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MATHEMATICAL MODELING AND SIMULATION OF MICROALGAE GROWTH IN SERIAL AIRLIFT PHOTOBIOREACTOR

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Abstract. Environmental impacts caused by greenhouse gas emissions are a global concern, for this reason, the search for ways to reduce these emissions has become a critical point in our society. While renewable energy sources represent 14% of the global energy matrix, in Brazil, this percentage is 46.1%, with emphasis on biofuels, which represent 6.9%. The production of biodiesel through microalgae appears as an alternative to conventional production that depends on soy or other agricultural products. Microalgae can be grown in compact photobioreactors that have a high production rate in a small area. Microalgae can also be used in the treatment of combustion gases, since those gases accelerate microalgae growth. Even so, large scale production processes face problems such as low productivity in the case of ponds and high energy cost in the case of compact tubular photobioreactors. In order for microalgae production to become attractive, it is necessary to develop an economically competitive process and for this purpose, the objective of this research is to develop a high efficiency airlift reactor with a volume large enough to treat emission gases on a large scale and still produce quality biofuels. A mathematical model of the airlift reactor will be presented and validated using experimental data from other studies. The model will take into account the kinetics of microalgae growth according to the following parameters: oxygen concentration, carbon dioxide concentration, nitrate concentration, phosphate concentration, temperature and luminosity. Mass balance will be applied at each component participating in the reaction following the kinetic growth and the mass transfer laws between the feeding gas and the microalgae culture. The parametric analyzes conducted indicate a strong dependence of the CO₂ mass transfer constant on the growth rate of the microalgae, the more efficient the addition of dissolved CO₂ to the culture, the faster it will grow. Another parametric

analysis conducted indicates that the addition of greater amount of nitrate in the culture medium used means greater amount of final biomass produced. Although it was not possible to collect experimental data from the proposed system, the present study has already shown that the suggested mathematical model works. Once these data can be collected, it will be possible to apply modeling and simulation tools to produce microalgae in the proposed photobioreactor with high efficiency, minimizing operating costs.

Keywords: Microalgae, Photobioreactor, Biodiesel, Mathematical modeling.

1. INTRODUCTION

Microalgae are unicellular beings that can be found in aquatic environments such as rivers, lakes, seas and oceans. They are photosynthetic organisms, therefore, in presence of light they convert carbon dioxide (CO₂) into oxygen (O₂), thus obtaining the carbon and energy necessary for their metabolic activities (Sajjadi *et al.*, 2018). Microalgae biomass has a high content of lipids and carbohydrates, so it can be used in the production of biofuels such as biodiesel and ethanol. In addition, microalgae biomass can contain high protein value and can be used in animal feed and food supplements. Microalgae are also used in the production of pigments, carotenoids and other high value metabolites (Ho *et al.*, 2011).

The production of biofuels using microalgae appears as an alternative to conventional production that depends on soy or other agricultural products. Unlike agricultural products used in the production of biofuels, microalgae do not participate in the food chain and also do not have production limitations in terms of seasonality, that means it can be produced all year long (Siaut *et al.*, 2011).

Microalgae can be cultivated in compact photobioreactors that have a high production rate occupying a small area, in addition they can be used to treat flue gases, accelerating their growth (Balmant *et al.*, 2016). Even so, large-scale production processes face problems such as low efficiency in the case of lagoons, high energy cost in the case of compact tubular photobioreactors and high maintenance demand in the case of airlifts tubular photobioreactors (Singh and Sharma, 2012).

For the production of microalgae to become attractive, it is necessary to develop economically competitive processes that can be associated with other energy plants, such as thermoelectric plants, for example. The design of photobioreactors that are more efficient and that can be scaled to engineering projects is one of the great challenges for the production of microalgae. In this context, modeling and simulation tools are very important to analyze a process and verify which variables can be controlled to produce microalgae with high productivity and more efficiently.

The objective of this work is to model and simulate an airlift photobioreactor with serial tubes on a pilot scale to produce microalgae more efficiently in a system that can be scaled up for engineering projects.

2. MATHEMATICAL MODEL

The development of the serial airlift photobioreactor system will be carried out at the NPDEAS (Sustainable Energy Research and Development Center) located in the Federal University of Paraná in Curitiba. The system was built with 50 mm diameter transparent PVC tubes, each airlift module is formed by 2 vertical tubes of 2.6 m in height, one of which receives air supply (riser) and the other does not receive (downcomer). At the top of the riser there is a gas outlet that extends another 0.5 m vertically. The reactor consists of 10 airlift modules allocated in two rows with a total volume of approximately 100 L. At the downcomer at one end there is a sample collector. The compressed air that feeds the reactor it will be supplied by a screw compressor continuously connected, the air supply system has a barometer and valves for pressure control, the air dispersion is done with a metal screen placed on each entrance at the bottom of the reactor.

