A CFD-VOF based model to address intensive photobioreactor design

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Abstract

The design and optimization of photobioreactors for intensive microalgal cultures are key issues to increase process performance. A model to assess the photosynthetic performance of tubular, bubble column and flat photobioreactors is presented. The model has coupled microalgal light distribution, photosynthesis kinetics and gas-liquid hydrodynamics. A lumped kinetic parameter model of photosynthetic unit (PSU) has been adopted for photosynthetic reactions. The dynamics of a microalgal cell has been described according to the gas-liquid flow of a bubble column. The flow field induced by liquid turbulence and bubbles uprising throughout the photobioreactor have been simulated with ANSYS-FLUENT. A representative domain of the flat photobioreactor has been selected by adopting proper periodic boundary conditions. Turbulence dispersion fields have been assessed by numerical simulations for several bubble size. A random-walk model developed in MATLAB has been adopted to microalgal cells to assess the irradiance experienced by the PSU-cell in the photobioreactors. The photobioreactor performances - expressed in terms of global photosynthesis rate – have been assessed. Irradiance level and biomass concentration have been changed in the range of operating conditions typically adopted for known processes.

Keywords: flat photobioreactor, microalgae, CFD, photosynthesis, random walk, VOF

1. Introduction

The photosynthesis process to convert light and carbon dioxide in chemical energy is the base of the microalgal metabolism. Microalgae are nowadays cultivated in open ponds and closed photobioreactors [1]. The design of photobioreactors are voted to maximize the so called light-to-biomass yield. For this reason the main guideline to design the cultivation system is to have high surface to volume ratio and many geometries have been proposed in lab and pilot investigations: tubular photobioreactor, flat panel, bubble column and airlift and more advanced configurations [2]. The microalgal growth is characterized by several process with different time-scales ranging from the photon capture (few milliseconds), the gas exchange within the system (some minutes), the dynamic of the irradiance fluctuation according to the circadian cycle (24 h) and to seasonal cycle (months).

The mathematical models of the photosynthesis available in the literature are based on the lumping of a large number of biochemical reactions into simple steps and into hypothetical concepts [3-11]. Many models are based on the concept of the photosynthetic unit (PSU). The main hypothesis is that the PSU has a manifold of states that depend on the photon flux and only few simple steps are considered to approximate the photosynthesis process: light-capture, photochemical and non-photochemical quenching, photoinhibition and PSU repairing. Most of them are triggered by the actual exposition of the PSU to the light, which is is affected: 1) light field throughout the liquid culture and 2) the hydrodynamic of the microalgal cells. The light decays inside the photobioreactor depending on several phenomena as reflection, refraction, and absorption on the microalgal cells [12-14]. Instead the hydrodynamic tend to move the microalgal cell between light and dark zones. The hydrodynamic is a function of the reactor design (flat, tubular, annular, cylindrical) and of the adopted operating conditions (single-/two-phase, laminar/turbulent flow, gas and liquid flow rate, …) [15-16] In the last years, the Computation Fluid Dynamics (CFD) has frequently been adopted to characterize the photobioreactor hydrodynamics under classic and novel configurations [17-21].

Models have been proposed to couple the photosynthesis kinetics, the light intensity field, and the photobioreactor hydrodynamics [22-30]. However, many of them are characterized by criticisms because of the large difference in the time-scale of the kinetic and the hydrodynamic processes.

This work aims at describing the average performance of a base case photobioreactor (flat panel) coupling a detailed hydrodynamic simulation and a simplified kinetic model to describe the photosynthesis dynamics. A CFD-VOF model has been adopted to track the microalgal flow. The effect of a critical parameter as the bubble diameter, biomass concentration and wall irradiance on both the hydrodynamic and the kinetic of the process has been investigated.

2. Model setup

The wide spectrum of time-scales characteristic of the investigated process has required to adopt a computation strategy. On one side, the light-capture and photochemical

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quenching processes are characterized by time-scales of few milliseconds and they require a small computational time step to be described. On other hand, photoinhibition and repairing processes are characterized by time-scale of hundreds of seconds and they require a large computational time step to obtain statistically meaningful results. In addition, the light in high-concentrated cultures decays in few millimetres so very fine spatial- and/or time-discretization for Eulerian and Lagrangian models are necessary at least in this part of the computational domain.

