SIMULATION OF HOLLOW FIBRE MEMBRANES PHOTOTBIOREACTOR

A Thesis

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In Partial Fulfillment of the Requirements for the Degree of

Master of Science

by

Cheng Fu

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ABSTRACT

Microalgae fix inorganic carbon (CO_2) into biomass that can be used as biofuels through photosynthesis. In microalgae-based photobioreactors, the poor distribution of light and CO_2 source often limit the production. A promising solution for these problems is applying light waveguides to deliver the light uniformly and introducing hollow fibre membranes (HFMs) which can increase the interfacial contact area for gas transfer.

There are several parameters that have impact on the efficiency of HFM reactor, such as light, temperature, gas velocity in fibre, inlet concentration of CO_2, and distance between HFM arrays. Our research goal is using simulation methods to test those parameters, make predictions and help to simplify further experiments.

The numerical model we used to approach the microorganisms in photobioreactors system, Monod equation model, has several empirical coefficients which need to be determined by experiments. Our group members have done the experiment testing how the fibre distance influences the algae growth. We redid the experiment on computer using COMSOL Multiphysics 4.3b, and the result matched well, which verified the reliability of the simulation model. Then we tested the effect of inlet concentration of CO_2 and the gas velocity.

BIOGRAPHICAL SKETCH

Cheng Fu earned his Bachelor of Science degree in Physics from Peking University, Beijing, China in 2012. After graduation, he came to Cornell University and joined the Master of Science program in School of Applied Physics.

Cheng received Outstanding Student Award from School of Physics, Peking University regarding to his academic record and participation in campus activities. In addition to his academic studies, Cheng joined the Student Union in Peking University. He coordinated and organized several activities as the vice-president of the Literature and Art Department.

While pursuing his undergraduate degree, Cheng began to participate in research projects to practice what he learned from class. He applied finite difference time domain (FDTD) method to simulate and design a double-slit surface plasmon sensor in Professor Jiasen Zhang's group. During his graduate study, Cheng joined Professor David Erickson's group in a biofuel reactor project in Cornell University. He studied the bioreactor by simulation methods.

Cheng's thesis, entitled "Simulation of Hollow Fibre Membranes Photobioreactor" was supervised by Dr. David Erickson in Sibley School of Mechanical and Aerospace Engineering.

I would like to dedicate this thesis to my family, my friends and

to my supervisor, Professor David Erickson.

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I could not write this thesis without the help and support of the kind people around me, and I would like to mention them here.

Above all, I would like to thank my parents and my dear friends for their great patience and personal support. My words and expressions of thanks could not suffice for their great support.

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Last but not the least, I thank my friends, both in Ithaca and elsewhere for their support and encouragement.

For any errors or inadequacies that may remain in this work, of course, the responsibility is entirely my own.

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CHAPTER 1

INTRODUCTION AND MOTIVATION

Biofuels produced from microalgae have drawn widespread interest as a solution to problems arising from the usage of fossil fuel, such as climate change, energy security and CO_2 emissions [1]. Microalgae can fix CO_2 with an efficiency 10–50 times greater than that of terrestrial plants [2]. Thanks to genetic engineering technology, many kinds of usable product, such as hydrogen [3], ethanol [4], and other valuable products [5], can be secreted directly by microalgae. However, the economic viability of microalgae-based photobioreactors has been limited by some well-documented weaknesses, such as poor distribution of light and CO_2 source within the reactor, low algae concentration, and large water and energy consumption [6].

Applying Hollow fibre membranes (HFMs) can improve the gas delivery and product extraction within the reactor [7]. And reactors can get uniform light penetration by introducing light waveguides. Our motivation is driven by the applications of bioreactors integrating with HFMs and waveguides. There are several parameters that have impact on the efficiency of this kind of reactor, such as gas velocity in fibre, inlet concentration of CO_2, distance between fibres, light wavelength, light intensity and temperature etc.

It takes time and money to test all those parameters by experiment. Our research goal is using simulation methods to test those parameters, make predictions to simplify further experiments. Among these parameters, the light and temperature were

tested by other group members by experiment. Our simulation only focuses on gas velocity, inlet concentration of CO_2 and fibre distance. Both gas velocity and inlet concentration of CO_2 relate to the cost and energy. Fibre distance determines the size and output of our reactor.

In order to simulate the algae growth in reactor, we decided to apply Monod equation model [8]. However, Monod equation has several empirical coefficients which differ between species and environmental conditions. As a result we need experiment results to verify those coefficients in the simulation. Our group members have done the experiment testing the fibre distance and published their results [9]. By matching the simulation and the experiment results, we can confirm the reliability of our simulation, and then predict the scale and impact of other parameters. Since the experiment contains other environment factors and errors and our simulation based on several assumptions for simplification, the result cannot predict precise values. But we can still get the right relationship and an expectation range of those parameters we concern, which is useful and valuable for further experiments.

We will introduce the physics behind the simulation in Chapter 2 in details. In Chapter 3, we will cover the previous experiment work which our simulation result relies on, and discuss the setup of our simulation program. Then we will show our simulation result in Chapter 4, and conclude with our summary in Chapter 5.

CHAPTER 2

THEORETICAL BACKGROUNDS

In this chapter, we will first review the state-of-art of photobioreactors, and then introduce the simulation approach to the reactor system by showing the physics behind the project.

2.1 Photobioreactors

Photobioreactors [10] are reactors that employ photosynthetic microorganisms to convert light and CO_2 into usable and valuable biomass. By applying genetic engineering technology, microalgae have been reported being able to produce many kinds of usable product. The key advantage of a photobioreactor is that it can control the supply of environmental conditions for specific species, which allows much higher growth rates and purity levels than in natural or habitats similar to nature. Due to the high density of microorganisms and high value of the product, microalgae-based photobioreactors have attracted increasing concerns. There are many different designs, two most common industrial microalgae-based photobioreactors are open air pond type and closed type tube reactors [11]. Despite their easy construction, there are several well-documented weaknesses as we mentioned in chapter 1.

2.1.1 Light distribution within the reactor

Light distribution within traditional pond and tube/plate type reactors is inherently poor [12]. Shaded by the organisms that live closer to the illuminated surface, the organisms at the bottom do not get sufficient light exposure.

Our solution to this challenge owes to the fact that the increased efficiency of techniques for coupling solar energy into light guiding elements. By inserting low-cost solid state slab waveguides into the algae sink, we can increase the light distribution within the sink, because more light can penetrate into the deeper part of the reactor. Some of our group members are working on improving the uniformity of light distribution along those waveguides.

2.1.2 Nutrient delivery within the reactor

In order to get high productivity, it is necessary for photobioreactors to have the CO_2 delivered and products, such as O_2 and ethylene, extracted efficiently. If the light illumination is sufficient to the algae, the diffusion of CO_2 and O_2 to and from the organisms will become the key factor that limits the productivity [13].

As a promising solution to the problems mentioned earlier, hollow fiber membranes (HFMs) can increase the surface area for mass transfer and control the CO_2 retention time and concentration inside of a reactor. HFMs enable gas transfer by exploiting partial pressure differences across the membrane. So the membrane can deliver CO_2

and remove O_2 and other product simultaneously. The HFMs we used in our experiment is purchased from Mitsubishi Rayon Co. Ltd, and model number was MHF304KM.

2.1.3 Synechococcus elongates

In order to evaluate and compare our photobioreactor to current benchmark production levels, we used *Synechococcus elongatus* as our model photosynthetic organism. *S. elongatus* is one of the most abundant cyanobacteria in marine and fresh water, and it requires only water, minimal salts, CO_2, and vitamins for growth. Therefore it has been studied for biofuel production. The Liao Lab in the Department of Chemical and Biomolecular Engineering at UCLA engineered the wild-type strain *S. elongatus* PCC7942 into *S. elongatus* SA665 by adding a pathway for the production of isobutyraldehyde [14].