The hypotheses raised for mathematical modeling were:

- Homogeneous reactor;
- Each airlift module behaves like a perfectly agitated reactor;
- Adiabatic system;
- Average ambient temperature is the same as the reactor;
- The composition of atmospheric air: 78.98% N₂, 21% O₂ and 0.02% CO₂.

For the development of the mathematical model, the equations used in Mass Balance and Growth Kinetics will be presented separately.

The photobioreactor can be seen in Figure 1.

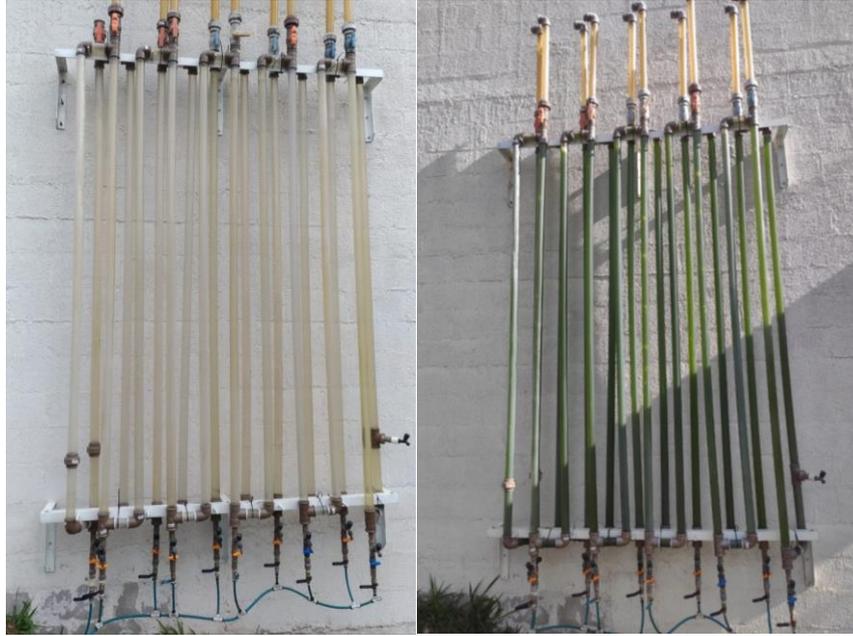


Figure 1. Serial airlift photobioreactor.

2.1 Mass Balance

The mass balance was performed taking into account biomass, total nitrate, total phosphate, carbon dioxide and oxygen. The reactor was divided into 10 control volumes, each of which represents an airlift reactor. The current containing the culture that enters the reactor i is equal to the current that leaves the reactor $i-1$, the culture current that leaves reactor i is equal to the current that enters reactor $i+1$, in addition to each of the volumes of control there is atmospheric air inlet and a gas outlet.

The mass balance for biomass is described in the Eq. (1).

$$\frac{dX_i}{dt} = \frac{Q}{V} \cdot (X_{i-1} - X_i) + \mu \cdot X_i, \quad (1)$$

Where Q is the current flow, V the volume of each airlift, X_i is the biomass concentration and μ is the conversion rate of the biomass formation reaction.

The mass balance for nitrate is described in Eq. (2).

$$\frac{d[NO_3]_i}{dt} = \frac{Q}{V} \cdot ([NO_3]_{i-1} - [NO_3]_i) - Y_{\frac{NO_3}{X}} \cdot \mu \cdot X_i, \quad (2)$$

Where $[NO_3]$ is the nitrate concentration and $Y_{\frac{NO_3}{X}}$ is the stoichiometric ratio of the biomass formation reaction between nitrate and biomass.

The mass balance for phosphate is described in Eq. (3).

$$\frac{d[PO_4]_i}{dt} = \frac{Q}{V} \cdot ([PO_4]_{i-1} - [PO_4]_i) - Y_{\frac{PO_4}{X}} \cdot \mu \cdot X_i, \quad (3)$$

Where $[PO_4]$ is the phosphate concentration and $Y_{\frac{PO_4}{X}}$ is the stoichiometric ratio of the biomass formation reaction between phosphate and biomass.

