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OPTIMAL CONTROL OF ALGAE BIOFILM GROWTH IN WASTEWATER TREATMENT USING COMPUTATIONAL MATHEMATICAL MODELS

by

Gerald Benjamin Jones

**Capstone submitted in partial fulfillment of
the requirements for graduation with**

University Honors

with a major in
Mathematics

in the Department of Mathematics & Statistics

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Abstract

Microalgal biofilms are comprised of a syntrophic consortium of microalgae and other microorganisms embedded within an extracellular matrix. Despite significant processes in the application of microalgal biofilms in wastewater treatment, mechanistic understanding and optimization of microalgal biomass yield and productivity under environmental constraints is still lacking. This paper identifies theoretical insights on this challenging biological problem by leveraging novel mathematical and computational tools. In particular, through a computational mathematical model to advance the understanding of microalgal biofilm growth kinetics under environmental constraints through a systematic parameter study. Moreover, design of algae biofilm reactors for optimal biomass yield and productivity in wastewater treatment under different environments is explored. The proposed model could be further calibrated to generate reliable predictions that can improve the design, operation, and management of microalgal biofilms in wastewater treatment.

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Optimal Control of Algae Biofilm Growth in Wastewater Treatment using Computational Mathematical Models

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1 Introduction

Microalgae have attracted considerable interest worldwide due to their renewable and sustainable properties; they are economical and environmental-friendly sources for biofuels and bioactive products. The past decade has witnessed new applications of microalgae in renewable energy, biopharmaceutical, and nutraceutical industries. Among the applications of microalgae, scientists have been using microalgae in wastewater treatment due to the capability of consuming greenhouse gases, such as carbon dioxide CO_2 , from the atmosphere and converting pollutants (such as nitrogen and phosphorus) into biomass. The biomass can be used as feedstock for engineered processes producing useful products such as bioplastics, biocrude, and other bioactive metabolites. Thus, microalgae can contribute to novel solutions to some of the significant challenges for the 21st century. A schematic illustration of the microalgae cultivation system in wastewater treatment is shown in Figure 1. However, the productivity of suspended microalgal growth cultivation systems is usually limited.

One solution to increase productivity is to use biofilm-based algae cultivation on attached substrates [4, 11]. This approach has drawn attention as a way to optimize algae yield in wastewater treatment systems [15, 10, 5, 7]. Microalgae-based biofilms are composed of eukaryotic and prokaryotic photoautotrophic microorganisms and heterotrophic bacteria entrapped in a gel-like

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matrix known as extracellular polymeric substances (EPS) that are cultivated on a solid support (substratum) in aquatic environments. Algae-biofilm cultivation systems for wastewater treatment have several potential advantages including their variable chemical compositions dependent on their cultivation medium, biomass biodiversity, high tolerance of extreme environmental conditions (temperature, salinity, and water quality), ability to remove pollutants such as nitrogen and phosphorus from liquid waste streams and CO_2 from the atmosphere. Algae biofilms offer the benefits of phytoremediation, with a harvesting mechanism that eliminates energy-intensive solid-liquid separation processes including centrifugation, filtration, and sedimentation. Despite the significant progress and promising applications of the algae-biofilm cultivation systems in wastewater treatment, the algae biofilm technology platform presents several challenges that need to be addressed adequately for both pilot-scale and full-scale implementation. In particular, algae-biofilm productivity optimization under various environmental and operational parameters (including the selection of proper microalgal strain(s); nutrient uptake; light quality; temperature; pH ; CO_2 ; attaching substrate/material; flow velocity; the presence of other microorganisms) remains a crucial challenge. The lack of insights on these parameters becomes a bottleneck to predicting the performance of the technology and to scale-up of the technology from laboratory scale to pilot to full-scale.

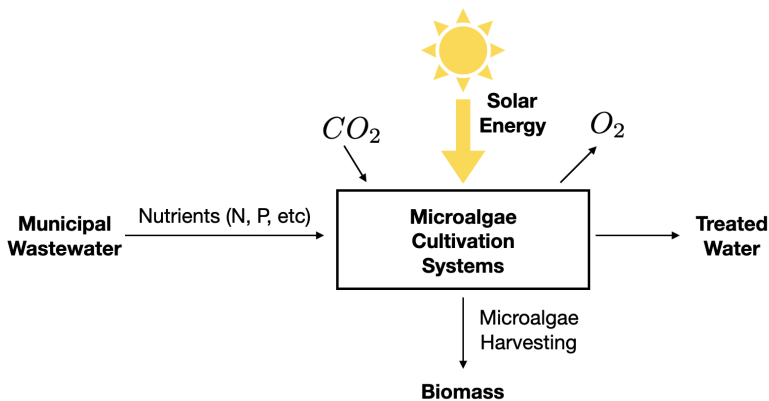


Figure 1: A schematic illustration of microalgae cultivation systems for wastewater treatment. There are rich nutrients such as nitrogen and phosphorus in the wastewater. The microalgae cultivation system will remove the nutrients and convert them, along with the solar energy, into biomass such as biofuels and bio-products.

Due to the complexity of the algae biofilm cultivation system and the confounded nature of environmental factors on biomass productivity, predictive mathematical models will be desirable to provide insights. Unfortunately, this is nontrivial, as many factors shall be considered appropriately [6]. Light and temperature are the major factors for algae biofilm growth. The algal biofilm will not effectively produce when light is limited and will be inhibited when the light is too strong [13, 22]. Therefore, understanding algal biofilm under various light access conditions is one major issue in mathematical modeling. Among the many inspiring mathematical models in understanding photosynthesis for microalgae [14, 13, 22, 23] that have been broadly used to investigate the photosynthesis dynamics in algae biofilms, Bechet et al. provide a comprehensive review of existing mathematical models to assess biomass productivity affected by light and temperature in [2]. In particular, they categorize the existing mathematical models for photosynthesis in well-mixed dense cultures into three types with a list of relevant models summarized in the tables in [2]. Also, most

of these existing models focus on mass action principles, and the spatial resolutions are ignored for simplicity. In reality, the sunlight fails to penetrate deep into the algae biofilm as the light energy will be absorbed by the algal cultures. Thus, the thickness of algae biofilms needs to be considered in the mathematical models. Some other factors that are also important include the hydrodynamic stress [9, 8], nutrient supply and mass transport through the biofilms [20, 18], and the substrate properties [12]. To date, there is limited theoretical work on modeling algal biofilms in wastewater treatment. Some seminal work is described in [1, 2, 3, 17]. So far, no quantitative model exists to predict biofilm productivity that agrees with experimental data at laboratory and pilot scales.

In this paper, we propose a computational mathematical model to discover the underlying mechanics of algae biofilm growth in wastewater treatment. The photosynthesis process of algae biofilm development and the impact of light inhibition have been considered in the model formulation. In addition, to accurately model the light effect, the biofilm thickness is also embedded in the model. With the newly proposed model, we conduct a systematic study on various environmental factors on algae biofilm growth and identify optimal control strategies to improve biomass productivity. This model will serve as guidance for designing an algal biofilm cultivation system with adjustable rotation speed or exposure rates to optimize biomass productivity. The objectives of the research reported here include (1) description of the mathematical model developed to predict algae-based biofilm productivity; (2) demonstration of the influence of light intensity, peripheral velocity, and light exposure time (fraction) on productivity; and (3) determination of the effect of harvesting frequency on productivity and on efficiency.

The rest of this paper is organized as follows. In Section 2, we introduce the rotating algae biofilm reactor and derive the computational mathematical model. Afterward, we introduce the numerical setups, numerical schemes, and provide a thorough numerical study on algal biofilm growth under various environmental factors with the proposed model. In the end, we draw a brief conclusion and discuss some future work.

