Spatial Effects in Microbial Mats

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I would like to dedicate this thesis to my parents and to my brother; they have always supported and encouraged me.
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Abstract

The patterns typically found in microbial mats consist of stratification of the mat into layers which are stacked on top of each other in the vertical direction and the temporal oscillations which are a result of daily light cycles. Motivated by experimental findings, the possibility of other types of spatiotemporal patterns are considered in a two dimensional microbial mat. A model is proposed which consists of a system of reaction diffusion equations which describe the dynamics of the concentrations of phototrophic and heterotrophic microbes in the mat as well as the concentrations of the metabolites they consume: oxygen, carbon dioxide, and biomass. The system is first studied without diffusion and the fixed points and their stability are considered for a range of parameters. Diffusion is then reintroduced and the system is studied in one spatial dimension using numerical simulations with a central region illuminated and the outer regions in the dark. It is found that fronts in the concentrations of phototrophs, heterotrophs, and oxygen may form at the light/dark boundary.
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Chapter 1

Introduction

1.1 Microbial Mats

Microbial mats have existed on Earth for more than 3 billion years and have played a significant role in altering the composition of the atmosphere through their production of O$_2$, H$_2$, and CH$_4$ [1]. Microbial mats are communities of microbes which are typically found in aquatic environments and which interact to produce a series of biofilms embedded in an exopolysaccharide matrix resulting in a layered structure which is visible to the naked eye as depicted in Fig. 1.1 [1].

The different microbial species typically stratify due to light and chemical gradients in the mat which may lead to a series of colorful layers. These chemical gradients are created and sustained by the interactions of the constituent microbes [2]. The overlapping chemical gradients result in microenvironments which are favorable to different functional classes of microbes [1].

The top layer of microbial mats is typically comprised of oxygenic phototrophs which act as the primary producers in the community while the layers below contain microbes such as anoxic phototrophs, heterotrophs, and sulfur bacteria[3]. The phototrophs are the primary producers in the mats since they use the energy from light to fix carbon in the form of biomass which can then be consumed by heterotrophic microbes. Although microbial mats may contain hundreds of different types microbes, typically only a small fraction of these microbes comprise most of mat by mass.
The environmental conditions on Earth have changed dramatically over the last 3 billion years and microbial mats have been able to adapt and survive in a wide range of environmental conditions [1]. For example, microbial mats can be found today in extreme environments such as those which are hypersaline, sulfuric, or at high temperature [1]. Due to the large diversity in microbial mats and their resilience to a wide range of environmental conditions, the study of microbial mats is important for developing a better understanding of the ways in which communities of microbes interact and evolve in order to survive in many different environments.

1.2 Microbial Mat Dynamics in 2D Film

In an experiment described in [4], a sample from a microbial mat was collected and well mixed into a homogeneous slurry. The slurry was spread onto an oxygen detector which was placed into a sealed chamber. A circular region in the center of the slurry was illuminated periodically with the light being turned on and off every 90 minutes.

After 22 days, it was found that in a ring-shaped region just inside the light dark boundary, the oxygen concentration was higher than everywhere else.

Since diffusion is acting to smooth out the oxygen distribution, the inhomogeneities in the oxygen distribution are most likely due to differences in the concentration of microbes which consume oxygen relative to those which produce oxygen. This would imply that there is a relative abundance of oxygen producing organisms at the light/dark boundary.

The distribution of oxygen observed in the experiment indicates that the microbial dynamics in this two dimensional microbial mat are subject to some non-trivial edge effects. In the next section, a simple model of microbial dynamics in two dimensions is proposed in order to understand the effects of the light/dark boundary.
Chapter 2

Description of Model

2.1 Reaction Diffusion Equations

Reaction diffusion equations have been used in describing a wide range of biological phenomena from morphogenesis to protein-ligand binding. These equations take the form

$$\partial_t u = f(u) + D\nabla^2 u$$

(2.1)

where $u$ represents the quantity of some compound involved in the reaction $f(u)$. The diffusion coefficient of the compound $u$ is denoted by $D$.