The mass balance for carbon dioxide dissolved in the liquid phase is described in Eq. (4).

$$\frac{d[CO_2]_i}{dt} = \frac{Q}{V} \cdot ([CO_2]_{i-1} - [CO_2]_i) - Y_{\frac{CO_2}{X}} \cdot \mu \cdot X_i + h_{mCO_2} \cdot ([CO_2]^* - [CO_2]_i), \quad (4)$$

Where $[CO_2]$ is the concentration of carbon dioxide dissolved in the liquid phase, and $Y_{\frac{CO_2}{X}}$ is the stoichiometric ratio of the biomass formation reaction between carbon dioxide and biomass, h_{mCO_2} is the mass transfer coefficient and $[CO_2]^*$ is the concentration of carbon dioxide at the interface, which can be determined by Henry's Law described in Eq. (5).

$$[CO_2]^* = H_{CO_2} \cdot p_{CO_2}, \quad (5)$$

Where H_{CO_2} is Henry's constant for CO_2 and p_{CO_2} is the partial pressure of carbon dioxide in the gas entering the reactor.

The mass balance for dissolved oxygen in the liquid phase is described in Eq. (6).

$$\frac{d[O_2]_i}{dt} = \frac{Q}{V} \cdot ([O_2]_{i-1} - [O_2]_i) + Y_{O_2} \mu \cdot X_i + h_{mO_2} \cdot ([O_2]^* - [O_2]_i), \quad (6)$$

Where $[O_2]$ is the concentration of dissolved oxygen in the liquid phase, and Y_{O_2} is the stoichiometric ratio of the biomass formation reaction between oxygen and biomass, h_{mO_2} is the mass transfer coefficient and $[O_2]^*$ is the oxygen concentration at the interface, which can be determined analogously to the carbon dioxide concentration at the interface.

2.2 Growth Kinetics

Growth kinetics take into account temperature, light intensity, dissolved carbon dioxide, dissolved oxygen, total nitrate and total phosphate as shown in Eq. (7) (Balmant et al., 2011).

$$\mu = \mu_{max} \cdot \mu(T) \cdot \mu(I_0) \cdot \mu(CO_2) \cdot \mu(O_2) \cdot \mu(N_{Tot}) \cdot \mu(P_{Tot}), \quad (7)$$

Where each term in the equation represents the influence of these variables on the reaction rate. The equations to determine each of the components of Eq. (7) can be seen in Table 1.

Table 1. Growth kinetics equation terms.

Constant	Term	Equation	Fonte
Temperature	$\mu(T)$	$\mu(T) = a \cdot T^2 + b \cdot T + c$	Balmant <i>et al.</i> , 2011.
Light intensity	$\mu(I_0)$	$\mu(I_0) = \frac{I_0}{\left(K_{I_0} + I_0 + \frac{I_0^2}{k_{I_0}}\right)}$	Aiba, 1982.
Carbon dioxide	$\mu(CO_2)$	$\mu(CO_2) = \frac{CO_2}{\left(K_{CO_2} + CO_2 + \frac{CO_2^2}{k_{CO_2}}\right)}$	Andrews, 1986.
Oxygen	$\mu(O_2)$	$\frac{A}{\left(1 + \left(\frac{O_2\%}{B}\right)^C\right)}$	This work.
Total nitrate	$\mu(N_{Tot})$	$\mu(N_{Tot}) = \frac{N_{Tot}}{\left(K_{N_{Tot}} + N_{Tot}\right)}$	Araújo <i>et al.</i> , 2009.
Total phosphate	$\mu(P_{Tot})$	$\mu(P_{Tot}) = \frac{P_{Tot}}{\left(K_{P_{Tot}} + P_{Tot}\right)}$	Araújo <i>et al.</i> , 2009.

The validation of the mathematical model will be done by applying the model to the experimental data from Toledo-Cervantes *et al.* (2013), where the growth of the microalgae *Scenedesmus obtusiusculus* is analyzed with CO_2 concentrations in the inlet gas of 0.4 vvm and 0.8 vvm and also experimental data from Ho *et al.* (2012) in which the growth of the microalgae *Scenedesmus obliquus* is analyzed with a total nitrate amount of 120 mg/L. In addition, the mathematical model will be applied to experimental data collected from the proposed reactor, comparing the experimental biomass production to the theoretical biomass production.

All simulations will be performed using MATLAB® software. To solve the system of ordinary differential equations, the routine *ode23s* from the Matlab library was used. This is a routine that uses an implicit 2nd/3rd order method with adaptive step.

Then, it is possible to carry out a parametric analysis of the project variables, determining their impact and identifying possible optimization opportunities. Uncertainty analyzes must be carried out according to error propagation methodologies.

