TRANSIENT MODELING AND SIMULATION OF COMPACT PHOTOBIOREACTORS

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ABSTRACT

In this paper, a mathematical model is developed to make possible the simulation of microalgae growth and its dependency on medium temperature and light intensity. The model is utilized to simulate a compact photobioreactor response in time with physicochemical parameters of the microalgae *Phaeodactylum tricornutum*. The model allows for the prediction of the transient and local evolution of the biomass concentration in the photobioreactor with low computational time. As a result, the model is expected to be a useful tool for simulation, design, and optimization of compact photobioreactors. Numerical solutions of the mathematical model are presented for the visualization of biomass concentration and total production. Several simulations were performed with temperatures ranging from 274 K to 300 K, and the maximum biomass production was achieved with an operating temperature of 294 K.

Keywords: Numerical Simulation, Microalgae Growth, Temperature, Light Intensity.

NOMENCLATURE

C Biomass concentration, (gm^{-3})
μ Specific growth rate, (h^{-1}) h^{-1}
m Specific maintenance rate, $h^{-1}(h^{-1})$
D Dilution rate, $h^{-1}(h^{-1})$
μ_{MAX} Maximum specific growth rate, $h^{-1}(h^{-1})$
$I, I(C)$ Mean light intensity, $(\mu E m^{-2} s^{-1})$
R Vessel radius, (m)
S Distance from vessel surface to an internal point, (m)
ϕ Angle of the light path
I_0 Incident light intensity on culture surface, $(\mu E m^{-2} s^{-1})$
C_0 Initial Biomass concentration, (gl^{-1})
I_k Constant representing the affinity of algae to ligth, $(\mu E m^{-2} s^{-1})$
K_a Biomass absorption coefficient, $m^2 g^{-1} (m^2 g^{-1})$
Y_b Absorption coefficient normalized to pigment – free biomass, $m^2 g^{-1}$ $(m^2 g^{-1})$
Y_p' Absorption coefficient normalized to total pigment content, $m^2 g^{-1}$ $(m^2 g^{-1})$
a, b, c Parameters to be defined
K_i Measure of photo inhibition, $(\mu E m^{-2} s^{-1})$
A_1, A_2 Factors frequency, $[(h]^{-1})$
E_a , E_b Activation energy, $kcal\ mol^{-1}$ $\left(\frac{kcal}{mol}\right)$
T Medium temperature, (K) T_0 Initial temperature, (K)

INTRODUCTION

In recent years microalgae cultivation has been the subject of scientific research in several countries such as Brazil, United States, China, Italy, and Spain due to expected high oil productivity when compared with crops. Microalgae can be used in many important applications such as to obtain compounds of interest in food, chemicals and pharmaceuticals. The cultivation of microalgae in photobioreactors is an effective way of producing microalgae biomass. Inside the bioreactor, it is possible to control the cultivation conditions inducing the production of higher concentrations of some products of interest for a particular application, such as proteins, pigments, fatty acids and carbohydrates.

The microalgae are present in all aquatic systems where the incidence of sunlight occurs. This happens because the light is a factor of great importance for its growth. Because of its high biodiversity there are many characteristics that are attributed to the microalgae. In some cases, like the *Phaeodactylum tricornutum* (Bacillariophyceae), the main characteristic is the high density of lipid in its structure (Xu, 2006). Due to the fact that microalgae are capable of producing more tons of vegetable oil per hectare per year than any oleaginous (Pérez, 2007) a large amount of research has been concentrated on it. Many companies have been investing time and money on microalgae technology, allowing the researchers to enhance the production in large scales reactors. The oil produced with the algae biomass can be used in different ways.

The development of a mathematical model to predict the growth of microalgal through the numerical solution is of great importance for the development of knowledge in this area of science. The present model takes into account temperature, light intensity, design and engineering of photobioreactor.

The model is applied to a tubular photobioreactor of semi-continuous cultivation, where the growth of microorganisms is a function of the average light intensity inside the pipe. When physical parameters such as pH, CO_2, phosphorus and others are not limiting the growth of biomass, light intensity and temperature become the most important factors.

Richmond (1992) noted that the availability of light for each cell in a photoautotrophic culture is a function of: a) the intensity and duration of the incident light, and b) the concentration of cells, or population density, which affects the process of mutual growth through shading. Serenotti et al. (2004) comment that under appropriate conditions of light, cells can store energy and produce intermediate products (such as ATP) which are used for the fixation of carbon dioxide and the biomass synthesis.