As a matter of fact, no more than 10 s of flow real time can been simulated by the CFD and a longer conversion time – hundreds of seconds - is required to assess microalgal photosyntheis performance in the photobioreactor.

The simulation model has been structured in five sequential section:

2.1. CFD-VOF

The two-phase gas-liquid flow was simulated by using ANSYS Fluent commercial package and adopting the VOF scheme [31] to describe the bubble gas-liquid interface. The simulation looked at a 3D parallelepiped region of the photobioreactor (Figure 1): planes normal at the z axis are the reactor walls. Periodic boundary conditions were adopted for planes normal at the x and y axis. No-slip condition was adopted at the photobioreactor walls. The domain was discretised using a uniform cubic elements mesh: 168000 cells of 0.25 mm size. The time step was set at 10-4 s. Initial conditions were: one single spherical bubble at the centre of the domain; still liquid and gas phases. The bubble started to rise and to change its shape since the beginning of the simulation. The bubble velocity was calculated by averaging the gas-velocity in cell where the void fraction was larger than 0.5. The simulation was considered representative of the two-phase flow when the system approached a quasi-steady behaviour in term of bubble path and velocity.

2.2. Turbulence characterisation

The main results of the section I were the velocity fields ($v_i(x,y,z,t)$ where i=x, y, z) and of gas volume fraction ($\varepsilon_G(x,y,z,t)$). The turbulent behaviour of the flow was characterised in term of statistical data - the velocity variance, the Lagrangian integral time scale, and the turbulent dispersion – referred to the three component x,y,z according to Roberts [32] and calculated in each computational cell:

$$v_i'^2(x,y,z) = \int \left(v_i(x,y,z,t) - \langle v_i(x,y,z) \rangle_t \right)^2 dt \qquad (1)$$

$$T_{L\,i}(x,y,z) = \int_0^{+\infty} \int_0^{+\infty} \frac{v_i(x,y,z,t) \cdot v_i(x,y,z,t+\tau)}{v_i'^2} dt d\tau \qquad (2)$$

$$D_{T\,i}(x,y,z) = v_i'^2(x,y,z) \cdot T_{L\,i}(x,y,z) \qquad (3)$$

Data assessed by Eqs (1), (2) and (3) were averaged over the x and y axis according to the periodic behaviour imposed at the boundary walls normal to these axis:

$$v_i'^2(z) = \iint v_i'^2(x,y,z) dxdy \qquad (4)$$

$$T_{L\,i}(z) = \iint T_{L\,i}(x,y,z) dxdy \qquad (5)$$

$$D_{T\,i}(z) = \iint D_{T\,i}(x,y,z) dxdy \qquad (6)$$

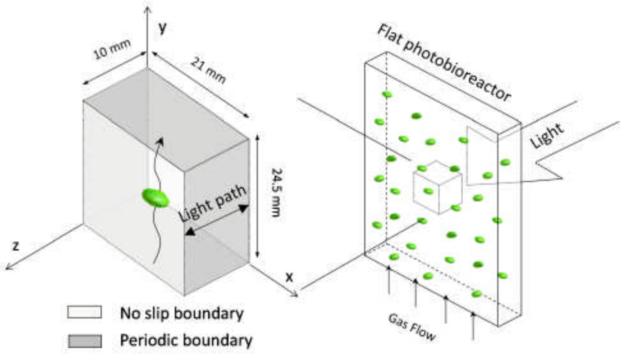

Figure 1 – System domain and boundaries for the CFD-VOF simulation

2.3. Random walk scheme

The average turbulent characteristics (function of z) were used to assess the flow of microalgae. The microalgal displacement was simulated by adopting a random walk according to the Langevin scheme [33]. The velocity (u_x,u_y,u_z) and the position (x,y,z) of a microalgal cell as a function of the time t was calculated:

$$du_i = \left(-\frac{u_i}{T_{i\,L}} + \frac{1}{2}\left(1 + \frac{u_i^2}{v_i'^2}\right) v_i'^2 \right) dt + \sqrt{\frac{2 v_i'^2 dt}{T_L}} \xi_i \qquad (7)$$

$$(x,y,z)_{t+dt} = (x,y,z)_t + (u_x, u_y, u_z) \cdot dt \qquad (8)$$

where (ξ_x, ξ_y, ξ_z) is a Wiener isotropic process.