3. RESULTS

3.1 Validation

The validation of the mathematical model was carried out using experimental data from two other works: Toledo-Cervantes *et al.* (2013) and Ho *et al.* (2012).

The results of the validation of the model with the study by Toledo-Cervantes *et al.* (2013) were performed with the carbon dioxide gas input of 0.4 vvm and 0.8 vvm. The input parameters for these simulations can be seen in Table 2.

Table 2. Input parameters from Cervantes *et al.* (2013).

Parameter	Description	Value	Units
X_i	Initial biomass concentration	550	mg.L ⁻¹
$[NO_3]_i$	Initial nitrate concentration	1000	mg.L ⁻¹
$[PO_4]_i$	Initial phosphate concentration	348	mg.L ⁻¹
$[CO_2]_i$	Initial dissolved CO ₂ concentration	0.6	mg.L ⁻¹
$[O_2]_i$	Initial dissolved O ₂ concentration	8.7	mg.L ⁻¹
P_{CO_2}	CO ₂ partial pressure	0.02	bar
P_{O_2}	O ₂ partial pressure	0.21	bar
h_{mCO_2}	CO ₂ mass transfer coefficient	72.62 for 0.4 vvm 200 for 0.8 vvm	day ⁻¹
h_{mO_2}	O ₂ mass transfer coefficient	0.037 for 0.4 vvm 0.5 for 0.8 vvm	day ⁻¹
K_{CO_2}	CO ₂ saturation constant	1.05×10^{-6}	-
K_{NO_3}	O ₂ saturation constant	922.39	-
K_{PO_4}	PO ₄ saturation constant	85.07	-
A	Adjustment constant A for O ₂	1	-
B	Adjustment constant B for O ₂	33,182.42	-
C	Adjustment constant C for O ₂	99.32	-
μ_{max}	Maximum conversion rate	0.934	-
Y_{CO_2}	CO ₂ stoichiometric coefficient	1.8	-
Y_{O_2}	O ₂ stoichiometric coefficient	1.96	-
Y_{PO_4}	PO ₄ stoichiometric coefficient	0.05	-
Y_{NO_3}	NO ₃ stoichiometric coefficient	0.325	-
Q/V	Inverse retention time	10	day ⁻¹
nr	Number of reactors	10	-

The graphic representing the growth of the microalgae biomass for a gas inlet with 0.4 vvm of CO₂ showed satisfactory results, as shown in Figure 2.

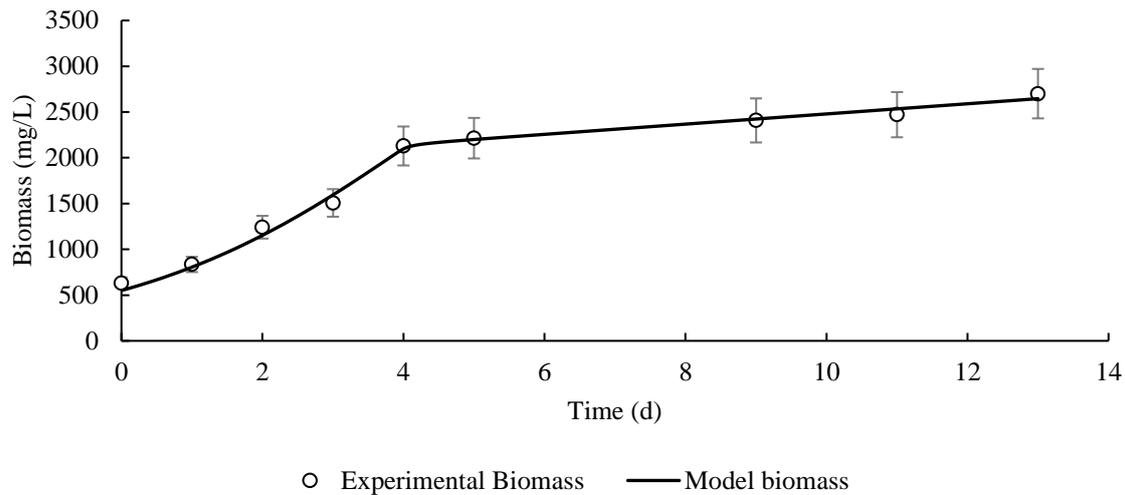


Figure 2. Experimental biomass data with 0.4 vvm CO₂ compared to theoretical model.

In the same simulation, the growth curve for biomass with 0.8 vvm CO₂ in the inlet gas was obtained, which also presented good results when compared to the experimental data as can be seen in Figure 3.