The temperature of cultivation, in addition to the rate of illumination, is another important aspect when working with the heterotrophic cultivation of microalgae. Like any organism, microalgae can grow at different temperatures. When the temperature is different from the optimum temperature growth, the microalgae present a lower growth (at low temperatures) or inhibition and death (in the case of high temperatures). However, the algae can adapt to different growing conditions since the increase or decrease in temperature occurs gradually. Sudden increases in temperature will invariably provide cell death. Apart from directly affecting cell metabolism and cause a slowdown in growth and reproduction of algae, temperature, as described in several studies in the literature, promotes a change in the composition of fatty acids present in lipids synthesized, in particular the lipids from membrane (Chen et al., 2008). This fact is explained by the changes imposed by temperature on the fluidity of cell membrane. With higher temperatures, the membrane lipids are replaced with lipids with more unsaturated fatty acids, presenting a more compact structure which, give in this case, lower plasma membrane fluidity. The opposite occurs in the case of lower temperatures, i.e., the substitution of saturated fatty acids by unsaturated fatty acids in these lipids membrane allowing the membrane fluidity even at low temperatures. This same behavior is repeated in other organisms such as bacteria and even in mammals.

In the present work, the mathematical model was conceived for a photobioreactor that was designed to work on a plant where the produced oil will be processed into biodiesel and consumed in an internal combustion engine driven generator (genset). Part of the energy produced will be used to supply the plant needs characterizing in this way, a sustainable energy unit. As a result, this study develops a mathematical formulation for investigating the design and operating conditions for microalgae cultivation in the photobioreactor. The methodology takes into account the temperature and light intensity during a 120 hours growth simulation.

MATHEMATICAL MODEL

Several mathematical models of photobioreactors based in the scheme of light decay can be found in literature. The general problem of photobioreactor design considering light attenuation is extensively discussed by Bernardez et al. (1987). Several mathematical descriptions of photobioreactors had taken into consideration the distribution of light in the volume of the culture, either using an averaged value of the illuminance, or averaging the growth rate (Dermoun, 1992; Evers, 1991; Fernández, 1998; Frohlich, 1983; Grima, 1994).

In this study, the mathematical model is based on the work of Grima *et al.* (1994) with the modifications made by Fernandez (1998) that include the photoinhibition phenomenon in the

original formulation. Since growth is also inhibited or stopped out of a certain temperature range, which depends on the selected species, the Arrhenius equation model for temperature, as presented by Pérez (2007), was added to the current formulation. Taking into account these modifications, the maximum specific growth rate is no longer constant, but varies with photobioreactor temperature.

The variation of biomass concentration versus time is given by Eq. (1).

$$\frac{dC}{dt} = C(\mu - m - D) \quad (1)$$

where C is the concentration of biomass [$\frac{m^2}{g}$], μ the specific growth rate [h^{-1}], m the maintenance rate [h^{-1}] and D the dilution rate [h^{-1}].

The temperature and average light intensity in the photobioreactor are considered independent variables. The light availability inside the culture is determined by the solar irradiance, the design of the reactor, the biomass concentration, and the pigment content in the culture, which leads to the self-shading effect (Grima, 1994). Therefore, the resulting expression for the specific growth rate of biomass (μ) is

$$\mu = \frac{\left(A_1 e^{\left(\frac{E_a T - T_0}{RT\ T_0}\right)} - A_2 e^{\left(\frac{E_b T - T_0}{RT\ T_0}\right)}\right) I^{b+\frac{c}{I_0}}}{\left(I_k\left(1+\left(\frac{I_0}{K_i}\right)^a\right)\right)^{b+\frac{c}{I_0}} + I^{b+\frac{c}{I_0}}} \quad (2)$$

where I_k is a constant affinity of the algae with light $(\mu E m^{-2} s^{-1})$, I the average light intensity of the pipes in the photobioreactor $(\mu E m^{-2} s^{-1})$, I_0 the light intensity on the surface of the tubes of the photobioreactor $(\mu E m^{-2} s^{-1})$, K_i a measure of photo inhibition $(\mu E m^{-2} s^{-1})$, *a*, *b*, *c* and *n* are parameters to be defined, A_1 and A_2 are the frequency factors $[(h)^{-1}]$, E_a and E_b are the activation energies $\left(\frac{kJ}{mol}\right)$, R is the universal gas constant $\left(\frac{kJ}{mol}\right)$, T is absolute temperature (K) and T_0 is the initial temperature (K).

