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Mechanistic model for design, analysis, operation and control of microalgae cultures: Calibration and application to tubular photobioreactors

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ABSTRACT

Closed photobioreactors (PBRs) are usually used for the production of high-value microalgae biomass at higher productivities than in open ponds. A large variety of different PBRs have been developed to optimize the biomass productivity and photosynthesis efficiency. At the same time mathematical models for PBRs are also increasing in popularity for design of new systems and for improving understanding of the complex processes occurring inside. The aim of the present study is to calibrate of the new mechanistic model for microalgae growth using experimental data from two different tubular photobioreactors. Hydrodynamic and light attenuation through the medium were added in the model to obtain a realistic representation of photobioreactor. Furthermore, the model was able to predict microalgae production under different climatic conditions and the oxygen accumulation throughout the photobioreactor.

1. Introduction

Industrial production of microalgae can be accomplished in open or closed photobioreactors. Open systems are shallow channels in the shape of race tracks (raceway reactors) and have been extensively studied in the past [8,13]. Though open photobioreactors represent an efficient economic solution in front of closed photobioreactors, they can be easily contaminated by microorganisms and difficult to control. These disadvantages make closed photobioreactors more suitable when high-value products are the target of the culture. Closed systems strictly control chemical, physical and biological factors and can improve conditions for microalgae growth by optimizing light absorption due to turbulent conditions in the culture [8,9,25,26].

Closed photobioreactors (as well as open raceways) are sensitive to carbon limitations and pH variations that could limit photosynthesis and therefore biomass production [14]. Carbon and pH limitations can be corrected by supplying carbon dioxide (CO_2^-) in order to maintain high photosynthesis rates and pH control. However the two most critical issues of closed photobioreactors are the risk of overheating and their potential for oxygen accumulation and subsequent growth inhibition [18]. To prevent overheating, closed photobioreactors often require cooling as well as degasser systems [27]. Concentrations of dissolved oxygen (DO) in the culture above 250% air saturation can dangerously inhibit microalgae activity [10].

Over the last few decades, mathematical models have proven to be useful tools for the design, analysis, operation and control in multiple engineering problems [5]. Nowadays, models have become essential tools for understanding complex processes, such as those occurring in photobioreactors. In the case of microalgae cultures, models are less developed than those seen in other fields. When models contain too few parameters, they risk the capability of not capturing the complexity of microalgae cultures in long-term scenarios, and therefore can be unreliable. Having this in mind, Solimeno et al. (2015) [22] developed a complete mechanistic mathematical model that includes crucial physical and biokinetic processes that describe microalgae growth in different types of cultures, particularly in wastewater (where growth is controlled by carbon and nitrogen limitations). This model was calibrated with data from a complete stirred culture fed with simulated treated wastewater using a 0D domain [22]. A global sensitivity analysis was carried out using the same set of data [23]. In the present paper we intend to go beyond our previous work, calibrating the model with data from two different pilot scale tubular closed photobioreactors fed with different types of medium culture. In this present case, a 2D domain, which represents the hydrodynamics of the system (i.e., transport of diluted species and mass transfer phenomena), is coupled with the

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previous mechanistic model [22]. The resulting model has been implemented into the COMSOL Multiphysics™ software, which solves equations using the finite elements method (FEM).

The aim of the present study is to calibrate the new and more complex mechanistic model of Solimeno et al. (2015) [22] using experimental data from two different tubular photobioreactors. The potential of the model is demonstrated by means of practical study cases in which we simulate oxygen concentrations (the most critical growth inhibition factor of closed photobioreactors) and predict microalgae production as a function of temperature and light intensity. Simulations show the potential of photobioreactor configurations to optimize microalgae production. The overall objective of this model is to become a reference to simulate physical, chemical and biokinetic microalgae processes in different types of photobioreactors fed with different types of medium cultures.

2. Methods

2.1. Pilot closed photobioreactors and experimental data

Both photobioreactors were located in Spain, one in "Estación Experimental Las Palmerillas", property of Fundación CAJAMAR in Almeria, and the other in "Agropolis", property of Universitat Politècnica de Catalunya-BarcelonaTech in Barcelona (Fig. 1). The vertical tubular photobioreactor (PBR) in Almeria includes a loop solar receiver made of transparent plastic tubes of 0.09 m diameter with a total horizontal length of 400 m, and a 0.4 m diameter bubble column with 3.5 m of height, and has a total working volume of 3000 L. The PBR unit is used to produce the microalgae *Scenedesmus almeriensis*, which is characterized by a high growth rate and tolerance temperatures up to 45 °C and pH values up to 10 [1,20]. The PBR works by creating continuous flow of culture between loop and bubble column by means of a centrifuge pump located at the bottom of the column. The pump provides a constant flow velocity of 0.8 m s^{-1} inside the loop. The pH of the culture is controlled by injection of pure CO_2 at 5 L min^{-1}. In the bubble column, excess DO is removed by a constant airflow rate of 140 L min^{-1}. The culture temperature is maintained by passing cooling water at 1500 L/h through an internal heat exchanger located inside the bubble column. When fresh culture medium is poured into the system, the culture is harvested through an overflow located on top of the column. Temperature, pH and DO are measured at several locations along the tube using Crison probes (Crison Instruments, Spain) connected to a control-transmitter unit MM44 (Crison Instrument, Spain). Liquid and gas flow rates are measured using digital flowmeters (PF2W540 and PF2A510, from