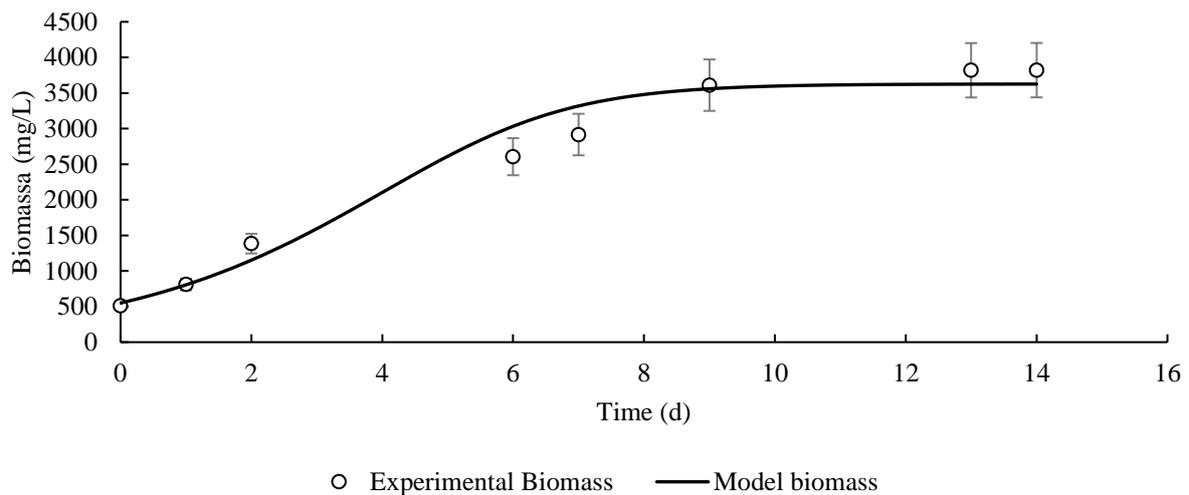


Figure 3. Experimental biomass data with 0.8 vvm CO₂ compared to theoretical model.

The results of model validation using experimental data from Ho *et al.* (2012) were carried out by verifying the biomass production curve and the nitrate consumption curve. Input parameters for these simulations can be seen in Table 3.

Table 3. Input parameters from Ho *et al.* (2012)

Parameter	Description	Value	Units
X_i	Initial biomass concentration	59	mg.L ⁻¹
$[NO_3]_i$	Initial nitrate concentration	117	mg.L ⁻¹
$[PO_4]_i$	Initial phosphate concentration	348	mg.L ⁻¹
$[CO_2]_i$	Initial dissolved CO ₂ concentration	0.6	mg.L ⁻¹
$[O_2]_i$	Initial dissolved O ₂ concentration	8.7	mg.L ⁻¹
P_{CO_2}	CO ₂ partial pressure	0.02	bar
P_{O_2}	O ₂ partial pressure	0.21	bar
h_{mCO_2}	CO ₂ mass transfer coefficient	74.8	dia ⁻¹

h_{mO_2}	O ₂ mass transfer coefficient	5.8	dia ⁻¹
K_{CO_2}	CO ₂ saturation constant	2.87	-
K_{NO_3}	O ₂ saturation constant	68.83	-
K_{PO_4}	PO ₄ saturation constant	75.48	-
A	Adjustment constant A for O ₂	1	-
B	Adjustment constant B for O ₂	33,182.42	-
C	Adjustment constant C for O ₂	99.32	-
μ_{max}	Maximum conversion rate	3.395	-
Y_{CO_2}	CO ₂ stoichiometric coefficient	1.8	-
Y_{O_2}	O ₂ stoichiometric coefficient	1.96	-
Y_{PO_4}	PO ₄ stoichiometric coefficient	0.05	-
Y_{NO_3}	NO ₃ stoichiometric coefficient	0.027	-
Q/V	Inverse retention time	10	dia ⁻¹
nr	Number of reactors	10	-

The biomass curve represented in Figure 4 presented good results when compared to the experimental data, the nitrate curve also presented good results mainly at the beginning and at the end of cultivation, as shown in Figure 5.

