**Comprehensive computational model for combining fluid
hydrodynamics, light transport and biomass growth in a Taylor vortex
algal photobioreactor: Lagrangian approach**

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Abstract

A comprehensive quantitative model incorporating the effects of fluid flow patterns, light distribution, and algal growth kinetics on biomass growth rate is developed in order to predict the performance of a Taylor vortex algal photobioreactor for culturing *Chlorella vulgaris*. A commonly used Lagrangian strategy for coupling the various factors influencing algal growth was employed whereby results from computational fluid dynamics and radiation transport simulations were used to compute numerous microorganism light exposure histories, and this information in turn was used to estimate the global biomass specific growth rate. The simulations provide good quantitative agreement with experimental data and correctly predict the trend in reactor performance as a key reactor operating parameter is varied (inner cylinder rotation speed). However, biomass growth curves are consistently over-predicted and potential causes for these over-predictions and drawbacks of the Lagrangian approach are addressed.

Keywords: Photobioreactors; Taylor-Couette flow; Microalgae; CFD; Simulation; Radiation Transport

1. Introduction

In order to optimize the design and to reliably scale up photobioreactors, it is necessary to accurately simulate the complex interplay between physical, chemical and biological phenomenon that occur on multiple-time and length scales. For example, Figure 1 depicts some important relationships between hydrodynamics, mass transport, radiation transport, and algal growth kinetics. However, obtaining quantitatively accurate and reliable models for each of the fundamental processes governing global reactor performance can be challenging or computationally expensive. For example, accurate simulation of fluid mixing and mass transport requires at a minimum the use of validated gas-liquid fluid flow simulations. Accurate simulation of radiation transport in photobioreactors is also a difficult and computationally expensive endeavor for realistic geometries involving curved reactor walls (Kong and Vigil, 2014).

In addition to challenges associated with developing suitable models for fluid flow, radiation transport, and microorganism growth, an efficient computational scheme for capturing the interplay between these processes is required. A comprehensive model should in principle account for all mutual interactions between these basic processes. However, several justifiable assumptions can significantly reduce computational costs, for example by neglecting the effect of biomass loading on hydrodynamics. However other phenomena, particularly insofar as they impact the amount and manner of light delivery to microorganisms, must be carefully simulated as irradiance of microorganisms is known to be the most critical factor affecting photobioreactor performance. Specifically, fluid mixing patterns that shuttle microorganisms periodically between light and dark regions of the

reactor can substantially enhance both biomass productivity and light utilization efficiency (Hu and Richmond, 1996; Ugwu *et al.*, 2005; Sobczuk *et al.*, 2006; Kong *et al.*, 2013). Consequently, the essential elements of a comprehensive model of photobioreactor performance should include (a) accurate prediction of radiation distribution in the reactor as a function of biomass concentration, (b) a photosynthetic growth model that accounts for temporal variations in light exposure experienced by microorganisms, and (c) a hydrodynamic model capable of accurately predicting flow patterns, mixing, and the spatial trajectories of microorganisms.

The most common approach for integrating hydrodynamic, radiative, and kinetic growth models to predict global reactor behavior is to (1) compute velocity fields in the reactor, (2) compute microorganism spatial trajectories (Lagrangian particle tracking), (3) generate temporal light exposure trajectories by mapping microorganism position-time data to predictions for the photon flux obtained from a radiation model, and (4) use light exposure trajectories to integrate an algal biomass kinetic growth equation. However, as has been demonstrated by Pruvost *et al.* (2008), such an approach requires that the Lagrangian particle tracks be consistent with a spatially uniform distribution of biomass for consistency with energy conservation. Although others have made use of the Lagrangian simulation approach to simulate photobioreactor performance, the coupling of detailed multiscale sub-models for hydrodynamics, radiation transport, and algal growth kinetics into a comprehensive modeling tool is novel. Furthermore, the use of experimentally validated and rigorous hydrodynamic and radiation transport sub-models enables analysis and new insights into limitations and weaknesses of the Lagrangian simulation approach. The comprehensive model described

here is applied for the first time to a reactor with more complex hydrodynamics and distribution of radiative flux than is found in more familiar flat panel or tubular reactors.

