



Numerical multiphase modeling of CO₂ absorption and desorption in microalgal raceway ponds to improve their carbonation efficiency



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ABSTRACT

The carbonation efficiency in raceway ponds was improved by modeling CO₂ desorption and absorption between the pond and the atmosphere. The Euler–Euler two-fluid method was used to model gas–liquid flow mixing with mass transfer in the raceway pond. The average gas hold-up, mass transfer coefficient, dissolved CO₂ concentration, CO₂ desorption rate to the atmosphere, and CO₂ absorption rate from the atmosphere were investigated using the effects of sump configuration, pond geometry, and gas–liquid hydrodynamic properties. The carbonation efficiency of the entire raceway pond was investigated by considering the effects of sump geometrical design, aspect ratio, water depth, paddle wheel rotational speed, gas bubble size, and gas mass flux. The CO₂ desorption and absorption rates were estimated using novel equations from the literature. Results showed that the CO₂ desorption rate was low in wide and shallow raceway ponds. The gas–liquid mass transfer increased in ponds with a low aspect ratio and small water depths. The high rotational speeds of the paddle wheel enhanced gas dissolution, and large amounts of CO₂ were desorbed to the atmosphere. Moreover, sump configuration as well as geometrical and gas–liquid hydrodynamic properties significantly affected the carbonation efficiency and algal productivity.

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1. Introduction

Microalgae convert CO₂ from the atmosphere into carbon compounds (e.g., carbohydrates) during photosynthesis to be utilized in biofuel production. The conversion process of CO₂ to organic compounds by microalgae is called carbon fixation. Microorganisms, such as microalgae, that grow by fixing carbon are called autotrophs. The cultivation of microalgae (autotrophs) has two main modes: photoautotrophic and heterotrophic [1]. In photoautotrophic cultivation, microalgae use sunlight and CO₂ as energy and carbon sources, respectively. Photoautotrophic cultivation is widely used to cultivate microalgae in raceway ponds and photobioreactors [2]. Heterotrophic cultivation uses organic compounds (e.g., sugars) as energy and carbon sources. The fermenter is an application of heterotrophic cultivation. Heterotrophic cultivation is expensive because of its high maintenance cost [3]. Raceway ponds and photobioreactors are only suitable for large-scale microalgae cultivation [4–6]. The constructional and operational

expenses of a photobioreactor are approximately 100 times those of an outdoor raceway pond. Therefore, the cost of algal biomass (per kg) produced from the photobioreactor is twice that from the raceway pond. Raceway ponds also consume less energy and are easily operated with low capital and production costs [7,8]. Atmospheric CO₂ is inefficiently dissolved from air to water, and insufficient CO₂ in raceway ponds can negatively affect algal productivity. Moreover, only 5% of the required carbon is directly transferred from the atmosphere to raceway ponds [9–11]. Therefore, supplying CO₂ through an external source (e.g., a gas sparger or sump) is an effective approach to increase the CO₂ concentration in outdoor raceway ponds. The placement of a sump increases the depth of a pond, thereby significantly increasing gas hold-up, residence time, and the gas–liquid mass transfer rate [12–14]. The release of a major portion of supplied CO₂ in the atmosphere is called decarbonation or desorption. This process significantly reduces the carbon fixation efficiency by decreasing the available carbon in the pond. The CO₂ loss rate to the atmosphere mainly depends on the depth, mixing velocity, and friction coefficient of the pond. These parameters can be used to determine the mass transfer coefficient [13,15–17]. Increasing gas flow rates also increase the mass transfer coefficient and dissolved CO₂

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concentration in the pond. However, increasing the dissolved CO₂ concentration decreases the CO₂ fixation efficiency because of high CO₂ loss to the atmosphere, which consequently decreases the microalgae productivity [18]. The mass transfer coefficient is higher in the paddle wheel and sump than in the other sections of the pond. Large gas bubbles decrease the mass transfer coefficient because of low gas–liquid mixing. High mass transfer coefficients increase the algal productivity and power consumption of the pond [19].

Numerous researchers placed a vertical baffle in the center of the sump to equally divide the pond into downflow and upflow sections. This design of the sump enhances the gas–liquid mixing and transfer rate by allowing water to flow in a counter-clockwise direction with respect to gas [14,19]. Increasing the liquid and gas velocities increases the mass transfer coefficient values. The dissolved CO₂ concentration and mass transfer rate decrease when using a sump with a vertical baffle [15]. Previous studies were limited because only a single sump design (vertical central baffle) was used. Therefore, the sump design must be improved to enhance gas–liquid mixing and reduce decarbonation in raceway ponds [20]. Several alternative raceway designs have been developed to produce CO₂ bubbles in ponds without using a sump [21–23]. Moreover, novel relationships have been proposed to estimate the loss rates of CO₂ to the atmosphere and the CO₂ uptake by the raceway pond from the atmosphere [23]. However, these designs require a large amount of energy and are not feasible for mass microalgal cultivation [15,18]. In addition to sump design and gas–liquid hydrodynamic properties, the geometry of the pond can also affect gas–liquid flow mixing and carbonation efficiency. The effects of different sump designs as well as hydrodynamic and geometrical properties on carbonation efficiency are difficult to investigate. However, with the advancements in commercial computational fluid dynamics (CFD) tools, cost-effective modeling of large-scale complex multiphase flow systems has become feasible. Numerical studies involving multiphase flow systems (photobioreactors, bubble column, and airlift reactors) were conducted using the prominent Euler–Euler two-phase model [24–30]. Drewry et al. [31] modeled the exchange of CO₂ between the atmosphere and pond in the absence of a carbonation sump; however, their study disregarded the effects of hydrodynamic and geometrical properties of the pond [31]. Therefore, numerical studies regarding modeling the CO₂ exchange between raceway pond and the atmosphere while considering the effects of sump design, hydrodynamic properties, and pond geometry remain limited.