It was discovered by Turing that a pair of reaction diffusion equations describing the dynamics of a pair of compounds (morphogens) may lead to a variety of spatial patterns in the concentrations of those compounds (morphogens) such as 'dappled' patterns and standing waves [5]. If a system with three or more morphogens is considered, even more patterns such as traveling waves are possible [5].

Due to the relatively simple form of these equations and their ability to describe many types of instabilities, equations of the form (2.1) are plausible candidates for describing the oxygen distribution pattern found in [4]. In the rest of Chapter 2, a system of partial differential equations of the form (2.1) is developed to understand microbial dynamics in two dimensions.

2.2 The Model

Despite the fact that microbial mats typically contain many different types of microbes with a wide variety of metabolic processes, we may simplify these many complex metabolic interactions by considering two general classes of organisms: phototrophs and heterotrophs.
Phototrophs use energy from light to produce organic material and oxygen and heterotrophs metabolize organic material through cellular respiration. The metabolism of the phototrophic and heterotrophic microbes may be described by the reactions

\[
\text{Phototrophs: } \text{light} + \text{CO}_2 + \text{H}_2\text{O} \rightarrow \text{CH}_2\text{O} + \text{O}_2 \tag{2.2}
\]

\[
\text{Heterotrophs: } \text{O}_2 + \text{CH}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2\text{O} \tag{2.3}
\]

Since water is assumed to be readily available in the microbial mat, the only metabolites which will be considered are carbon dioxide (CO\(_2\)), oxygen (O\(_2\)), and biomass (CH\(_2\)O).

Although this description of the microbial metabolisms found in mats is greatly simplified, it captures the idea that the phototrophic microbes use the energy from light to produce compounds which are crucial to the metabolisms of the heterotrophic microbes.

In order to understand the potential interactions between phototrophic and heterotrophic microbes in a two-dimensional microbial mat, consider the following system of partial differential equations:

\[
\partial_t p = p \left[ \mu_p (l) \frac{[\text{CO}_2]}{[\text{CO}_2] + K_{\text{CO}_2}} - \tau_p - ch \right] + D_p \nabla^2 p \tag{2.4}
\]

\[
\partial_t h = h(1 - f) \left[ \mu_h \frac{[\text{O}_2]}{[\text{O}_2] + K_{\text{O}_2}[\text{CH}_2\text{O}] + K_{\text{CH}_2\text{O}}} - \tau_h \right] + D_h \nabla^2 h \tag{2.5}
\]

\[
\partial_t [\text{CO}_2] = h f A_{\text{CO}_2}^p \left[ \mu_p \frac{[\text{O}_2]}{[\text{O}_2] + K_{\text{O}_2}[\text{CH}_2\text{O}] + K_{\text{CH}_2\text{O}}} - p A_{\text{CO}_2}^h \frac{[\text{CO}_2]}{[\text{CO}_2] + K_{\text{CO}_2}} \right] + D_{\text{CO}_2} \nabla^2 [\text{CO}_2] \tag{2.6}
\]

\[
\partial_t [\text{O}_2] = p A_{\text{O}_2}^p \left[ \mu_p \frac{[\text{CO}_2]}{[\text{CO}_2] + K_{\text{CO}_2}} \right] - h f A_{\text{O}_2}^h \left[ \mu_h \frac{[\text{O}_2]}{[\text{O}_2] + K_{\text{O}_2}[\text{CH}_2\text{O}] + K_{\text{CH}_2\text{O}}} \right] + D_{\text{O}_2} \nabla^2 [\text{O}_2] \tag{2.7}
\]