2. Comprehensive Reactor Model

2.1. Gas-Liquid Two-Phase Flow CFD Model

In this work, our previously validated two-fluid flow model was used to simulate multiphase flow dynamics in a Taylor vortex reactor (Gao *et al.*, 2015a; 2015c; Gao *et al.*, 2016a). Microalgal growth in this high biomass concentration system is not limited by gas-liquid interphase mass transfer, and therefore no interphase mass transfer model is required (Gao *et al.*, 2015b; Ramezani *et al.*, 2015). The axisymmetric equations of continuity and conservation of momentum equations are given by:

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \vec{u}_k) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}(\alpha_k \rho_k \vec{u}_k) + \nabla \cdot (\alpha_k \rho_k \vec{u}_k \vec{u}_k) = -\alpha_k \nabla p + \nabla \cdot (\overline{\overline{\tau_k}} + \overline{\overline{\tau_k^{Re}}}) + \alpha_k \rho_k \vec{g} + \vec{F}_{Ik} \quad (2)$$

Here, α_k and $\vec{u}_k$ are the phase volume fraction and the phase velocity for liquid ($k = l$) and gas ($k = g$), respectively. The phase stress and Reynolds stress tensors are represented by $\overline{\overline{\tau_k}}$ and $\overline{\overline{\tau_k^{Re}}}$. The liquid-gas momentum exchange term, $\vec{F}_{lg}$ can be decomposed into five independent interphase forces: drag, lift, virtual mass, wall lubrication, and turbulent dispersion forces. The interested reader can find expressions for the constitutive relations and model parameters in Gao *et al.* (2015c).

2.2. Lagrangian Particle Tracking Simulations

The photosynthesis rate depends on cell light exposure history which in turn depend upon microorganism spatial trajectories and light distribution. A Lagrangian particle tracking model coupled with the gas-liquid CFD model described above was employed to compute

thousands of cell trajectories by integrating Newton's law for random cell initial positions.

The equation of motion for microorganisms in the reactor could in general include many interphase forces such as drag, buoyancy, virtual mass and lift. However, due to the small characteristic size ($\sim 5 \mu\text{m}$) of the microorganism considered in this work (*Chlorella vulgaris*), the drag force is dominant so that particle trajectories can be computed by integrating the following equations (ANSYS Fluent, 2012):

$$m_p \frac{d\vec{u}_p}{dt} = \vec{F}_D \quad (3)$$

$$\frac{d\vec{X}_p}{dt} = \vec{u}_p \quad (4)$$

where $\vec{X}_p$ is the particle position vector. The drag force $\vec{F}_D$ can be expressed as (Schiller and Naumann, 1935) by assuming that the algal cells are spherical:

$$\vec{F}_D = \frac{\pi d_p^2}{8} \rho_l C_D (\vec{u}_l - \vec{u}_p) |\vec{u}_l - \vec{u}_p|$$

where the drag coefficient C_D is given by

$$C_D = \begin{cases} \frac{24}{\text{Re}_p} (1 + 0.15 \text{Re}_p^{0.687}) & \text{Re}_p \leq 1000 \\ 0.44, & \text{Re}_p > 1000 \end{cases} \quad (6)$$

Here, Re_p is the particle Reynolds number. Note that the drag force exerted on algal cells

depends upon the turbulent continuous liquid phase velocity $\vec{u}_l$. This quantity can be

decomposed into time-averaged and fluctuating components, such that

$$(7) \quad \vec{u}_l = \overline{\vec{u}_l} + \vec{u}'_l$$

where $\vec{u}'_l$ is the fluctuating liquid eddy velocity given by

$$(8) \quad \vec{u}'_l = \xi_i \sqrt{\frac{2k}{3}}$$

Here k is the turbulence kinetic energy and ξ_i is the zero mean unit variance Gaussian random value. Particles (algal cells) remain under the influence of the eddy until either (1) the