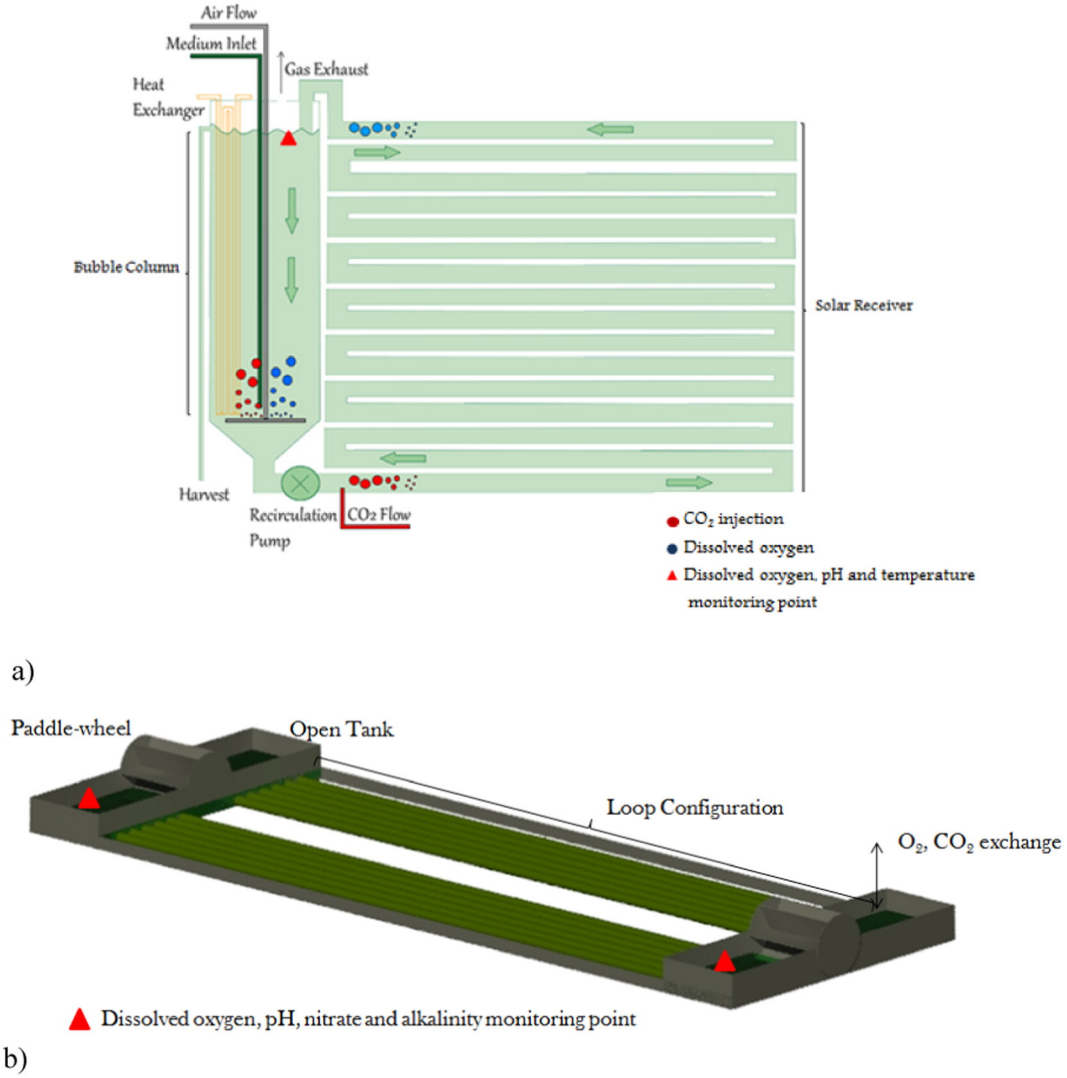

Fig. 1. a) Tubular vertical photobioreactor located in Almeria (Spain) with details of the solar receiver (a continuous tubular loop) and a mixing unit (a bubble column). The culture is continuously recirculating from one to the other part using airlift and mechanical pumps [14]. b) Tubular horizontal photobioreactor located in Barcelona (Spain) with details of the two open-air tanks and the loop configurations (6 tubes per each flow direction). Mechanical paddlewheels promote the recirculation of the culture through the system.

Table 1
Agricultural runoff characteristics during batch experiment in the tubular horizontal photobioreactor located in Barcelona (Spain).

Parameter	Agricultural runoff
pH	8.4
Dissolved oxygen (g m^{-3})	6.6
NO_3^--N (g m^{-3})	0.6
Alkalinity (g $CaCO_3$ m^{-3})	42

SMC, Japan). All of these monitoring systems are in turn connected to a control computer through a data acquisition device NI Compact FieldPoint (National Instruments, USA) [13]. Data for the present study were obtained at the end of a two month experiment in which the photobioreactor was operated in continuous mode, medium flow rate of 1020 L d^{-1}, and under controlled pH (7.8) and temperature (lower than 35 °C). As a result, the amount of microalgae biomass was kept fairly constant. Culture medium used was Mann&Myers, prepared using agricultural fertilizers. Collected data were retrieved in batch mode by switching off the feeding for 24 h (at the end of the two months). Dissolved oxygen and pH data were recorded every 30 min, while temperature and irradiance were measured every hour.

The horizontal tubular photobioreactor in Barcelona is composed of two open-air tanks made of polypropylene and is 1.8 × 1 × 0.4 m (L × W × H) in size. These tanks include paddlewheels that provide enough head pressure to move the culture through 12 (6 per each flow direction) transparent 0.125 m diameter polyethylene tubes (each 50 m length). Culture flows from one tank to the other at a constant velocity of 0.125 m s^{-1}. Tanks also allow release of exceeding oxygen accumulated along tubes. The PBR has an effective volume of 8.5 m^3. Note that in this PBR there is no CO_2 injection or pH control. Data used for the present work were retrieved from a three days batch experiment and measured in each tank. For this experiment the PBR was filled with 8 m^3 of agricultural runoff from a nearby agriculture canal which were inoculated with 0.5 m^3 of inoculum with microalgae from a previous experiment (Table 1). The PBR contained different microalgae species belonging to the genus *Pediastrum* sp., *Chlorella* sp. and *Scenedesmus* sp.

The horizontal PBR has dissolved oxygen and pH online sensors in each tank that record data every hour, and temperature and irradiance online sensors that record data every two to three hours. Gathered data are stored using a Programmable Logic Controller (PLC) that is connected to a computer with supervisory control and a data management system (Green web manager 2.0). During the three days of experiments, offline samples were taken every two-three hours and analyzed in the laboratory for nitrates and alkalinity. Analysis of nitrate ion chromatography was accomplished using a Thermo Finnigan chromatograph with a metallic detector TCD (thermal conductivity detector). Alkalinity was analyzed using conventional titrimetric procedures indicated in Standard Methods [3]. Note that bicarbonate was calculated using alkalinity measurements, pH, and equilibrium constants of carbon species (Eq. (1)).

$$\text{Alkalinity} = 50 * \left[\frac{S_{HCO3}}{12} + 2 * \frac{S_{CO3}}{12} + S_{OH} - S_H\right] \quad (1)$$

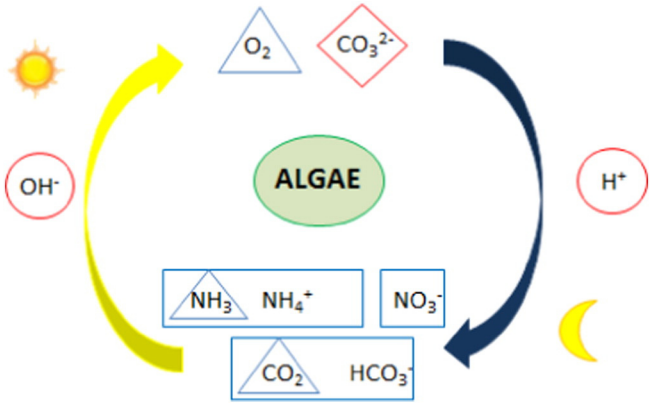

Fig. 2. General schematic representation of the conceptual model by Solimeno et al. (2015) [27]. Microalgae (green ellipse), substrates (rectangles), gaseous species (triangles) and species depending on algal activity which are neither substrates nor gases (diamonds and circles). Other nutrients (e.g. phosphorus) and micronutrients are not limiting factors. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

2.2. Conceptual model

The new mechanistic model presented by Solimeno et al. (2015) [22] considers crucial physical, chemical and biokinetic processes for the description of microalgae growth in different types of cultures, particularly in wastewaters. The main relevant feature of the model, respect to any previous model for microalgae production [4,6,19], consists in the inclusion of a carbon limitation on the growth of microalgae, as well as a dynamic model for photosynthesis, photolimitation, light attenuation, and photorespiration. In the model, microalgae grow with light, consume nutrients (i.e., carbon and nitrogen), and release oxygen (Fig. 2).