\[
\partial_t [\text{CH}_2\text{O}] = p \tau_p + h \tau_h + c p h - h A_{\text{CH}_2\text{O}}^{\text{h}} \left[ \mu_h \frac{[\text{O}_2]}{[\text{O}_2] + K_{\text{O}_2}[\text{CH}_2\text{O}] + K_{\text{CH}_2\text{O}}} \right] + D_{\text{CH}_2\text{O}} \nabla^2 [\text{CH}_2\text{O}] \tag{2.8}
\]
where $p$, $h$, $CO_2$, $O_2$, and $CH_2O$ represent the concentrations of phototrophs, heterotrophs, carbon dioxide, oxygen, and biomass respectively; $D$ represents the diffusion coefficient of each quantity; $K$ represents the half rate constant of each reaction, and $c$ represents the rate at which heterotrophs are killing phototrophs. The death rates of phototrophs and heterotrophs are denoted by $\tau_p$ and $\tau_h$. The ratio of the amount of each metabolite used or produced in each reaction to the amount of phototrophs or heterotrophs present is given by the coefficients $A$; the subscript represents the metabolite being produced/consumed and the superscript indicates whether it is being produced/consumed in the phototrophic or heterotrophic reaction.

In the heterotrophic reaction, some of the carbon from the biomass will be incorporated into the heterotrophs while the rest will be released as $CO_2$. The fraction of carbon which is released as $CO_2$ is denoted by $f$.

The coefficients $\mu_p$ and $\mu_h$ denote the maximum growth rate for phototrophs and heterotrophs. Note that $\mu_p$ in equation (2.1) is dependent on the amount of light, $l$.

Although the system studied in [4] was a two dimensional system, we assume radial symmetry so that the system may be studied as function of the time $t$ and a single spatial variable $x$.

To simplify the notation, define $\phi([CO_2])$ and $\psi([O_2],[CH_2O])$ as

$$\phi([CO_2]) = \frac{[CO_2]}{[CO_2]+K_{CO_2}}$$

$$\psi([O_2],[CH_2O]) = \frac{[O_2]}{[O_2]+K_{O_2}} + \frac{[CH_2O]}{[CH_2O]+K_{CH_2O}}$$

### 2.2.1 Parameters and Scaling

In order to simplify this system of partial differential equations, the following simplifying assumptions are made. Since phototrophs and heterotrophs are both much larger than the other compounds considered in the model, we may assume that there are only two diffusion coefficients: $D_1$ will denote the diffusion coefficient for phototrophs and heterotrophs and $D_2$ will denote the diffusion coefficient for carbon dioxide, oxygen, and biomass ($CH_2O$). Since it is reasonable to assume that the death rates of phototrophs and heterotrophs are comparable, we choose $\tau_p = \tau_h = \tau$. To simplify the notation, define the following dimensionless
quantities:
\[
\gamma_1 = A_h^{\text{CO}_2} \frac{K_{\text{CH}_2\text{O}}}{K_{\text{CO}_2}} \quad \gamma_3 = A_{O_2}^{p} \frac{K_{\text{CH}_2\text{O}}}{K_{O_2}}
\]
\[
\gamma_2 = A_{h}^{\text{CO}_2} \frac{K_{\text{CH}_2\text{O}}}{K_{\text{CO}_2}} \quad \gamma_4 = A_{h}^{p} \frac{K_{\text{CH}_2\text{O}}}{K_{O_2}}
\]

Now, let the primed quantities denote the rescaled variables and define

\[
t' = t \mu_h
\]
\[
D'_1 = \frac{D_1}{\mu_h}
\]
\[
D'_2 = \frac{D_2}{\mu_h}
\]
\[
\tau' = \frac{\tau}{\mu_h}
\]
\[
c' = \frac{c}{\mu_h} K_{\text{CH}_2\text{O}}
\]
\[
p' = \frac{p}{K_{\text{CH}_2\text{O}}}
\]
\[ h' = \frac{h}{K_{CH_2O}} \]
\[ \alpha = \frac{\mu_p}{\mu_h} \]
\[ [CH_2O]' = \frac{[CH_2O]}{K_{CH_2O}} \]
\[ [CO_2]' = \frac{[CO_2]}{K_{CO_2}} \]
\[ [O_2]' = \frac{[O_2]}{K_{O_2}} \]