integration time exceeds the eddy life time (t_e), or (2) the distance between the center of an eddy and a particle exceeds the eddy length (L_e). In the eddy lifetime model the particle interaction time (t_i) is assumed to be equal to the smaller of the eddy lifetime and the eddy crossing time and is given by

$$(9) \quad t_i = \min(t_e, t_c)$$

When this time is reached, a new value of the instantaneous velocity is obtained by applying a new value of ξ_i . The characteristic lifetime and length scale of an eddy can be estimated as (Gosman and Loannides, 1983):

$$t_e = C_e \frac{k}{\epsilon}, \quad L_e = C_e \sqrt{\frac{3}{2}} \frac{k^{3/2}}{\epsilon}$$

where the constant C_e is typically assumed to be in the range 0.2-0.56 (Yeoh and Tu, 2010).

In this work, C_e was taken as 0.3. The particle eddy crossing time is given by (Gosman and Loannides, 1983):

$$t_c = -\tau_p \ln \left[1 - \exp \left(-\frac{L_e}{\tau_p |\vec{u}_l - \vec{u}_p|} \right) \right]$$

where the particle relaxation time is given by:

$$(12) \quad \tau_p = \frac{4\rho_p d_p}{3\rho_l C_D |\vec{u}_l - \vec{u}_p|}$$

2.3. Algal Biomass Growth Model

Most dynamic biological models having the ability to incorporate the effects of light gradients and light/dark exposure cycles are based on the photosynthetic unit (PSU) construct which envisions light absorbing reaction centers in microorganisms occupying various states and considers transitions between these states (Eilers and Peeters, 1993; Camacho Rubio *et al.*, 2003; García-Camacho *et al.*, 2012, Nikolaou *et al.*, 2015). The Eilers-Peeters model, as revised by Wu and Merchuk (2001), was employed here to simulate microalgal growth rates.

This 3-state model considers PSUs to be in either a resting, active, or inhibited state. The kinetic expressions used to describe the evolution of the distribution of PSUs in the three states are given by (Wu and Merchuk, 2001):

$$\begin{aligned} \frac{dx_1}{dt} &= \alpha I x_1 + \gamma x_2 + \delta x_3 \\ \frac{dx_2}{dt} &= \alpha I x_1 - \gamma x_2 - \beta I x_2 \\ (14) \quad x_1 + x_2 + x_3 &= 1 \\ (15) \quad \mu &= k\gamma x_2 - M \end{aligned}$$

In the above equations, x_1 , x_2 , and x_3 represent the fractions of PSUs occupying the resting, active, and inhibited states, respectively. The instantaneous photon flux received by microalgae is given by I . The remaining parameters α , β , γ , δ , and k are in general both species and temperature-dependent. The specific growth rate is given by μ , and M is the maintenance coefficient describing requirements for internal metabolism and allowing for negative growth in low light conditions (Papáček *et al.*, 2014). By sampling thousands of cell light history trajectories and integrating Eqs. (13)-(15), the reactor mean specific growth rate $\bar{\mu}$ can be estimated and used to compute the instantaneous dry biomass concentration provided that the system is only limited by light and not by nutrients so that (Wu and Merchuk, 2001)

$$(16) \quad \frac{dC_b}{dt} = \bar{\mu} C_b.$$

2.4. Radiative Transport Simulation

In previous work, Kong and Vigil (2014) developed and validated a numerical solution of the following radiative transport equation:

$$\frac{dI_\lambda(\vec{r}, \vec{s})}{ds} = (a_\lambda + \sigma_{s,\lambda}) I_\lambda(\vec{r}, \vec{s}) = \frac{\sigma_{s,\lambda}}{4\pi} \int_0^{4\pi} I_\lambda(\vec{r}, \vec{s}') \Phi_\lambda(\vec{r}, \vec{s}') d\Omega \quad (17)$$

In the above expression, I_λ is the wavelength-dependent radiance, $\vec{r}$ is the position vector, $\vec{s}$ is the ray direction vector, $\vec{s}'$ is the scattering direction vector, s is the path length, a_λ is the wavelength-dependent absorption coefficient, $\sigma_{s,\lambda}$ is the wavelength-dependent scattering coefficient, Φ_λ is the wavelength-dependent phase function and Ω' is the solid angle. All modeling methods and parameters used here were identical to those reported by Kong and Vigil (2014), who applied their model to the same concentric cylinder geometry. It should be noted that the model assumes (1) algal cell concentration is uniformly distributed in the annular reaction zone and (2) the effect of gas bubbles on radiation distribution can be neglected. As will be discussed in sections 4, gas-liquid CFD simulations provide some justification for both of these assumptions.