Note that other nutrients (e.g., phosphorus) and micronutrients are not considered to be limiting factors because are usually highly available in wastewaters (which is the type of culture mainly addresses by the model) [17]. Dependency of microalgae growth on phosphorus could easily be implemented in the model by creating a limiting Monod function, similar how the other nutrients (i.e., carbon and nitrogen) were represented. In the model, as a result of microalgal activity in the presence of light, hydroxide ions concentration and pH increase. Increases in pH displace the equilibrium of the carbon species towards the formation of carbonates (which are not bioavailable for growth). Note that this model assumes that carbon dioxide as well as bicarbonate are bioavailable for growth. In darkness, endogenous respiration of microalgae release carbon dioxide, the concentration of hydrogen ions increase and the pH decreases. With decreasing pH, the carbon equilibrium shifts and carbonate turns into bicarbonate, which can be used as substrate again in the presence of light [25]. A detailed description of the model, including components, and processes can be found in Solimeno et al. (2015) [22]. A list of the processes included in the model, the equations describing their rates and the matrix of stoichiometric parameters are shown in Supplementary Tables (4–5).

2.3. Model domain

The photobioreactor's configuration was assumed to have a 2D geometry. The domain was divided into two sub-domains (D1 and D2) corresponding to the loop configuration and the bubble column for the vertical system in Almeria, and to the open-air tanks and the tubes for the horizontal system in Barcelona (Fig. 3). In the case of the vertical system, D1 was 400 m long in the longitudinal direction and 0.09 m in diameter, while in the horizontal system it was 50 m long and 0.125 m in diameter. D2 domains were designed allocating the volume of the bubble column (vertical system) and open-air tank (horizontal system) along a surface interface area where gases were transferred to the atmosphere, fixing the corresponding D1 diameter. Thus, the bubble column is 3.3 m long and 0.09 m deep, while the tank is 5.76 m long and 0.125 m deep. These simplifications allow to simulate of hydrodynamics within the system. Note that in the present model it was necessary to divide the domain into two sub-domains due to the different domain conditions. Transfer of gases to the atmosphere took place exclusively in the bubble column and open-air tanks. A periodic condition was applied at

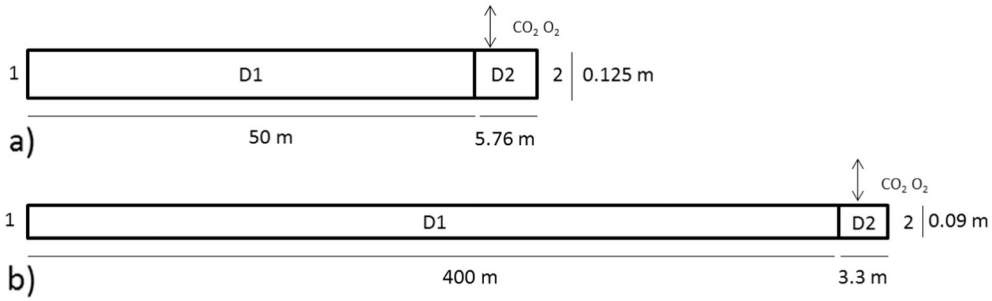

Fig. 3. Schematic representation of the model domain, a) simplification of the horizontal photobioreactor located in Barcelona (Spain), b) simplification of the vertical photobioreactor in Almeria (Spain). D1 represents the loop configuration of both PBRs and D2 is the total volume of open-air tank (a) and bubble column (b) respectively for horizontal and vertical photobioreactor. A periodic condition was applied at boundaries 1 and 2 to reproduce the continuous culture flow.

boundaries 1 and 2 to reproduce the continuous culture flow from domain 2 to 1 (degasser to loop and tank to tube).

2.4. Hydrodynamics of the system, light attenuation and temperature

In our previous work [22], the calibration of the model was conducted in a complete mixed reactor represented by a 0D domain in order to simplify hydrodynamic's complexity. In the present work, as a result of the motion of the culture through the tubes and bubble column or open-air tank, a 2D domain was needed, which include hydraulic and transport equations. On the other hand, in the previous work [21], it was assumed that microalgae cells captured photons at all depths (light attenuation was neglected due to 0D domain). The present work incorporates light attenuation due to the presence of microalgae.

In the model microalgae processes are influenced by temperature [22]. It is known that the growth rate of microalgae is highly dependent on temperature; it increases when optimum temperature is reached and drastically decreases when optimum temperature is exceeded [12]. In the present study, microalgae production was simulated in a study case at different temperatures, showing the dependence of microalgae growth on temperature.

Hydrodynamics of system was modeled through the COMSOL Multiphysics™ software, previously used for the calibration of the microalgae model in a completely stirred experiment, which solves differential equations using the finite elements method (FEM).

2.4.1. Hydraulic considerations

In the PBR used in this work the culture is set in motion by an external pump (vertical system) or by paddlewheels (horizontal system), and enters the model domain with a certain velocity. To predict the flow regime without starting a simulation, the Reynolds number was firstly calculated. The Reynolds number quantifies the ratio of inertia to viscous forces, characterizing the flow regime (Eq. (2)):

$$Re = \frac{\rho * v * d}{\mu} \tag{2}$$

where ρ is the culture density (assumed to have the same density as water, 1000 kg m^{-3}), v is the culture velocity (m s^{-1}), d is the tube diameter (0.09 m and 0.125 m for vertical and horizontal systems, respectively), and μ is the dynamic viscosity of the culture (assumed to be the same as water 0.003 kg m^{-1} s^{-1}). The Reynolds number was calculated to be approximately 27,000 for the vertical system and 5000 for the horizontal. Note that in tubes with a flow with a Reynolds number above 4000 is already considered turbulent [24], and in these conditions transversal variations of culture properties (temperature, dissolved oxygen, biomass concentration, etc.) may be neglected and Navier-Stokes equations can be solved directly. With such high Reynolds number's temperature does not significantly influence the motion because viscous forces (μ) are very small when compared to inertial forces (v).

For turbulent flow, COMSOL Multiphysics™ solves the Navier-Stokes as well as continuity equations. Turbulent effects are modeled using "Turbulent Mixing" interfaces for "Transport of Diluted Species" physics. In "Turbulent Mixing" models the additional mixing caused by turbulence is estimated by adding turbulent diffusivity to the molecular diffusivity considering:

$$D_T = \nu_T / Sc_T \tag{3}$$

where D_T is the turbulent diffusion, ν_T is the turbulent kinematic viscosity at 20 °C (1.004E-06 m^2 s^{-1}) and Sc_T is the turbulent Schmidt number (0.7).

Table 2
Dissolved and particulate components considered in the model.