In general, the physics behind the bioreactor is simple. Although it is hard to numerically simulate the process of photosynthesis, the part of the reaction we focused on is quite obvious. The microalgae consume the inlet CO_2, grow, and emit O_2 and ethylene. Simulating a mechanism by which the amount of ethylene can increase coupled with decreasing amount of CO_2 is easy, because it only refers to several variations of numbers. The complicated part in our project is to find formulas and models to describe and determine the algae growth and mass transfer in the system.

2.2 Growth of microalgae

Microalgae fix the CO_2 through photosynthesis, which is a growing process for the microorganism. The more microalgae we have, the more product can we get. However, in a closed photobioreactor, the environment for algae is limited. The living space, the distribution of light and nutrient, the extraction of waste are all important factors which can influence the growth of algae. As mentioned before, the light part will not be considered in our simulation. We simplify the situation where only nutrient and space are taken into consideration.

The growth of microorganisms can be described by Monod equation [15].

$$\mu = \mu_{\max} \frac{S}{K_s + S} \tag{2.1}$$

where μ is the specific growth rate of the microorganisms, μ_{max} is the maximum specific growth rate of the microorganisms, S is the concentration of the limiting substrate for growth and Ks is the "half-velocity constant"—the value of S when μ/μ_{max} equals to 0.5. Both μ_{max} and K_s are empirical coefficients. They differ between species and depend on the ambient environmental conditions. In our simulation, S is the concentration of CO_2, which is the only nutrient in our reactor. The value of μ_{max} and K_s need to be determined by matching the simulation with experiment results.

The number of microorganisms in a culture will increase exponentially until an essential nutrient is exhausted, the growth rate μ is defined as:

$$N(t) = N(0)e^{\mu t} \tag{2.2}$$

Where *N(t)* is number of algae at time t, *N(0)* is the initial amount of the strain, *t* is the time.

The Monod equation can describe the growth of algae, but the death of algae is complicated to be predicted by simulation method. Since it is influenced by many factors, we did not find a function or equation that can describe the death of microorganisms properly. We tried to assume a death rate which was determined by several parameters, but lacked of theoretical proof and failed in simulation. As a result, we decided not to numerically consider the death of algae in our system.

We still need to artificially set a maximum value for the algae concentration referred to the closed living space. Even we assumed they never died, they couldn't grow to infinity because the space was limited. When the result of algae concentration reached the maximum it would stop increasing.

2.3 Convection–diffusion equation

Our bioreactor contains an algae sink (a liquid environment where algae live) and hollow fibre membranes (only gas in those fibres). We inlet CO_2 into the HFMs, let them diffuse into the sinks where microalgae absorb those CO_2 and emit O_2 and ethylene. Then those product will diffuse back into the HFMs and flow out of our system. The motion of these gas molecules in the sink, fibre and through the membranes contains two processes: diffusion and convection. We need a formula to calculate those concentrations in our system.

The convection–diffusion equation is a combination of the diffusion and convection (advection) equations, and describes physical phenomena where particles, energy, or other physical quantities are transferred inside a physical system due to those two processes. It is widely used in many fields as a numerical simulation method, so it has many simplified forms. In general [16],

$$\frac{\partial c}{\partial t} = \nabla \cdot (D\nabla c) - \nabla \cdot (vc) + R \tag{2.3}$$

where c is the species concentration, D is the diffusion coefficient of the species, v is the average velocity of the species moving, R is the source. The first term on the right hand side is the diffusive term which describes the diffusion process in a system caused by the concentration gradient. The second term is convective term, which is usually forced by pressure or temperature gradient. The last term is the source, including exterior forces and reactions.

In our simulation, the diffusion coefficients, velocity and source terms are known. We can separate the space into many small cubes and couple three of Equation 2.3 (one for algae, one for CO_2 and the other for ethylene) in each cube to calculate their concentrations.

2.4 *COMSOL Multiphysics*

COMSOL Multiphysics is a finite-element analysis, solver and simulation software. It contains many packaged models for various math, physics and engineering

applications. COMSOL Multiphysics can work with MATLAB for optimizing parameters. It can run on many operation platforms like Windows, Mac and Linux.

In our simulation, we used the Chemical Reaction Engineering Module from COMSOL Multiphysics version 4.3b. This module includes the basic formulas which can describe our system: Mass transfer in a liquid (algae sink) and gas (fibre) environment with given boundary conditions (geometric boundaries of our reactor). By applying the Reacting Flow in Porous Media model which is packaged as a sub interface in this module, we can define diffusion barriers (the surface of HFM), flows (in algae sink and inside HFMs) and boundary conditions. The kinetic expressions for the reacting system are automatically defined in the module. What we have to do is just set the values of constants and give the initial value to the variables.

More details about the simulation setup will be shown in section 3.3.

CHAPTER 3

EXPERIMENTAL PROCESS

As the theoretical background is clear, it is time to introduce the experimental process. We will cover the setup of the reactor, the experiment process done by previous group members and our simulation details in this chapter.

3.1 Reactor setup

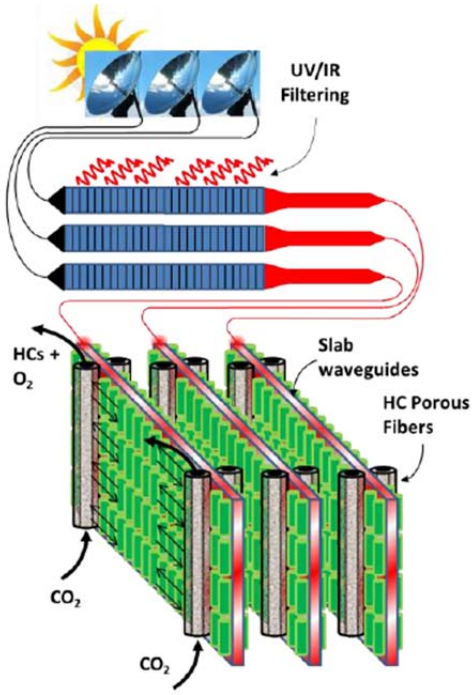

Figure 3.1 Layout for integrated reactor.

Figure 3.1 shows the ideal prototype of our bioreactor. First we select the useful wavelength from sunlight. Then deliver the light along low-cost solid state slab waveguides to supply microalgae the energy for their photosynthesis process. For a

single bioreactor we intend to integrate 10 waveguides held by a 3D printed frame. The algae live in the sink between the waveguides in a liquid environment. At the same time, we pump CO_2 gas through the hollow fibre membranes. These fibres allow gas to diffuse through but algae not. The concentration of CO_2 in the fibre is higher than the concentration in the sink, so carbon dioxide will diffuse into the algae sink, then get absorbed by the algae and converted into O_2, ethylene and other biomass. The O_2 and ethylene will diffuse back into the HFMs, since there is a concentration gradient between the inside and outside the fibres. These gases come out from the other end of the fibres with some remaining CO_2. By applying some industrial methods, we can separate these gas mixtures and gather the ethylene, which can be used as biofuel.

There are several parameters influencing the reactor production, such as the light wavelength, the light intensity, the size of the reactor, the algae we use, etc. We were separated into several sub-groups to solve these challenges. Our simulation focuses on the velocity and concentration properties.

3.2 Previous work

As mentioned before, the reliability of our simulation depends on experiment results, because several constants in the numerical model are empirical. So here we have to introduce the previous work done by other group members. The geometric size of our simulation model is based on the reactors in this experiment.