Inserting the rescaled variables and parameters into equations (2.4)-(2.8) we obtain

\[ \partial_t p' = p' \left[ \alpha \phi \left( [CO_2]' \right) - \tau' - c'h' \right] + D'_1 \partial_x^2 p' \]
\[ \partial_t h' = h' \left[ (1 - f) \psi \left( [O_2]' , [CH_2O]' \right) - \tau' \right] + D'_1 \partial_x^2 h' \]
\[ \partial_t [CO_2]' = \gamma_1 h' f \psi \left( [O_2]' , [CH_2O]' \right) - \gamma_2 p' \alpha \phi \left( [CO_2]' \right) + D'_2 \partial_x^2 [CO_2]' \]
\[ \partial_t [O_2]' = \gamma_3 p' \alpha \phi \left( [CO_2]' \right) - \gamma_4 h' f \psi \left( [O_2]' , [CH_2O]' \right) + D'_2 \partial_x^2 [CO_2]' \]
\[ \partial_t [CH_2O]' = \tau' p' + \tau' h' + c'h' p' - h' A_{CH_2O}^h \psi \left( [O_2]' , [CH_2O]' \right) + D'_2 \partial_x^2 [CH_2O]' \]

where now
\[ \phi \left( [CO_2]' \right) = \frac{[CO_2]'}{1 + [CO_2]'} \]
\[ \psi \left( [O_2]' , [CH_2O]' \right) = \frac{[O_2]'}{1 + [O_2]'} \frac{[CH_2O]'}{1 + [CH_2O]'} \]
Since these equations contain a large number of parameters, we will simplify the equations by considering only the region of parameter space for which \( \gamma_1 = \gamma_2 = \gamma_3 = \gamma_4 = 1 \) and \( A_{CH_2O}^h = 1 \). Dropping the prime notation and setting each of the \( \gamma \) to 1, we have the following system of partial differential equations:

\[
\frac{\partial t}{\partial t} p = p \left[ \alpha \phi(\text{CO}_2) - \tau - ch \right] + D_1 \partial_x^2 p \tag{2.9}
\]

\[
\frac{\partial h}{\partial t} = h \left[ (1 - f) \psi\left(\text{O}_2, [\text{CH}_2\text{O}]\right) - \tau \right] + D_1 \partial_x^2 h \tag{2.10}
\]

\[
\frac{\partial t}{\partial t} [\text{CO}_2] = hf \psi\left(\text{O}_2, [\text{CH}_2\text{O}]\right) - p\alpha \phi(\text{CO}_2) + D_2 \partial_x^2 [\text{CO}_2] \tag{2.11}
\]

\[
\frac{\partial t}{\partial t} [\text{O}_2] = p\alpha \phi(\text{CO}_2) - hf \psi\left(\text{O}_2, [\text{CH}_2\text{O}]\right) + D_2 \partial_x^2 [\text{CO}_2] \tag{2.12}
\]

\[
\frac{\partial t}{\partial t} [\text{CH}_2\text{O}] = \tau p + \tau h + chp - h \psi\left(\text{O}_2, [\text{CH}_2\text{O}]\right) + D_2 \partial_x^2 [\text{CH}_2\text{O}] \tag{2.13}
\]

\section{2.3 Numerical Methods}

Since it is difficult to gain much insight from equations (2.11)-(2.15) with analytical techniques, numerical simulations were used to study the possible dynamics which they describe. In order to simulate these dynamics, the forward Euler (explicit) method was used. As an example of how this method was used, consider the equation

\[
\frac{\partial t}{\partial t} z = f(z) + \partial_x^2 z \tag{2.14}
\]

Discretizing both space and time and letting the lower index denote the temporal coordinate and the upper index denote the spatial coordinate we then have the equation

\[
\frac{z_{j+1}^i - z_j^i}{\Delta t} = f(z_j^i) + \frac{z_j^{i-1} + z_j^{i+1} - 2z_j^i}{\Delta x^2} \tag{2.15}
\]

To obtain a formula for \( z \) at time \( j + 1 \), equation (2.17) can be solved for \( z_{j+1}^i \) to obtain

\[
\frac{z_{j+1}^i - z_j^i}{\Delta t} = f(z_j^i) + \frac{\Delta t}{\Delta x^2} \left( z_j^{i-1} + z_j^{i+1} - 2z_j^i \right) \tag{2.16}
\]
If $z$ is taken to be a vector whose components are the dependent variables in equations (2.11) - (2.15) and $f(z)$ is taken to be the right hand side of those equations excluding the diffusion term, then equation (2.18) describes the numerical scheme used in simulating the dynamics of those equations.