Component	Description	Units
Dissolved components		
S_{NH4}	Ammonium nitrogen	gN-NH_4 m^{-3}
S_{NH3}	Ammonia nitrogen	gN-NH_3 m^{-3}
S_{NO3}	Nitrate nitrogen	gN-NO_3 m^{-3}
S_{CO2}	Carbon dioxide	gC-CO_2 m^{-3}
S_{HCO3}	Bicarbonate	gC-HCO_3 m^{-3}
S_{CO3}	Carbonate	gC-CO_3 m^{-3}
S_{O2}	Dissolved oxygen	gO_2 m^{-3}
S_H	Hydrogen ions	gH m^{-3}
S_{OH}	Hydroxide ions	gH-OH m^{-3}
Particulate component		
X_{ALG}	Microalgae biomass	gTSS m^{-3}

Table 3
Initial concentrations of the components in the vertical photobioreactor of Almeria (Spain) and horizontal photobioreactor of Barcelona (Spain).

Components	Concentrations		Units
	Vertical PBR	Horizontal PBR	
X_{ALG}	774.14	251	gTSS m^{-3}
S_{NH4}	14	–	gN-NH_4 m^{-3}
S_{NH3}	0.684	–	gN-NH_3 m^{-3}
S_{NO3}	4.2	0.6	gN-NO_3 m^{-3}
S_{CO2}	1.59	0.068	gC-CO_2 m^{-3}
S_{HCO3}	100	7.59	gC-HCO_3 m^{-3}
S_{CO3}	0.62	0.085	gC-CO_3 m^{-3}
S_{O2}	7.2	6.64	gO_2 m^{-3}
S_H	6.31E-6	3.55E-6	gH m^{-3}
S_{OH}	1.58E-3	2.82E-3	gH-OH m^{-3}

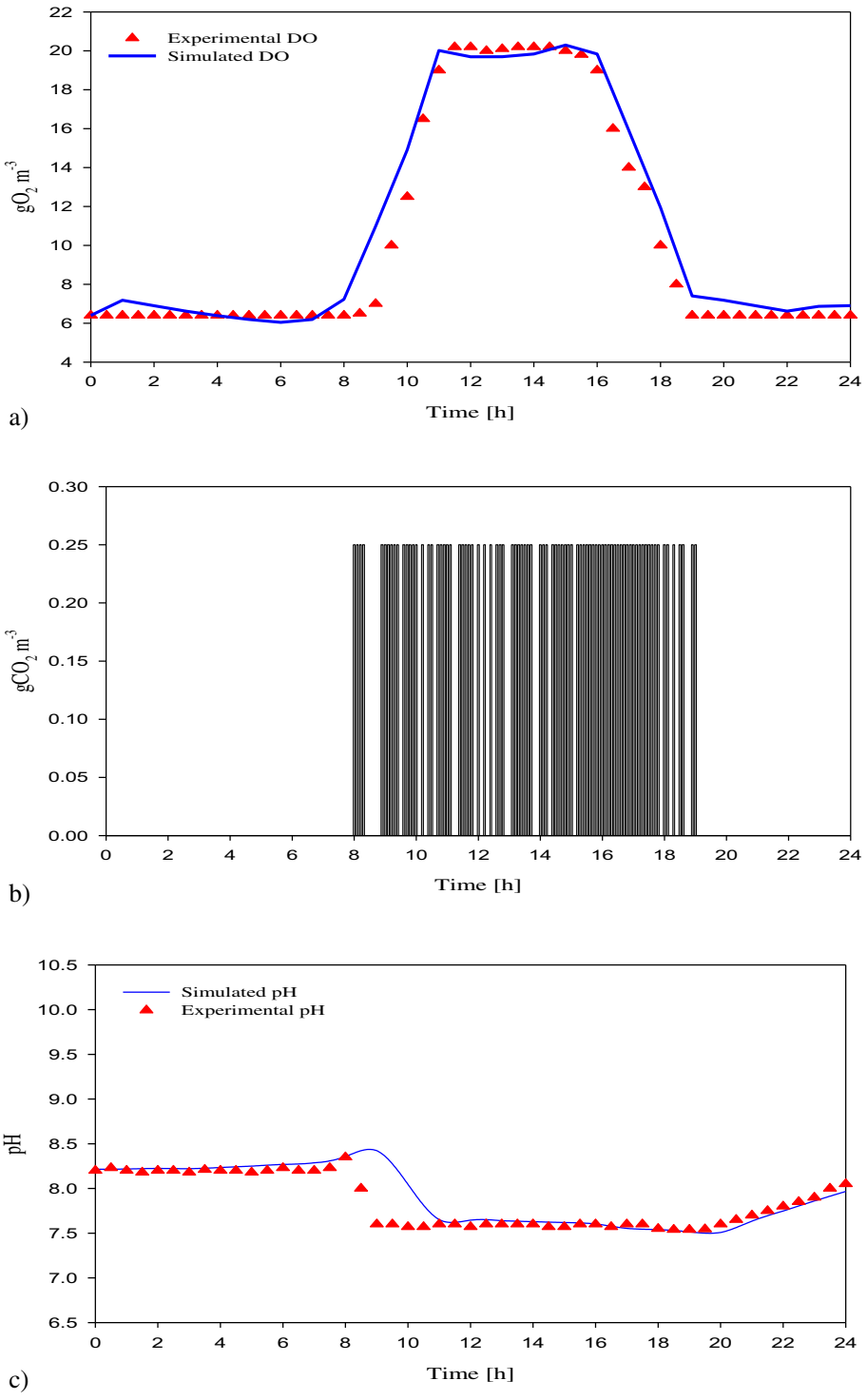

Fig. 4. Experimental (red triangles) and simulated (blue line) (a) dissolved oxygen (DO) and (c) pH values as a function of CO_2 injection (b) over the 24 h in the vertical photobioreactor in Almeria (Spain). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

2.4.2. Transport of dissolved and particulate components

Transport of diluted and particulate components with a concentration S_i [g m^{-3}] by convection and diffusion is given by:

$$\frac{\delta Si}{\delta t} + (-D_T \cdot S_i) + \mathbf{u} \cdot c_i = r_i \quad (4)$$

$$r_i = \sum_j v_{j,i} * \rho_j \quad (5)$$

where i = 1, 2…m are the different components considered (Table 2), and j is the number of processes shown in Supplementary Table (4); u [m s^{-1}] is the vector of velocity, r_i [g m^{-3} s^{-1}] is the reaction rate, ρ [g m^{-3} s^{-1}] is the process rate corresponding to the biokinetic and chemical j processes described in Solimeno et al. (2015) [22] and $v_{j,i}$ is the stoichiometric coefficient. Mathematical expressions of the stoichiometric coefficient and values of biokinetic, physical and chemical parameters are shown in Supplementary Tables (6–9).