This work has already been published [9].

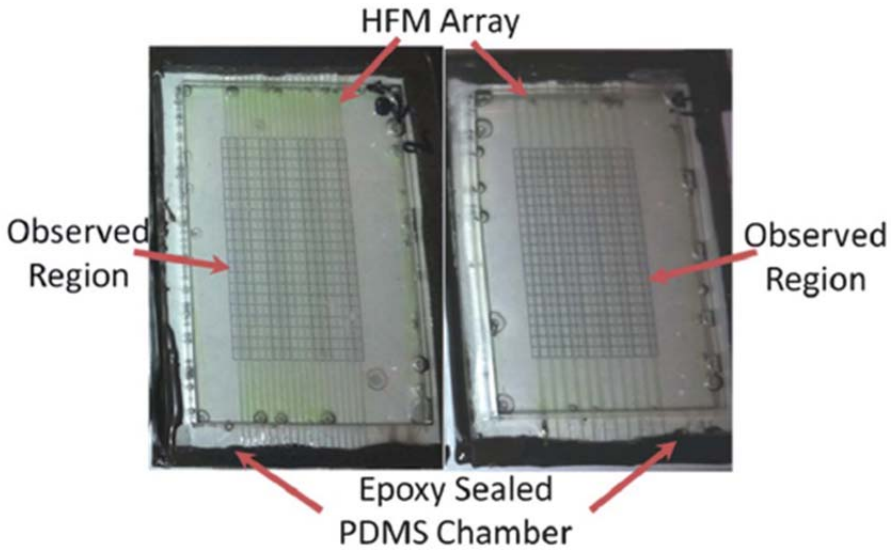

Figure 3.2 Photographs of the two types of reactors tested: 3-diameter unit-cell (left) and 6-diameter unit-cell (right). *RSC Adv., 2014, 4, 1460.*

Figure 3.2 shows the basic setup in this experiment. The goal of this work is to study of the growth of algae under different fibre distances and the effect of aeration method. So the experiment setup is quite simple compared to the ideal model. Rather than integrating 10 slabs waveguides, each of these reactors contained two large cover slides (75 mm×50 mm×1 mm). The area of the reactor was 58 mm×38 mm×6 mm.

The gas aerated in the fibre was air. The edges of the reactors were sealed by polydimethylsiloxane (PDMS), which could prevent the air leaking into the reactor and influencing the algae growth. In order to make CO_2 the only nutrient source for the *S.elongatus*, several steps were performed to the strains. According to the author, the *S. elongates* SA665 first lived in modified BG-11 medium, and then they were sparged with N_2 for 30 min in an anaerobic serum bottle before re-suspension and

inoculation. The reactors were placed under two fluorescent lamp strips (American Fluorescent Plug-in Light Strip), which provided a photon flux density of 75 $\mu E/m^2 \cdot s$. The temperature in the laboratory was 25°C. The ends of the fibres opened to the atmosphere to allow passive gas exchange to occur through the lumens of the fibres.

They first tested 2 fibres, not arrays, by setting the distance as 3 fibre-diameters, 6 fibre-diameters and 12 fibre-diameters. The result showed that with the increasing fibre distance, the algae grew more slowly. So in the fibre array test, they only tested 3 and 6 fibre-diameter setups. 3 reactors of each type were fabricated. By imaging the fluorescent light from the algae in 30 days, the growth distribution around the fibre array was recorded. Then those images were stitched together to produce the surface density maps of algae.

After testing the fibre distance, they pumped air into the HFMs and observed how the algae growth influenced by the aeration method. All the other conditions were kept the same, and they built a setup to actively aerate the reactors at a pressure of 3.45 kPa, which corresponded to a flow rate of 50 mL/min. Again, the fluorescent light image was taken as a record for surface density of algae.

3.3 Simulation setup

Based on the work introduced in Section 3.2, we built up our simulation model by COMSOL Multiphysics Version 4.3b.

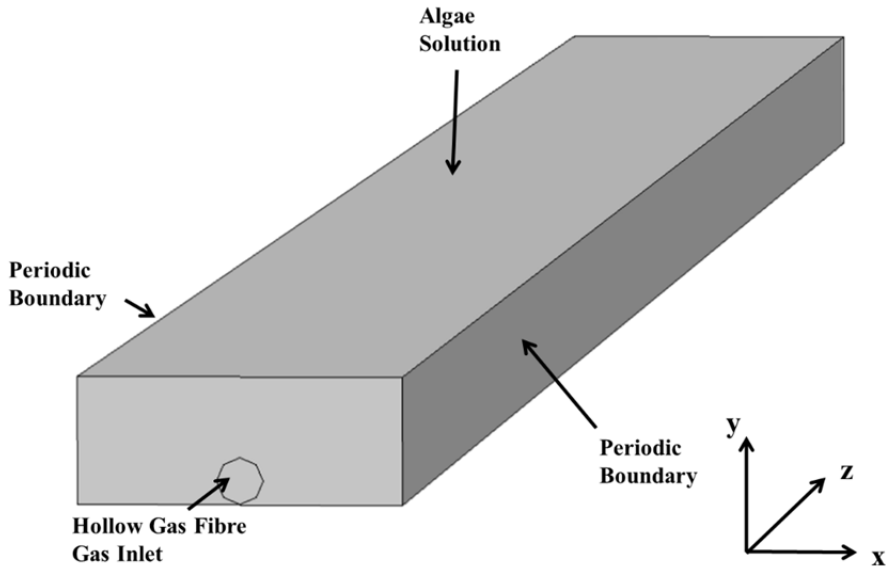

Figure 3.3 Basic setup of reactor model.

The basic setup is shown as Figure 3.3. The diameter of fibre was set to 290 μm according to the specifications from Mitsubishi Company. The length of the reactor was 58mm, which was the effective length of the reactor. The depth of the reactor did not affect much in our reactor since we assumed the light is sufficient. Because the larger the model the longer time it would take the computation, we just chose the depth about 800μm, which was high enough for the fibre. The width of the reactor would be changed for different fibre distance tests. In Figure 3.3, the width of the reactor was set to the length of 7 fibre diameter, corresponded to a 6 fibre diameter gap between two fibres.

By choosing the interface of Species Transport in Porous Media under Chemical Reaction Engineering Module, we could set specific conditions to our system. Since we intended to simulate a HFMs array, along the x direction we set the periodic boundary conditions. In simulation language, it means:

$$c_{i,inside} = c_{i,outside} \tag{3.1}$$

$$-\vec{n}_{inside}\vec{N}_{i,inside} = \vec{n}_{outside}\vec{N}_{i,outside} \tag{3.2}$$

Equation 3.1 shows that the concentrations are the same at both sides of the periodic boundaries, and Equation 3.2 confirms that the number of particles flowing out of the boundary is the same with the number of flowing in, i.e. the net flux is zero. $\vec{n}$ is the normal direction of the boundary, and $\vec{N}$ is the particle number with the direction of their speed. The subscript *i* indicates for different species.

Open boundary condition was set to the end of the fibre when the gas velocity in the fibre was not zero. The numerical form for Open boundary is shown below:

$$\begin{aligned} -\vec{n}\cdot D_i \nabla c_i &= 0 \qquad && if\ \ \vec{n}\cdot\vec{u} \geq 0 \\ c_i &= c_0 && if\ \ \vec{n}\cdot\vec{u} < 0 \end{aligned} \tag{3.3}$$

When the velocity has the direction pointing out of the fibre, the concentration gradient is zero which indicates the gas flow out of the fibre. When velocity is pointing into the fibre, there should be a constant concentration treated as an exterior source.