2 Computational Mathematical Model Formulation

2.1 Rotating algae biofilm reactor (RABR)

This paper is focused on a particular biofilm-based algae cultivation system: the rotating algae biofilm reactor (RABR) [4, 5, 16]. The RABR removes nutrients from wastewater by producing algae biomass that transfers nutrients from a liquid phase (wastewater) to a solid phase (biomass) that can be used in bioproduct production. The RABR consists of rope coiled around a cylinder rotating through a growth substrate, i.e., wastewater, to produce an attached algal biofilm on the rope surface and remove nutrients from the wastewater. The produced algal biofilms can be mechanically harvested and transformed into value-added bioproducts, such as biofuels, animal feed, bioplastics, and fertilizers. There is extensive experimental research in the literature on the RABR at laboratory and pilot scales. However, there are limited theoretical results concerning how to integrate the environmental and management control factors into a framework for understanding and for predicting biomass yield and productivity. In preparation for scaling up and industrial applications of the RABR technology, a theoretical/mathematical model describing the system must be developed. Due to high nitrogen and phosphorus concentrations in the growth substrate from the anaerobic digestion process at the Central Valley Water Reclamation Facility (CVWRF) in Northern Utah and high summertime light intensity, the algal biofilm system is often light inhibited. In this paper, we propose a computational model inspired by [1] that describes light-limited algae growth. The process discussed below also shows promise for mitigating harmful algal

blooms through encouraging and controlling algae production in a water reclamation facility before discharge of the wastewater to a receiving environment such as a lake or reservoir. Compared to standard raceway ponds that cultivate algae in suspension, the RABR increases productivity up to 300% [4]. Further, the RABR has a lower economic cost with a relatively inexpensive harvest procedure and small electricity demand.

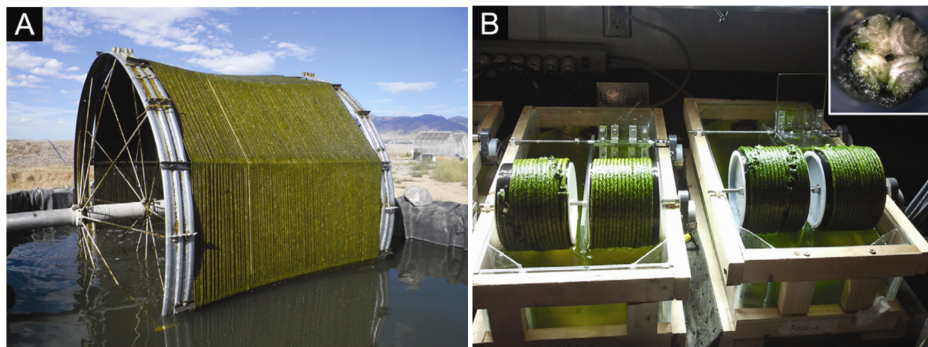


Figure 2: Rotating algal biofilm Reactors (RABR) developed in the Sustainable Waste to Bioproducts Engineering Center (SWBEC) laboratory, represents a novel microalgal biofilm cultivation system for wastewater treatment. RABR removes nutrients from wastewater by cultivating an algal biofilm on the rope-substratum surface that is rotated to alternately expose the growth surface to the wastewater to acquire nutrients and then to the air/sunlight for microalgae uptake of nutrients with biomass production. The harvested biomass can be utilized for renewable diesel, soil fertilizer, and high-value bioproducts. (A) Pilot-scale; (B) Lab-scale.

Over the last decade, many iterations of the RABR have been created and tested. Original versions of the RABR consisted of growing a biofilm on rope wrapped around a cylinder-shaped structure, including a barrel (see Figure 2). One version of the RABR was used to study biofilm formation on a flat surface that formed the sides of slowly rotating disks [19]. Compared to its barrel counterparts, the disk RABR may increase the ratio of the surface area of the biofilm to the volume of the tank and use less electrical power [6]. However, unlike the disk RABR, the barrel RABR has an automated harvesting procedure to separate biofilm algae from the wastewater that provides an energy-efficient mechanism to lower the total system energy cost.

2.2 Computational model formulation

In this section, we propose a computational model for the RABR system. A schematic is shown in Figure 3. In this computational model, the rope on the RABR is partially immersed in the water and partially exposed to the natural sunlight. The algal biofilm on the rope will go through photosynthesis and convert the solar energy and nutrients into biomass. If solar energy is too strong, photosynthesis will be inhibited. In this simple case, the nutrient in the wastewater is assumed sufficient, so the mass transfer and nutrient removal dynamics are not considered. Only biomass growth is investigated.

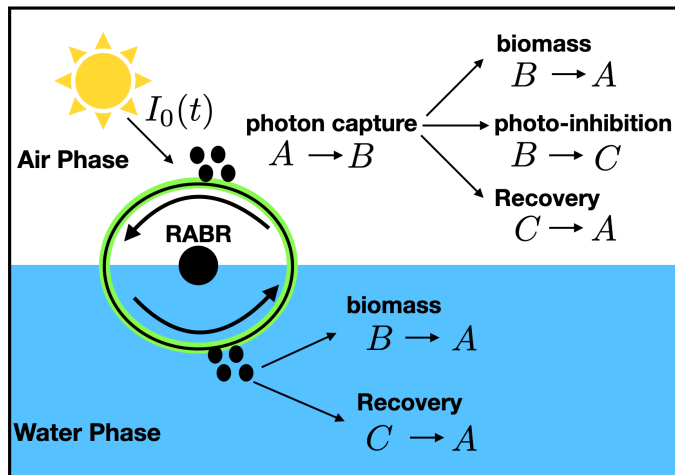


Figure 3: A schematic illustration of the proposed computational model for the rotating algal biofilm Reactors (RABR). The rope on the RABR is rotating in and out of water and the photon will be captured and converted into biomass.

2.2.1 Photosynthetic process

There are two widely used systems in the literature to model the reactive kinetics of the photosynthetic process. A schematic illustration of these two systems is shown in Figure 4. Mainly, it is assumed that there are three physiological states for the photosynthetic process: the open (or reactive) state, the closed (or activated) state, and the inhibited state. Their volume fractions are denoted by A , B , and C , respectively. Specifically, the open state is ready to observe photons, and the closed state is processing solar energy into chemical energy. The inhibited state is dormant due to intense solar radiation. However, there is a significant difference between the two reactive kinetics. In Figure 4(a), it is assumed the inhibited state will recover to an open state, while the inhibited state will recover to an activated state in Figure 4(b).

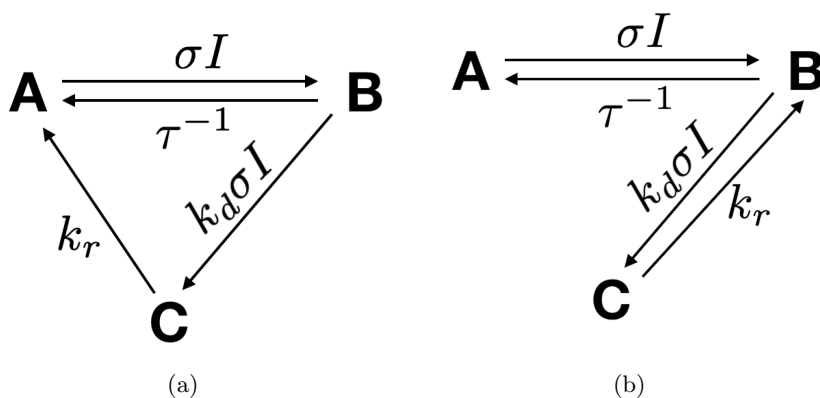


Figure 4: Reactive kinetics for the photosystem during photosynthesis and photoinhibition processes. (a) the reactive kinetics from [22]; (b) the reactive kinetics from [13]. Here k_r is the repair rate, k_d is the damage rate, I is the light intensity, τ is the turnover time of the electron transport chain, σ is the effective absorption cross-section per unit of photosynthetic units.

