E be denoted by \bar{E} and the boundary

of E is denoted by ∂E . For each point $P = (x^*, t^*)$ in \bar{E} , let

$$U_\epsilon(P) = \{(x, t) : 0 < t^* - t < \epsilon \text{ and } |x - x^*| < \epsilon\}.$$

The parabolic interior of \bar{E} , denoted by \tilde{E} , is the set of points where

$$U_\epsilon(P) \subset E$$

for some $\epsilon > 0$. The parabolic boundary, Γ , is the set $\bar{E} \setminus \tilde{E}$ (See Figure 2).

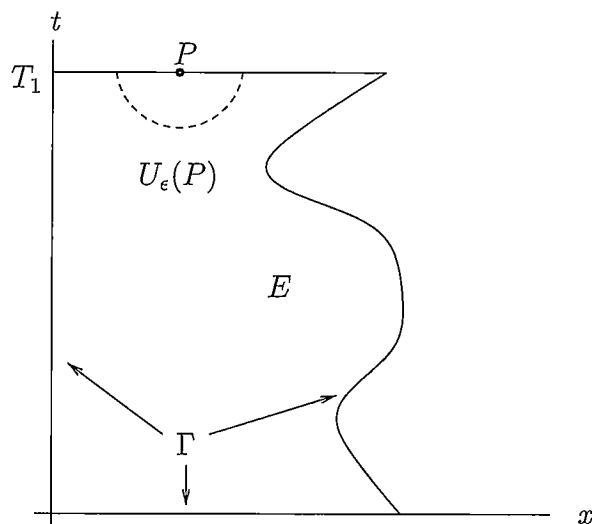


Figure 2. The sets E , Γ and $U_\epsilon(P)$.

Let $Z(E)$ be the set of continuous functions, u , on \bar{E} where $\frac{\partial u}{\partial x}$, $\frac{\partial u}{\partial t}$ and $\frac{\partial^2 u}{\partial x^2}$ are also continuous on E . A function is admissible if it is a member of this set. For this class of functions, we define the linear operator L acting on u as

$$L[u] = a(x, t) \frac{\partial^2 u}{\partial x^2} + b(x, t) \frac{\partial u}{\partial x} - \frac{\partial u}{\partial t} \quad (3.1)$$

where a, b are bounded functions on \bar{E} with $a(x, t) \geq 0$. L is called a parabolic operator. If there exists a $\mu > 0$ such that $a(x, t) \geq \mu > 0$ for all (x, t) in E , then L is said to be uniformly parabolic. Also consider the operator B acting on u in $\Gamma \setminus \{(x, t) : t = 0\}$ as

$$B[u] = c(x, t)u + d(x, t)\frac{\partial u}{\partial n} \quad (3.2)$$

where c and d are non-negative functions on Γ , n is an outward normal direction and $c^2 + d^2 > 0$ for all points in Γ . B is the boundary operator.

Suppose L is a uniformly parabolic operator and consider a function h on E such that $h \leq 0$. Suppose u is an admissible function which satisfies the differential inequality

$$(L + h)[u] = a(x, t)\frac{\partial^2 u}{\partial x^2} + b(x, t)\frac{\partial u}{\partial x} + h(x, t)u - \frac{\partial u}{\partial t} \geq 0. \quad (3.3)$$

Theorem 1. *Let P be a point on ∂E where the normal derivative at P is not parallel to the t axis. Let $U(P)$ be a closed ball where $U(P)$ is tangent to ∂E at P and the interior of $U(P)$ is contained in E . If $M = \max_E u$ is attained at P and $u < M$ in $U(P)$ except at P , then for any outward direction of E denoted by ν*

$$\frac{\partial u}{\partial \nu}(P) > 0.$$

Theorem 2. *If $M = \max_E u$ is attained at some point P in the parabolic interior of E and $M \geq 0$, then $u \equiv M$ on all line segments where t equals a constant which lie directly below this point.*

The next theorem provides a maximum principle for solutions of (3.3) when h is bounded above. The theorem, as stated below, is found in [1].

Theorem 3. (Maximum Principle) Suppose u is an admissible function which satisfies (3.3) where $h(x, t) \leq K < +\infty$ and u also satisfies the inequality $B[u] \leq 0$.

If $u(x, 0) \leq 0$, then $u(x, t) \leq 0$ in \bar{E} .

Furthermore, either

$$u(x, t) < 0 \quad (3.4a)$$

in E or there exists some $t^* \leq T_1$ such that

$$u(x, t) \equiv 0 \quad (3.4b)$$

for all $t \leq t^*$.

Proof. Consider the function $v = u(x, t)e^{-\lambda t}$ where $\lambda > K$. Notice that,

$$\begin{aligned} (L + h - \lambda)[v] &= a(x, t) \frac{\partial^2 v}{\partial x^2} + b(x, t) \frac{\partial v}{\partial x} + h(x, t)v - \lambda v - \frac{\partial v}{\partial t} \\ &= a(x, t)e^{-\lambda t} \frac{\partial^2 u}{\partial x^2} + b(x, t)e^{-\lambda t} \frac{\partial u}{\partial x} + h(x, t)ue^{-\lambda t} + \\ &\quad - \lambda ue^{-\lambda t} - \frac{\partial u}{\partial t} e^{-\lambda t} + \lambda ue^{-\lambda t} \\ &= (L + h)[u]e^{-\lambda t} \geq 0 \end{aligned}$$

Since $h - \lambda < 0$, the conclusions of Theorem 1 and 2 hold. Let $\bar{M} = \max_{\bar{E}} v$.

Assume, to reach a contradiction, that $\bar{M} > 0$. Since v is continuous, it must attain its maximum on \bar{E} . Let P be the point where $v(P) = \bar{M}$.