Thin Diffusion Barrier Condition was set to the surface of the cylinder which indicated the HFM. We assume that:

$$\begin{aligned} -\vec{n}\cdot D_{i,barrier}\nabla c_{i,inside} &= \frac{D_{i,barrier}}{d}(c_{i,inside} - c_{i,outside}) \\ -\vec{n}\cdot D_{i,barrier}\nabla c_{i,outside} &= \frac{D_{i,barrier}}{d}(c_{i,outside} - c_{i,inside}) \end{aligned} \tag{3.4}$$

$D_{i,barrier}$ is the diffusion constant of the gas passing through the fibre. According to Mitsubishi Company, the diffusion coefficient of their fibre is quite small. So we set the rate that the gas passing through the fibre 10^6 times less than their diffusion rate in air. And the algae would never diffuse into the fibre. *d* is the thickness of the fibre, we set it to 3μm.

All the other surface boundaries were chosen to be No flux:

$$-\vec{n}_i \cdot \vec{N} = 0 \tag{3.5}$$

Free flow condition was defined both in the fibre and outer block, which referred to the algae sink. The so called "Free flow" condition is described by convection and diffusion equation as Equation 2.3.

$$\frac{\partial c}{\partial t} = \nabla \cdot (D\nabla c) - \nabla \cdot (vc) + R \tag{2.3}$$

There were three variables which we concerned, the algae growth, the concentration of CO_2 and the concentration of ethylene. Inside the fibre, we only had to calculate the ethylene and CO_2, because the algae would not diffuse into the fibre. In the sink, we had to calculate all the three variables. *D*, *v* and *R* were known to us.

We used mol/m^3 as the unit of concentration of CO_2 and ethylene in the numerical setup for simplification. In order to study the algae, we defined the concentration of algae from 0.0001 to 0.01. Because in the experiment they used surface density as the measurement of algae growth and it was hard to use the unit of mol/m^3 to describe organisms, we just set the algae concentration to a dimensionless quantity. The maximum value (0.01) was artificially set according to the experiment results.

The diffusion coefficient of algae in the sink was set to be 10^{-17} cm^2/s, assuming them not moving in the sink due to their habit. The diffusion coefficients of the gases are shown in Table 3.1 [17], which corresponds to the *D* values in Equation 2.3.

Values(cm^2/s)	Description (solute/solvent)	Values(cm^2/s)	Description (solute/solvent)
1.65×10^{-1}	CO_2/ air	1.62×10^{-1}	Ethylene/air
1.92×10^{-5}	CO_2/water	1.87×10^{-5}	Ethylene/ water

Table 3.1 Diffusion Coefficients

For the term v in Equation 2.3, the liquid velocity in the sink was zero, while the gas velocity in the fibre would be varied.

The initial value of CO_2 and ethylene were 0 both in the sink and fibre, and for algae the initial concentration in sink was 0.0001. We defined a Source at the inlet end of the fibre which acted as the air. It would be changed during the study of the effect of different concentration of inlet CO_2.

The source term in Equation 2.3 refers to the change rate of the concentration of each variable. For simplification, we will use the terms [CO_2], [ETH] and [A] indicating the concentration of CO_2, ethylene and algae, respectively, and RCO2, RETH and RA for the source term for [CO_2], [ETH] and [A], in the following text.

The source terms for [CO_2] and [ETH] are quite simple. Based on basic chemistry knowledge, the reaction rate depends on concentration, solvent, catalyst, etc. In our system, however, only concentration has to be concerned. So the source terms for [CO_2] and [ETH] are:

$$RCO2 = -[A] \cdot [CO_2] \tag{3.6}$$

$$RETH = 0.02 \cdot [A] \cdot [CO_2] \tag{3.7}$$

There is a minus sign for CO_2 because it keeps decreasing by consumption. The 0.02 in Equation 3.2 is due to the conversion efficiency of the algae. Since it was a dimensionless quantity, the amplitude of the algae concentration could act as a scaling number which can scale the reaction speed.

The growing rate of algae is quite different since it is not a simple reactant, so we need to derive from Monod equation for its changing rate. We can convert S (concentration of nutrient) term into $[CO_2]$ in Monod equation (2.1), and substitute the *N* (number amount of algae) in exponentially increasing Equation 2.2 by the concentration of algae (*[A]*), which make them suitable in our simulation.

$$\mu = \mu_{\max} \frac{[CO_2]}{K_s + [CO_2]} \tag{3.8}$$

$$[A] = [A(0)]e^{\mu t} \tag{3.9}$$

$$\Rightarrow \frac{d[A]}{dt} = \mu[A(0)]e^{\mu t}$$

$$= \mu_{\max} \frac{[CO2]}{K_s + [CO2]}[A]$$

$$\Rightarrow RA = \frac{\mu_{\max} \cdot [CO_2]}{K_s + [CO_2]}[A] \tag{3.10}$$

The source term for algae is shown as Equation 3.10, where μ_{max} and K_s are two empirical constants. We need to fit the simulation result to the experiment record in order to choose their values.

Since the living space for algae was limited, algae couldn't keep growing exponentially to infinity as predicted by Equation 2.2. After comparing to the experiment result, we decided to limit the concentration of algae from 10^{-4} to 10^{-2}, i.e. a growth about 100 times. When the *[A]* reaches 0.01 it will stop increasing artificially.

So far we have finished introducing the whole setup of our simulation. The results will be soon covered in next chapter.

CHAPTER 4

RESULT AND DISCUSSION

In this chapter, we will show our result and discussion. First we shall cover the previous work with which our simulation matched, because the empirical constants could be only determined by an experiment record. The good match up confirms the reliability of our prediction simulation, as will be shown after the first part.

4.1 Redo previous work

In our group members' previous work [9], they tested the effect of fibre distance and the aeration methods by imaging and plotting the surface density variation during couple of days. Our simulation just did the same, by choosing different value of those empirical constant, we fit the result with the experiment record.

4.1.1 Fibre distance test

In the previous work our group members first tested the impact of different fibre distance. According to their experiment, they tested 3 fibre diameter and 6 fibre diameter spaced reactors. They imaged the fluorescent light from algae as a measurement of surface density on the 0, 3^{rd}, 5^{th}, 10^{th}, 17^{th} and 31^{st} day. We found these data valuable for our simulation to match up with.