In this paper, we adapt the case in Figure 4(a) from [22]. Therefore, through the mass action principle, the reactive kinetics for the three photosynthetic states are given as

$$\begin{aligned}\frac{dA}{dt} &= -\sigma IA + \frac{B}{\tau} + k_r C, \\ \frac{dB}{dt} &= \sigma IA - \frac{B}{\tau} - k_d \sigma IB, \\ \frac{dC}{dt} &= -k_r C + k_d \sigma IB.\end{aligned}\tag{1}$$

Using the compatible condition $A + B + C = 1$, we can simplify the reactive kinetics in (1) as

$$\begin{aligned}\frac{dB}{dt} &= \sigma I - \sigma IC - \left(\sigma I + k_d \sigma I + \frac{1}{\tau}\right)B, \\ \frac{dC}{dt} &= -k_r C + k_d \sigma IB.\end{aligned}\tag{2}$$

We remark that the authors in [1] introduce a seminal work on modeling the light effects on rotating algal biofilms, where they have embraced the reactive kinetics in Figure 4(b) and introduced the biofilm thickness. In addition, they assumed the dynamics of A is in a faster time scale and reaches steady state i.e. $\frac{dA}{dt} = 0$ in their case. However, in our case, as shown in (1), the equation for A has a $k_r C$ term. We cannot assume that A reaches rapidly to its steady state.

2.2.2 Biofilm thickness

Furthermore, if the biofilm thickness is taken into account, $A(z, t), B(z, t), C(z, t)$ would be a function of z and t , where $z \in [0, h(t)]$ with $h(t) > 0$ the biofilm thickness. Let $X(t)$ denotes the areal biomass concentration with unit g/m^2 . The area biofilm growth could be proposed as

$$\frac{dX}{dt} = \left[\frac{1}{h} \int_0^h \mu(z, t) dz \right] X(t),\tag{3}$$

with $\mu(z, t)$ the net growth rate, proposed as

$$\mu(z, t) = k \frac{B(z, t)}{\tau} - R(t),\tag{4}$$

based on the reactive kinetics in (1) with $R(t)$ the death rate and k a constant to scale the growth rate. Here we assume $R(t) = R$ a constant for simplicity. We remark that the net growth rate in (4) differs from the one in [1]. In their case, the growth rate is defined as $\mu = k\sigma IA - R$, where the first term for μ is based on the fact $\sigma IA = \frac{B}{\tau}$ when A reaches steady state. In our case, $\sigma IA = \frac{B}{\tau}$ is not valid any more.

In addition, if we assume the biofilm is isotropic, i.e it has a constant density ρ among all different depths and areas, $X(t)$ could be represented as

$$X(t) = \rho h(t),$$

with $h(t)$ the height of the biofilm. Substituting it into (3), we obtain

$$\frac{dh(t)}{dt} = \int_0^h k \frac{B(z, t)}{\tau} dz - Rh(t).\tag{5}$$

2.2.3 Governing equations

Overall, we extend the reduced reactive kinetics in (2) with spatial (biofilm-height) dependence and combine them with the biofilm height evolution in (5). Then, the governing model for the algal biofilm growth on the rotating algal biofilm reactors (RABR) reads as

$$\begin{cases} \frac{\partial B(z,t)}{\partial t} = \sigma I(z,t) - \sigma I(z,t)C(z,t) - \left(\sigma I(z,t) + k_d \sigma I(z,t) + \frac{1}{\tau} \right) B(z,t), & z \in [0, h], \\ \frac{\partial C(z,t)}{\partial t} = -k_r C(z,t) + k_d \sigma I(z,t) B(z,t), & z \in [0, h], \\ \frac{dh(t)}{dt} = \int_0^h k \frac{B(z,t)}{\tau} dz - Rh(t). \end{cases} \quad (6)$$

This is a differential-integral equation with free surface. Notice there is a big difference between the proposed model (6) with the model in [1]. In particular, A is not assumed to reach the steady state in (6), which might lead to different numerical results.

For a close comparison, we also derive the model when A reaches steady state in (6), which are given as

$$A = \frac{1-C}{1+\tau\sigma I} + \frac{k_r\tau C}{\underline{1+\tau\sigma I}}, \quad B = \frac{\sigma I\tau(1-C)}{1+\tau\sigma I} - \frac{k_r\tau C}{\underline{1+\tau\sigma I}}. \quad (7)$$

For such case, the net growth rate $\mu(z,t)$ can be calculated as

$$\mu = k \frac{B}{\tau} - R = (1-C) \frac{k\sigma I}{1+\tau\sigma I} - \frac{kk_r}{\underline{1+\tau\sigma I}} C - R. \quad (8)$$

Then, the governing model with the biomass thickness reads as

$$\begin{cases} \frac{dh(t)}{dt} = \int_0^h \left[(1-C(z,t)) \frac{k\sigma I(z,t)}{1+\tau\sigma I(z,t)} - \frac{kk_r}{\underline{1+\tau\sigma I(z,t)}} C(z,t) \right] dz - Rh(t), \\ \frac{\partial C(z,t)}{\partial t} = -\left(\beta(z,t) + \underline{\eta(z,t)} + k_r \right) C(z,t) + \beta(z,t), \\ \beta(z,t) = k_d\tau \frac{(\sigma I(z,t))^2}{\tau\sigma I(z,t) + 1}, \quad \underline{\eta(z,t)} = k_d\tau \frac{k_r I(z,t)}{\tau\sigma I(z,t) + 1}, \quad 0 < z < h. \end{cases} \quad (9)$$

Here the differences between the model in (9) and the model in [1] are marked with underlines. In particular, from equation (7), we observe the steady states for both A and B are altered with an extra factor (as marked with underlines), and the growth rate is affected with an extra decay term as shown in (8).

2.2.4 Light intensity

To complete the model, we need to identify the light distribution $I(z,t)$. The light distribution through biofilm could be modeled using the Beer-Lambert law [1]

$$I(z,t) = I(t)e^{-b(h-z)}, \quad z \in [0, h], \quad (10)$$

where $I(t)$ is the surface light intensity at time t .

As the RABR rotates, part of the rope will be exposed to the sunlight, and the rest will be immersed under the water. Then, we introduce the light exposure factor $\eta = \frac{l_*}{L}$ with L the total rope length and l_* the exposed rope length. We denote the peripheral velocity of the RABR as v ,

and the period of the RABR as T . Then the peripheral velocity v , length L , and period T have the relation:

$$T = \frac{L}{v}. \quad (11)$$

In this paper, we fix the rope length L and set the peripheral velocity v and light exposure factor η as free variables. The actual light intensity can be modeled by a square wave defined as

$$I(t) = I_0(t) \frac{1 + \text{sign}(\frac{T}{N} - \text{mod}(t, T))}{2}, \quad (12)$$

with $I_0(t)$ the maximum light intensity.

There are several approaches to approximate $I_0(t)$. For our model, we utilize existing light intensity data on April 25th, 2018 from the Sustainable Waste-to-Bioproducts Engineering Center (SWBEC). The light intensity is measured as photosynthetically active radiation (PAR) every 15 minutes for 24 hours. We then fit the PAR data with a smooth function $I_0(t)$ as shown in Figure 5 for a range of one day. Moreover, we assume each day has the same light pattern when we simulate for a longer time period.