Suppose P lies in the parabolic interior of E . From Theorem 2, $v \equiv \bar{M}$ for all horizontal line segments where t equals a constant below P including $t = 0$. However, this implies $u(x, 0) > 0$ for some x . If P does not occur in the parabolic interior of E , it must lie on Γ .

Since $u(x, 0) \leq 0$, P can not occur on Γ where $t = 0$. Now suppose that P is on Γ where $t \neq 0$. By Theorem 1, the outward normal derivative of v is

$$\frac{\partial v}{\partial n}(P) > 0.$$

At this same point, the function u and its outward normal derivative are positive. Since either $c(P) > 0$ or $d(P) > 0$, the boundary operator at this point is

$$B[u](P) = cu(P) + d\frac{\partial u}{\partial n}(P) > 0$$

which contradicts the assumption that $B[u] \leq 0$. Therefore, v cannot attain its maximum on \bar{E} ; which is a contradiction. Thus $\bar{M} \leq 0$ and it follows that $u \leq 0$ on \bar{E} .

To establish the last conclusion of the theorem, suppose $u(P) = 0$ for some P in E . At this point, $v(P) = 0$. Since $v \leq 0$ on \bar{E} , v attains its maximum at an interior point. From Theorem 2, we conclude that $v \equiv 0$ for all $t \leq t^*$ which implies $u = 0$ for all $t \leq t^*$. □

Theorem 3 leads to a comparison theorem for a special class of non-linear parabolic equations. We will use this theorem to prove that the solutions are bounded.

Theorem 4. (Comparison Theorem) Consider the differential operator P .

Define P acting on an admissible function u as

$$P[u] = a(x, t) \frac{\partial^2 u}{\partial x^2} + b(x, t) \frac{\partial u}{\partial x} + h(x, t, u) - \frac{\partial u}{\partial t}$$

where $a(x, t) \geq \mu > 0$ and continuous; $b(x, t)$ is a bounded continuous function and h is a continuous function that is locally Lipschitz in u .

Suppose u_1 and u_2 are admissible functions where

$$P[u_2] \leq P[u_1] \text{ on } E$$

and

$$B[u_1] \leq B[u_2] \text{ on } \Gamma \setminus \{(x, t) : t = 0\}.$$

If $u_1(x, 0) \leq u_2(x, 0)$, then $u_1(x, t) \leq u_2(x, t)$ for all $0 \leq t \leq T$. Furthermore, either $u_1(x, t) < u_2(x, t)$ on E or there exists a $t^* \leq T$ such that $u_1(x, t) \equiv u_2(x, t)$ for all $0 \leq t \leq t^* \leq T$.

Proof. Let $v = u_1 - u_2$ and consider the linear operator $L + \bar{h}$ where

$$\bar{h}(x, t) = \begin{cases} \frac{h(x, t, u_1(x, t)) - h(x, t, u_2(x, t))}{u_1(x, t) - u_2(x, t)} & u_1 \neq u_2 \\ 0 & u_1 = u_2 \end{cases}.$$

Since h is locally Lipschitz in u , \bar{h} is bounded above. The conclusions follow by applying Theorem 3 to v . □

Solution Bounds

In this section, we will provide bounds on S , f , v and L . Although G and R are usually defined as

$$G(S) = \frac{S}{1+S}$$

and

$$R(S) = \frac{S}{1+S} - \beta,$$

the results of this section do not depend on these specific functions. Recall from Chapter 2, both functions are C^1 , $G'(S)$, $R'(S) \geq 0$ for $S \geq 0$ and $G(0) = 0$.

To use the theorems from the previous section, we must identify the sets E and Γ (See Figure 3). Recall, we assume that solutions exist and are unique.

The solution curve of (2.26c) will define one of the boundaries of E . However, E must be a bounded set in the xt plane and we will only consider sets where $x \geq 0$. If $L(t)$ is the solution to (2.26c), then $L(t)$ is a C^1 function. L corresponds to the thickness of a biofilm where we assume that $L(0) \neq 0$. Let $T_2 = \sup\{0 < t < T_1 | L(t) > 0\}$. By continuity, $T_2 \neq 0$. For any finite time, T , where $0 < T < T_2$, let

$$\Omega_t = (0, L(t)) \times \{t\} \tag{3.5}$$

and define the set E as

$$E = \bigcup_{0 < t < T} \Omega_t. \tag{3.6}$$

The sets $\overline{\Omega}_0$, $\{0\} \times [0, T]$, $\overline{\Omega}_T$ and $\{(L(t), t) | 0 \leq t \leq T\}$ are the boundary of E where $\overline{\Omega}_0$ and $\overline{\Omega}_T$ represent the closure of Ω_0 and Ω_T . The parabolic interior of E is

$$\tilde{E} = \bigcup_{0 < t \leq T} \Omega_t. \quad (3.7)$$

The parabolic boundary, Γ , is the union of the sets $\overline{\Omega}_0$, Γ_0 and Γ_L where

$$\Gamma_0 = \{0\} \times [0, T),$$

and

$$\Gamma_L = \{(L(t), t) | 0 \leq t < T\}.$$

Notice that Γ_0 is a straight line and Γ_L is a C^1 curve in the xt plane. Thus every point in these sets satisfy the hypotheses of Theorem 1.