2.4. Irradiance field

Assuming the Lambert-Beer law, the coefficient K of light exponential decay from the wall irradiance I° through a photobioreactor depends on the light-path (LP), the dry weight specific absorption coefficient (a^*_{DW}) and biomass concentration (X). The instantaneous level of irradiance on the tracked algal cell can be calculated as

$$I(t) = I^0 e^{-a^*_{DW} X \cdot z(t)} \qquad (9)$$

2.5. Photosynthesis rate

The lumped kinetic model of photosynthesis proposed by Eilers and Peeters [3] and Camacho-Rubio et al. [8] has been adopted in the present simulation. The PSU is characterized by three states: open or resting (x_1), activated or closed (x_2), and damaged or non-functional (x_3). x_1, x_2 and x_3 are the fraction of PSU in each state (Figure 1). The PSUs in open state is activated by the photons capture (PC) process. The fate of activated PSUs depends on the probability to be further irradiated. The natural fate is to transfer the fixed energy to the successive photosynthetic pathway, a step identified by Camacho-Rubio et al.

[8] and known as the photochemical quenching (PQ) process. A second possible fate of the activated PSU is the non-photochemical quenching (NPQ): the extra photons may be discharged by means of the dissipative process without state change. The photoinhibition (PI) process occurs if the NPQ process is not sufficient to dissipate the exceeding irradiance: a x_2-PSU irradiated by an extra photon is inhibited, and it assumes the damaged state x_3. The x_3–PSU does not participate to the photosynthesis process and the PSU may recover the open state according to a repair (REP) mechanism. Figure 2 reports a sketch of the state flow and kinetics. According to Eilers and Peeters [3], the adopted photosynthetic model is:

$$\begin{aligned} \frac{dx_1}{dt} &= -\alpha I x_1 + \gamma x_2 + \delta x_3 \\ \frac{dx_2}{dt} &= \alpha I x_1 - \gamma x_2 - \beta I x_2 \\ \frac{dx_3}{dt} &= \beta I x_2 - \delta x_3 \end{aligned} \quad (10)$$

The photosynthesis rate Φ has been assumed proportional to the PQ rate. Therefore, the value of x_2 is the ratio between Φ and the maximum photosynthesis rate Φ^{MAX}, associated to the condition of all the PSUs activated. The kinetic parameters of Wu and Merchuk [26] have been adopted: $\alpha=1.935\cdot10^{-3}$ m^2 /μE, $\beta=5.7848\cdot10^{-7}$ m^2 /μE, $\gamma=0.146$ s^{-1}, $\delta=4.796\cdot10^{-4}$ s^{-1}.

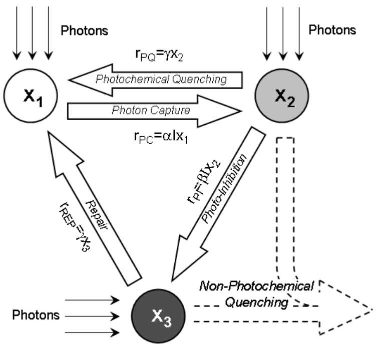

Figure 2: The lumped kinetic model of photosynthesis after Eilers and Peeters [3].

3. Results and discussion

3.1. Two-phase hydrodynamic and average turbulent field

Figure 3 reports snapshots of the bubble path along the domain picked during the last 5 s of the simulation. The shape and the path of the bubble strongly depend on the bubble diameter: A) d_B=3 mm, the bubble mainly fluctuates between the two walls keeping an ellipsoidal shape; B) d_B= 6mm, the bubble oscillates mainly along the horizontal direction x between the two periodic boundaries; C) d_B= 8 mm, the bubble assumes a sort of wobbling shape and the walls strongly affect its capacity to fluctuate in the x,z direction.