2.5. Model Component Coupling Method

The overall strategy (depicted in Figure 2) for computing biomass growth curves in photobioreactors includes performing CFD and particle tracking simulations to obtain spatial particle trajectories, computing spatial light distribution in the reactor by numerically solving Eq. (17), and lastly computing algal growth rate using Eqs. (13-16).

3. Computational Details

3.1. Growth rate model parameters

The PSU model parameters that appear in Eqs. (13)-(15) are species specific, and have not previously been reported for *Chlorella vulgaris*, which is the organism used to generate experimental data for comparison with our model predictions. Consequently, experimental data obtained by Dauta *et al.* (1990), who investigated the growth rate of *Chlorella vulgaris* over a wide range of light intensities was used to fit the PSU model parameters using the

method developed by Wu and Merchuk (2001). The results of this fitting procedure demonstrate that PSU model predictions compare favorably with experimental data for growth of *Chlorella vulgaris* at 35 °C. The fitted parameters are as follows ($R^2=0.9685$): $\alpha = 7.253 \times 10^{-4} \text{ m}^2/(\mu\text{E})$, $\beta = 1.703 \times 10^{-8} \text{ m}^2/(\mu\text{E})$, $\delta = 9.968 \times 10^{-6} \text{ s}^{-1}$, $\gamma = 0.009485 \text{ s}^{-1}$, $k = 0.004511$, $M = 9.913 \times 10^{-6} \text{ s}^{-1}$.

3.2 Algebraic Representation of Light Distribution

Rather than generating new solutions to the computationally demanding radiative transfer equation (17) at each time step of the simulation, an algebraic expression to represent the photon flux was developed by fitting various trial function to numerical solutions of the general radiative transport equation (17) for several biomass loadings (0.25, 0.5, 1.0, 2.0, and 4.0 g/L). By finding a suitable algebraic expression in this manner, the photon flux can be accurately interpolated for any radial position and biomass concentration. After testing many functions, the following expression was found to closely approximate computed photon flux distributions in the Taylor vortex reactor:

$$I = I_o \exp \left[\left(aC_b + b \right) \frac{r}{r_o} + c \right] \left(\frac{r}{r_o} \right)^{dC_b + e} \quad (18)$$

Here, $I_o = 592.7 \mu\text{E}/\text{m}^2\cdot\text{s}$, r_o is the outer cylinder radius, C_b is the dry biomass concentration (g/L), r is radial position (m), and best fit ($R^2 = 0.9981$) values for the parameters in Eq. (18) are given by $a = -0.02431 \text{ L/g}$, $b = 8.234$, $c = -8.351$, $d = 19.22 \text{ L/g}$, $e = -9.567$.

3.3 Taylor Vortex Photobioreactor

A Taylor vortex photobioreactor was used to culture *Chlorella vulgaris*. Details concerning the experimental apparatus and measurements can be found in Gao *et al.* (2015b). The rotating inner cylinder has a radius of 3.81 cm and the fixed transparent acrylic outer cylinder has an inner radius of 5.08 cm, resulting in a gap width of 1.27 cm. The length of the

reactor is 50.8 cm and the reactor is filled to a height of $h = 48$ cm, producing a total liquid working volume of 1.70 L. The density and viscosity of the culture media are 1036 kg/m^3 and $7.22 \times 10^{-4} \text{ kg/m}\cdot\text{s}$, respectively. The density of algal cells was taken to be identical with the culture media, and the mean cell diameter is $5 \text{ }\mu\text{m}$.