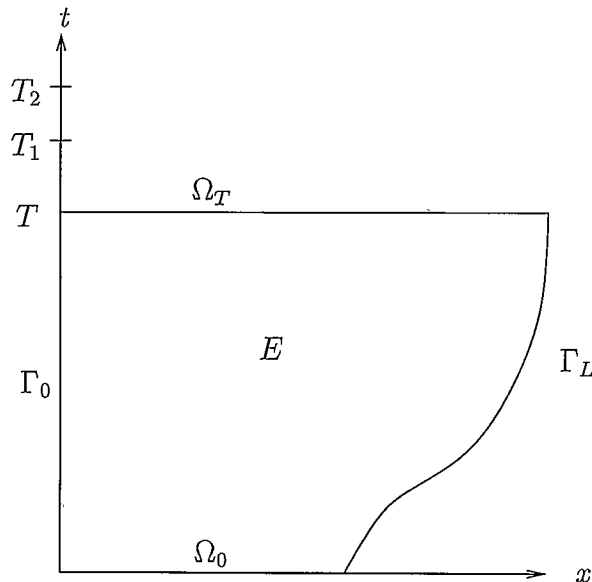


Figure 3. The sets E , Ω_0 , Ω_T , Γ_L and Γ_0 .

Bounds on S

On the sets E and Γ define the operator P acting on an admissible function u as

$$P[u] \equiv \frac{1}{\epsilon} \frac{\partial^2 u}{\partial x^2} + \frac{1}{\epsilon} g(x, t, u) - \frac{\partial u}{\partial t} \quad (3.8)$$

where the function g is

$$g(x, t, u) = \begin{cases} -\frac{1}{\varphi^2} G(u) f(x, t) & u \geq 0 \\ 0 & \text{otherwise} \end{cases} \quad (3.9)$$

Since $G(0) = 0$, g is a continuous function. The following lemma shows that g is in fact locally Lipschitz in u .

Lemma 1. *The function $g(x, t, u)$ defined by (3.9) is locally Lipschitz in u .*

Proof. Let $u_1 < u_2$. g is differentiable in the u argument except at $u = 0$. If 0 is not in the interval $[u_1, u_2]$, let

$$K = \frac{|f(x, t)|}{\varphi^2} \begin{cases} \max_{[u_1, u_2]} G'(u) & u_1 > 0 \\ 0 & u_2 < 0 \end{cases}$$

Notice that $K = \max_{[u_1, u_2]} |g_u(x, t, u)|$. By the Mean Value Theorem, there exists \tilde{u} in the interval $[u_1, u_2]$ such that

$$\begin{aligned} \frac{|g(x, t, u_2) - g(x, t, u_1)|}{|u_2 - u_1|} &= \left| \frac{g(x, t, u_2) - g(x, t, u_1)}{u_2 - u_1} \right| \\ &= \left| \frac{\partial g}{\partial u}(x, t, \tilde{u}) \right| \\ &\leq K. \end{aligned}$$

If 0 is in the interval of $[u_1, u_2]$, let $K = \frac{|f(x, t)|}{\varphi^2} \max_{[0, u_2]} G'(u)$. Since $u_1 \leq 0 \leq u_2$, the Mean Value Theorem can be used again to show

$$\begin{aligned} \frac{|g(x, t, u_2) - g(x, t, u_1)|}{|u_2 - u_1|} &= \frac{|g(x, t, u_2)|}{u_2 - u_1} \\ &= \frac{|f(x, t)|}{\varphi^2} \frac{G(u_2)}{u_2 - u_1} \\ &< \frac{|f(x, t)|}{\varphi^2} \left(\frac{G(u_2) - G(0)}{u_2 - 0} \right) \\ &= \frac{|f(x, t)|}{\varphi^2} G'(\tilde{u}) \end{aligned}$$

for some $0 \leq \tilde{u} \leq u_2$. □

Now define the boundary operator B acting on u defined on $\Gamma \setminus \Omega_0$ as

$$B[u] \equiv c(x, t)u(x, t) + d(x, t) \frac{\partial u}{\partial n}(x, t) \quad (3.10)$$

where n is the outward normal direction and the functions c and d are

$$\begin{aligned} c(x, t) &= \begin{cases} 1 & (x, t) \in \Gamma_L, \\ 0 & \text{otherwise,} \end{cases} \\ d(x, t) &= \begin{cases} 1 & (x, t) \in \Gamma_0, \\ 0 & \text{otherwise.} \end{cases} \end{aligned}$$

The operators P and B satisfy the hypotheses of Theorems 4. Using these two operators, the following proposition provides conditions for bounds on the S solution.

Proposition 1. Let \bar{S} be a solution to

$$\begin{aligned} \epsilon \frac{\partial \bar{S}}{\partial t} &= \frac{\partial^2 \bar{S}}{\partial x^2} + g(x, t, \bar{S}) && \text{for all } (x, t) \in E \\ \frac{\partial \bar{S}}{\partial x}(0, t) &= 0, \quad \bar{S}(L(t), t) = S_b && \text{for } 0 < t < T \\ \bar{S}(x, 0) &= S_b && 0 < x < L_0 \end{aligned}$$

If $S_b > 0$, then $0 < \bar{S}(x, t) \leq S_b$ for all $(x, t) \in E$.

Proof. If \bar{S} is a solution to the system above, then $P[\bar{S}] = 0$ and $B[\bar{S}] = 0$. Notice that for the functions $u_1 = 0$ and $u_2 = S_b$

$$P[0] = 0,$$

$$P[S_b] = -\frac{1}{\epsilon \varphi^2} G(S_b) f(x, t),$$

$$B[0] = 0,$$

$$B[S_b] = \begin{cases} 0 & \text{on } \Gamma_0, \\ S_b & \text{on } \Gamma_L, \end{cases}$$

hence $P[S_b] \leq P[\bar{S}] \leq P[0]$ and $B[0] \leq B[\bar{S}] \leq B[S_b]$. By Theorem 4, it follows that $0 \leq \bar{S} \leq S_b$. Since $S_b \neq 0$, the second condition of Theorem 4 cannot hold. Therefore, \bar{S} is strictly greater than zero. \square

From this proposition, it follows that $0 < S \leq S_b$. Since $\bar{S} > 0$,

$$g(x, t, \bar{S}) = -\frac{1}{\varphi^2} G(\bar{S}) f(x, t) \text{ which implies } \bar{S} = S.$$

Bounds on f

Unfortunately Theorem 4 can not be applied to the f equation. If, however, we assume that biomass diffuses in the biofilm, the f equation is parabolic and Theorem 4 can be applied.