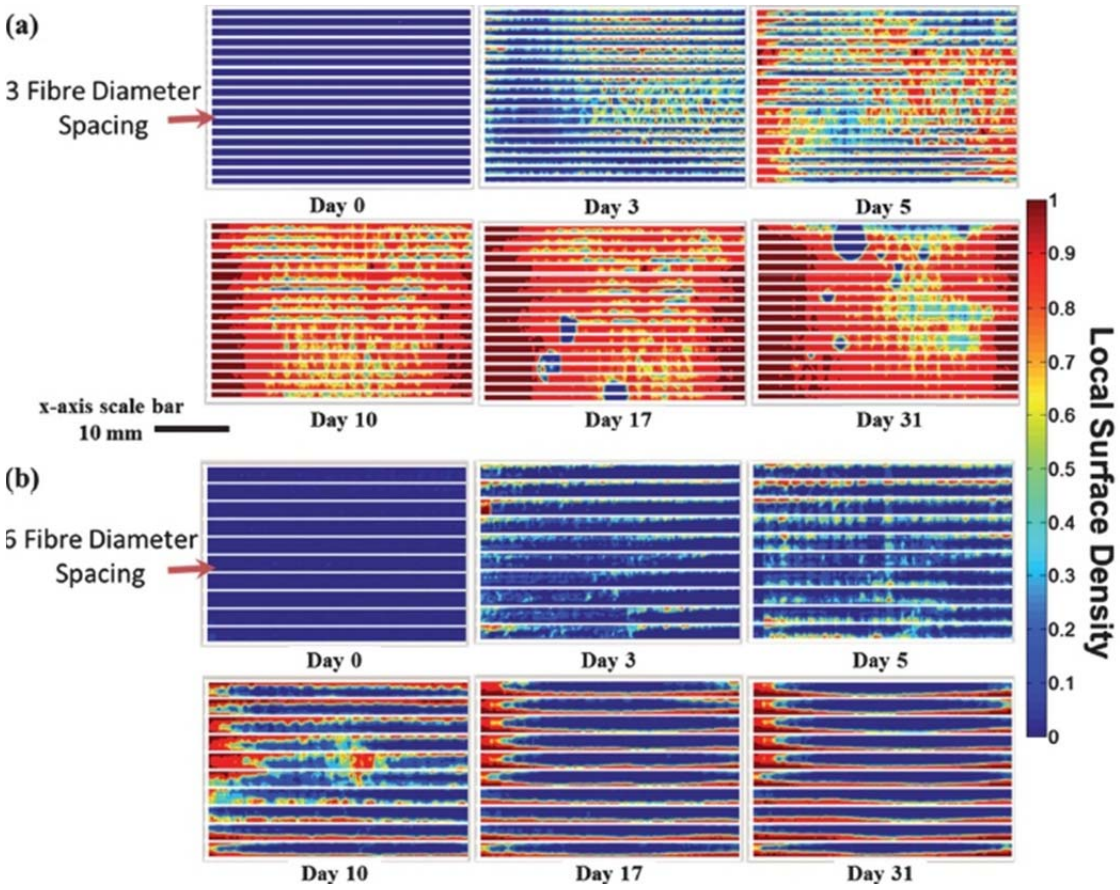

Figure4.1 Surface density maps for two types of arrays over the course of 30 days: local surface density for the (a) 3 fibre diameter spaced array and (b) 6fiber diameter spaced array.

Figure 4.1 was the fluorescent surface density map from the experiment. The white lines in those pictures were the HFMs and the color indicated the amount of algae. The surface density calculated in the experiment was recorded by the fluorescent light from the algae and normalized to the darkest region. Compared to this, the surface density calculated in our simulation was the average value of *[A]* normalized to its max value, 0.01. This was the reason why we set the maximum for the algae growth to a 100 times. By calculating the average of all three reactors for each fibre distance

setup, our group members recorded the value of the total surface density for algae in these reactors, which was found as a valuable result for our simulation to match up.

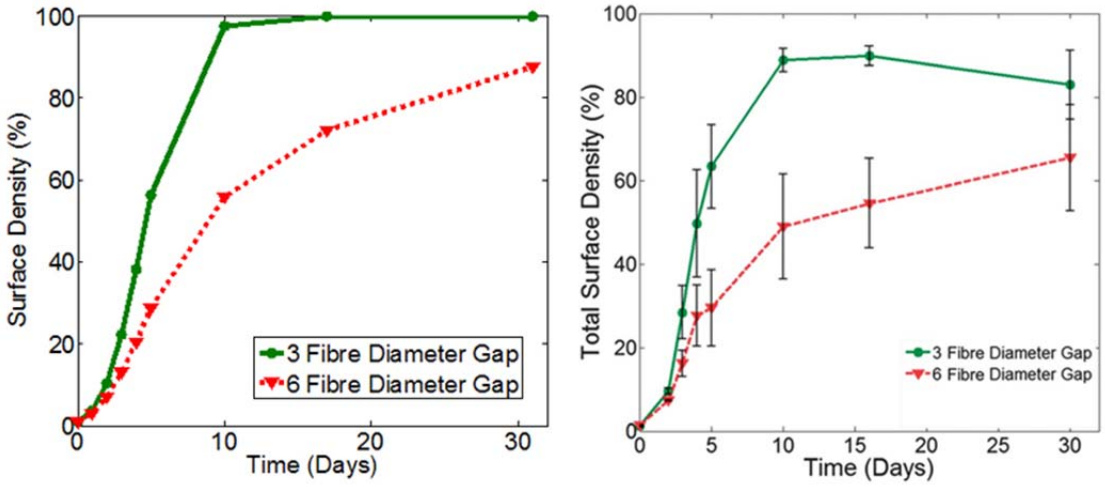

Figure 4.2 Total surface density for the 3 fibre diameter spaced and 6 fibre diameter spaced reactors: Left: Simulation result; Right: Experiment result.

Figure 4.2 shows the result matchup between our simulation and experiment. We can see from Figure 4.1, due to the CO_2 leakage at the sealed region (dark red regions especially on 10^{th}, 17^{th} and 31^{st} day of 3 fibre diameter setup), the surface density in experiment was normalized to those very dark regions. As a result, there was no surprise that in experiment plot of Figure 4.2 (right), the peak surface density was around 90% instead of 100%. So we didn't have to care about the value of 90% and set our peak for our simulation to 100% was reasonable. The decrease of surface density after 17^{th} day of the 3 fibre diameter setup in the experiment was probably due to the death of algae which we mentioned earlier that we didn't considered in our simulation. So we didn't have to fit that part of the curve.

After studying this curve, we decided to choose the result of the surface density on day 5 and day 10 to matchup with, which was shown as the green curve on the right of

Figure 4.2. On 5th day the surface density of 3 fibre diameter spaced reactor should reach about 50%-60%, and on the 10th day it should reach 90%-100%. Based on these two conditions, we ran many simulations and finally set our empirical parameters. After this fixation, we did not change any of the fundamental parameters setup for the following simulations in order to keep it reliable. We have to note that, the constants were not unique. If we changed them a little the curve would not change much and still matched the experiment result.

The first prediction form our simulation was the surface density of 6 fibre diameter gap reactor. The red curve in the left plot in Figure 4.2 was our simulation results, compared to the red curve in the right plot which came from the experiment records. There was a decrease of increasing rate from 17th day to 30th day comparing to the days before 17. Because some of the algae had already reached their peak value around day 17 and stopped growing, not all of them kept increasing exponentially. As a result the total surface density, which was the average value for all the algae in the measured plane, had a reduced increasing rate. The algae in 6 diameter gap reactors grew faster in the simulation than in the experiment results. But the trend and shape of those curves, which were the most important characteristics, were the same. So we decided to use this setup in the following simulations.

Then we imaged our surface density maps for 3 and 6 fibre diameter spaced reactors, comparing with the experiment pictures shown in Figure 4.1.

The comparison of 3 diameter gap reactors was shown in Figure 4.3. We copied our simulation image and put them together to show a whole picture for the HFM arrays.

It was reasonable because we applied periodic boundaries. Our simulation results indicated that, since the gas velocity in fibres was zero and both ends of the HFMs were open to the air, the algae grew from the two ends towards to the center, which was the same as in the experiment. Because it took lots of time for CO_2 diffusing into the middle part of the fibre, the algae in the middle of the reactor could not get enough CO_2 for growth. There were some bubbles in the experiment which could not be concerned in simulation.