Since the chamber in the experiment in [4] was sealed around the outer edges, no-flux boundary conditions are used in the simulations.

The time step used in the simulations was $\Delta t = 0.001$ and the spatial step used was $\Delta x = 0.1$. The numerical values used for the diffusion coefficients are $D_1 = 0.01$ and $D_2 = 0.1$. The simulations were carried out with Python 3.5.

Although using the implicit method rather than the explicit method would guarantee convergence for larger time steps, the numerical simulations carried out using the explicit method with the time step specified above converged and ran in a reasonable amount of time.
Chapter 3

Results

3.1 Properties of the Model with No Diffusion

3.1.1 Fixed Points

To gain an intuition for the dynamics described by equations (2.11)-(2.15), we begin by solving for the steady state solutions of these equations without including the diffusion terms. Without diffusion, equations (2.11)-(2.15) become

\[
\frac{\partial t}{t} p = p \left[ \alpha \phi \left( [\text{CO}_2] \right) - \tau - ch \right] \tag{3.1}
\]

\[
\frac{\partial t}{t} h = h \left[ (1 - f) \psi \left( [\text{O}_2], [\text{CH}_2\text{O}] \right) - \tau \right] \tag{3.2}
\]

\[
\frac{\partial t}{t} [\text{CO}_2] = h f \psi \left( [\text{O}_2], [\text{CH}_2\text{O}] \right) - p \alpha \phi \left( [\text{CO}_2] \right) \tag{3.3}
\]

\[
\frac{\partial t}{t} [\text{O}_2] = p \alpha \phi \left( [\text{CO}_2] \right) - h f \psi \left( [\text{O}_2], [\text{CH}_2\text{O}] \right) \tag{3.4}
\]

\[
\frac{\partial t}{t} [\text{CH}_2\text{O}] = \tau p + \tau h + chp - h \psi \left( [\text{O}_2], [\text{CH}_2\text{O}] \right) \tag{3.5}
\]
Due to the symmetries in equations (3.1)-(3.5), we have the following two conserved quantities

\[ \partial_t [O_2] + \partial_t [CO_2] = 0 \implies [CO_2] + [O_2] = \text{constant} \equiv \nu \]

\[ \partial_t p + \partial_t h + \partial_t [CO_2] + \partial_t [CH_2O] = 0 \implies p + h + [CO_2] + [CH_2O] = \text{constant} \equiv \delta \]

To find the steady state solutions, the time derivatives are set to 0 and we are left with the following system of equations

\[ p \left[ \alpha \phi ([CO_2]) - \tau - ch \right] = 0 \quad (3.6) \]

\[ h \left[ (1-f) \psi ([O_2],[CH_2O]) - \tau \right] = 0 \quad (3.7) \]

\[ hf \psi ([O_2],[CH_2O]) - p \alpha \phi ([CO_2]) = 0 \quad (3.8) \]

\[ \tau p + \tau h + chp - h \psi ([O_2],[CH_2O]) = 0 \quad (3.9) \]

\[ [CO_2] + [O_2] = \nu \quad (3.10) \]

\[ p + h + [CO_2] + [CH_2O] = \delta \quad (3.11) \]

Using Mathematica, the system of equations (3.6)-(3.12) may be solved for various combinations of parameters. Although there will always be a solution for which \( p = h = 0 \), we are interested primarily in the nontrivial solutions to the system of equations. Additionally, the system of equations typically has solutions for which at least one of the concentrations is negative. Since it is unphysical to have negative concentrations, only the solutions for which all of the concentrations are positive are considered.