Assuming that biomass diffuses inside the biofilm, a new flux \mathbf{J}_i for biomass is

$$\mathbf{J}_i = v\rho_i - D_i \frac{\partial \rho_i}{\partial x}.$$

Here ρ_i is either the active or inactive cell density and D_i is the diffusion coefficient. If it is assumed that the inactive biomass diffuses at the same rate as the active biomass, the dimensionless equations found in (2.26) become

$$\epsilon \frac{\partial S}{\partial t} = \frac{\partial^2 S}{\partial x^2} - \frac{1}{\varphi^2} G(S)f, \quad (3.12a)$$

$$\frac{\partial f}{\partial t} = d \frac{\partial^2 f}{\partial x^2} + (R(S)(1-f) - \alpha)f - v \frac{\partial f}{\partial x}, \quad (3.12b)$$

$$\frac{dL}{dt} = v(L(t), t) \quad (3.12c)$$

where

$$v(x, t) = \int_0^x R(S(\xi, t))f(\xi, t) d\xi. \quad (3.12d)$$

If D_f is the diffusion constant of f then the parameter d is defined as

$$d = \frac{D_f}{D}. \quad (3.13)$$

The definition of the variables and other parameters remains unchanged. We will assume that the parameter $d \ll 1$ and is small compared to the other parameters in

the model. If biomass does not interact or pass through the substratum, the no-flux boundary condition at $x = 0$ is

$$v(0, t)f(0, t) - d\frac{\partial f}{\partial x}(0, t) = 0.$$

Since $v(0, t) = 0$, this reduces to

$$\frac{\partial f}{\partial x}(0, t) = 0.$$

With the addition of the diffusion, a boundary condition at $x = L$ must be placed on f . For example, if we assume that the cell density at the interface is a prescribed function of t , then the boundary condition for f at $x = L$ is

$$f(L, t) = a(t) \tag{3.14}$$

where $a(t)$ is a non-negative function and $a(t) \leq 1$ for all t . Other types of boundary conditions, like no-flux or a Robin type condition could also be applied. For these linear boundary conditions, the results of the proposition below still hold.

Proposition 2. *Suppose f solves*

$$\begin{aligned} \frac{\partial f}{\partial t} &= d\frac{\partial^2 f}{\partial x^2} - v(x, t)\frac{\partial f}{\partial x} + (R(S)(1 - f) - \alpha) f && \text{for all } (x, t) \in E \\ \frac{\partial f}{\partial x}(0, t) &= 0 \quad f(L(t), t) = a(t) && \text{for } 0 < t < T. \end{aligned}$$

If $0 \leq f(x, 0) \leq 1$ for all $x \in \Omega_0$, then for all $(x, t) \in E$, $0 \leq f(x, t) \leq 1$.

Proof. Consider the operator P acting on an admissible function u as

$$P[u] \equiv d\frac{\partial^2 u}{\partial x^2} - v(x, t)\frac{\partial u}{\partial x} + (R(S)(1 - u) - \alpha) u.$$

Since $0 < S \leq S_b$, R is continuous and bounded. Notice that the non-linear term is quadratic in u and hence continuously differentiable in the u argument. Therefore, the operator P satisfies the hypotheses of Theorem 4. Now define on $\Gamma \setminus \Omega_0$ the boundary operator as

$$B[u] = c(x, t)u(x, t) + d(x, t)\frac{\partial u}{\partial n}$$

where the functions c and d are

$$c(x, t) = \begin{cases} 1 & (x, t) \in \Gamma_L, \\ 0 & \text{otherwise,} \end{cases}$$

$$d(x, t) = \begin{cases} 1 & (x, t) \in \Gamma_0, \\ 0 & \text{otherwise.} \end{cases}$$

B also satisfies the hypothesis of Theorem 4.

Notice for $u_1 = 0$ and $u_1 = 1$,

$$P[0] = 0,$$

$$P[1] = -\alpha,$$

$$B[0] = 0,$$

$$B[1] = \begin{cases} 1 & (x, t) \in \Gamma_L, \\ 0 & (x, t) \in \Gamma_0. \end{cases}$$

Thus, $P[1] \leq P[f] \leq P[0]$ and $B[0] \leq B[f] \leq B[1]$. Therefore by Theorem 4, $0 \leq f(x, t) \leq 1$ for all $(x, t) \in E$. □

Typically $f(x, 0)$ is a non-zero constant function. Using arguments that are similar to those used for the S equation, it follows that $f(x, t) > 0$.

Bounds on v and L

The S solution is bounded and with the addition of diffusion to the f equation, the f solution is also bounded. Since the v and L equations are integrals involving functions of S and f , bounds can be derived for v and L provided diffusion is included in the f equation.