This study primarily aims to improve the carbonation efficiency of a raceway pond by modeling CO₂ desorption and absorption between the pond water and the atmosphere. The modeling will be conducted while considering the effects of sump design, pond geometry, and gas–liquid hydrodynamic properties. The study also suggested optimized values of the aforementioned hydrodynamic and geometric properties to enhance the microalgae carbon fixation efficiency. The microalgae productivity can be increased with improved CO₂ fixation based on the optimized hydrodynamic and geometric properties. The Euler–Euler two-phase numerical approach was used to model the gas–liquid flow mixing with mass transport in the entire raceway pond with carbonation sump. The gas–liquid flow mixing of CO₂ and pond water was initially modeled with the effects of atmospheric air and a paddle wheel. The velocity fields from the gas–liquid modeling were used to solve equations of the mass transfer model to compute for the dissolved CO₂ concentration and mass transfer coefficient. Novel equations from the literature were also used to estimate the CO₂ desorption rate to the atmosphere and the CO₂ absorption rate from the atmosphere as influenced by the sump [23]. Various sump designs,

gas mass flux values, paddle wheel rotational speeds, and gas bubble sizes were applied to investigate their effects on microalgae productivity and CO₂ fixation efficiency. The average or overall values of the gas hold-up, mass transfer coefficient, dissolved CO₂ concentration, CO₂ desorption rate to atmosphere, and CO₂ absorption rate from atmosphere of an entire raceway pond were calculated. Different aspect ratios and pond depths were considered to analyze the effects of pond geometry on the preceding parameters without considering the algal cells.

2. Mathematical modeling

A 2D paddle wheel (diameter = 0.6 m) with six blades (0.55 m × 0.04 m) was used to generate turbulent flow in the 3D raceway pond with a length (*L*) of 23 m and a channel width (*W*) of 2.25 m (Fig. 1). A boundary-connected coupling methodology was used to import the turbulent pulsatile flow effects of the 2D paddle wheel in the 3D raceway pond [32–34]. CO₂ was supplied to the raceway pond by using a basic carbonation sump (length (*L_s*) = 0.65 m, width (*W_s*) = 2.25 m, and depth (*d_s*) = 1 m) and was placed 1.8 m downstream of the paddle wheel, as shown in Fig. 1 [19]. Various possible sump configurations were presented to improve the gas–liquid flow mixing and carbonation efficiency of the raceway pond (Fig. 2). Fig. 2(a) shows the canvas type gas diffuser used in the experiment of Weissman et al. [13] and was placed at the bottom of the pond to supply CO₂. Model (b) represents the basic sump design (rectangular shaped) used in Mendoza et al. [19] to increase gas–liquid contact time (Fig. 2(b)). A vertical central baffle (thickness = 0.1 m) was used to split the sump into upflow and downflow sections to increase the CO₂ transfer to the liquid (Fig. 2(c)). The vertical baffle (thickness = 0.1 m) was tilted in a counter-clockwise direction (CCW) at a 15° angle to enhance gas–liquid mixing (Fig. 2(d)). The baffle thickness of model (d) was further increased to 0.15 m to examine its effects on carbonation efficiency (Fig. 2(e)). The sump (f) configuration was modeled with the baffle (thickness = 0.1 m) placed in a clockwise direction (CW) at a slanting angle of 15° (Fig. 2(f)). Another sump configuration was introduced by increasing the baffle thickness of model (c) to 0.25 m (Fig. 2(g)).

The study performed an economic analysis of the different aforementioned sump configurations by estimating the hydraulic power consumption of the raceway pond. Hydraulic power is defined as the power consumed by the paddle wheel to circulate water in the raceway pond. Hydraulic power is a function of the water flow rate and water depth in the raceway pond [13,32]. The governing equation of the hydraulic power consumption (*P_h*) is represented as follows:

$$P_h = \gamma n^2 U_l^3 d^{-0.33} \quad (1)$$

where *P_h* is the hydraulic power (W/m²), *γ* is the water specific weight (N/m³), *n* is the roughness coefficient (1), *U_l* is the liquid velocity (m/s), and *d* is the water depth (m).

The aspect ratio is a dimensionless parameter that significantly affects the flow characteristics in an open channel flow, as can be found in an algal raceway pond [35,36]. Therefore, this study used the aspect ratio (*AR*) to study the effects of the geometry or size of the pond on gas–liquid flow and mass transfer properties:

$$AR = \frac{\text{Channel width}(m)}{\text{Water or pond depth}(m)} = \frac{W}{d} \quad (2)$$

This study employed three different *AR* values (i.e., 5, 10, and 15) with different sump configurations, paddle wheel rotational speeds, pond depths, gas mass fluxes, gas bubble sizes to examine

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