As an example of a fixed point solution which was computed in Mathematica, for the choice of parameters \( \alpha = 3, \ c = 0.3, \ \tau = 0.12, \ f = 0.643, \ \nu = 7.2, \ \text{and} \ \delta = 25.8 \) the only fixed point which is nonzero and positive is

\[ p = 0.687274, \ h = 8.28682, \ [CO_2] = 6.61508, \ [O_2] = 0.584921, \ [CH_2O] = 10.2108 \]
3.1.2 Linearization and Stability of Fixed Points

To study the stability of the steady state solutions, the system of equations is linearized to see if small perturbations about the fixed point will grow or diminish with time. If we define the quantity

\[ \vec{\xi} = (p, h, [CO_2], [O_2], [CH_2O]) \]

and denote the fixed point by \( \xi^* \) then the rate of change of a small perturbation \( \Delta \vec{\xi} \) around the fixed point is given by

\[
\frac{\partial}{\partial t}(\Delta \vec{\xi}) = h(\vec{\xi}^*) + \Delta \vec{\xi} J(\vec{\xi}^*) \]

\[
= \Delta \vec{\xi} J(\vec{\xi}^*)
\]

where \( h \) denotes the right hand side of equations (3.1)-(3.5) and \( J \) is the Jacobian matrix. The eigenvalues of the Jacobian matrix are computed using Mathematica and if the real parts of all of the eigenvalues are negative, then the fixed point is stable.

For all the values of the parameters that were studied, there are either three real eigenvalues and one pair of complex conjugate eigenvalues or five real eigenvalues. The signs of the real parts of the eigenvalues depend on the choice of parameters.

To see how the stability of the eigenvalues is affected by varying the parameter \( \alpha \), we fix the values of the other parameters as follows

\[ \tau = 0.12 \] (3.12)

\[ f = 0.643 \] (3.13)

\[ \nu = 7.2 \] (3.14)

\[ \delta = 25.8 \] (3.15)

For certain parameter values, the Solve and Nsolve commands in Mathematica were unable to find solutions to the system of equations (3.6)-(3.12) despite the fact that numerical simulations in Python revealed the existence of steady state solutions for those parameter values. The parameter values above were chosen in part because Mathematica was able to solve the system of equations with those values.
For several values of $c$, the real and imaginary parts of the pair of complex conjugate eigenvalues is plotted in Fig 3.1.

![Graphs showing real and imaginary parts of eigenvalues for different values of $c$.](image)

Fig. 3.1 Dependence of real and imaginary parts of the complex conjugate pair of eigenvalues on $\alpha$ for several values of $c$.

For all of the parameter values depicted in Fig. 3.1, the three real eigenvalues are all negative. Therefore, for the values of $c$ and $\alpha$ for which the real part of the complex conjugate pair of eigenvalues is negative, the steady state solutions are stable.

To visualize for which values of $c$ and $\alpha$ the fixed point is stable, a phase diagram depicting the regimes of stability/instability is shown in Fig. 3.2. When $\alpha$ is very small compared to $c$, the fixed point for which $p = h = 0$ becomes stable and nonzero initial concentrations of phototrophs and heterotrophs will tend towards extinction.
Fig. 3.2 Phase diagram depicting values of $c$ and $\alpha$ for which the fixed point is stable or unstable. If $\alpha$ is very small compared to $c$, then the fixed point for which $p = h = 0$ becomes the stable fixed point. The other parameters are as specified in (3.12)-(3.6).

3.1.3 Phase Plots for Phototrophs and Heterotrophs

Now that the stability of the fixed points has been determined for a particular choice of parameters by linearizing the equations, the dynamics of the system are simulated.

First, we simulate the dynamics for a choice of parameters that corresponds to a stable fixed point. The parameters used are $\alpha = 3$, $c = 0.3$, and all other parameters are the same as in (3.13)-(3.16). The initial conditions are $p = 2.6555$, $h = 2.037$, $[\text{CO}_2] = 6.629$, $[\text{O}_2] = 0.56094$, and $[\text{CH}_2\text{O}] = 14.471$. Although linearizing the equations is an approximation which is valid only in a neighborhood of the fixed point, initial conditions are chosen such that the system begins far from the fixed point. The results of this simulation are shown in Fig. 3.3.