Proposition 3. *Suppose diffusion of f is included in the model equations. If $L(t)$ solves the differential equation*

$$\frac{dL}{dt} = v(L(t), t)$$

$$L(0) = L_0$$

where

$$v(x, t) = \int_0^x R(S(\xi, t)) f(\xi, t) d\xi,$$

then for all $(x, t) \in E$

$$|v(x, t)| \leq |R(S_b)| x$$

and

$$L(t) \leq L_0 \exp |R(S_b)| t.$$

Proof. By Propositions 1 and 2, S and f are bounded below by zero and above by S_b and 1 respectively. Since $R'(S) > 0$, for all $(x, t) \in E$

$$|v(x, t)| = \left| \int_0^x R(S(\xi, t)) f(\xi, t) d\xi \right|$$

$$\leq x |R(S_b)|.$$

Thus for all $0 < t < T$

$$\frac{dL}{dt} = v(L(t), t) \leq L(t) |R(S_b)|$$

and solving this differential inequality leads to the bound for $0 \leq t \leq T$

$$L(t) \leq L_0 \exp(|R(S_b)| t).$$

□

Behavior at the Interface

Consider the solution curve for the differential equation

$$\begin{aligned} \frac{dx}{dt} &= v(x(t), t) \\ x(0) &= x_0 \in \Omega_0 \end{aligned}$$

where

$$v(x, t) = \int_0^x R(S(\xi, t)) f(\xi, t) d\xi.$$

Let \dot{F} denote the derivative of F along the solution curve. On this curve,

$$\dot{f} = \frac{\partial f}{\partial t} + \frac{dx}{dt} \frac{\partial f}{\partial x} = \frac{\partial f}{\partial t} + v(x, t) \frac{\partial f}{\partial x}$$

and using (2.26b) this leads to the differential equation

$$\dot{f} = (R(S)(1 - f) - \alpha) f. \quad (3.15)$$

Along the curve that corresponds to the interface, S is equal to a constant, S_b .

So at the interface, a simple first order differential equation

$$\dot{f} = (R(S_b)(1 - f) - \alpha) f \quad (3.16)$$

holds. The equilibria solutions of this ODE are summarized in the lemma below.

Lemma 2. *Consider the first order initial value problem*

$$\dot{x} = (a_1(1 - x) - a_2)x, \quad (3.17a)$$

$$x(0) = x_0 \quad (3.17b)$$

where the parameter a_2 is non-negative. Solutions exist and are unique for all parameter values. If $a_1 = a_2$ or $a_1 = 0$ a bifurcation occurs and (3.17a) has one equilibrium solution, $x = 0$. Solutions of (3.17) decay to zero if $x_0 > 0$ and approach $-\infty$ if $x_0 < 0$. Otherwise, (3.17a) has two equilibrium solutions, $x = 0$ and $x = 1 - \frac{a_2}{a_1}$. For parameter values where $a_1 > a_2$, $x = 0$ is unstable and $x = 1 - \frac{a_2}{a_1}$ is stable. If $a_1 < a_2$, then $x = 0$ is stable and $x = 1 - \frac{a_2}{a_1}$ is unstable.

Proof. Notice that the right-hand side of (3.17a) is quadratic in x , hence it's locally Lipschitz in x . Therefore, a unique solution of (3.17) exists.

If $a_1 = 0$ equation (3.17a) reduces to

$$\dot{x} = -a_2x \quad (3.18)$$

and if $a_1 = a_2$ then (3.17a) reduces to

$$\dot{x} = -a_2x^2. \quad (3.19)$$

In both cases, there is only one equilibrium solution. Also, $\dot{x} < 0$ for all non-zero x values in both equations. If $x_0 > 0$, the solutions of (3.18) or (3.19) are decreasing functions and bounded below zero. Thus, the solutions must limit on zero. If $x_0 < 0$, the solutions are strictly decreasing and are not bounded below. These solutions will approach $-\infty$.

For all other values of a_1 and a_2 , the two equilibrium solutions can easily be found by setting the right-hand side of (3.17) to zero and solving for x . Notice that the derivative of the right-hand side is

$$F'(x) = a_1(1 - x) - a_2 - a_1x.$$

An equilibrium solution is stable provided $F'(x) < 0$. If $F'(x) > 0$ the equilibrium solution is unstable. Evaluating this at the equilibrium solutions gives

$$F'(0) = a_1 - a_2$$

and

$$F'\left(1 - \frac{a_2}{a_1}\right) = a_2 - a_1.$$

The stability conditions follow directly from these equations. □

Notice that in the region where $x = 1 - \frac{a_2}{a_1}$ is stable, it also holds that

$$0 < 1 - \frac{a_2}{a_1} \leq 1.$$

In the set of parameter values where $x = 1 - \frac{a_2}{a_1}$ is unstable, it follows $1 - \frac{a_2}{a_1} > 1$ if $a_1 < 0$ and $1 - \frac{a_2}{a_1} < 0$ if $a_1 > 0$.

Applying this to equation (3.16), it follows that the value of f at $x = L(t)$ approaches $1 - \frac{\alpha}{R(S_b)}$ if $R(S_b) > \alpha$ and approaches zero if $R(S_b) < \alpha$. This result indicates that the cell net growth rate must exceed the inactivation rate for a viable cell population to exist at the interface. It follows that f is bounded at $x = L(t)$ between 0 and 1 for all parameter values.

CHAPTER 4

STEADY-STATE SOLUTIONS

The initial formation of a biofilm is not well understood. It is known by experimentation that with a small amount of biomass present, the biofilm quickly increases in size and stabilizes at a thickness that ranges from 20 to 500 microns [2]. Active organisms are always present in these biofilms. In the model, this behavior corresponds to a stable steady-state solution with $f \geq 0$. The existence of steady-state solutions and the stability of those solutions are studied in this chapter.

In this chapter, we will assume that the functions R and G are

$$G(S) = \frac{S}{1+S},$$
$$R(S) = \frac{S}{1+S} - \beta.$$

Only solutions with $f \geq 0$ are considered. Since biofilms typically have active organisms present, a steady-state solution with $f \equiv 0$ is considered a trivial steady-state solution.