. The average light intensity, *I*, is given as a function of concentration as follows:

$$I(C) = \frac{I_0}{\pi R}\int_0^R \int_0^{\pi} exp\left(-CK_a\left((R-S)\cos\phi + \sqrt{R^2 - (R-S)^2 \sin^2\phi}\right)\right) d\phi \quad (3)$$

$$K_a = Y_p'(1{,}12.10^{-2} - 8{,}6.10^{-6}C + 1{,}6.10^{-8}C^2) + Y_b \quad (4)$$

where K_a is the biomass absorption coefficient [$m^2 g^{-1} biomass$], R the radius [m], S the distance from vessel surface to an internal point [m] and φ is the angle of incidence of the path of light.

NUMERICAL SIMULATION

The computational model uses data related to the microalgae *Phaeodactylum tricornutum* studied by Grima et al. (2001) and Fernández et al. (2000), and the photobioreactor parameters proposed by Vargas (2007). These are summarized in Table 1.

A Fortran 95 code was developed for the computational implementation of the mathematical model given by Eqs (1) – (4), while the Gnuplot [*http://www.gnuplot.info*] application is used for an interactive graphical plot of results. The Gnuplot is loaded from inside the Fortran routine.

An important innovation of this study is the fact that the current computational model simulates day light cultivation cycle with 12 hours of light and 12 hours in the dark. During the 12 hours of darkness there is only the loss of biomass caused by the rate of maintenance. A sine function is used to describe the light intensity over 12 hours of the day on the surface of the tubes of the photobioreactor.

Table 1. Parameters used in the numerical simulations.

$C_0 = 200\frac{g}{m^3}$	$Y_b = 0.\frac{0105m^2}{g}$
$t_f = 120\ h$	$Y_p' = 2.\frac{99m^2}{g}$
$m = 0.00385h^{-1}$	$I_k = 94.3\mu Em^{-2}s^{-1}$
$I_0 = 2500\mu Em^{-2}s^{-1}$	$D_i = 0.04\ h^{-1}$
$a = 3.04$	$b = 1.209$
$c = 514.5$	$T_0 = 293\ K$
$A_1 = 0.26\ h^{-1}$	$A_2 = 0.18\ h^{-1}$
$E_a = 117040\ Jmol^{-1}$	$E_b = 163020\ Jmol^{-1}$
$Point_M = 500\frac{g}{m^3}$	$Point_D = 520\frac{g}{m^3}$
$Point_R = 480\frac{g}{m^3}$	$K_i = 2000\ \mu Em^{-2}s^{-1}$

A semi-continuous culture was simulated numerically. The cell concentration was maintained between two reference points: the dilution point and the recovery point. The dilution point was taken as the simulation starting point, whereas the recovery point marked the end of the dilution process, i.e., the moment when the cells concentration started to increase again. This interval was selected in order to guarantee a high growth rate. A third parameter, the midpoint concentration, is the concentration rate calculated as the arithmetic average between the concentration values at the dilution and recovery points. The overall process is summarized as: i) the cells concentration grows up to the dilution point; ii)

from this point and on, the dilution starts and the system renovates, and iii) this occurs until the cells concentration reaches the recovery point and the dilution is interrupted.

A parametric analysis was conducted by varying the medium temperature. The dilution point was set as $520\frac{\mathbf{g}}{\mathbf{m^3}}$ and the recovery point was set as $480\frac{\mathbf{g}}{\mathbf{m^3}}$. Simulations were performed for $274\ K \leq T \leq 300\ K$ with a temperature step of $1\ K$.

Equation (1) predicts the microalgae growth in the photobioreactor with respect to time. The equation was solved with a fixed step 4th order Runge-Kutta method. Equation (3) is a double integral and was approximated by a Riemann sum algorithm, as follows:

$$I'(C) = \frac{I_0}{\pi R^2}\sum_{i=1}^{m}\sum_{j=1}^{n} exp\left(-CK_a\left((R-S_i)\cos\phi_j + \sqrt{R^2-(R-S_i)^2\sin^2\phi_j}\right)\right)\Delta\phi\Delta S \quad (5)$$

where $m = \frac{R}{\Delta S}$ and $n = \frac{\pi}{\Delta\phi}$.

RESULTS AND DISCUSSION

Results of the computational simulation for the microalgae biomass production in a period of 5 days (120 hours) of semi-continuous culture and at different temperatures, are presented in Table 2.

Table 2. Production during the 5 days of semi-continuous culture, in different temperatures.