The initial conditions may appear unnatural since they are specified to several decimal points, however, they were chosen by adding and subtracting integer values from the fixed points solutions computed using Mathematica.

The fixed point which is approached in this simulation agrees with the steady state solution found by solving the system of equations (3.6)-(3.12).
Fig. 3.3 The concentration of heterotrophs versus phototrophs (above) and the concentrations of heterotrophs and phototrophs versus time (below) as they approach a stable fixed point.
Next, we simulate the dynamics for a choice of parameters corresponding to an unstable fixed point. The choice of parameters used in the simulation is \( \alpha = 1.2, \ c = 0.3, \) and all other parameters are the same as in (3.13)-(3.16). The initial conditions are \( p = 0.6555, \ h = 4.037, \ \text{[CO}_2\text{]} = 6.629, \ \text{[O}_2\text{]} = 0.56094, \) and \( \text{[CH}_2\text{O]} = 14.471. \) The results of this simulation are depicted in Fig. 3.4

![Graphical representation of the unstable fixed point and its evolution over time.](image)

Fig. 3.4 The concentration of heterotrophs versus phototrophs (above) and the concentrations of heterotrophs and phototrophs versus time (below) as they move away from an unstable fixed point.

The value of the fixed point at the center of the spiral in Fig. 3.4 agrees with the value of the fixed point found by solving equations (3.6)-(3.12). Although the phototroph and heterotroph concentrations initially move away from the unstable fixed point, they are eventually attracted towards a limit cycle and oscillate around the fixed point.
For the same combination of parameters but with the initial conditions $p = 2.6555$, $h = 5.037$, $[\text{CO}_2] = 6.629$, $[\text{O}_2] = 0.56094$, and $[\text{CH}_2\text{O}] = 11.471$, the trajectory begins outside of the limit cycle in the phototroph-heterotroph plane and spirals inwards towards it. Therefore, the limit cycle in Fig. 3.4 attracts trajectories from both its interior and exterior in the phototroph-heterotroph plane.

Finally, we simulate the dynamics for a choice of parameters for which the real part of the complex conjugate eigenvalues is 0. This corresponds to a fixed point which is right at the boundary of instability and stability, i.e. it is the point at which the Hopf bifurcation occurs. The choice of parameters in this simulation is $\alpha = 1.55$, $c = 0.3$, and all other parameters are the same as in (3.13)-(3.16). The initial conditions are $p = 0.6555$, $h = 4.037$, $[\text{CO}_2] = 6.629$, $[\text{O}_2] = 0.56094$, $[\text{CH}_2\text{O}] = 14.471$. The results of this simulation are depicted in Fig. 3.5.

Fig. 3.5 The concentration of heterotrophs versus phototrophs (above) and the concentrations of heterotrophs and phototrophs versus time (below) as they oscillate around the fixed point.
The phototroph and heterotroph concentrations in Fig. 3.5 exhibit small amplitude oscillations around the fixed point, as is expected. The value of the fixed point which the phototroph and heterotroph concentrations are oscillating around again agrees with the value for the fixed point found by solving equations (3.6)-(3.12).

The three principal categories of behavior found by simulating the dynamics of the system are illustrated in Figs. 3.3, 3.4, and 3.5. In the stable regime, trajectories from all over the phase space are attracted towards the fixed point. As the system crosses from the stable regime to the unstable regime, the system begins to exhibit small amplitude oscillations in the neighborhood of the fixed point. Once the system has passed into the unstable regime, a larger amplitude limit cycle appears which attracts trajectories both from near the fixed point and from far away from the fixed point.

3.2 Properties of the Model with Diffusion Included

3.2.1 Formation of Fronts at the Light/No-Light Boundary

Now that the properties of the model have been studied without the diffusion terms, the diffusion terms are reintroduced and we consider how the system will behave when a central region of the spatial axis is illuminated and the outside regions are dark as in the experiment in [4].