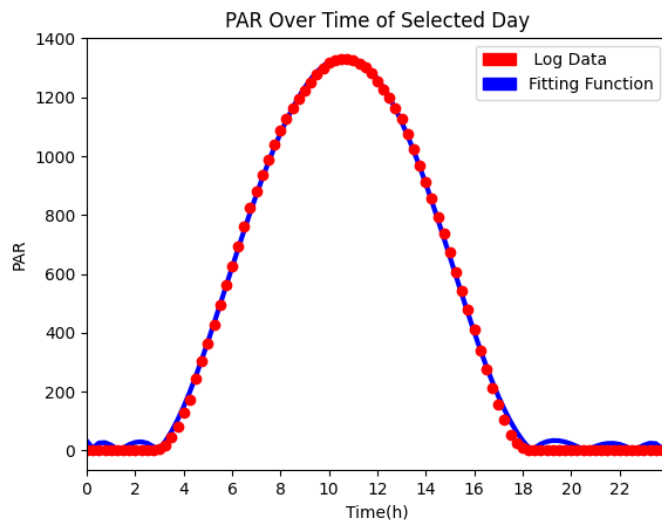


Figure 5: Light intensity over time. This figure shows the PAR data over a 24 hour period as red dots. The data is fitted with a continuous function shown as a blue line. The continuous function will be used for later simulations.

2.2.5 Biomass productivity optimization

Harvesting strategy. The algal biofilm grows rapidly when it is thin, and the growth either stops or significantly slows down once a certain thickness is reached. For instance, as biofilm thickness increases, biomass becomes “self-shading” and sunlight cannot penetrate the entire biofilm depth with the result that photosynthesis will be limited and nutrient uptake decreases. In a process known as sloughing, the algal biofilm will spontaneously detach from the rope substratum as the attachment surface becomes anaerobic due to heterotrophic respiration minus photoautotrophic activity. Eventually, the algal biofilm growth becomes equal to or less than the losses experienced through respiration, cell death, parasitism, and disease to reduce algal biofilm activity.

Therefore, after the biofilm height reaches a particular value, harvesting must occur to provide conditions for new growth. To maximize productivity, one must optimize the time points of harvest with respect to the current height of the biofilm. There are a few considerations: (a) at what value of biofilm thickness is a harvest appropriate? (b) when a harvest is appropriate and occurs, how much biofilm should remain on the substrate? and (c) what biomass growth rate is best to harvest? We intend to answer these questions by conducting various numerical experiments with our proposed computational models.

RABR rotating speed. Sunlight availability is crucial for microalgal biofilm photosynthesis. Nevertheless, in reality, sunlight is quite variable from season to season, day to day, and even minute to minute. At high PAR values, if the reactor is rotating too slowly, photo-inhibition may result and lower the biomass yield; at low PAR values, if the reactor is rotating too rapidly, there may be insufficient light penetration into the inner biomass for photosynthesis. Additionally, the periodic immersion in wastewater and air exposure is critical for gas exchanges (uptaking CO_2 and releasing O_2) to maintain proper microalgal biofilm development. Hence, identifying the optimal reactor rotating speed with respect to other environmental factors, in particular light intensity, is crucial for better biomass productivity.

Optimal control. With the model in (6), we are able to evaluate the biomass growth and manipulate controlling factors to optimize biofilm productivity. Here, we evaluate the averaged biomass productivity in the unit $gm^{-2}d^{-1}$, i.e. gram per square meters per day, during a period $t \in [t_0, t_1]$ by

$$P = \frac{1}{t_1 - t_0} \rho(h(t_1) - h(t_0)), \quad (13)$$

and the total productivity of the RABR is LS_0P , where S_0 is the rope surface area per unit length and L is the total length of the rope, such that LS_0 represents the total surface of the rope for algal biofilm growth. Here t_0 and t_1 are the starting and ending time of algal biofilm growth so that $h(t_1) - h(t_0)$ is the accumulated height difference of the biomass during the time period $t_1 - t_0$. One major goal in this paper is to solve the optimal control problem

$$\arg \max_{v, \eta} P(v, \eta; I_0(t)). \quad (14)$$

3 Numerical Results and Discussion

3.1 Numerical setups

Model parameters. In this sub-section, all of the model parameters are summarized. First we list the fixed variables in Table 1. The parameter values are chosen based on existing literature [1, 14, 3, 13].

Table 1: Parameter table with fixed parameter values.

Symbol	Value	Units	Description
σ	0.0019	$m^2/\mu mol$	effective absorption cross-section per unit of photosynthetic units
τ	6.849	s	turnover time of the electron transport chain
k_d	2.99×10^{-4}	s^{-1}	damage rate
k_r	4.8×10^{-4}	s^{-1}	repair rate
k	3.6467×10^{-4}	-	constant (link between photosystem dynamics and growth rate)
R	0.12	d^{-1}	respiration rate
b	1400	m^{-1}	light attenuation factor
ρ	140000	gm^{-3}	dry biomass density
p	6	-	number of simulated layers of biofilm
S_0	1/7	m^2	surface area of a 1-meter-length rope
L	7	m	total RABR rope length
h_0	1.1×10^{-4}	m	initial height of biofilm
C_0	0.2	-	initial proportion of biofilm in the photosynthesis process state of inhibited.

The parameters with undetermined values are summarized in Table 2. Their values will be specified in the corresponding numerical examples.

Table 2: Parameter table with undetermined parameter values.

Symbol	Units	Description
T	s^{-1}	period of the RABR
v	m/s	substrate (rope) line speed, with formula $v = \frac{L}{T}$
$I(t)$	$\mu mol/(m^2s)$	light intensity, as a function of time
η	-	light exposure percentage, rope length (exposed to sunlight) over total rope length
$h_{harvest}$	m	height of biofilm to remain after each harvest
$t_{harvest}$	s	time lags between consecutive biofilm harvests

Numerical schemes. The proposed model (6) is a free surface problem, with a coupled system of integral differential equations. In order to solve it numerically, we discretize the spatial domain $[0, h]$ into $p \in \mathbb{N}$ equally distanced intervals: $0 < z_1(t) < z_2(t) < \dots < z_p(t) < h(t)$, such that

$z_i(t) = \frac{i-\frac{1}{2}}{p}h(t)$. If we approximate the dynamics with p layers, we obtain the following discrete system of equations to represent the dynamics in each layer:

$$\begin{cases} \frac{d}{dt}B_i = \sigma\hat{I}_i(t) - \sigma\hat{I}_i(t)C_i(t) - \left(\frac{\sigma\hat{I}_i(t)\tau + k_d\sigma\hat{I}_i(t)\tau + 1}{\tau}\right)B_i(t), & i = 1, 2, \dots, p, \\ \frac{d}{dt}C_i = -k_rC_i(t) + k_d\sigma\hat{I}_i(t)B_i(t), & i = 1, 2, \dots, p, \\ \frac{d}{dt}h(t) = \sum_{i=1}^p \frac{k}{\tau}B_i(t)\frac{h(t)}{p} - Rh(t), \end{cases} \quad (15)$$

where $B_i(t)$ and $C_i(t)$ represent the value at $z = z_i(t)$, and the light intensity is approximated by

$$\hat{I}_i(t) = \frac{p}{h} \int_{z_i}^{z_{i+1}} I(z, t) e^{-b(h(t)-z)} dz, \quad i = 1, 2, \dots, p.$$

Then, the semi-discrete system in (15) is an ODE system. We introduce the notation

$$\Phi(t) = [B_1(t) \ B_2(t) \ \dots \ B_p(t) \ C_1(t) \ C_2(t) \ \dots \ C_p(t) \ h(t)]^T,$$

and denote the ODE system in (15) as

$$\begin{cases} \frac{d}{dt}\Phi(t) = F(\Phi(t)), \\ \Phi(0) = \Phi_0. \end{cases} \quad (16)$$

The ODE system is then solved by the built-in numerical time-integration solver in Python.

We remark that we use the assumption that $C_0 = 0.2$ for all of our numerical simulations in this paper. Also, in the rest of this paper, we initialize our values of A, B, and C by

$$B = \frac{\tau\sigma I(1-C)}{1+\tau\sigma I}, \quad A = \frac{1-C}{1+\tau\sigma I},$$

for our numerical calculations. This is compatible with the steady-state solution for the model in [1]. Another initial condition could be equation (7).