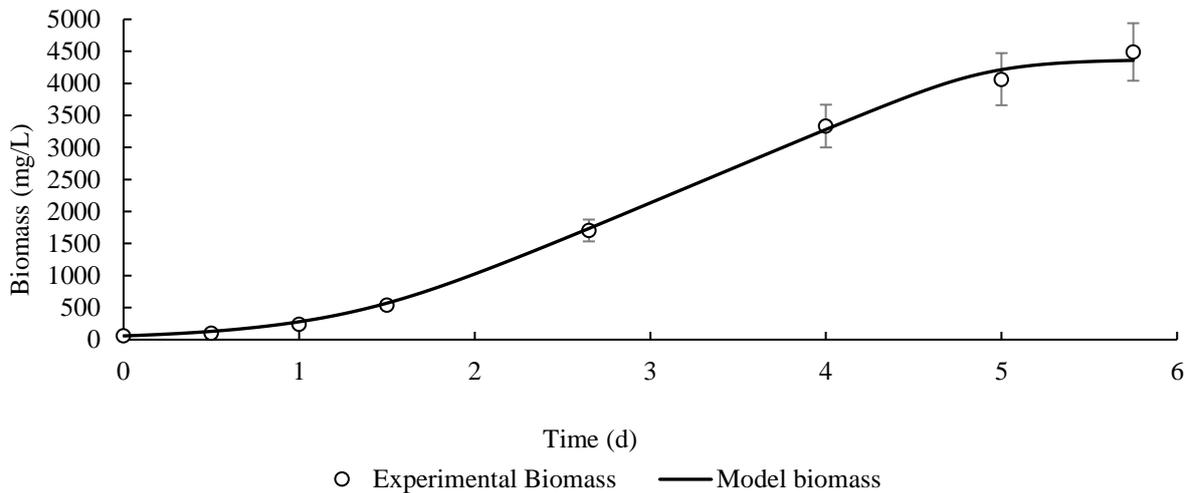


Figure 4. Experimental data of biomass production compared to theoretical model.

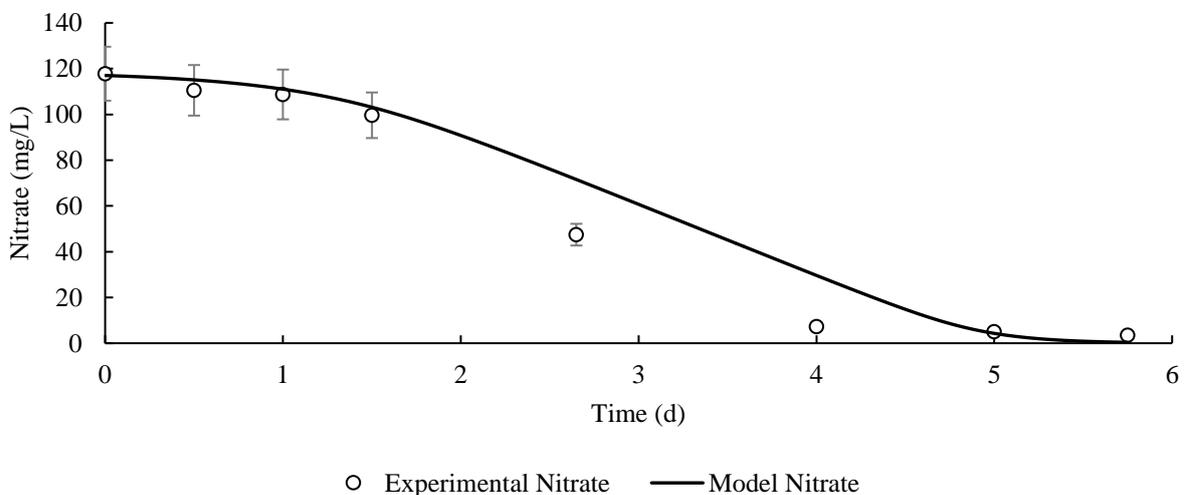


Figure 5. Experimental data of total nitrate compared to theoretical model.

The input parameters used to do the comparison between the experimental data from the proposed reactor and the mathematical model are shown in Table 4. The biomass curve from this simulation is shown in Figure 6.

Table 4. Input parameters from this work.

Parameter	Description	Value	Units
X_i	Initial biomass concentration	98.3	mg.L ⁻¹
$[\text{NO}_3]_i$	Initial nitrate concentration	182	mg.L ⁻¹
$[\text{PO}_4]_i$	Initial phosphate concentration	148	mg.L ⁻¹
$[\text{CO}_2]_i$	Initial dissolved CO ₂ concentration	0.6	mg.L ⁻¹
$[\text{O}_2]_i$	Initial dissolved O ₂ concentration	8.7	mg.L ⁻¹
P_{CO_2}	CO ₂ partial pressure	0.02	bar
P_{O_2}	O ₂ partial pressure	0.21	bar
h_{mCO_2}	CO ₂ mass transfer coefficient	45.29	dia ⁻¹
h_{mO_2}	O ₂ mass transfer coefficient	8.29	dia ⁻¹
K_{CO_2}	CO ₂ saturation constant	3.32	-
K_{NO_3}	O ₂ saturation constant	3.57	-
K_{PO_4}	PO ₄ saturation constant	169.37	-
A	Adjustment constant A for O ₂	21.76	-
B	Adjustment constant B for O ₂	220.54	-
C	Adjustment constant C for O ₂	1804.73	-
μ_{max}	Maximum conversion rate	0.032	-
Y_{CO_2}	CO ₂ stoichiometric coefficient	1.8	-
Y_{O_2}	O ₂ stoichiometric coefficient	1.96	-
Y_{PO_4}	PO ₄ stoichiometric coefficient	0.05	-
Y_{NO_3}	NO ₃ stoichiometric coefficient	0.117	-
Q/V	Inverse retention time	10	dia ⁻¹
nr	Number of reactors	10	-