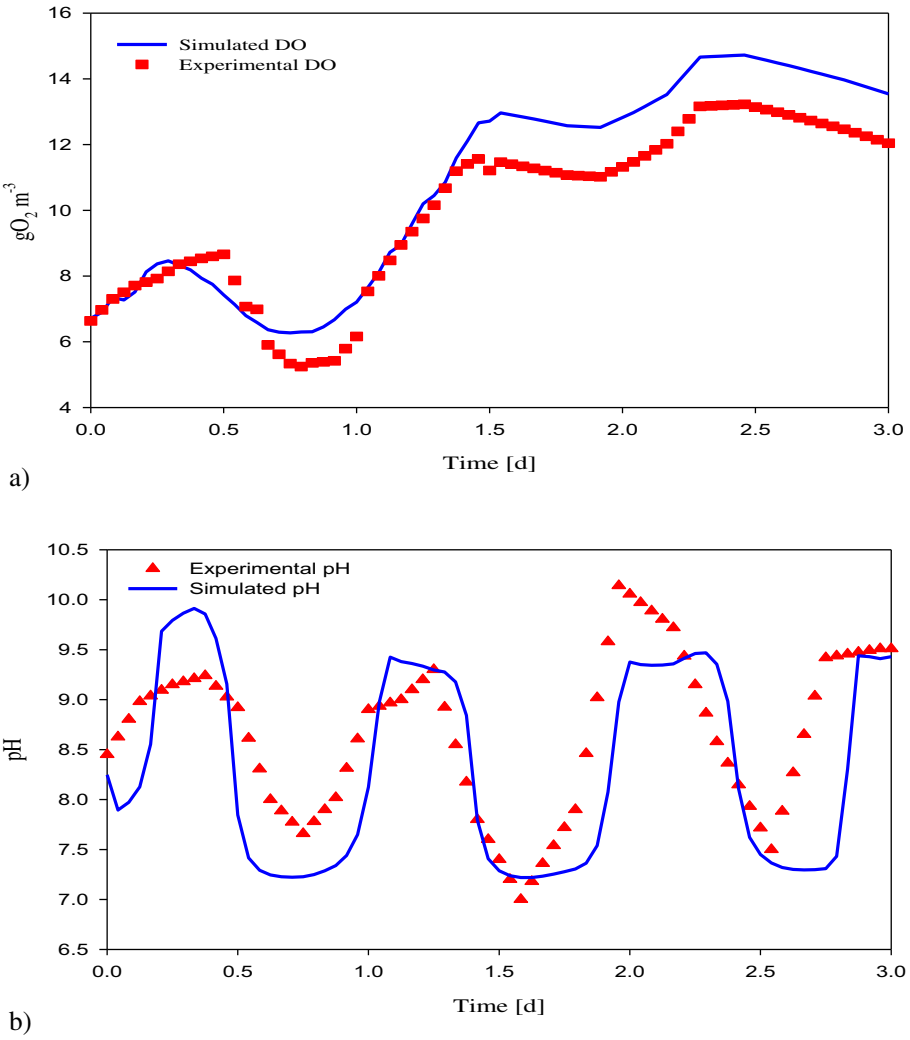

Fig. 5. Experimental (red triangles) and simulated (blue line) (a) dissolved oxygen (DO) and (b) pH values over the three days in the horizontal photobioreactor in Barcelona (Spain). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

2.4.3. Light attenuation

In the present study light intensity decay was described using Lambert-Beer's Law, which dictates that intensity decreases exponentially as it penetrates into a perfectly homogeneous section of culture with a short penetration pathway [20], as it is the case of both PBR. In this case light is attenuated by the presence of microalgae inside the reactors. The average light intensity (I_{av}, [μmol m^{-2} s^{-1}]) at any point within the culture is therefore calculated as [15]:

$$I_{av} = I_o \cdot \psi \, (1 - \exp(k_i \cdot X_{ALG} \cdot d)/(k_i \cdot X_{ALG} \cdot d) \quad (6)$$

where I_o [μmol m^{-2} s^{-1}] is the incident light intensity, k_i is the extinction coefficient for microalgae biomass [0.1 m^2 g^{-1}] [7], X_{ALG} is the concentration of microalgae, ψ is the solar irradiance fraction available in the reactor and d [m] is the diameter of tube.

2.4.4. Temperature

In our model, the influence of temperature on microalgae activity was implemented by the thermic photosynthetic factor ($f_{T,FS}$), which takes into account the effects of temperature on microalgae growth, endogenous respiration and inactivation processes (1a, 1b, 2 and 3 in Supplementary Table 4, respectively). Water temperature varies both on hourly and daily scales, affecting microalgal photosynthesis and respiration rates. The thermic photosynthetic factor is represented in the model following the work of Dauta et al. (1990) [12]:

$$f_{T,FS}T = e^{-\frac{T-Topt^2}{s}} \quad (7)$$

where T_{opt} (optimum temperature) was assumed to be 25 °C [12] and s equal to 13 [12] (it is a parameter value for empirical fitting).

2.5. Calibration procedure

Model output results are highly sensitive to the maximum specific growth rate of microalgae (μ_{ALG}), mass transfer coefficient for oxygen ($K_{a,O2}$), and carbon dioxide ($K_{a,CO2}$). The mass transfer coefficients depend on the extension of the surface interface and photobioreactor design [22]. Therefore, these parameters were calibrated in the two different tubular photobioreactors. The model was first calibrated using experimental data obtained from the vertical photobioreactor located in Almeria (Spain). Dissolved oxygen, pH, temperature and irradiance were monitored for 24 h on February 28th, 2012. Afterwards, the model was calibrated with experimental data from the horizontal photobioreactor located in Barcelona (Spain). Data used for this calibration were retrieved from three days batch experiment from April 16th, 2012 to April 19th, 2012. Available data used for the calibration procedure are shown in Supplementary Tables (1–2). The initial concentrations of components in the vertical and horizontal photobioreactors at