Figure 4 reports results of the simulations in terms of bubble velocity along the y vertical axis ($v_{y\,B}$) as a function of the time. The time series refer to three simulations carried out with different initial bubble diameter (d_B): 3, 6 and 8 mm. After 2-3 s the bubble velocity starts to fluctuate and approaches a constant average value. The average bubble velocity slightly decreases from 0.18 m/s to 0.15 m/s when the bubble diameter increases from 3 to 8 mm. The time series calculated during the last 5 second of each simulation have been used for the turbulence analysis of the velocity fields.

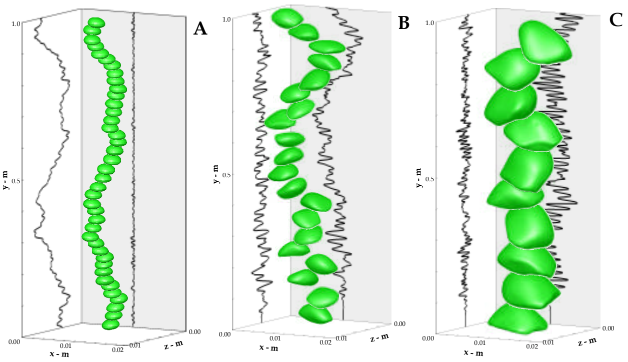

Figure 4 – Simulation results: bubble path along the domain (A – d_B=3 mm; B – d_B=6 mm; C – d_B=8 mm)

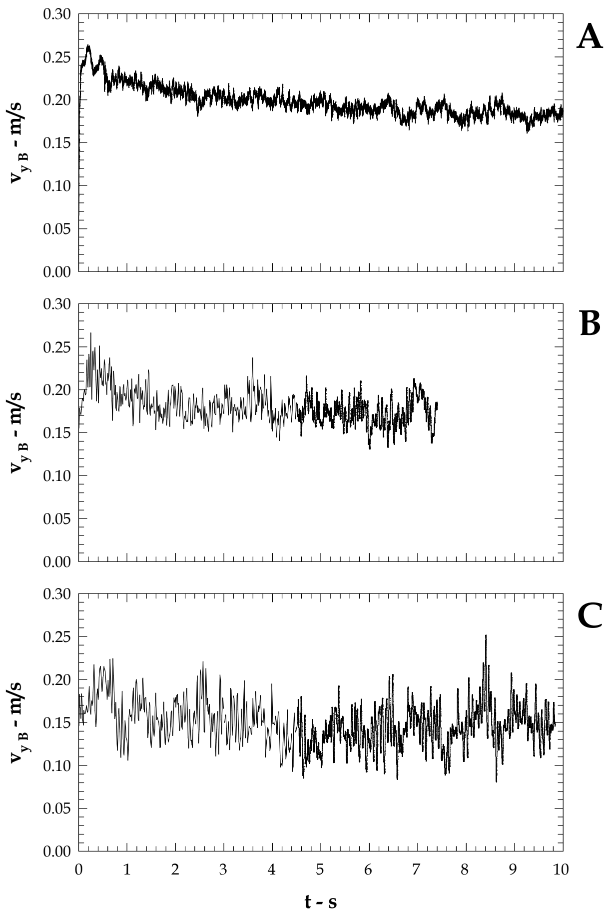

Figure 4 – Simulation results: vertical bubble velocity as a function of the time. (A – d_B=3 mm; B – d_B=6 mm; C – d_B=8 mm)

Figure 5 reports the map of the average values of the turbulent dispersion of the liquid phase assessed for the flux along the three axis x,y,z as a function of the z position. It is possible to observe that the highest turbulence level regards the y direction. This dominant turbulence may be interpreted taking into account the presence along this direction of the driving force of the bubble flow. The D_T in z direction changes remarkably with the bubble diameter from 3 to 6 mm and does not change anymore with a further increase of d_B to 8 mm.