Since $\mu_p$ and hence also $\alpha$ are functions of the amount of light, the darkness condition is equivalent to setting $\alpha = 0$. The dynamics of the system are simulated with $\alpha = 1.8$ in the illuminated region, $c = 0.27$, $\tau = 0.12$, $f = 0.643$, $v = 7.2$, and $\delta = 25.8$. The initial conditions used are $p = 0.6555$, $h = 4.037$, $[\text{CO}_2] = 6.629$, $[\text{O}_2] = 0.56094$, and $[\text{CH}_2\text{O}] = 14.471$. In the case without diffusion, this combination of parameters was found to correspond to a stable fixed point. The results of the simulation are shown in Fig. 3.6.
Fig. 3.6 The concentration of phototrophs (left), heterotrophs (center), and oxygen (right) as the system approaches the steady state. The vertical black dashed lines indicate the boundary between light and dark.

Fig. 3.7 The concentration of carbon dioxide (left) and biomass (right) as the system approaches the steady state. The vertical black dashed lines indicate the boundary between light and dark.
The oxygen profile in Fig. 3.6 has the same peaks just inside the light/dark boundary as the oxygen profile observed in the experiment in [4]. Although these results correspond to a particular choice of parameters, the same general shape for the oxygen profile was found in other simulations for a large range of parameter values and initial conditions.

To understand why the oxygen profile takes this shape, first note that its shape is very similar to the shape of the phototroph profile since the phototrophs are the oxygen source. Since the concentrations of biomass, carbon dioxide, and oxygen are rescaled by their respective half-rate constants, it is evident from Figs. 3.6, 3.7 that the system is saturated everywhere with carbon dioxide and biomass and the concentrations of carbon dioxide and biomass will not have any significant effect on the shape of the phototroph or heterotroph profiles as the system approaches its steady state.

Since the phototrophs cannot grow outside of the illuminated region, no oxygen will be produced there. The heterotrophs are only limited by oxygen so they will grow much more rapidly in the light region than in the dark region and will diffuse slowly outwards into the dark region. As the heterotrophs diffuse outwards, their concentration will begin to drop just inside of the light/dark boundary. Since the heterotrophs are killing the phototrophs, as the heterotroph concentration drops towards the edge of the light region this allows for the phototroph concentration to increase resulting in peaks in the phototroph concentration just inside the light/dark boundary. As the phototrophs grow more rapidly near the boundary, more oxygen will be produced near the boundary than in the center of the light region resulting in peaks in the oxygen concentration just inside the light/dark boundary.

Although in the experiment in [4] the light was turned on and off every 90 minutes and in the simulation the light was kept, a very similar profile for oxygen concentration appeared.

For the simulation whose results are shown in Figs. 3.6, 3.7, the profiles first assumed the general shape shown in Fig. 3.6 after which they exhibited damped oscillations as they approached the steady state. Although most of the profile oscillated in phase, the profiles in the center of the illuminated region in between the two peaks oscillated with different amplitude and phase than the rest of the profile.

The central region which oscillated separately from the rest of the profile has a length scale which is likely determined by the choice of parameters or by the width of the illuminated region. For similar simulations in which the parameters were chosen so that the oscillations of the overall profile were undamped, the oscillations in the central region were then undamped as well.
3.3 Outlook

Despite the fact that the model used to describe the microbial dynamics in a two dimensional system was a very simple one, it was able to reproduce the general shape of the oxygen profile observed in the experiment in [4]. If the effects observed with this model were the same as those responsible for the oxygen profile observed in [4], then one would expect to see the same profile emerge if the light were kept on constantly rather than being turned on and off every 90 minutes.

As a next step in studying this model, the presence of instabilities at finite wave number may be considered. If an instability at a particular wavenumber were found, the wavenumber at which the instability appeared would describe a characteristic length scale for the oscillations discussed at the end of section 3.2.1.
References