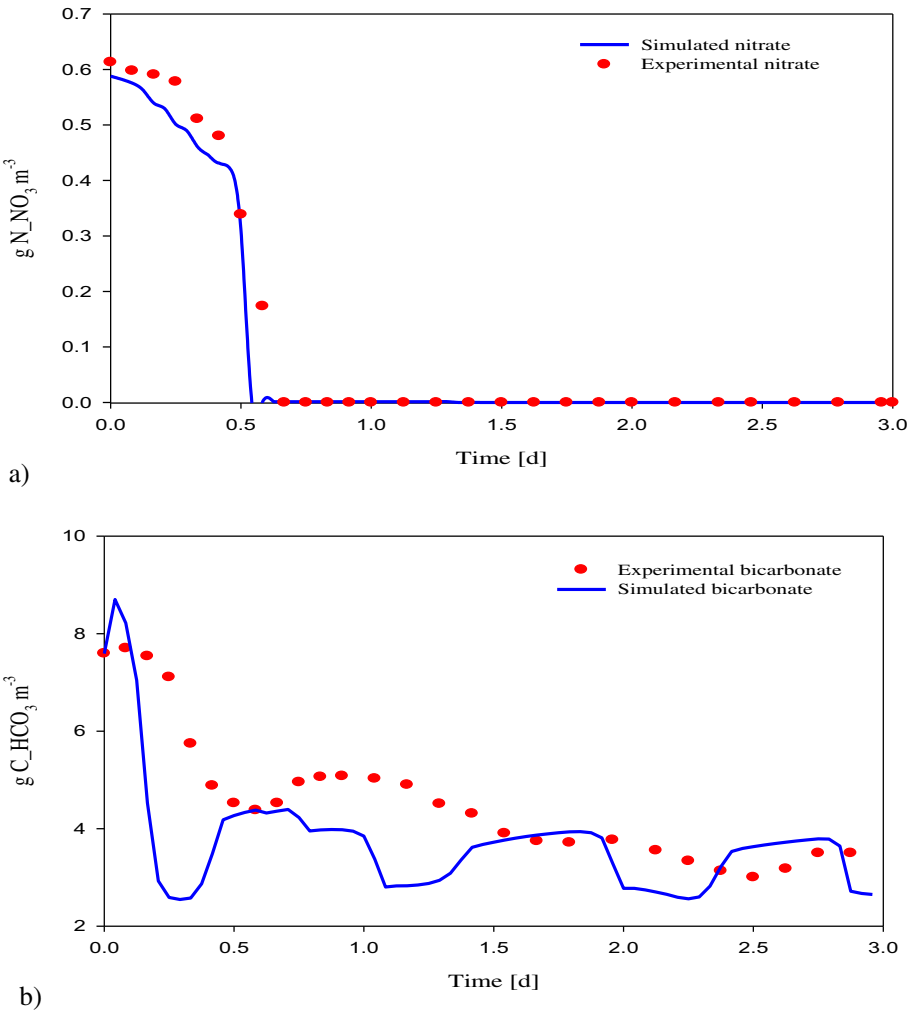

Fig. 6. Experimental (red dots) and simulated (blue line) (a) nitrate and (b) bicarbonate concentrations over the three days in the horizontal photobioreactor in Barcelona (Spain). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the beginning of the experiments are shown in Table 3. In the horizontal PBR the concentrations of NH_4^+ and NH_3 were lower than the analytical method's detection limit and therefore considered to be zero for this model. Note the difference in initial concentrations of microalgae (X_{ALG}) between the two PBRs due to their different operating conditions

2.6. Study cases

Practical study cases have been done to evaluate the influence of both temperature and irradiance on microalgae production, and the effect of oxygen concentration in the loop. The vertical photobioreactor of Almeria (Spain) was selected as reference for these studies.

Starting from the initial concentrations used for calibration of the model in the vertical photobioreactor, average daily microalgae production was simulated using daily temperature and irradiance variations from 17th day of each month of year. Two scenarios were evaluated. In the first set of simulations the vertical photobioreactor was under controlled temperature by passing cooling water at 1500 L/h through an internal heat exchanger located in the bubble column of the photobioreactor. In a second set of simulations, temperature was obtained from meteorological annals of Almeria (Spain). These two scenarios were compared and an estimation of the total annual production using monthly irradiance variations was calculated. Irradiance, expressed as photosynthetically active radiation (PAR), was estimated for Almeria (Spain) from the mathematical equations presented in Supplementary Table 10 [2].

Moreover, oxygen concentration throughout the 400 m of vertical photobioreactor was evaluated while maintaining the reactor under controlled temperature, Dissolved oxygen profile in the loop configuration was simulated at noon in the months of July and January, when the highest and lowest temperature, respectively, were recorded.

3. Results

In this work simulations for two different photobioreactors were studied. First we present the results of the model calibration for the vertical photobioreactor. Fig. 4 shows that the model was able to accurately match DO and pH trends over the course of one day inside the system, with decreasing pH due to CO_2 injection (which displaces the equilibrium of carbon species).

Fig. 5 shows the results of the calibration in the horizontal photobioreactor. Experimental and simulated dissolved oxygen and pH values inside the open-air tanks of the horizontal photobioreactor are presented. As can be seen, the wavelike trend of pH varied due to microalgae activity, which is quite well simulated by the model. Moreover, Fig. 6 shows the experimental and simulated nitrate (N_NO_3) and bicarbonate (C_HCO_3) concentrations in the horizontal system. The model was able to reproduce quite well the trend of experimental data. In absence of ammonia species, only nitrates are used as nitrogen substrates for microalgae growth. The low concentration of nitrate in the culture medium limited the activity of microalgae. As can be seen, microalgae consumed nitrate concentrations quickly in the first hours

Table 4
Values of calibrated parameters in the vertical and horizontal photobioreactors.

Parameter	Description	Value	
		Vertical PBR	Horizontal PBR
μ_{ALG}	Maximum specific growth rate of microalgae	1.7 d^{-1}	1.7 d^{-1}
$K_{a,O2}$	Mass transfer coefficient for oxygen	2.9E-03 s^{-1}	9.2E-03 s^{-1}
$K_{a,CO2}$	Mass transfer coefficient for carbon dioxide	2.8E-03 s^{-1}	9.0E-03 s^{-1}

of experiment (Fig. 6). Likewise, Fig. 6 shows that bicarbonate concentrations decreased faster in the first hours due to intense microalgae activity. After 22 h, in absence of nitrate, daily variations of bicarbonate are related to changes in equilibrium species of carbon.

Note that, in general, simulations of the vertical PBR were more accurate than those of the horizontal due to in the horizontal system there was some growth of other microorganisms different from microalgae (e.g., bacteria and protozoa). This was to be expected as the culture water was from an irrigation channel. The activity of these microorganisms affected simulated factors though it is not known to what extent, because unfortunately we do not have values for these organisms.

Table 4 presents the values of the parameters that were calibrated in each photobioreactor. Note that maximum specific growth rate (μ_{ALG}) and the transfer of gases to the atmosphere ($K_{a,O2}$ and $K_{a,CO2}$) were also calibrated in our previous works [22,23]. In this previous work the model output results are very sensitive to these parameters [22, 23], and therefore should be calibrated with great accuracy. Furthermore, gas transfer parameters depend on the extension of the surface interface. Due to different PBRs design, modifications of these parameters were considered worthwhile.

4. Discussion

4.1. New features of the model

In comparison to our previous work [22], where a 0D domain was applied, here 2D domain was used to represent the two tubular photobioreactors. The domain was divided in two sub-domains (D1 and D2), where different conditions from the tubes (D1) to the open body (D2) of the photobioreactors were applied. According to the function of bubble column in the vertical system and the open-air tank in the horizontal system, the transfer of gases to the atmosphere was only applied to the D2 domain that corresponds to the total volume of these specific parts.

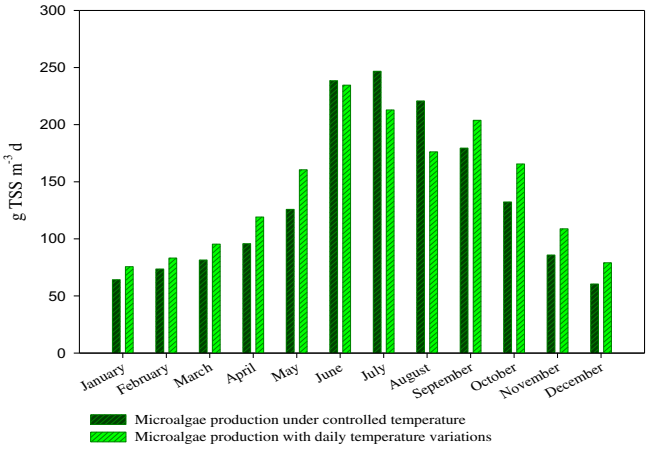

Fig. 7. Average daily microalgae production for each month of the year under controlled temperature and with daily temperature variations.

