Numerical Simulation of Two-phase Laminar Flow for CO₂ and Microalgae Suspension in the HLTP

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Abstract: This paper proposes a mathematical model of two-phase flow for carbon-dioxide and microalgae suspension in an Horizontal Loop Tubular Photo-bioreactor (HLTP) taking into account the light irradiance. The model with no-slip condition on the wall and zero outward normal stress at the outlet of the HLTP is used to simulate the fluid phenomena inside the HLTP. The viscosity of the algal suspension is considered as a function of relative viscosity related to concentration and growth rate of the microalgae. The simulation is carried out on the seventh day of the culture. The effect of average irradiance in a day on the viscosity is investigated. The results show that the two-phase flow model can capture the real behavior of the microalgae culture in the HLTP.

Key Words: Microalgae, HLTP, Growth rate, Light irradiance, Simulation, Scale up.

1 Introduction

Microalgae based biodiesel production has drawn keen interest due to the global warming concern and the depleting sources of petroleum fuel [1, 2]. Open ponds and closed photobioreactors are two widely known cultivation systems for microalgae. In the closed Photobioreactor (PBR) system, the mass transfer rate and the shear stress distribution are two important factors considered for improving the performance of PBR [3]. In the microalgae cultivation process, CO₂ is needed for photosynthesis. As CO₂ and microalgae suspension flow together, gas-liquid phases show different flow regimes depending on the reactor geometry and operating conditions [4]. Moreover, the gas hold-up distribution and the flow regimes are controlled by the domain size and the volumetric gas flow rate or mass transfer respectively [5]. Since microalgae are photosynthetic microorganisms, light regime is one of the most important limiting factors for their rapid growth [6]. It is known that the sun radiation is the largest source of energy among the entire abundant sources including fossil fuel. To convert the solar energy into a usable energy is really a challenging task. In a natural biological process, microalgae can use sunlight to convert CO₂ into biomass for bio-fuel production and other sectors, for example, food, medicine and cosmetic production [7, 8].

Extensive research has been carried out since last five decades on microalgae cultivation and their wide variety of applications. But most important results are achieved recently due to improvement of high performance computer. In 2002, Babcock et al. [9] studied the hydrodynamics and mass transfer for an airlift photo-bioreactor. They have found that the efficiency of light penetration in culture is affected by the geometry and the mixing conditions which are controllable via design and operations. However, their study was focused only on single-phase flow and the role of CO₂ is neglected. Ugwu et al. [10] indicated that gas-bubble velocity was a measure of culture flow rates in tubular reactors since algal suspension were circulated along with gas bubble. Recently, Sato et al. [11] proposed a computational model for two-phase microalgae flow taking into account flashing light effect in a virtual photo-bioreactor. In their study, the viscosity of the culture medium was fixed. Findings from the most studies of the two-phase flow indicate that air-water material is used to represent CO₂- algal suspension. In existing models, the growth rate of microalgae is not taken into account [6].

In this study, we focus on the microalgae suspension and CO₂ flow in a HLTP. A mathematical model for two-phase flow is proposed to investigate the hydrodynamics phenomena in the HLTP. The growth rate of microalgae due to the effect of light is considered. The effect of average irradiance on the cell concentration for the seventh day of the culture is also investigated.
2 Mathematical Model

In this study, an airlift driven HLTP is considered in microalgae cultivation. Due to various substances including microalgae and CO$_2$ occupied in the HLTP, the turbulent flow appears. The uniform mixture of algal suspension and CO$_2$ is considered as an incompressible two-phase Newtonian fluid and the flow problem is assumed to be laminar.

2.1 Computational Domain and Meshes

The photo-bioreactor considered in our study is so-called Horizontal Loop Tubular Photo-bioreactor (HLTP), as depicted in Fig.1. Its radius is 0.025 m and length is 32 m. The surface area and working volume are 4.946 m$^2$ and 0.06119 m$^3$, respectively. A fine mesh design is considered for our simulation with 376,057 elements and 3,033,933 degrees of freedom.

