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

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ABSTRACT

A comprehensive Eulerian approach for integrating a three-phase CFD model, a sophisticated detailed model for radiation transport, and a transport equation for algal growth kinetics is developed and utilized to predict the performance of a Taylor vortex algal photobioreactor. Simulation predictions are compared with corresponding experimental data and with simulation predictions obtained using the more commonly employed Lagrangian particle tracking method. The Eulerian simulations correctly predict the experimental trend that biomass productivity increases with increased rates of mixing, and they also suggest that there are limits to these productivity increases as the mixing rate becomes very large. Simulation over-prediction of biomass productivity at high azimuthal Reynolds numbers can be attributed to the fact that at high biomass loadings most radiation is absorbed near illuminated reactor surfaces, and it becomes increasingly important, but also more difficult, to properly resolve the thinning hydrodynamic and radiative boundary layers.

1. Introduction

Interest in cultivation of phototrophic microalgae has been driven by possible large-scale applications such as for production of biofuels, chemicals, human and animal nutrition, cosmetics, medicine and other value added products [1]. Computational fluid dynamics (CFD) has been used to simulate the performance of algal photobioreactors as a means of reducing design costs and improving reactor efficiency [2]. Such simulations present many challenges such as formulating and solving accurate, quantitative models for the physical and biological processes that determine reactor performance, including multiphase hydrodynamics and mass transport (gas-liquid-solid flow), radiation transport, and microalgae biological function, some important interactions are depicted in Fig. 1. At present, computational simulations of algal growth in photobioreactors incorporating all these factors are limited [3], in part due to the fact that the relevant phenomena are highly coupled and interact across widely separated timescales [4].

At high biomass concentrations, light penetration decays sharply with distance from irradiated surfaces in photobioreactors due to microalgae self-shading. As a result, cells may receive sufficient or even excess radiation near irradiated surfaces and insufficient or no radiation in other regions of the reactor. Hence, microorganism exposure to light is usually the most important and limiting factor controlling performance of photobioreactors [5]. However, since fluid mixing governs the movement of cells in the reactor and thereby determines the light exposure that they experience, accurate simulation of hydrodynamics is a crucial component of any model predicting photobioreactor performance. Indeed, reactors that provide flow structures that induce coherent light-dark cycles significantly improve microalgal growth rate [6–11].

In view of the above discussion, it is evident that in addition to accurate models for fluid flow, radiation transport, and biomass growth kinetics, a computational framework for coupling models for the governing phenomena is required in order to predict photobioreactor performance [12]. The most common approach for coupling fluid mixing, radiation transport, and algal growth kinetics employs the following general algorithm: (1) independently solve the equations of motion for fluid flow and radiative transport, (2) use computed fluid flow velocity field predictions to perform Lagrangian particle tracking simulations for numerous algal cell trajectories with random starting positions, (3) use the resulting cell spatial trajectories and results from light distribution simulations to compute temporal cell light exposure histories, and (4) use the cell light exposure trajectories to compute biomass growth rate.

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Notation

C_D	drag coefficient, dimensionless
d_s	diameter of algae cell, m
$D_{s,L}$	Laminar diffusion coefficient of algae cell, $m^2\ s^{-1}$
$D_{s,t}$	turbulent diffusion coefficient of algae cell, $m^2\ s^{-1}$
F	inter-phase forces, kg $m^{-2}\ s^{-2}$
g	gravitational acceleration, m s^{-2}
L	cylinder height, m
p	pressure, Pa
r	cylinder radius, m
Sc_t	Turbulent Schmidt number, dimensionless
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 inhibited state, dimensionless

Greek letters

α	volume fraction
μ_t	turbulent viscosity, Pa s
ρ	density, kg m^{-3}
$\overline{\overline{\tau}}$	phase stress tensor, N m^{-2}
$\overline{\overline{\tau^{Re}}}$	phase Reynolds stress tensor, N m^{-2}

Subscripts

l	liquid
g	gas
s	solid

In our previous paper [13], we employed detailed CFD, radiation, and a photosynthetic unit (PSU) model of algal growth to carry out Lagrangian simulations for biomass accumulation in a Taylor vortex photobioreactor. A comparison of simulation predictions with experiments demonstrated reasonably good quantitative agreement for several reactor operating conditions, but biomass yield was consistently over-predicted. The error can be attributed in part to an inherent weakness of Lagrangian particle tracking, namely the difficulty in accurately computing cell trajectories near reactor surfaces [13,14].