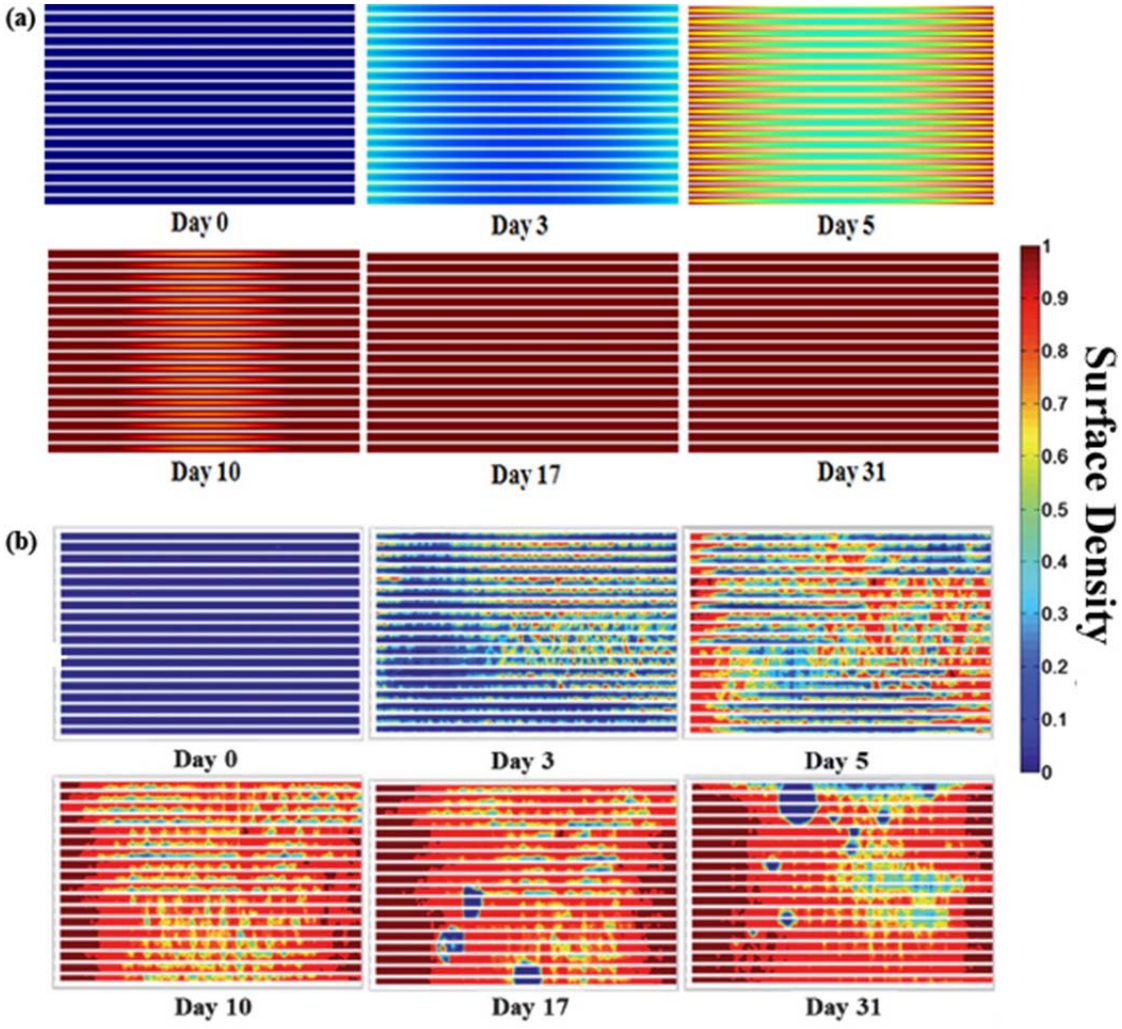

Figure 4.3 Surface density maps of algae for 3 fibre diameter spaced array over 30 days: (a) Simulation result and (b) Experiment result.

The same comparison was made with 6 fibre diameter array in Figure 4.4.

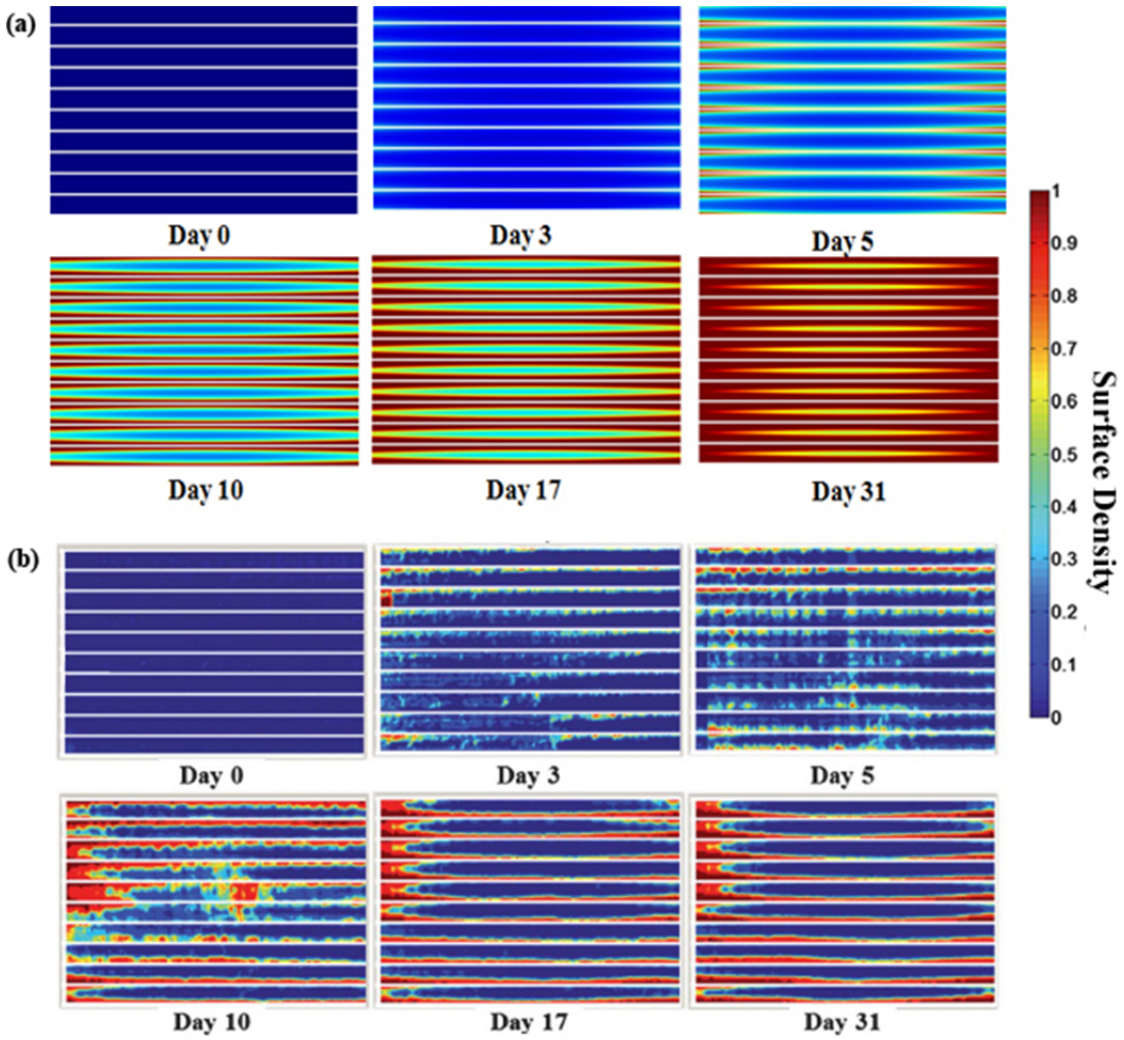

Figure 4.4 Surface density maps of algae for 6 fibre diameter spaced array over 30 days: (a) Simulation result and (b) Experiment result.

As can be seen in the experiment for 6 fibre diameter spaced array in Figure 4.4, the phenomenon that the algae near the fibre grew much faster was predicted by the simulation. We have to note here that in the experiment the algae only grew from one side of the fibre due to experiment environment errors we could not explain, maybe was gravity. And also, the 31st day image in experiment didn't match the result of a

total surface density about 60%. This was probably because it was one of the three reactors, and it was the slowest one among the others.