In [13], numerical simulations showed that the active volume fraction and substrate profiles were non-negative. However, the model also predicted unbounded growth unless a detachment function was included in the biomass equations or a sloughing term was added to the biofilm thickness equation. We will prove that if the inactivation rate is non-zero then only a trivial steady-state solution will exist. We

will also show that if the inactivation rate is zero, then under certain conditions a non-trivial steady solution exists. Finally, we will prove that the trivial steady-state solution is linearly unstable for certain parameter values.

Existence of Steady-State Solutions

The steady-state equations are given by (see equations (2.26))

$$\frac{d^2 S}{dx^2} = \frac{1}{\varphi^2} \frac{S}{1+S} f, \quad (4.1a)$$

$$v \frac{df}{dx} = \left(\left(\frac{S}{1+S} - \beta \right) (1-f) - \alpha \right) f, \quad (4.1b)$$

$$\int_0^L \left(\frac{S(\xi)}{1+S(\xi)} - \beta \right) f(\xi) d\xi = 0 \quad (4.1c)$$

where

$$v(x) = \int_0^x \left(\frac{S(\xi)}{1+S(\xi)} - \beta \right) f(\xi) d\xi. \quad (4.1d)$$

The corresponding boundary conditions for this problem are

$$\frac{dS}{dx}(0) = 0, \quad S(L) = S_b, \quad v(0)f(0) = 0. \quad (4.2)$$

The parameter α controls which steady-state solutions are possible. The first proposition shows that if α is positive, then only a trivial steady-state solution exists.

Proposition 4. *For $\alpha > 0$, the solution $S(x) \equiv S_b$, $f(x) \equiv 0$ and any real number L is the only solution of (4.1) where $f(x) \geq 0$.*

Proof. Notice that if equation (4.1b) is integrated from 0 to L and integration by parts is applied, we obtain

$$\begin{aligned}\int_0^L v \frac{df}{dx} d\xi &= v f \Big|_0^L - \int_0^L f \frac{dv}{dx} d\xi \\ &= - \int_0^L f \frac{dv}{dx} d\xi.\end{aligned}$$

Now using equation (4.1b) and equation (4.1d) the expression above leads to

$$\int_0^L \left(\left(\frac{S(\xi)}{1+S(\xi)} - \beta \right) (1-f(\xi)) - \alpha \right) f(\xi) d\xi = - \int_0^L \left(\frac{S(\xi)}{1+S(\xi)} - \beta \right) f^2(\xi) d\xi.$$

Simplifying this expression results in the integral equation

$$\int_0^L \left(\left(\frac{S(\xi)}{1+S(\xi)} - \beta \right) f(\xi) - \alpha f(\xi) \right) d\xi = 0,$$

which by using equation (4.1c) implies

$$\alpha \int_0^L f(\xi) d\xi = 0.$$

If $f \geq 0$, the calculation above shows that $f \equiv 0$. Thus the integral condition in (4.1c) will be satisfied for any S or L . Furthermore, if $f \equiv 0$ is substituted into equation (4.1a), the boundary conditions on S imply that S must be the constant function $S(x) = S_b$. So $S(x) = S_b$, $f(x) = 0$ and any real valued L satisfies that steady state equations. \square

It should be pointed out that a similar argument could be applied to a higher dimensional model with more than one species present. Recall from Chapter 2, if ρ_i is the density of some organism in the biofilm then the mass balance principles state

$$\frac{\partial}{\partial t} \int_{\Omega} \rho_i d\sigma + \int_{\Omega} \rho_i \mathbf{v} \cdot \mathbf{n} d\sigma = \int_{\Omega} F_i d\sigma$$

where Ω is an arbitrary volume and \mathbf{n} is the outward normal direction of Ω . If Ω is the entire biofilm, then this equation at steady-state is

$$\int_{\partial\Omega} \rho_i \mathbf{v} \, d\tau = \int_{\Omega} F_i \, d\sigma.$$

However, at steady-state the velocity is zero on the substratum and interface. The periodic boundary conditions will cancel out the remaining integrals on $\partial\Omega$. Therefore, the integral on the right-hand side is zero. If F_i is non-negative, then F_i must be identically zero. Furthermore, if F_i is proportional to ρ_i or some other biomass density, we conclude that this density is identically zero. This argument is not valid if a detachment term or some other function that models removal of biomass is included in F_i ; in this situation, F_i may change sign.

We now consider the case $\alpha = 0$. For any β , there is a constant steady-state solution, namely $S(x) = S_b, f(x) = 0$ and L any real number. Other solutions exist for certain β values. The conditions for the existence of these steady-state are summarized in the next theorem.

Theorem 5. (*Existence of Steady-State Solutions*) *The existence of solutions to (4.1) fall into two categories.*

If $\beta < \frac{S_b}{1 + S_b}$, then two steady-state solutions exist; the constant steady-state solution: $S(x) \equiv S_b, f(x) \equiv 0$ and L any real number and the solution $f(x) \equiv 1, \tilde{L} < \infty$ and \tilde{S} where \tilde{S} and \tilde{L} solve the differential equation

$$\frac{d^2 \tilde{S}}{dx^2} = \frac{1}{\varphi^2} \frac{\tilde{S}}{1 + \tilde{S}} f \tag{4.3a}$$

with boundary conditions

$$\frac{d\tilde{S}}{dx}(0) = 0, \quad \tilde{S}(\tilde{L}) = S_b. \quad (4.3b)$$

If $\beta > \frac{S_b}{1+S_b}$, then only one steady-state solution, the constant steady-state will exist.