2.2 Governing Equations

As the microalgae suspension and CO$_2$ mixture is considered as an incompressible two-phase Newtonian fluid and the flow is laminar, the governing equations are the continuity equation and the Navier-Stokes equations as follows:

$$\nabla \cdot \mathbf{u} = 0,$$

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot [-pI + \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \rho \mathbf{g} + \mathbf{F}_{st},$$

where $\mathbf{u}$ denotes the velocity of the mixture, $\rho$ and $\eta$ are its density and viscosity which will be given later, $\mathbf{g}$ is the gravity, $I$ is the identity matrix, $p$ is the pressure and $\mathbf{F}_{st}$ is the surface tension force. The separation of the two-phase flow is described by the Cahn-Hilliard advection-diffusion equation \[12\]:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \frac{\gamma \lambda}{\epsilon_{pf}^2} \nabla \psi,$$

where $\phi$ is the dimensionless phase field variable, $\epsilon_{pf}$ is a parameter controlling interface thickness, $\gamma$ is the mobility, $\lambda$ the mixing energy density. The function $\psi$ is given by following equations:

$$\psi = -\nabla \cdot \epsilon_{pf}^2 \nabla \phi + (\phi^2 - 1)\phi + \epsilon_{pf}^2 \frac{\partial f}{\partial \phi},$$

$$\lambda = \frac{3\epsilon_{pf}\sigma}{\sqrt{8}},$$

$$\gamma = \chi \epsilon_{pf}^2,$$
where the term \( \frac{\partial f}{\partial y} \) denotes the phi-derivative of external free energy, \( \sigma \) is the surface tension coefficient and \( \chi \) is the mobility tuning parameter. The density and viscosity of the mixture are function of volume fraction of microalgae suspension \( V_l \). The volume fraction of microalgae suspension is \( V_l = (1 + \phi) / 2 \) and the volume fraction of CO\(_2\) gas is \( V_g = (1 - \phi) / 2 \). For the two phase flow model, the density and viscosity are defined to vary smoothly over the interface according to E. Molina’s study \([16]\) by the following equation:

\[
\rho = \rho_l + (\rho_l - \rho_g)V_l, \quad \eta = \eta_l + (\eta_l - \eta_g)V_l, \tag{7}
\]

where the subscripts \( l \) and \( g \) are used for the algae suspension and CO\(_2\) gas, respectively. The surface tension force in (2) is defined as

\[
F_{st} = G \nabla \phi, \tag{9}
\]

where \( G \) is the chemical potential (\( J m^{-3} \)) given by

\[
G = \frac{\lambda \psi}{\epsilon^2 \rho f}, \tag{10}
\]

The viscosity \( \eta_l \) in (8) is given by \( \eta_l = \eta_0 \eta_r(t) \). Occurrence of microalgae cell proliferation changes the concentration and subsequently the viscosity of the algal suspension. A microalgae cell is assumed to be a small sphere in our study \([13]\). Then relative viscosity relating to concentration is determined by Einstein’s relative viscosity equation as follows:

\[
\eta_r(t) = 1 + \varepsilon C(t), \tag{11}
\]

where \( \varepsilon \) is Einstein’s coefficient \([14]\). Based on the experimental data obtained by Hon-nami and Kunito \([15]\), the cell concentration \( C(t) \) in (11) depending on the growth rate \( \mu \) can be expressed by the following logistic function

\[
C(t) = C_0 + \frac{a}{1 + b \exp(-\mu t)}; \tag{12}
\]

where \( C_0 \) is the initial concentration of the suspension, and \( a \) and \( b \) are constant. Since the light availability is an important limiting factor for biomass production, we then consider that the specific growth rate of microalgae depends on average light irradiance according to E. Molina’s study \([16]\) by the following equation:

\[
\mu = \frac{\mu_{\text{max}} I_{\text{av}}}{I_k + I_{\text{av}}}, \tag{13}
\]

where \( \mu_{\text{max}} \) is the maximum growth rate of microalgae, \( I_k \) is a constant depending upon microalgae culture condition. By ignoring the dynamical and physiological properties of algae cell, the average irradiance \( I_{\text{av}} \) depends mainly on incident irradiance \( I_0 \) available on the surface of the PBR and is given by

\[
I_{\text{av}} = \frac{I_0}{D K_a C_0^2} \left[ 1 - \exp(-D K_a C_0) \right], \tag{14}
\]

where \( K_a \) is the extinction coefficient of the biomass, \( D = \frac{d_r}{r} \) is the diameter of the PBR tube and \( \theta \) is the angle of incidence of direct radiation depending on a function of five parameters including the declination (\( \delta \)), solar hour (\( sh \)), geographic latitude (\( \varphi \)), surface slope (\( \beta \)), and surface azimuth angle (\( \tau \)), and the hour angle (\( \omega \)) \([19]\) as:

\[
\cos \theta = \sin \delta \sin \varphi \cos \beta - \sin \delta \cos \varphi \sin \beta \cos \tau + \cos \delta \cos \varphi \cos \beta \cos \omega + \cos \delta \cos \varphi \sin \beta \cos \tau \cos \omega + \cos \delta \sin \beta \sin \tau \sin \omega \tag{15}
\]