With the harvesting procedure described previously, there is one assumption we made worth considering. As the light intensity of a layer depends on how many layers are above it, once we remove the top layers of biofilm, the light intensity immediately changes for the biofilm, including A, B, and C values. In order to address this change, we reinitialize the A, B, and C values of the biofilm by (1) collecting the A, B, and C value of all layers of biofilm before harvest, (2) assigning the new top and bottom layers to have the same A, B, and C values as the old top and bottom layers, and then (3) interpolating what the A, B, and C values are for the intermediary layers.

3.2 Model comparisons

First of all, we conduct several numerical tests to compare the models. Here we name the model from [1] as Model I, the model in equation (9) as Model II (i.e., the proposed model with the assumption of A in steady-state), and the proposed model in equation (6) as model III. Systematic comparisons among the three models are summarized in Figure 6.

In figure 6(a), we observe a specific range of light intensity for better biomass productivity. The profile in Figure 6(a) seems appropriate. The three models also seem to have good agreement

in Figure 6. However, these three models demonstrate quite different results for the optimal rope exposure, as shown in Figure 6(b). Our proposed model suggests an optimal percentage of rope exposure for biofilm productivity for the given conditions. In contrast, Model I/II indicates that all the rope shall be exposed to sunlight, which is not the case in reality.

Furthermore, we comment that Figure 6(b) is a different setup with the numerical example in [1], where the authors have assumed the exposed rope length is fixed, and the total rope length changes with respect to the percentage of exposure. We argue that the case in [1] is problematic as with T fixed, longer rope means faster rotation such that the energy cost cannot be ignored.

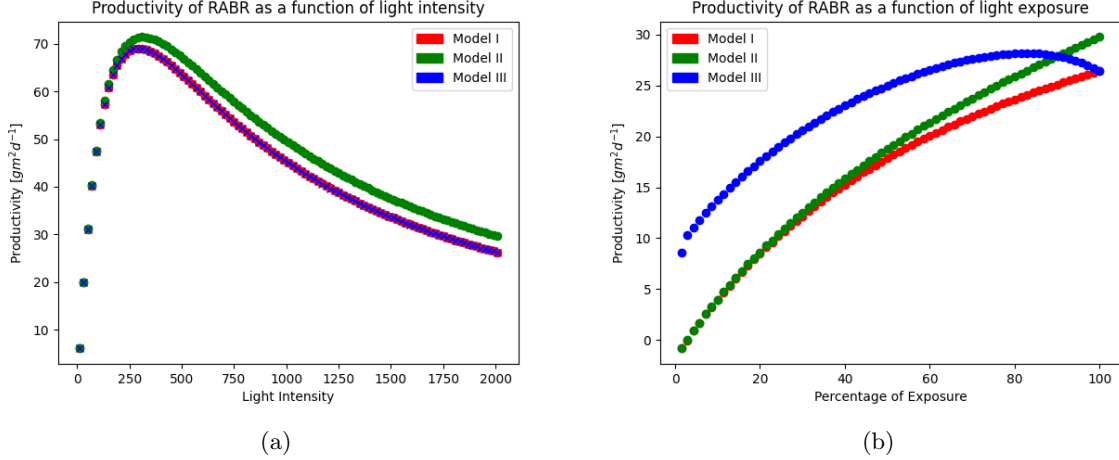


Figure 6: Algal biofilm productivity comparisons between different models. (a) algal biofilm productivity under various light intensity; (b) algal biofilm productivity at various percentages of rope exposure to sunlight. In this example, we have a fixed RABR rotation period of $T = 45\text{s}$ for both (a) and (b), with $\eta = 1$ in (a) and $I_0(t) = 2000\mu\text{mol}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ in (b).

From the previous comparisons, note that our proposed model in equation (6) provides realistic predictions. In the remainder of this paper, we provide a systematic investigation of the major controlling factors for improving algal-biofilm biomass yield.

3.3 Optimal control for biomass productivity

First of all, we take an in-depth look at three controlling factors affecting productivity: light intensity, RABR peripheral velocity, and exposure percentage of the RABR to sunlight. Given the complexity of this problem, it is not practical to simultaneously visualize the phase diagram for multiple variables. Thus, we provide three visualization sequences by fixing one of the three parameters while changing the other two in their physical ranges. In the remainder of this subsection, we fix the rope length $L = 7\text{ m}$ and use constant light for eight-hour-span simulations.

In the first case, we explore biomass productivity under various light intensities. The results of eight simulations are summarized in Figure 7. We observe that when the light intensity is low, in Figure 7(a), a large proportion of rope shall be exposed to gain higher biomass productivity. However, less rope shall be exposed to gain higher productivity when light intensity is high, observed in Figure 7(f). RABR peripheral velocity does not seem to have strong effects when the light intensity is low. Also, we observe that faster speed is favorable when the light intensity is strong,

as indicated in Figure 7(e).

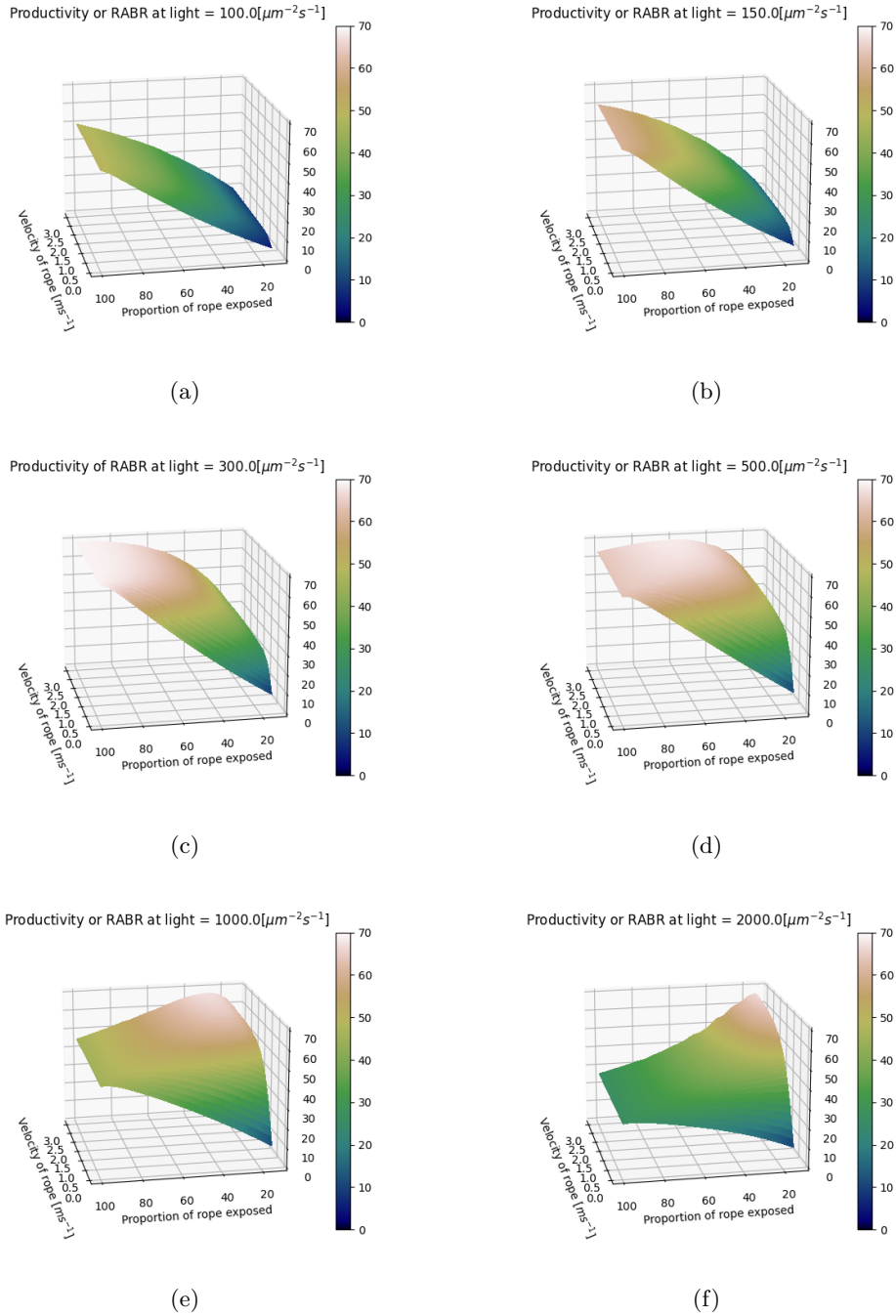


Figure 7: Algal biofilm productivity under varying light intensity situations. In this figure, the algal biofilm productivity over an eight-hour period are shown, under constant light intensity with $I_0 = 100, 150, 300, 500, 1000, 2000 \mu\text{mol m}^{-2} \text{s}^{-1}$.