A periodic condition was applied at boundaries 1 and 2 to reproduce the recirculation of flow from the loop configuration to the bubble column in the vertical system, and from the tubes to the open-tank in the horizontal system. Simulation results demonstrated that these simplifications were adequate to describe the specific parts of different tubular photobioreactors. Moreover, fluid flow and transport equations were added in the current model to obtain a realistic representation of the hydrodynamics in the photobioreactors.

In addition to the previous mechanistic model presented by Solimeno et al. (2015) [22] light attenuation through the medium was implemented. Light intensity decays exponentially due to microalgae biomass accumulation inside the reactors. Assuming a perfect mixing of medium, due to turbulent flow regime, an irradiance average I_{av} was used to represent any point within the reactor.

4.2. Calibration of the model

Results of the sensitivity analysis, reported in our previous work [23], had indicated that the maximum specific growth rate of microalgae (μ_{ALG}) and the mass transfer coefficient for oxygen ($K_{a,O2}$) and carbon dioxide ($K_{a,CO2}$) were the parameters with the greatest impact on simulation outputs. Therefore, calibration of these parameters must occur in each particular case.

The calibrated maximum specific growth rate of microalgae (μ_{ALG} = 1.7 [d^{-1}]) in the vertical photobioreactor fits well within literature range [0.4–2.0 d^{-1}]. Also, the mass transfer coefficient in the bubble column for oxygen which was $K_{a,O2}$ = 2.9E-03 s^{-1} fits into the range values for vertical photobioreactors [1.2E-03 to 7.7E-03 s^{-1}] [16]. The mass transfer coefficient for carbon dioxide ($K_{a,CO2}$ = 2.8E-03 s^{-1}) was consistent with range values [1.1E-03-7.0E-03 s^{-1}] for bubble column systems [16]. These same parameters were calibrated with experimental data over three days from the horizontal photobioreactor located in Barcelona (Spain). Likewise as in the previous calibration, the values generated for the maximum growth rate of microalgae (μ_{ALG} = 1.7 [d^{-1}]), the mass transfer of oxygen ($K_{a,O2}$ = 9.2E-03 [s^{-1}]) and carbon dioxide ($K_{a,CO2}$ = 9.0E-03 [s^{-1}]) were all in agreement with literature ranges for tubular photobioreactors [8].

Mass transfer coefficients depend on, temperature, mixing and most importantly, the extension of the surface interface. Thus, variable values of mass transfer coefficients from vertical and horizontal photobioreactors are due to different design and scale-up of bubble column and open-tanks, respectively.

Also the culture medium influences the mass transfer coefficients and the maximum growth rate of microalgae. In this work the horizontal photobioreactor was filled with agricultural runoff which could be contain few concentrations of bacteria and other microorganisms. The activity of these microorganisms could influence dissolved oxygen and carbon dioxide concentrations in the medium culture, and therefore could slightly affect the values of the calibrated parameters. However, single microscopic observations during the experiment indicated that their concentration was irrelevant in comparison to microalgae (as usual in this type of PBR), and thus their influence is considered very low or almost negligible. Calibrating the model in two different photobioreactors (e.g., horizontal and vertical) with different types of media has proved the robustness and resilience of the mathematical model to operate under variables conditions.

Table 5
Comparing total annual production under controlled temperature and daily temperature variations versus optimizing system using cooling water during summer.

Total annual production	Value
Optimizing system	
1796.86 gTSS m^{-3}	
Daily temperature variations	
1714.53 gTSS m^{-3}	
Under controlled temperature	
1604.48 gTSS m^{-3}	

4.3. Study case: microalgae production as a function of temperature and irradiance

Irradiance and temperature play an important role in microalgae production. These physical factors influence biokinetic and chemical processes related to microalgae growth. Irradiance is strictly correlated to photosynthesis rate. At high level of irradiance, microalgae become 'light saturated' because photosynthesis cannot process more photons. As result, the rate of photosynthesis progressively starts to stabilize [8,11]. Temperature influences the equilibrium of chemical species (carbon and nitrogen), uptake of nutrients, transfer of gases to the atmosphere, and especially the microalgae growth rates. The optimal temperature for microalgae growth ranges between 15 °C and 25 °C, depending on the species [5,17]. Temperature above or below this range negatively affects biomass yield.

Thanks to the model, previously calibrated with daily experimental data, has been possible to make predictions of microalgae production over long-term with different environmental factors, such as temperature and irradiance. Simulations of the average daily microalgae production at a monthly scale in the vertical photobioreactor are presented in Fig. 7. As can be observed simulations indicate that production is generally higher under daily temperature variations due to a more favorable temperature range (Supplementary Table 3). Table 5 presents the annual microalgae production comparing the two scenarios studied: under controlled temperature and with daily temperature variations. Although the growth of microalgae decreases with high temperature and irradiance during the months of June, July and August (when the highest temperatures of the year occur), total annual production of microalgae exposed to daily temperature variations is higher than the reactor under controlled temperature. To optimize production, it might be considered to only use cooling water during the hottest months (June, July and August). Moreover, simulations results show that during the summer the production is also inhibited due to high dissolved oxygen concentrations throughout loop configuration up to 250% of air saturation (see next section).

4.4. Study case: oxygen concentration

Fig. 8 shows the simulations of the dissolved oxygen profile throughout the 400 m length of the vertical photobioreactor at noon (when the highest temperature occurs) in the months of January and July. These two months were selected as they represent the minimum and maximum microalgae activity in a monthly basis time scale. As can be seen, the lower light intensity and temperature in January gives as a result lower dissolved oxygen concentrations in contrast to July. Also it can be observed in both months how dissolved oxygen concentration increases throughout the loop and decreases in the bubble column. In July, transfer of excess of dissolved oxygen to the atmosphere throughout the airlift permits to re-establish, at the beginning of loop configuration, the oxygen level under the maximum concentration of oxygen dissolved in water (32 gO_2 m^{-3}) equal 350% of saturation (9.07 gO_2 m^{-3}) [1,7]. This property of the photobioreactor design is especially important in warm months (such as July), when a high photosynthetic activity could cause inhibition due to oxygen accumulation.

The model presented in this work allows to simulate and study microalgae growth inhibition due to high dissolved oxygen concentrations thanks to the inclusion of a photorespiration factor $f_{PR}(S_{O2})$ [22]. The function ($f_{PR}(S_{O2})$) in Fig. 9 describes that for dissolved oxygen concentrations lower than the $250\%S_{O2}^{SAT}$ (22.67 gO_2 m^{-3}) the photosynthesis rate is reduced by 10%. Above this value, the photosynthesis rate decrease more quickly with a vertical asymptote and is equal at zero when dissolved oxygen reaches the 350% saturation limit (τS_{O2}^{SAT} = 32 gO_2 m^{-3}).