To carry out quasi-three-dimensional axisymmetric CFD simulations of flow in the Taylor vortex photobioreactor, a non-uniform rectangular mesh was employed to discretize the annular reaction zone. In previous work simulating mass transfer in the same reactor, three progressively finer meshes were tested and it was found that a mesh size of 32×480 (radial $\times$ axial grid points) is sufficient to capture the essential features of the flow (Gao *et al.*, 2015a). However, in this work the distribution of light is also important and at high biomass concentrations the photon flux drops dramatically with radial distance from the illuminated reactor surface. Hence, refinements to the hydrodynamic computational mesh were considered to better capture the effect of steep light gradients on algal growth. Specifically, a mesh size of 64×960 was employed, but since the resulting biomass concentration predictions using the finer mesh were nearly identical to those obtained using the 32×480 mesh, it was decided that no further mesh refinements were necessary.

Boundary conditions used to carry out CFD calculations were as follows. For gas and liquid phases, no-slip conditions were specified at wall boundaries and the azimuthal velocity of the inner cylinder was chosen to match experimental conditions. The inlet gas flow rate was 85 mL/min , also in accordance with the experiments. Pressure outlet boundary conditions were used for all fluid phases.

The commercial finite volume CFD code, ANSYS FLUENT 14.5 (Ansys Inc., US) was

used to solve the hydrodynamic equations. Transient CFD simulations were performed using an integration time step of 5×10^{-4} s. While typical algal growth experiments had a duration of approximately 120 hours, it is neither practical nor necessary to perform CFD simulations for that time period. Instead, fluid flow simulations were performed until fluid flow statistics reached steady values. Subsequently, particle trajectories were carried out for 10 seconds of real time.

Numerical integration of Eq. (16) to compute the reactor biomass concentration was performed using a time step $\Delta t = 0.05$ s. This value is much smaller than the characteristic light/dark cycle time scale. The initial biomass concentration was set to the initial condition in the experiments (0.1 g/L), and the initial values of the fractions of the three metabolic states were estimated to be similar to those found in the subculture used to seed the reactor. This subculture was under a photon flux density of $20 \mu\text{E}/\text{m}^2 \cdot \text{s}$, and values for the fractions of PSUs in each of these three states was estimated from steady-state solution of Eqs. (13) and (14) to be $x_1 = 0.3874$, $x_2 = 0.5924$, $x_3 = 0.0202$. Hence, very few PSUs are in the inhibited state at the start of the simulation.

4. Results and Discussion

4.1. Flow Hydrodynamics

Example contour plots for instantaneous simulated liquid phase stream function and gas volume fraction are shown in **Figure 3** for typical Taylor vortex photobioreactor operating conditions with an inner cylinder rotation speed of 400rpm and air flow rate of 0.05 vvm (85mL/min). It is obvious from **Figure 3(a)** that toroidal vortices are formed in the narrow annular gap, wherein fluid circulates between the inner and outer cylinder walls. Because

algal cells have a small Stokes number, they closely follow liquid phase streamlines and are rapidly and periodically shuttled between the relatively well illuminated regions near the outer cylinder and darker regions near the inner cylinder – a phenomenon that leads to improved light utilization and biomass growth rate (Miller *et al.*, 1964; Kong *et al.*, 2013).

Figure 3 (b) clearly demonstrates that gas bubbles (confirmed visually in experiments) preferentially distribute near the dark inner cylinder wall due to centrifugal forces. This observation, in tandem with the fact that the gas volume fraction in the reactor is very low ($< 2\%$), suggests that in this apparatus bubbles have negligible effect on radiation transport, as the small bubble volume resides in regions of the reactor where very little light is present. Hence, the assumption that the presence of gas bubbles can be neglected in the numerical solution of the radiative transport equation (17) is well justified.