To prove this theorem, it will be demonstrated that for $\beta \neq \frac{S_b}{1+S_b}$ the only solutions for (4.1b) are the constant solutions $f(x) = 0$ and $f(x) = 1$. Once this has been established, then (4.1) can be reduced to a differential equation for S and an integral equation involving L . The existence of a unique solution to this reduced problem is proved.

Lemma 3. If $\beta \neq \frac{S_b}{1+S_b}$ and $\alpha = 0$, then the only possible solutions to (4.1b) are $f(x) \equiv 1$ and $f(x) \equiv 0$

Proof. Notice that equation (4.1b) can be written as

$$\begin{aligned} v \frac{df}{dx} &= - \left(\frac{S}{1+S} - \beta \right) f^2 + \left(\frac{S}{1+S} - \beta \right) f \\ &= - \frac{dv}{dx} f + \frac{dv}{dx} \end{aligned}$$

which leads to

$$\frac{d(vf)}{dx} = \frac{dv}{dx},$$

which can be re-written as

$$\frac{d}{dx}(v(f-1)) = 0.$$

Since $v(0) = 0$,

$$v(x)(f(x) - 1) = 0$$

for all $x \in [0, L]$.

Two possibilities can occur: either $f(x) \equiv 1$ or $v(x) \equiv 0$. If $v(x) \equiv 0$ then it must also be true that

$$v'(x) = \left(\frac{S(x)}{1 + S(x)} - \beta \right) f(x) = 0$$

for all $x \in [0, L]$. If $\frac{S(x)}{1 + S(x)} - \beta = 0$, then at $x = L$

$$\frac{S_b}{1 + S_b} - \beta = 0$$

which is a contradiction. Thus if $v(x) \equiv 0$, it follows that $f(x) \equiv 0$. \square

Lemma 4. *If $f(x) \equiv 0$ and $\alpha = 0$, then the solution to (4.1a) is $S = S_b$ and (4.1c) is satisfied for any L .*

Proof. If $f(x) \equiv 0$ then equation (4.1c) is satisfied for any L and the boundary conditions on S can only be satisfied by the constant solution $S(x) \equiv S_b$. \square

The next two propositions consider the case of $f(x) \equiv 1$. When $f(x) \equiv 1$, (4.1) reduces to a differential equation and integral equation that must be satisfied simultaneously. The first proposition proves the existence and uniqueness of solutions to the differential equation. The second proves that a unique solution, with the addition of the integral equation will exist provided $\beta < \frac{S_b}{1 + S_b}$.

Proposition 5. *For any $l > 0$, there exists a unique solution to the differential equation*

$$\frac{d^2 S}{dx^2} = \frac{1}{\varphi^2} \frac{S}{1+S} \quad (4.4a)$$

with boundary conditions

$$\frac{dS}{dx}(0) = 0, \quad S(l) = S_b. \quad (4.4b)$$

Proof. Let $u = S$ and $w = \frac{dS}{dx}$. The two dimensional system equivalent to (4.4) is

$$u' = w \quad (4.5a)$$

$$w' = \frac{1}{\varphi^2} \frac{u}{1+u}. \quad (4.5b)$$

This system has one equilibrium solution $(0, 0)$ and the linearization about this equilibrium solution is

$$J = \begin{bmatrix} 0 & 1 \\ \frac{1}{\varphi^2} & 0 \end{bmatrix} \quad (4.6)$$

which has eigenvalues $\lambda_{\pm} = \pm \frac{1}{\varphi}$, hence $(0, 0)$ is a saddle point. Consider the phase portrait of (4.5) in the region $u \geq 0$. In this region let,

$$H(u, w) = \frac{w^2}{2} - \frac{1}{\varphi^2} (u - \ln(1+u)). \quad (4.7)$$

One can easily check that the level sets of (4.7) are invariant for the flow generated by (4.5).

The unstable manifold lying in the first quadrant is given by

$$w = \frac{\sqrt{2}}{\varphi} \sqrt{u - \ln(1+u)}. \quad (4.8)$$

Let R be defined as the following region in the phase portrait (see Figure 4)

$$R = \left\{ (u, w) : 0 < w < \frac{\sqrt{2}}{\varphi} \sqrt{u - \ln(1+u)} \text{ and } 0 \leq u \leq S_b \right\}. \quad (4.9)$$

Along $w = 0$, the vector field points to the interior of R . So a trajectory starting at

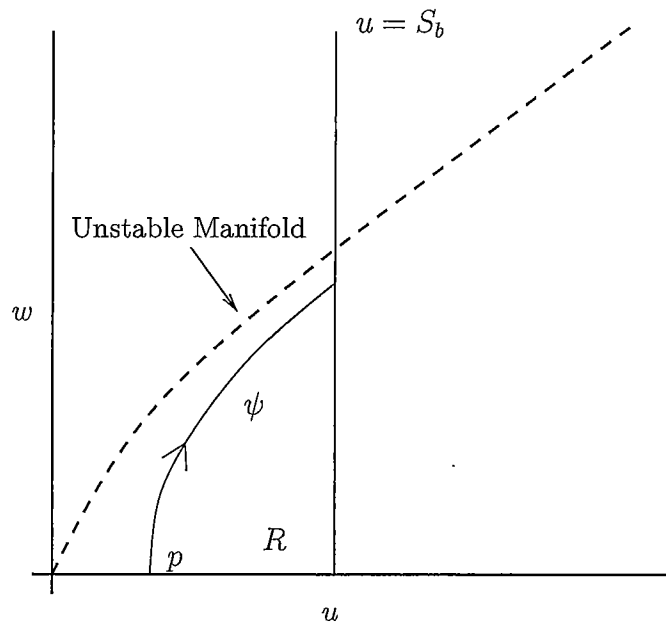


Figure 4. Region R and flow ψ .