According to Grima et. al.’s study \([17]\), we found that the horizontally placed tube absorbs higher irradiance with respect to change in solar hour. Thus, the surface slope \( \beta \) is set to zero degree \([18]\), which provides the following simplest form of (15), i.e.,

\[
\cos \theta = \sin \delta \sin \varphi + \cos \delta \cos \varphi \cos \omega, \tag{16}
\]

where the declination \( \delta \) is defined by

\[
\delta = 23.45 \sin \left[ \frac{360}{365} \left( 284 + N \right) \right], \tag{17}
\]

where \( N \) is the day of the year \([19]\). To calculate an hour angle \( \omega \), we follow the concept of Duffie and Beckman \([19]\). They considered that the angular displacement is 15 degree per hour for earth rotation from east to west, and the value is negative for morning hours and positive for afternoon hours. Thus an hour angle \( \omega \) can be determined by

\[
\omega = 15(sh - 12). \tag{18}
\]

In our simulation the geographical location for the HLTP is Phayathai, Bangkok, Thailand, where the value for the geographical latitude \( \varphi \) is \( 13^\circ 45'32'' \).

### 2.3 Boundary and Initial Conditions

It is important to specify initial and boundary conditions for a given system. In this study we considered no-slip boundary condition on the wall and zero normal stress at the outlet of the domain, which are given by:

\[
u = 0, \tag{19}
\]

\[
[-pI + \eta(t)(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)]
\mathbf{n} = 0. \tag{20}
\]

On the inlet surface \( |\mathbf{u}| = U_{in} \) and the volume fractions of microalgae suspension and CO\(_2\) are 0.95 and 0.05.
3 Numerical Results

In this study, we run our simulation using the COMSOL multiphysics package version 4.2a. The simulation is carried out on the seventh day of the culture. The model parameters $\frac{\partial f}{\partial \phi}$, $\mu_{\text{max}}$, $I_k$, $\varepsilon$, $C_0$, $a$, $b$, $K_a$, $\eta_g$, $\eta_0$, $\rho_g$ and $N$ are set to be 0.01, 0.063$h^{-1}$, 114.67$\mu E m^{-2}s^{-1}$, 2.5$m^3g^{-1}$, 0.55, 1, 200, 0.0369$m^2g^{-1}$, 0.0000625$Pa.s$, 0.001$Pa.s$, 0.001$799 kg/l$ and 172 respectively. The initial solution $u = 0$ is everywhere except at the inlet, where the inlet velocity $U_{in} = 0.5ms^{-1}$.

![Figure 2: Velocity magnitude of the fluid flow at the U-loop (a).](image1)

![Figure 3: Velocity magnitude at three different cross-sections for the U loop (a).](image2)

![Figure 4: Distribution of shear rate along the HLTP.](image3)

Fig.2 and Fig.3 present the velocity magnitude of the two-phase flow along the U-loop (a) of the HLTP, and at three cross-sections which are the beginning (C1), the middle (C2) and the end (C3) of the U-loop (a) respectively. The results show that the velocity magnitude is generally high at the middle of the tube. Comparing the magnitude of the velocity on the three planes, it is found that there is no significant different in the velocity magnitude. Compared to our previous study of the single-phase flow [20], the flow speed at the middle plane (C2) of the first U-loop is higher. It increases from 0.789$ms^{-1}$ to 0.933$ms^{-1}$. It indicates that mass transfer is increased due to bubble effect of $CO_2$ in the current simulation.

It is known that movement of fluids incur a shear stress on the domain boundary. In this context, we give special attention to the shear rate distribution for the straight and curve (U-Loop) portions of the HLTP. We found that the shear rate is uniform at the straight portion of the tube whereas it fluctuates positively along the U-loop as shown in Fig. 4. The result shows that the phase flow passes through the U-loop with...
Figure 5: Shear rate distribution at 06:00 and 18:00 along the inner and outer lines [see Fig.2] of the U-loop(a) : (i) inner line; (ii) outer line.

Figure 6: Dynamic viscosity of microalgae from 06:00 to 18:00 on the seventh day of the culture.

Figure 7: Pressure profile along the HLTP from the inlet to the outlet surfaces.

4 Conclusion

A CFD based mathematical model is developed to simulate the two-phase flow for CO$_2$ and microalgae suspension in the HLTP. We observed that the flow phenomena is quite dissimilar between straight and U-loop portions of the HLTP. Unlike the straight portion, the velocity magnitude and shear rate are higher at the U-loop portion. It is found that a high mass transfer rate is obtained in the two-phase flow model. A uniform linear pressure drop is found for the entire domain from the inlet to the outlet. The viscosity of the microalgae is increased in response to the light irradiance.

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