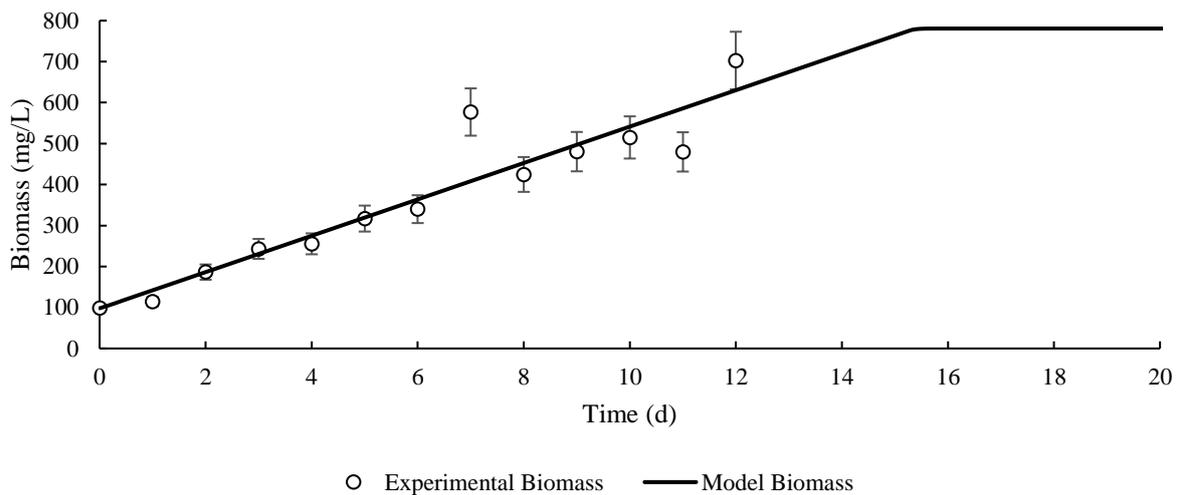


Figure 6. Experimental data of biomass production compared to theoretical model.

3.2 Parametric Analysis

Fixing the other variables, the value of the CO₂ mass transfer coefficient (h_{mCO_2}) was changed to verify what would be its effect on biomass production. Figure 7 shows biomass production by changing the order of magnitude of the mass transfer coefficient. The values tested were 150 day⁻¹, 1500 day⁻¹ and 15000 day⁻¹.