The same conclusion could be drawn from both simulation and experiment, that the 3 fibre diameter spaced reactor haf higher efficiency than 6 fibre diameter spaced reactor. When the space gap increased, it would be harder for CO_2 to diffuse far away from the fibre. The algae lived in the center of two fibre could not get enough CO_2, so the increased fibre distance reduced the algae growth.

4.1.2 Aeration test

Our group member only used 3 fibre diameter spaced reactor for testing the influence of gas velocity on algae growth, so did our simulation.

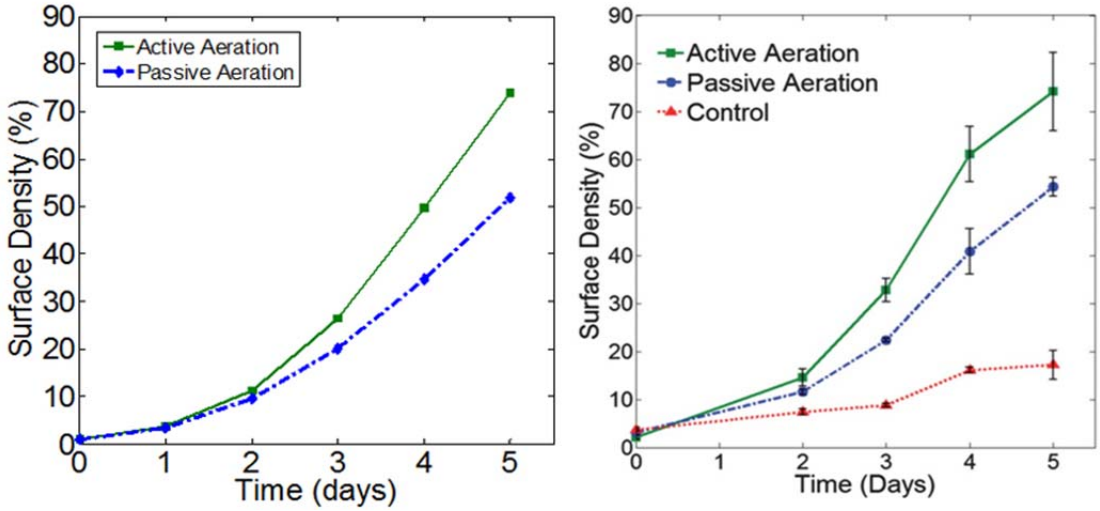

Figure 4.5 Surface density for the actively aerated (12.6m/s) and passively aerated (0 m/s): Left: Simulation result(no control group); Right: Experiment result.

The second prediction made by our simulation was the surface density plot of the algae under an active aeration in 5 days, as compared in Figure 4.5. The active

aeration was made by a flow rate of 50 mL/min air into the fibre. The same value was used in our simulation. The shape and trend of our simulation result, the green curve on the left of Figure 4.5 matched well with the surface density curve from experiment (green curve on the right), which confirmed the reliability of our simulation. Since active aeration brought more CO_2 into the reactor, the surface density under active aeration should definitely higher than the passive one.

Note that, in the experiment our group members also tested a control group (red line in right figure of Figure 4.5) without fibres in the reactor. Due to some CO_2 leakage and nutrient left in the culture the algae still grew under that condition, which our simulation was not able to predict.

4.2 Predictions

The good matchup between our simulation and the experiment records confirmed the reliability of our program. The goal of our study is to make some predictions by simulation method and help to simplify our further experiment. So now we will continue to cover the simulation result of those parameters which were not tested by experiment.

We have to note that, due to those factors we ignored and experimental errors, the simulation result will never be exactly the same as we got in the experiment. Also, it cannot predict a precise value for the parameters we tested. What we can get is the

shape and trend of the relationship we concern, and an expectation range for those parameters. These are also meaningful and reliable for our further experiments.

4.2.1 Effect of gas velocity in the fibre

The first parameter we concern a lot is the gas velocity in the fibre. If we increase the speed of gas in the fibre, we can bring CO_2 along our reactor and extract the production gas, like O_2 and ethylene, more quickly. It can improve the production of our reactor to some level, but also mean more energy consumption. On the other hand, since the high velocity cannot increase the concentration of CO_2 very much, the reaction speed may not increase very much. Consequently, the ethylene production may mainly depend on the extraction rate rather than the reaction rate when the velocity is high. It seems that there should be a balance between the velocity and algae growth and that is what we want to find out. By choosing the velocity range from 0.01m/s to 10m/s, we ran our simulation for both 3 and 6 fibre diameter spaced reactors. We chose the CO_2 source to be air.

To calculate the ethylene production, we first multiplied the gas velocity and the area of the fibre end to get the gas volume we could get per second, then timed the concentration of ethylene at the end of the fibres. The production was calculated for one fibre. We only tested the value until the 5^{th} day from the beginning, since it was enough to see the trend of the curve and it could save much time for the computing. The unit of production we used was mol/sec. It was simple for our calculation, but

might not be a very convenient number for industry application. Since we focused on the effect and compact of those experiment parameters, the most valuable result was the trend and variation of the product, not the value or number. So we decided to keep using mol/sec in the records.

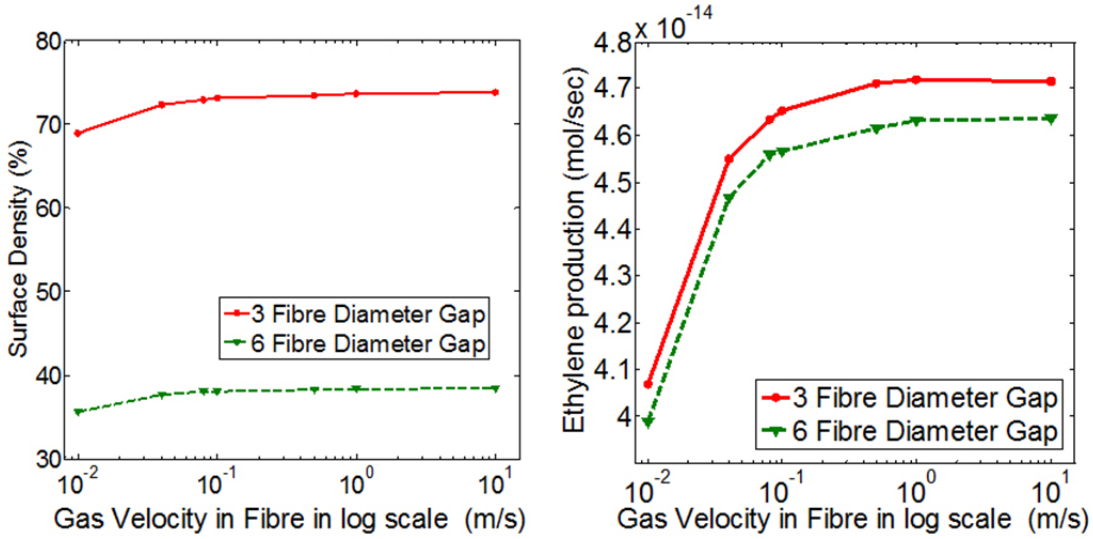

Figure 4.6 Simulation results for both 3 and 6 fibre diameter spaced reactors with the gas velocity in fibre increasing. Left: Surface density of algae vs velocity; Right: Ethylene production vs velocity. Velocity is shown in log scale.

As can be seen in Figure 4.6, we found the balance point for our reactor. For both fibre distance setups, the algae growth reached its maximum at a speed of 0.1 m/s, while the ethylene production peaked after 0.5 m/s. This difference was a result of the balance between the speed of reaction and speed of production extraction as discussed at the beginning of Section 4.2.1.