Next, we investigate the algal biofilm growth under various peripheral velocities. The simulation results are summarized in Figure 8. From Figure 8, we observe that less rope exposure is preferred

when the light intensity is strong, in order to obtain higher biomass productivity. This result is consistent with the results in Figure 7. Figure 8(d) shows a clear nonlinear correlation between light intensity and rope exposure for optimal productivity when the RABR is rotating fast. When the RABR is rotating very slowly, as in Figure 8(a), the RBAR will not be able to take full advantage of the sunlight, and the more rope exposure is always favorable for higher productivity.

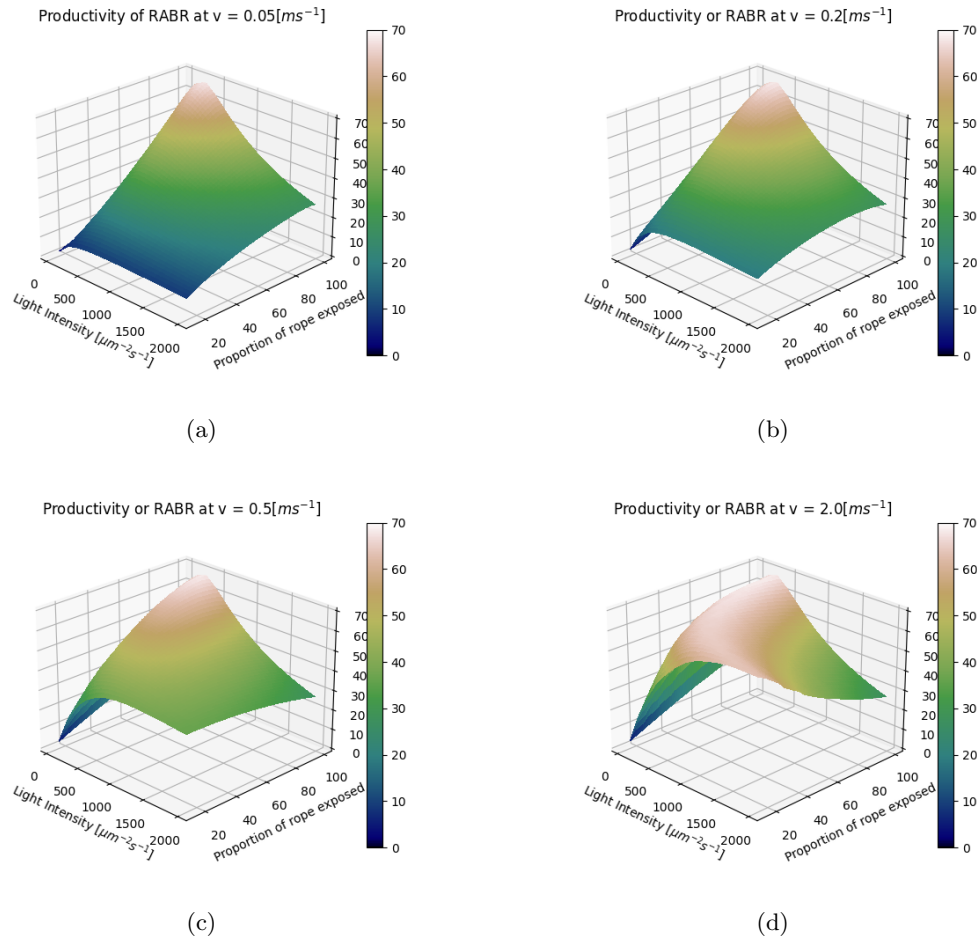


Figure 8: Algal biofilm productivity with various RABR peripheral velocities. Here the algal biofilm productivity are shown, with various RBAR peripheral velocity $v = 0.05ms^{-1}$, $0.2ms^{-1}$, $0.5ms^{-1}$ and $2ms^{-1}$.

In the discussions above, we provide a systematic investigation of productivity at various light intensities and rope line velocities. Next, we inspect the biomass growth at various rope exposure percentages. Here we fix the total rope length and vary the percentage of the rope exposed to the sunlight. The numerical results are summarized in Figure 9. We observe that the optimal productivity shifts to weaker light intensity and slower peripheral velocity, with more rope exposed to sunlight, which is agreeable with reality. The effects of peripheral velocity on biomass productivity become weaker with more rope exposed to the sunlight.

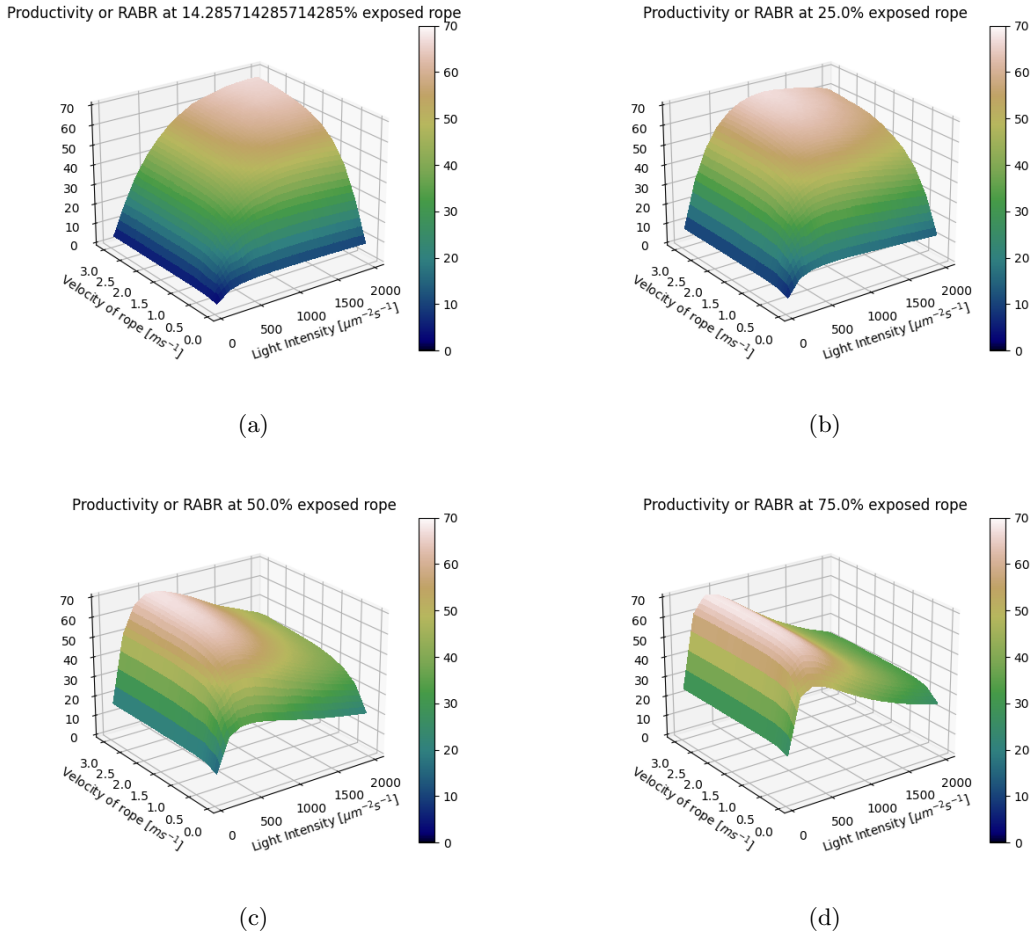


Figure 9: Algal biofilm productivity at various percentages of rope exposure. Here the biofilm productivity with light exposure percentage $\eta = \frac{1}{7}, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ are presented.