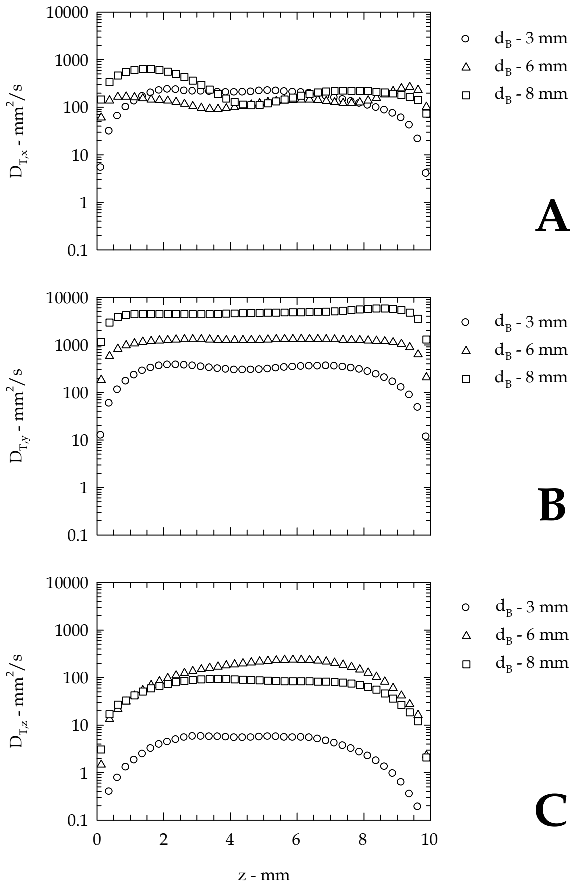

Figure 5 – Turbulent dispersion in the x (A) ,y (B) and z (C) direction for the value of the bubble diameter.

3.2. *Microalgal tracking and PSU dynamic*

The microalgal tracking has been carried out according to the Langevin approach assuming the v'^2 and T_L assessed by the CFD simulations. Figure 6 reports few seconds of the microalgal displacement on the y-z plane. According to the model, the microalgal has lost the memory of its path on the T_L time scale. Perfect reflection has been assumed at the photobioreactor wall.

Figure 6 – Microalgal path according to the Langevin scheme of random walk in 3 mm bubble flow.

The dynamics of the PSU has been simulated for a microalgal cell in the three-dimensional investigated domain swept by bubbles. The time-average values of $I(t)/I^0$, $x_1(t)$, $x_2(t)$ and $x_3(t)$ have been calculated and the simulation have been stopped when their standard deviation were smaller than 10^{-6}. Figure 7 A-C reports the time-average PSU states as a function of the biomass concentration X from 0.1 to 10 g/L at a wall irradiance I^0=2000 μE/(m^2 s) for d_B of 3, 6 and 8 mm.