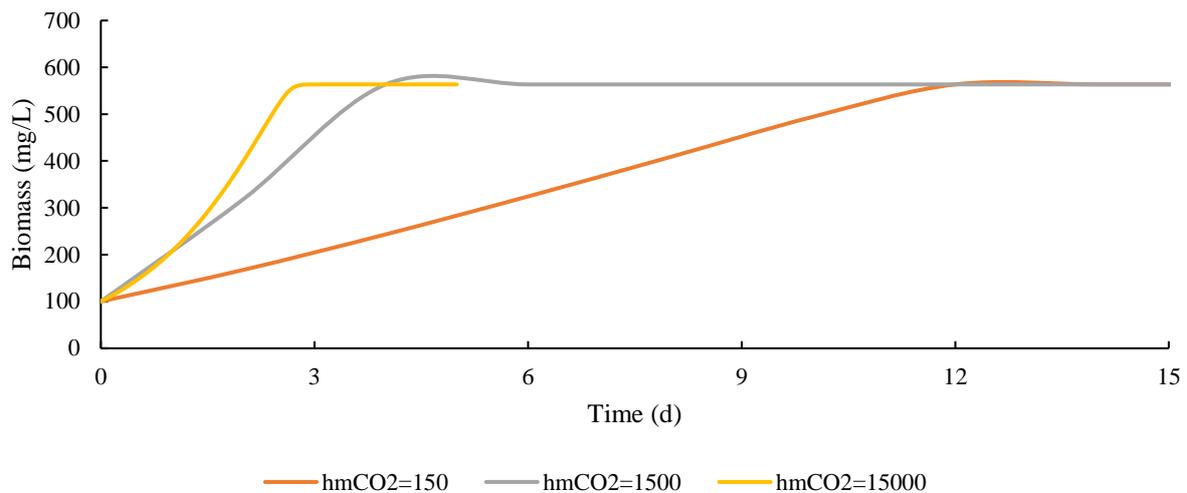


Figure 7. Variation of biomass production for different h_{mCO_2}

Note that the better the gas exchange, the faster the microalgae will grow. Although the value of 15000 day^{-1} does not represent a real value, it is possible to observe that from 1500 day^{-1} onwards there is not much gain in productivity, so forcing gas exchange by increasing the inlet gas flow can be beneficial to some extent limit, which, if exceeded, can only mean greater energy expenditure without a return in productivity.

The second analysis was carried out by varying the amount of nitrate available in the medium at the beginning of cultivation, obtaining the biomass growth profile as a function of time. The amounts of initial nitrate analyzed were 148 mg/L and 350 mg/L , the growth curves for these two values can be seen in Figure 8.

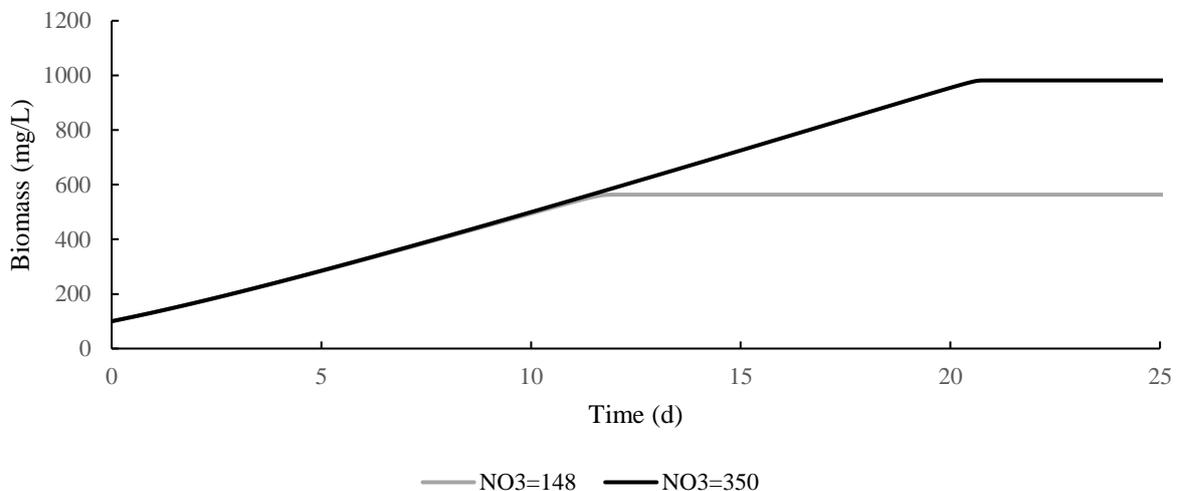


Figure 8. Variation of biomass production for different concentrations of NO_3 .

It is important to note that nitrate has no influence on the growth rate of the microalgae, it works as a growth limiting factor. Therefore, increasing the amount of nitrate will not increase productivity, but the amount of biomass produced.

4. CONCLUSION

According to the simulations and parametric analyzes performed in the MATLAB® software, it was possible to conclude that:

- The proposed mathematical model is valid because it satisfactorily simulated two sets of data from two different experiments;
- The mathematical model also works well with the data collected from the proposed reactor;

- The analysis carried out by varying the values of the CO₂ mass transfer constant highlighted the importance of this gas for the production of microalgae and highlighted the need to maximize the mass transfer in the reactor, as long as not much energy is spent on this process;

- The analysis carried out with variations in the initial concentrations of nitrate showed that the dosage of nitrate in the culture medium must be adequate for the amount of biomass to be produced, since little nitrate can result in a low final biomass and a lot of nitrate can mean a waste of this nutrient if the microalgae enters the decay phase before consuming all the available nitrate.

It has not yet been possible to carry out the experimental tests in the proposed photobioreactor, however, once these data can be collected, it will be possible to carry out other analyzes such as the analysis of the variation in the inlet pressure of gases and variations in the nutrients of the culture medium and its impacts on biomass production.

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