3.4 Harvesting strategies

To date, there is little information reported in the literature regarding exploring optimal harvesting strategies for algal biofilms in wastewater treatment. In this sub-section, we evaluate optimal harvesting frequency and height of biofilms remaining after harvesting to obtain the best algal biofilm productivity. Note the expense of harvest operations [10, 21] will not be considered in the current paper. We are also assuming a uniform thickness of biofilm remains on the rope after each harvest operation. A more realistic procedure with stochastic processes will be explored in our future work.

Several numerical investigations have been conducted. Here we present one case with fixed rope length $L = 7$ m and light intensity over every day (24 hours) in Figure 5. An eight week time span of RABR operations is simulated with various harvesting frequencies and remaining biofilm heights after harvesting. The numerical results are summarized in Figure 10. These results demonstrate how our current harvesting mechanism identifies strategies to increase biomass productivities during wastewater treatment. We observe that the biofilm productivity is low without harvesting and increases with more frequent harvesting operations. We also observe that a finite amount of biofilm

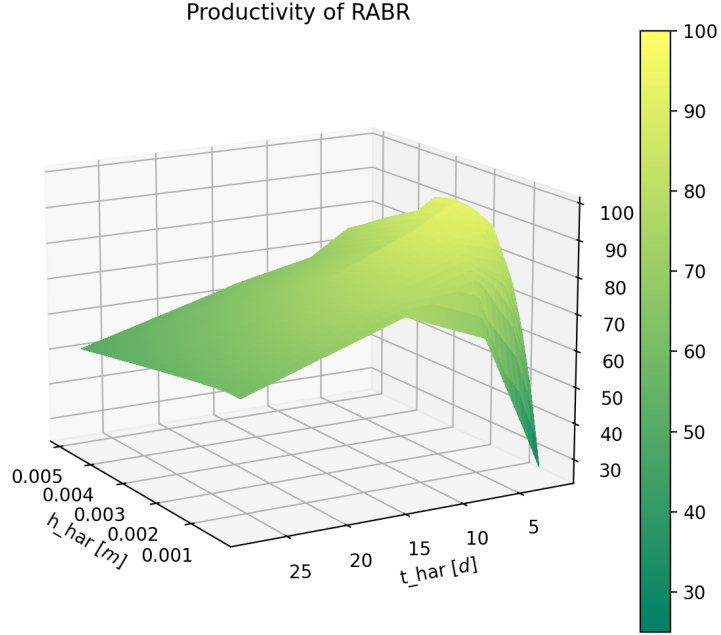


Figure 10: A surface plot of the RABR biomass productivity with various harvest strategies. Here $h_{harvest}$ is the biofilm height to achieve after harvest, and $t_{harvest}$ is the time interval between two consecutive harvest operations. This figure indicates that harvesting algal biofilms frequently with proper height left will increase the biomass yield. For this figure, we use $T = 45s$, $I_0(t)$ from Figure 5, and $\eta = \frac{1}{7}$.

shall serve as a residual after each harvest for algal biofilms to reproduce quickly.

We also present biofilm thickness at various times for comparison for four typical harvesting scenarios in Figure 11. We observe that the biofilm thickness keeps increasing and reaches a plateau without harvesting, as shown in Figure 11(a). For cases with harvesting given in Figure 11(b-d), the biofilm heights are periodic, synchronizing with the harvesting operations. Figure 11(b) has the minimum productivity in all four cases. A contributing factor to this result is that the procedure leaves less biofilm after each harvest as shown in Figure 11. Results presented in Figure 11 indicate that suitable biomass must remain after each harvesting to maintain optimal RABR biofilm productivity.

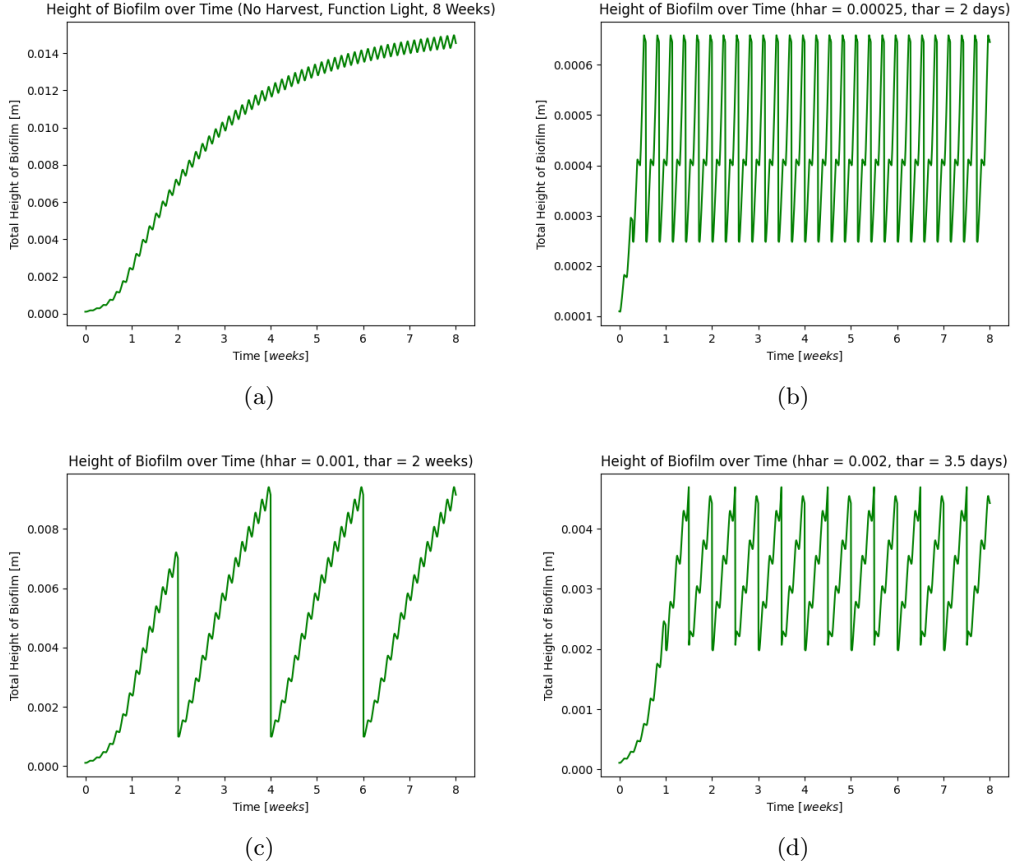


Figure 11: Algal biofilm heights over an eight-week period for different harvesting strategies. This figure shows the time sequence of biofilm thickness at four harvesting cases: (a) no harvest; (b) harvest every 2 days leaving $h_{harvest} = 0.00025m$ of biofilm; (c) harvest every 2 weeks with $h_{harvest} = 0.001m$; (d) harvest every 3.5 days with $h_{harvest} = 0.002m$. For this figure, we use $T = 45s$, $I_0(t)$ from Figure 5 and $\eta = \frac{1}{7}$.

4 Conclusion

In this paper, we have proposed a predictive computational model to investigate algal biofilm growth on rotating algal biofilm reactors (RABR). The effect of light intensity, peripheral velocity, and percentage of rope exposure on biomass productivity have been systematically investigated. Optimal harvesting strategies have also been explored. Our results show that optimal control of these factors to maximize biomass productivity is doable. The proposed model could be further calibrated to generate reliable predictions for nontrivial applications for investigating the efficient application of microalgal biofilms in wastewater treatment.