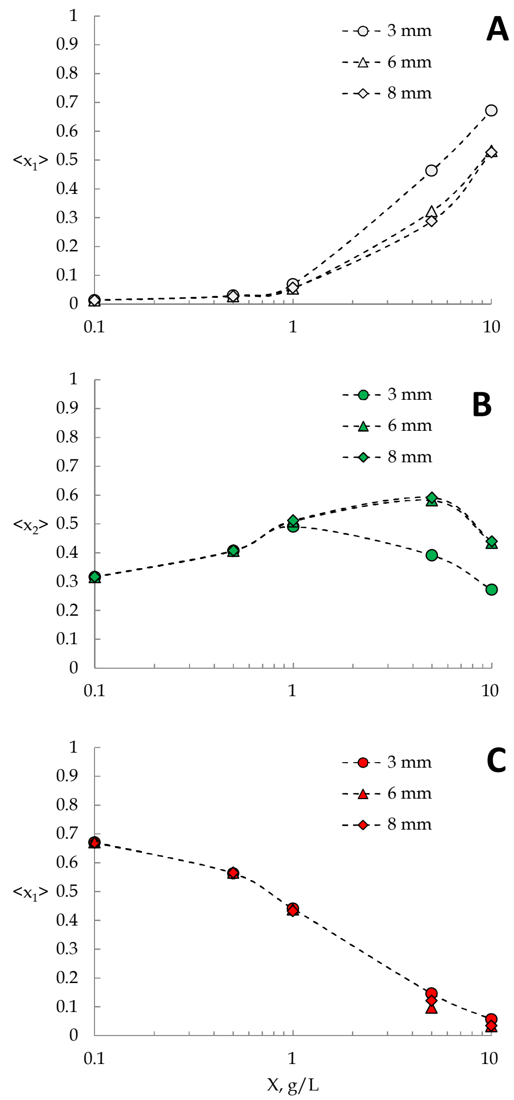

Figure 7 – Average PSU state as a function of the biomass concentration (X) for three different bubble diameter: 3 mm (A), 6 mm (B), 8 mm (C)

Since the photosynthesis rate is proportional to the PQ step of the PSU model, the extent of $<x_2>$ gives an indication of the value of the photosynthesis rate. According to that for X<1 g/L no difference can be found in the result induced by three different size of the bubbles. Instead for X>1 g/L, the turbulence induce by 6 mm bubbles enhance the photosynthesis rate more than in case of 3 mm bubbles. No further enhancement can be observed instead when 8 mm bubbles are flowing up through the domain. Olivieri et al., [35] found in their model accounting a simple homogenous and isotropic turbulence field, that the upper limit of x_2 is always related to the case of well mixed conditions when the turbulence has a characteristic time lower than the kinetic related to the PSU dynamic. In this case, the model has been improved taking into account a non-homogeneous and an-isotropic turbulence field. Even in this case the photosynthesis rate is maximised when the turbulence time scales are significantly larger than the characteristic kinetic times. A further increase of turbulence results only in a larger energy consumption due to pumping the bubbles throughout the photobioreactor.

Figure 8 shows the effect of the wall irradiance I0 on $<x_2>$ at different biomass concentrations.

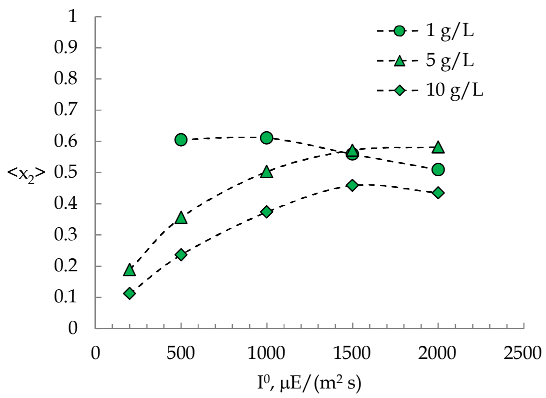

Figure 8 – $<x_2>$ as a function of the wall irradiance for different biomass concentration

The data are not trivial: for 1 g/L the phosynthesis rate is maximised at low value of I^0 meaning that the light decay is not so high to prevent photoinhibition. Instead increasing the biomass concentration gives better result at high value of wall irradiance: the increase in the light decay is now strongly reducing the photo-inhibition phenomena which are limited only in a small layer close to the irradiated wall. In addition, it seems that an optimal biomass concentration can be observed at 5 g/L, meaning that a further increase in the growth doesn't end in better photosynthesis rate.

If we assume that the specific growth rate is only limited by the photosynthesis, then the best biomass productivity is obtained at 5 g/L and high wall irradiance. According to Hu et al., [36] with further lowering the photobioreactor thickness, the photosynthesis rate should be maximised at higher biomass concentration.

4. Conclusions and future perspectives

The model of a thin flat photobioreactor coupling CFD, radiative transfer and photosynthesis dynamic has given significant insight in how to optimise the design and operation of this configuration. Results are in agreement with what found in literature and provide also indication on the level of gas sparging required to achieve the so called "light well mixed" condition reported previously [34]. Further confirmation of what postulated discussing figure 8 can come by using the model to characterise the effect of the light path in thin flat photobioreactor.

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