The amount difference of the algae growth and the ethylene production between two fibre distance setups were quite different. Although as shown in the left plot of Figure 4.6, the algae in 3 fibre gap reactors had the amount nearly twice of those in 6

fibre gap reactors, the ethylene production didn't differ much. This was because in 6 fibre gap reactors, the area of algae growth was twice of that in 3 fibre gap setups. As a result the total amount of algae in these two setups was nearly the same and there was not a huge gap between their ethylene productions.

We have to note that, this result depends on the geometric parameters of the reactor. We may have a different value if we have a longer fibre or another fibre distance set, but definitely we will have a curve with the same shape and trend. And the value of the balance point, around 0.5 m/s, should be reliable for a similar size reactor.

4.2.2 Effect of concentration of CO_2

The concentration of CO_2 is the main factor that determines the reaction rate. So it is an important parameter in our system. Values were still calculated on the 5th day.

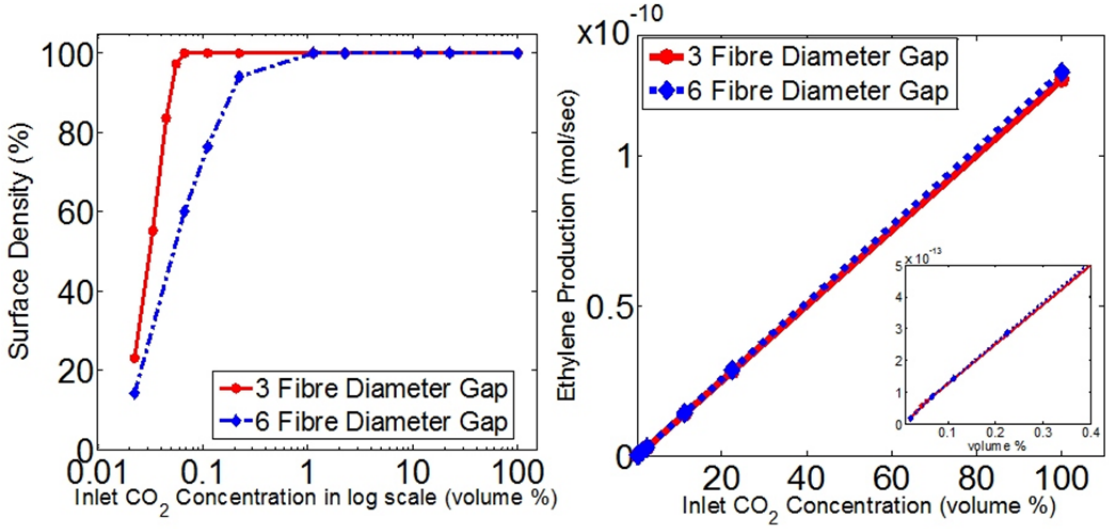

Figure 4.7 Simulation results for both 3 and 6 fibre diameter spaced reactors with the inlet CO_2 concentration increasing. Left: Surface density of algae vs CO_2; Right: Ethylene production vs CO_2.

From Figure 4.7 we could get the effect of changing concentration of CO_2. The algae could grow faster when increasing the carbon dioxide. For 3 fibre diameter spaced reactor, 0.07% CO_2 (volume percentage) was enough for the algae filling the space in 5 days. And for 6 fibre diameter spaced reactor, 1.12% (volume percentage) CO_2 could ensure the filling in 5 days. This difference was due to the diffusion of CO_2 in the algae sink. Things went slightly different for the ethylene production compared with Figure 4.6. When CO_2 concentration increased, the 6 fibre diameter gap reactor had more production than the 3 fibre diameter gap. Since in both setups the algae reached their maximum, the total amount of algae in 6-diameter reactor was more than that in 3-diameter setup and they could produce more ethylene. At low concentration, our experiment confirmed that the algae can consume and fix all the CO_2. But for higher concentration, we don't know whether *S. elongates* can deal with that much CO_2. So the result here needs further proof by experiment.

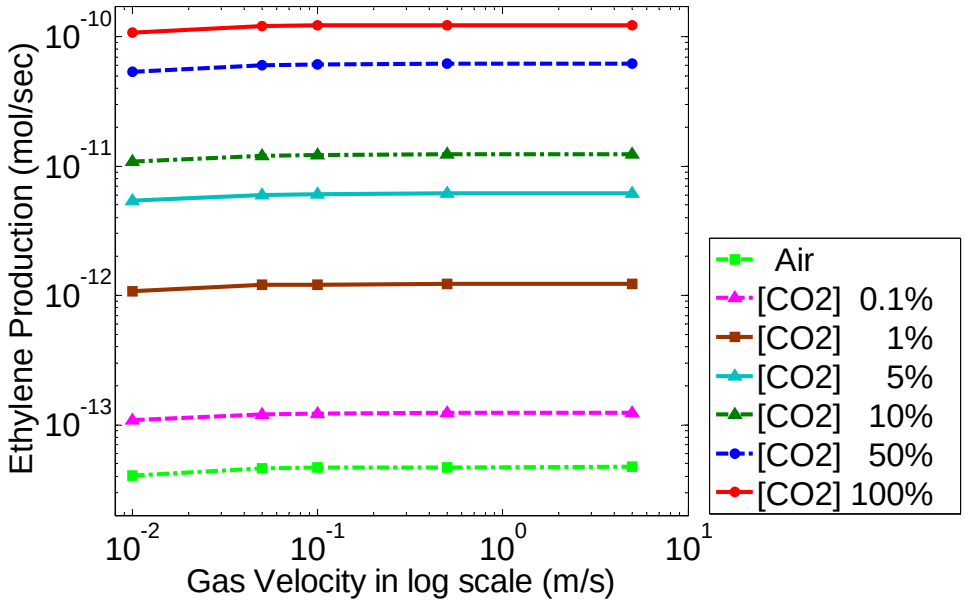

Figure 4.8 Relationship between production, gas velocity and CO_2 concentration.

For a better view of the effect of CO_2 concentration and gas velocity, we showed here in Figure 4.8 by integrating these two parameters in the same plot. Only 3 diameter gap setup was simulated, and the values were all calculated on the 5^{th} day. The concentration of CO_2 in the picture was measured in volume percentage. We varied the concentration from air, i.e. 0.02%, to 100%. For different concentrations of CO_2, the shape of the relationship between gas velocity and production looked the same. They shared the same relationship with increasing gas velocity and all reached their max value around 0.5 m/s.

CHAPTER 5

CONCLUSIONS AND FUTURE WORK

In this work, we have confirmed the value of numerical simulations for photobioreactor. The shape and trend of the curve of algae growth predicted by Monod equation can match the experiment very well, which can simplify the experiments and save much time on selecting those environmental parameters.

Meanwhile, proved by experiment results, our simulation is able to describe the reactor we designed, which ensures that its prediction is reliable and useful. We have shown that, both the algae growth and ethylene production may reach their maximum level when the gas velocity in fibre increases to a certain value. For a fibre about 6 cm long, the velocity for highest efficiency would be around 0.1 ~ 0.5 m/s. The effect of increasing inlet CO_2 concentration may keep improving the ethylene production to some level, and for algae growth, 0.07% (volume percentage) would be enough for a 3 fibre diameter spaced reactor and 1.12% (volume percentage) for a 6 fibre diameter spaced reactor. Again, we have to note that these values cannot be exactly accurate for experiments, but they are able to guide our choice during the further experiments.

Future work is necessary to integrate other parameters into the simulation, such as heat transfer and light intensity, for getting more comprehensive knowledge of this system and better predictions.

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