Here we describe an alternative approach for coupling models for hydrodynamics, radiation transport, and algal growth kinetics that does not require Lagrangian particle tracking. Specifically, we make use of the same models for radiation transport and algal growth kinetics employed in the Lagrangian simulations. However, particle tracking is avoided by solving a transport equation for the algal growth model within a three-phase (liquid-gas-solid) computational fluid dynamics (CFD) simulation in order to produce local predictions for algal growth rate, which in turn can be used to compute the global reactor performance. This Eulerian framework for incorporating hydrodynamics, radiation transport, and algal growth kinetics is then used to generate predictions for the performance of a Taylor vortex photobioreactor and these predictions are compared with those obtained using the Lagrangian approach and with corresponding experiments. Although the proposed Eulerian simulation method has significant advantages compared to the Lagrangian approach, it also suffers from some drawbacks at high biomass loadings due to difficulties in resolving the steep velocity and photon flux radial gradients that arise near the reactor illuminated surface (outer cylinder wall), as was previously reported for this reactor geometry [25]. Steep velocity gradients occur near both cylinder walls due to the no-slip boundary condition.

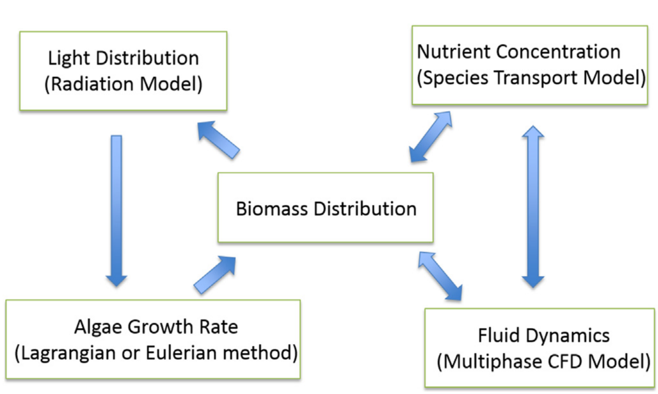

Fig. 1. Coupling of fluid dynamics, radiation transport and algal growth kinetics.

The remainder of the paper is organized as follows. In Section 2 model equations and computational methods are discussed. In Section 3, Eulerian simulation predictions for algal growth curves (*Chlorella vulgaris*) in a Taylor vortex photobioreactor are compared with those obtained from a Lagrangian simulation as well as with experimental data. Discussion of weaknesses of the two methods, as well as challenges associated with simulation of algal photobioreactors more generally, are presented in Sections 3 and 4.

2. Model equations and methods

2.1. Three-phase fluid flow model

The multiphase flow dynamics in a Taylor-Couette bioreactor are governed by interactions among three phases including gas bubbles, liquid culture media, and microalgal cells (solid). Here, the three-phase Eulerian approach was used, which was based on a validated two-fluid Eulerian-Eulerian model for bubbly Taylor-Couette flow [15]. In our previous work, the two-fluid model was validated by direct comparison of simulation predictions with velocity and phase distribution data from experiments performed by Murai et al. [16], who carried out studies of a vertical semi-batch gas-liquid Taylor-Couette reactor. The multiphase flow between two vertically oriented concentric cylinders was assumed to be axisymmetric, so that the quasi-two-dimensional mass and momentum equations include an axisymmetric azimuthal velocity component:

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

$$\frac{\partial}{\partial t}\left(\alpha_k\rho_k\vec{u}_k\right)+\nabla\cdot\left(\alpha_k\rho_k\vec{u}_k\vec{u}_k\right)=-\alpha_k\nabla p+\nabla\cdot\left(\overline{\overline{\tau}}_k+\overline{\overline{\tau}}_k^{Re}\right)+\alpha_k\rho_k\vec{g}+\vec{F}_{lk} \tag{2}$$

Here, α_k and $\vec{u}_k$ are the phase volume fractions and velocities for liquid ($k=l$), gas ($k=g$), and solid ($k=s$). The phase stress and Reynolds stress tensors are represented by $\overline{\overline{\tau}}_k$ and $\overline{\overline{\tau}}_k^{Re}$, respectively. Turbulence was simulated using the standard k − ω model [17], as this method has been shown to accurately predict fluid dynamics in turbulent Taylor-Couette flow [13,15,18].

In Taylor vortex algal photobioreactors the primary liquid growth medium is continuous whereas the low volume fraction secondary gas (<2%) and solid phases (<1%) are dispersed. Momentum exchange between the liquid and each dispersed phase is considered, whereas momentum exchange between the gas and solid dispersed phases is neglected. Based upon our previous work, the liquid-gas momentum exchange term, $\vec{F}_{lg}$, can be decomposed into five independent interphase forces including drag, lift, virtual mass, wall lubrication, and turbulent dispersion forces. The constitutive relations, model parameters, and thermal properties for the gas-liquid interactions can be found in