4.2. Particle Trajectory and Light Exposure History

Figures 4 (a) – (c) depict typical time series plots of algal cell radial position for different inner cylinder rotation speeds, as computed from the Lagrangian particle tracking model described previously. Increases in cylinder rotation speed produce more rapid shuttling of cells between the inner and outer cylinders by Taylor vortices as demonstrated by Figures 4(d) – (f). Specifically, it can be seen that when the boundary between light and dark regions of the reactor is located at the middle of the annular gap $(r - r_i) / (r_o - r_i) = 0.5$, histograms of the resulting light/dark cycle frequencies have mean values of 1.1 Hz, 2.2 Hz and 3.2 Hz for 200 rpm, 400 rpm and 600 rpm, respectively. It is worth noting that these mixing-induced light/dark frequencies are significantly higher than those produced in many commonly used photobioreactors (Janssen *et al.*, 2000; Pruvost *et al.*, 2002; Huang *et al.*, 2014; Olivieri *et al.*,

2015).

The effect of biomass loading on cell light exposure is an important factor for overall reactor performance. Specifically, at low biomass concentrations (such as 0.25 g/L) the photon flux variations experienced by microorganisms are relatively small no dark zone is observed.

At higher biomass concentrations, e.g. 1 g/L, the minimum photon flux experienced by microorganisms is nearly zero (dark zone) when cells approach the inner cylinder wall. Further increases in biomass concentration cause the boundary between light and dark regions of the reactor to shift towards the outer cylinder wall.

4.3. Biomass Growth Curves

Simulated Taylor vortex reactor biomass growth curves are compared with corresponding experimental data for three inner cylinder rotation speeds in Figure 5. The biomass density was compared rather than cell number density, as well-known correlations exist relating optical density, cell number density, and biomass concentration, such as those given by Kao et al., (2012). The simulations correctly predict the experimental trend of more rapid growth with increasing inner cylinder rotation speed, but in all cases biomass concentration is over-predicted by as much as 30% at longer culture times. For growth times less than approximately 60 hours, simulation predictions largely match the observed biomass concentration. As one would expect, both the simulations and the experiments show no significant effect of rotation speed on biomass growth curves when biomass concentration is sufficiently small so that no dark volume is present.

At least two causes can plausibly explain the discrepancy between experimental and simulated growth curves at long growth times. First, although biomass concentrations reach

relatively high values at long times and become light-limited, in the experiments the batch system may also become nutrient limited. Strong evidence for this problem is provided by Kong *et al.* (2013), who found that after the biomass concentration approaches an asymptote at long times, the addition of urea spurred renewed growth. In contrast, no nutrient limitation is considered in the simulations. Secondly, the Lagrangian approach employed here suffers computational difficulties that contribute to discrepancies between simulation predictions and experimental measurements. Specifically, in the absence of the fluctuating eddy velocity given by Eq. (8), cell trajectories become highly periodic because they closely follow liquid streamlines. As a result, cells do not sample radial positions near the cylinder walls where the light intensity is very high (outer cylinder) or very low (inner cylinder). This problem becomes particularly acute at high biomass concentrations because light gradients become very steep near the outer cylinder wall, and if cells cannot closely approach the outer cylinder, then light exposure (as well as specific growth rate) will be under-predicted. Although the inclusion of eddy velocity fluctuations overcomes this problem, it leads to another difficulty. In particular, algal cells become temporarily trapped at cylinder walls not due to any physical cause but because of the lack of submicron grid resolution required to properly model the motion of the microorganisms in the boundary layer near the wall. As a result, distortions in both the radial position-time and light history statistics are introduced. Specifically, unphysical trapping of cells on the outer cylinder wall leads to overestimation of the amount of light received by those cells. Similarly, cells trapped on the inner cylinder wall receive less light than they would had they not become trapped.

The problem of cells lingering near reactor wall surfaces is evident in **Figure 4** and can

be quantified by computing the radial cell concentration distribution from an ensemble average of thousands of “snapshots” of radial particle positions. Such an analysis demonstrates that algal cell concentration is uniformly distributed in the annular gap except near the cylinder walls, significant enhancement of cell concentration occurs. As a result, microorganisms spend too much time both in dark regions near the inner cylinder and bright regions near the outer cylinder. While these errors may be partially offsetting, cell concentration enhancement is greater near the outer cylinder, and as a result there may be net over-prediction of light delivery and algal growth rate.