$w = 0$ will immediately enter R . Let p be the point where the trajectory, ψ , enters R . This trajectory can not cross $w = 0$ at a later time since $u > 0$ in R . Furthermore, ψ must exit R in a finite amount of time. Since ψ cannot cross the unstable manifold, it must exit across $u = S_b$. This trajectory corresponds to a solution of (4.4) where \tilde{L} is the length of time ψ is in R and $S(0) = p$. The length of time ψ spends in R will depend on p . By integrating along ψ , the relationship between p and L can be

derived from H :

$$L(p) = \frac{\varphi}{\sqrt{2}} \int_p^{S_b} \frac{du}{\sqrt{F(u) - F(p)}} \quad \text{where } F(u) = u - \ln(1 + u). \quad (4.10)$$

As $p \rightarrow 0$, the trajectory ψ approaches the unstable manifold, thus

$$\lim_{p \rightarrow 0} L(p) = +\infty.$$

To calculate the limit as $p \rightarrow S_b^-$, let $r^2 = S_b - p$ and

$$I(p) = \int_p^{S_b} \frac{du}{\sqrt{F(u) - F(p)}}. \quad (4.11)$$

$I(p)$ can not be explicitly calculated; furthermore the integral has an integrable singularity. To work around this difficulty, a Taylor expansion for $I(S_b - r^2)$ about $r = 0$ will be calculated. Consider

$$g(u; p) = \sqrt{\frac{A(u-p)}{F(u) - F(p)}} \quad \text{where } A = \frac{p}{1+p}. \quad (4.12)$$

The expansion of (4.12) about $u = p$ is

$$g(u; p) = 1 - \frac{1}{4(1+p)p}(u-p) + O((u-p)^2). \quad (4.13)$$

It follows that

$$\begin{aligned} \frac{1}{\sqrt{F(u) - F(p)}} &= \frac{1}{\sqrt{A(u-p)}} \cdot g(u; p) \\ &= \frac{1}{\sqrt{A(u-p)}} - \frac{1}{4\sqrt{A}(1+p)p} \sqrt{u-p} + O\left((u-p)^{\frac{3}{2}}\right). \end{aligned}$$

By evaluating this expression at $p = S_b - r^2$ and integrating this equation, the expansion for $I(S_b - r^2)$ is

$$I(S_b - r^2) = 2\sqrt{\frac{1+S_b}{S_b}}r - \left(\frac{1}{S_b\sqrt{S_b(1+S_b)}} - \frac{1}{6S_b(1+S_b)} \right) r^3 + O(r^5) \quad (4.14)$$

and therefore

$$\lim_{p \rightarrow S_b^-} L(p) = 0.$$

Since $L(p)$ is continuous on $(0, S_b)$, for any $l > 0$ there exists a p such that $L(p) = l$. It follows that a solution to

$$\begin{aligned} \frac{d^2 S}{dx^2} &= \frac{1}{\varphi^2} \frac{S}{1+S}, \\ \frac{dS}{dx}(0) &= 0, \quad S(l) = S_b \end{aligned}$$

exists for each $l > 0$. We will now show that the function $L(p)$ is a monotone decreasing function of p by proving $L' < 0$.

Let $u = p + (S_b - p)\phi$, then (4.10) becomes

$$L(p) = \frac{\varphi}{\sqrt{2}} (S_b - p) \int_0^1 \frac{d\phi}{\sqrt{F(p + (S_b - p)\phi) - F(p)}}.$$

Set $G(\phi, p) = F(p + (S_b - p)\phi) - F(p)$ and let

$$I(p) = (S_b - p) \int_0^1 [G(\phi, p)]^{-\frac{1}{2}} d\phi.$$

It follows that

$$I'(p) = - \int_0^1 [G(\phi, p)]^{-\frac{1}{2}} d\phi - (S_b - p) \int_0^1 \frac{1}{2} [G(\phi, p)]^{-\frac{3}{2}} G_p d\phi$$

where

$$G_p = F'(p + (S_b - p)\phi) \cdot (1 - \phi) - F'(p).$$

Since

$$F''(u) = \frac{1}{(1+u)^2} > 0,$$

F' is a monotone increasing function, so we have

$$\begin{aligned} G_p &= F'(p + (S_b - p)\phi) \cdot (1 - \phi) - F'(p) \\ &\geq F'(p + (S_b - p)\phi) - F'(p) \\ &\geq 0. \end{aligned}$$

$G(\phi, p)$ is positive for any $0 < p < S_b$ and for all $0 < \phi < 1$, thus $I'(p) < 0$ for any $0 < p < S_b$. It follows that $L(p)$ is monotone decreasing and hence the solution to (4.4) is unique for each $l > 0$ □

Proposition 6. *If $\beta < \frac{S_b}{1+S_b}$ then there exists a unique L such that*

$$\frac{d^2 S}{dx^2} = \frac{1}{\varphi^2} \frac{S}{1+S}, \quad (4.16a)$$

$$\frac{dS}{dx}(0) = 0, \quad S(L) = S_b, \quad (4.16b)$$

$$\int_0^L \left(\frac{S(\xi)}{1+S(\xi)} - \beta \right) d\xi = 0. \quad (4.16c)$$

Proof. From (4.7), if a trajectory enters at point p and exits the region R at time L then

$$\frac{dS}{dx}(L) = \frac{\sqrt{2}}{\varphi} \sqrt{F(S_b) - F(p)}. \quad (4.17)$$

If equation (4.16a) is substituted into equation (4.16c), then (4.16c) is equivalent to an additional boundary condition

$$\frac{dS}{dx}(L) = \frac{1}{\varphi^2} \beta L. \quad (4.18)$$