However, due to the problem complexity, several additional investigations are required to design a RABR system that can automatically adjust its rotating speed and light exposure based on environmental factors such as light intensity and nutrient availability. In addition, biomass nutrient transfer shall be considered for a more realistic model. Optimal control will also be investigated for energy efficiency in biomass production.

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5 Reflective Writing Section

Since April of 2019, I have been actively participating in research. As a pure mathematics major with a minor in computer science, I wanted to push the boundaries of my academic knowledge as well as prepare myself for an eventual master's program. When beginning my research with Dr. Jia Zhao, I immediately saw the importance and significance of our work, as well as gain an understanding of the richness in opportunities such endeavors provide. It was my agreement to conduct research with Dr. Zhao that catalyzed my enrollment in the USU Honors Program; I did not know exactly where my research would take me, but I knew that wherever I landed I could complete the required capstone for the Honors Program. Following a summer of preparation, Dr. Zhao introduced me to the rest of our team for this project in September 2019. The team included; Dr. Ronald Sims and Dylan Ellis of the Biological Engineering Department and Ph.D. student Zengyan Zheng of the Mathematics Statistics Department. Together we have mathematically modeled algae biofilm growth for wastewater treatment. As a leading contributor to this project, I provided the code and numerical results for our models as well as led discussions in our weekly meetings on improving the model. While I have solely focused on interpreting the model in an ordinary differential equation context, Zengyan Zheng has started work on developing a partial differential equation model. Coming from the Biological Engineering Departments, Dr. Sims and Dylan Ellis offered crucial feedback and information to ensure our model reflected realistic results found in wastewater treatment. They also provided important literature to enrich our model in an engineering context. As my mentor, Dr. Zhao facilitated our weekly meetings and guided discussions and further research when necessary.

My capstone reflects this interdisciplinary effort.

Around September 2020, after nearly a year working on this project, Dr. Zhao was invited to submit a chapter in a topical volume titled "Contemporary Research in Mathematical Biology" and invited me to write about our work for the chapter. Over the course of the Fall 2020 semester, I collaborated with my colleagues to produce a manuscript that met the academic rigor necessary to be included in the book. As the first author, I wrote the rough draft of the manuscript as well as provided an outline of the results section. Once I generated all the necessary figures for our paper and wrote a rough draft of our results section, as a team, we polished the draft and added in more detail. As co-author, Dr. Zhao played a significant role in adding a level of detail that I could not have done alone in time for our December 15th deadline. Zengyan Zheng assisted in evaluating the formatting of the math equations in our paper as well as standardizing the references section in the paper. In order to have consistent terminology and concepts found in biological engineering, Dr. Sims and Dylan Ellis assisted in writing our background section as well as verified our diction in our results section. While I am the first author and have spearheaded this research through my code, numerical results, and writing, such an interdisciplinary endeavor would not have been possible without my other team members.

Due to the paper's interdisciplinary nature, I have been able to acquire and grow skills in a mathematical, computational, and engineering context. As our model is a series of ordinary differential equations, I have become much more versed in the connection of nonlinear dynamics in the context of univariate differential systems. As we begin to introduce additional variables into our model, I have utilized my work in MATH 6620 with Dr. Zhao, a course dedicated to numerically solving and understanding partial differential equations. From the extensive literature reviews conducted for this project, I have become educated on different modeling techniques as well as the theory behind them. With encouragement from Dr. Zhao, I enrolled in the GAMM Juniors' Summer School on Applied Mathematics and Mechanics to learn more about data-driven

methods of generating mathematical models.

Aside from math theory, I have refined my skills in computer science and programming. In tandem with learning numerical methods to solve our model, I have learned the necessary programming to write and execute the needed numerical methods. Along with proper coding etiquette, Dr. Zhao has guided me in learning the best way to catalog and store previous code to allow for easy retrieval and rereading. Over the last year, Dr. Zhao allowed me access to his server on campus to execute computationally heavy algorithms. I have learned how to preprocess, execute, and post-process data retrieved from his server for our model. When beginning my research, it would take nearly an hour to generate 8 data points for our figures in the manuscript. Towards the end of my capstone, I was able to generate nearly 400 data points in an hour.

One of the most rewarding aspects of this capstone has been the immersion I have experienced into the world of Biological Engineering and wastewater treatment. My research inspired me to become a member of the Institute of Biological Engineering. This has allowed me to present my research at the Intermountain Biological Engineering Conference twice. As our research improves the ability of wastewater treatment plants to reduce the creation of harmful algal blooms downstream, I have had the opportunity to visit and tour the Central Valley of Water Reclamation Facility (CVWRF), the largest wastewater treatment plant in Utah. I have also been given tours at WesTec Engineering Inc, our partners helping eventually construct pilot and full-scale RABRs for CVWRF. I was employed by Dr. Sims to conduct laboratory work over the Summer of 2020 to better prepare and facilitate data collection of laboratory-scale rotating algae biofilm reactors (RABRs). In addition to lab safety and diver's safety training, I learned basic and essential skills to harvest and record data on the algae in the RABRs. I am also taking a special topics course on bioreactors with Dr. Sims to further understand the mechanisms of a RABR. This is a first of its kind in the Biological Engineering Department as I am not an engineering major.

While there has been success in the analytical side of mathematically modeling algae biofilm, there have been significant challenges to obtaining a data-driven model as originally proposed in my capstone proposal. Due to COVID-19 restrictions, we had to postpone the construction of laboratory RABRs from Spring 2020 to Fall 2021. During the Fall semester, myself, Dr. Sims, and a handful of other biological engineer students constructed nine laboratory-scale RABRs. We have had issues of some RABRs not spinning, others becoming contaminated, and others spinning into the wall of their tank and spilling out following their six-week inoculation period to allow for initial algae growth. Unfortunately, the current state of the laboratory RABRs is not sufficient for proper data collection. However, I am deeply appreciative of the essential laboratory and mechanical skills I have acquired. After receiving a \$1.9 million grant from the Department of Energy, the Biological Engineering Department will be overseeing the construction of higher quality laboratory-scale RABRs in May 2021. I look forward to using the data from the upcoming RABRs to facilitate a data-driven model for mathematically modeling biofilm growth as I continue my studies as a USU graduate student.

This capstone has given me the opportunity to grow my skills as a researcher as well. I have had the opportunity to present my research on a local, statewide, national, and international scale. I have learned the process of writing proposals for grants and awards. From numerous edits and optimizations on our model, I have learned that research is a very iterative process. There have been a handful of times that, after making an optimization on our model, I look back to our earlier research and think, "How we did not come up with the idea earlier?". For example, weeks before publishing our paper, we noticed a critical division error that threw off all numerical results by a scalar factor and had to be rescaled. I have also learned throughout this project that research is often nonlinear. That is, there are periods with rapid developments and then others where

additional progress seems daunting.

After looking back on this previous year of research, I feel accomplished by what I have done even though it may be difficult from a day-to-day basis to see the progress. After hours of coding, reading, and discussing, my colleagues and I have developed an analytical model to predict algae biofilm growth. I have learned important skills as an academic and a researcher. I have been able to develop essential skills in both academia and industry within the fields of math, computer science, and biological engineering. I am eager to see where my future research takes me and am grateful for my experiences as an undergraduate at Utah State University.

6 Bibliography

Gerald Benjamin Jones has earned a bachelor's degree in mathematics and a minor in computer science at Utah State University (USU). He has conducted interdisciplinary research in the Mathematics & Statistics Department and the Biological Engineering Department at USU to mathematically model algae biofilm growth for wastewater treatment. He plans to return to USU for a masters degree and then will pursue a PhD in applied mathematics at a top research institution.