Further insight into the reactor biomass growth curves can be gained by considering the temporal evolution of an ensemble average (1000 trajectories) for each of the three PSU states, as is shown in Figure 6. When the reactor is inoculated at the beginning of the experiment, the algae experience a sudden increase in light exposure and the fraction of PSUs in the active state increases rapidly, for example increasing from 0.59 to 0.95 in only a few seconds. The inhibited fraction of PSUs also increases, but this increase occurs over a much longer timescale reaching a maximum after approximately 20 hours at which time the biomass concentration is still much less than 1 g/L and no dark volume yet exists near the inner cylinder. The increase in the fraction of inhibited PSUs comes at the expense of active state PSUs and also leads to an increase in the resting state fraction as inhibited PSUs recover. As the biomass concentration increases with time, reactor volume near the inner cylinder wall becomes dark (defined here as a photon flux of less than $10 \mu\text{E}/\text{m}^2\cdot\text{s}$, the approximate value of the photo compensation point), and consequently the fraction of PSUs in the resting state increases and the fractions of PSUs in the active and inhibited states declines as biomass

growth becomes increasingly limited by light availability.

5. Conclusion

A Lagrangian approach was used to simulate biomass growth curves in a Taylor vortex algal photobioreactor. Direct comparison of simulation predictions with corresponding experimental data for biomass growth curves demonstrates that the computational model correctly predicts that biomass can be more rapidly produced by increasing the Taylor vortex reactor inner cylinder rotation speed. Although the over-predictions of biomass concentration in the later stages may be partly explained by nutrient limitations present in the experiments but not considered in the simulations, computational limitations associated with the Lagrangian particle tracking approach also likely contributed to these discrepancies.

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Notation

C_d = drag coefficient, dimensionless

d_b = Sauter mean diameter of bubble, m

d_s = diameter of algae cell, m

F =inter-phase forces, $\text{kg m}^{-2}\text{s}^{-2}$

g = gravitational acceleration, m s^{-2}

L = cylinder height, m

p = pressure, Pa

r = cylinder radius, m

u = velocity, m s^{-1}

x_1 = mass fraction of resting state, dimensionless

x_2 = mass fraction of active state, dimensionless

x_3 = mass fraction of inhibitive state, dimensionless

X_p = particle position, m

Greek letters

α = volume fraction

ε = turbulent dissipation rate, m^2s^{-3}

μ_t = turbulent viscosity, Pa s

ρ = density, kg m^{-3}

τ = phase stress tensor, N m^{-2}

$\overline{\tau^{\text{Re}}}$ =phase Reynolds stress tensor, N m^{-2}

Subscripts

b = bubble

l= liquid

g= gas

p= particle

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Figure Captions

Figure 1. Coupling of fluid dynamics, radiation transport and algal growth kinetics.

Figure 2. Contour plot of (a) stream function of the liquid phase (kg/s) and (b) bubble volume fraction distribution at rotational speed of 400 rpm. In each plot, the inner cylinder wall is represented by the bottom boundary and the outer cylinder wall is represented by the top

boundary. In order to better show the results, the reactor length was scaled to half of the original length.

Figure 3. Schematic diagram of multi-timescale coupling method for Lagrangian simulation approach.

Figure 4. (a)-(c): Example radial position tracks for an algal cell at various reactor rotational speeds. (d)-(f): Light/dark cycle frequency at various reactor rotational speeds and for the specific condition when the light/dark boundary is located at normalized radial position $(r - r_i) / (r_o - r_i) = 0.5$.

Figure 5. Comparison of simulated biomass growth curves (lines) with experimental data (symbols) for different reactor inner cylinder rotational speeds.

Figure 6. Fraction of photosynthetic units in the (a) resting, (b) active, and (c) inhibited states as a function of time. The radial position of the light/dark boundary, based upon the photocompensation point, is shown in (d) as a function of time.

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6