In process design, the current model can be used to find the maximum photobioreactor length to avoid oxygen inhibition. For example, for the month of July, simulations were conducted using half the previous bubble column volume (from 0.44 m^3 to 0.22 m^3) in the vertical

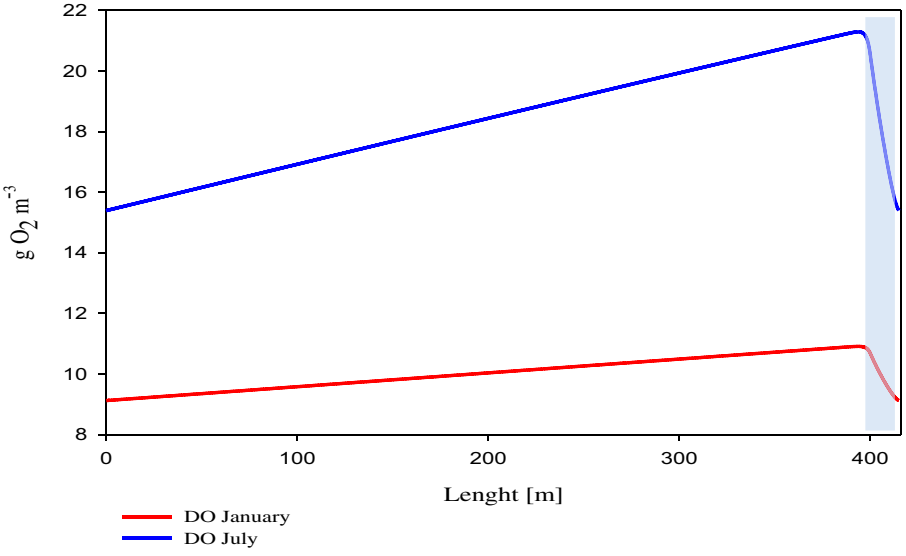

Fig. 8. Simulations of dissolved oxygen (DO) concentration profile throughout the vertical photobioreactor in Almeria (Spain) in the months of January and July. Bubble column position is represented by blue region. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

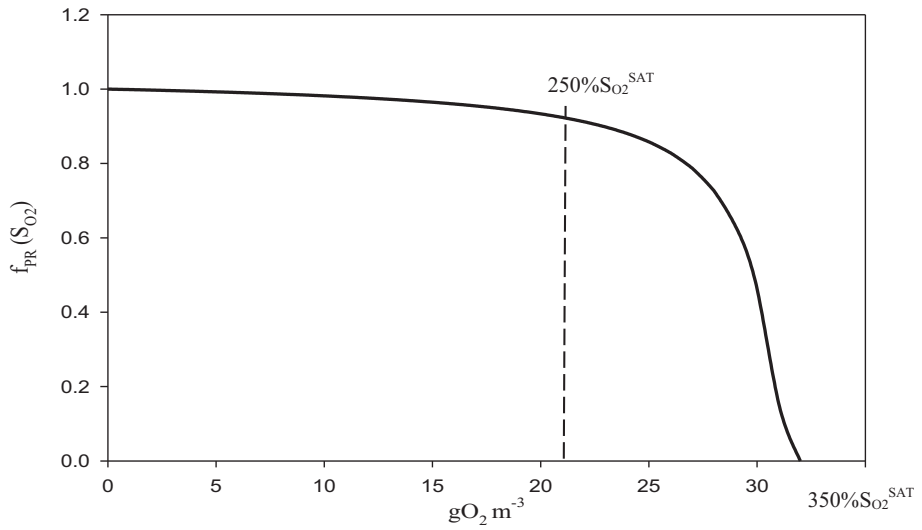

Fig. 9. Profile of photorespiration factor function for value of dissolved oxygen concentrations below the saturation limit (τS_{O2}^{SAT}).

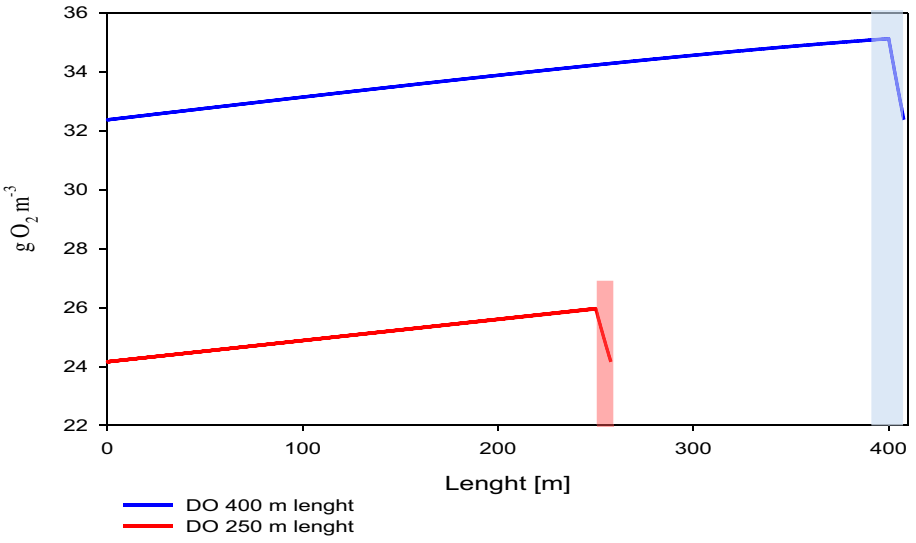

Fig. 10. Simulations of dissolved oxygen (DO) concentration profile throughout 400 m and 250 m length of the vertical photobioreactor in Almeria (Spain) in the months of July. Bubble column position is represented by blue and red rectangle, for 400 m and 250 m length of vertical photobioreactor, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

photobioreactors loops (400 m and 250 m). As seen in Fig. 10, reducing the volume of the bubble column and keeping the original loop configuration length (400 m), the simulation results show that the DO exceeds the saturation limit l inhibiting microalgae growth. The volume of bubble column is not enough to transfer the excess of dissolved oxygen to the atmosphere. On the contrary, simulations indicate that a 250 m length, photobioreactor greatly reduces the oxygen accumulation.

5. Conclusion

In this paper a new mechanistic model to simulate microalgae growth was calibrated in two different tubular photobioreactors. Fluid flow, transport equations and light attenuation were included in the model described in our previous work and implemented in COMSOL Multiphysics™ software. Uncertainty parameters from previous sensitivity analysis were calibrated in each photobioreactor. The results of calibration indicate that the mass transfer of gases and the maximum specific growth rate of microalgae fit well within literature ranges. Moreover, the developed model demonstrates potential prediction of oxygen accumulation throughout the loop configuration and daily microalgae production as a function of temperature and irradiance. The model proves to be an efficient tool for photobioreactor design and production optimization.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at http://dx.doi.org/10.1016/j.algal.2016.11.023.

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