Temperature	Production
274 K	0.0 $\frac{g}{m^3 h}$
275 K	**0.1** $\frac{g}{m^3 h}$
276 K	0.2 $\frac{g}{m^3 h}$
277 K	0.4 $\frac{g}{m^3 h}$
278 K	0.6 $\frac{g}{m^3 h}$
279 K	0.9 $\frac{g}{m^3 h}$
280 K	1.3 $\frac{g}{m^3 h}$
281 K	1.8 $\frac{g}{m^3 h}$
282 K	3.4 $\frac{g}{m^3 h}$
283 K	**6.9** $\frac{g}{m^3 h}$
284 K	9.9 $\frac{g}{m^3 h}$
285 K	15.8 $\frac{g}{m^3 h}$
286 K	20.2 $\frac{g}{m^3 h}$
287 K	24.2 $\frac{g}{m^3 h}$
288 K	30.9 $\frac{g}{m^3 h}$
289 K	36.2 $\frac{g}{m^3 h}$
290 K	40.7 $\frac{g}{m^3 h}$
291 K	44.7 $\frac{g}{m^3 h}$
292 K	47.8 $\frac{g}{m^3 h}$
293 K	49.6 $\frac{g}{m^3 h}$
294 K	49.7 $\frac{g}{m^3 h}$
295 K	47.3 $\frac{g}{m^3 h}$
296 K	41.0 $\frac{g}{m^3 h}$
297 K	27.6 $\frac{g}{m^3 h}$
298 K	3.8 $\frac{g}{m^3 h}$
299 K	0.0 $\frac{g}{m^3 h}$
300 K	0.0 $\frac{g}{m^3 h}$

Figure 1 illustrates the numerical results of all simulations for a semi-continuous microalgae cultivation considering the different temperatures listed in Table 2.

Figure 2 shows the total production for each temperature used in the simulation. Note that the production of biomass, using the midpoint set $\left(500\frac{\mathbf{g}}{\mathbf{m^3}}\right)$, is only possible with temperatures ranging from $282\ \mathbf{K}$ to $298\ \mathbf{K}$.

The higher biomass production found by the numerical solution, $49.7\frac{g}{m^3 h}$, was obtained at 294 K. Figures 3–5 show in detail the production of biomass, specific growth rate and the average light intensity inside the tubes of the photobioreactor, respectively, as a function of time at a temperature of 294 K.

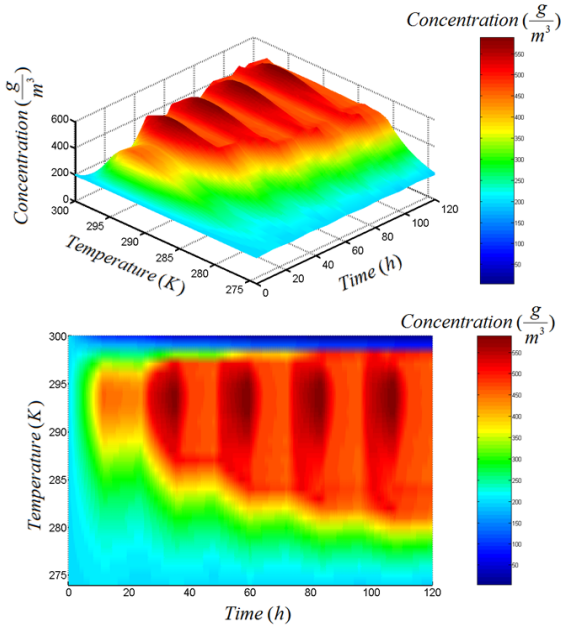

Figure 1. Microalgae biomass concentration versus simulation time and temperature for semi-continuous cultivation.

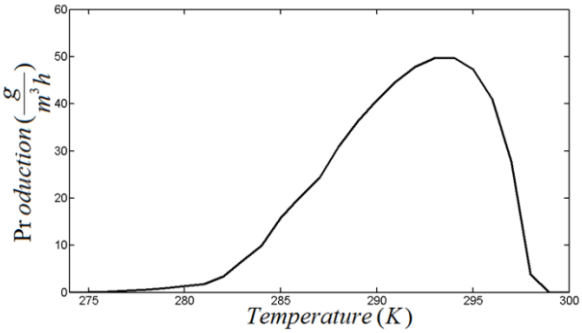

Figure 2. Production versus temperature for semi-continuous cultivation.

It is possible to notice in Fig. 4 the photoinhibition phenomenon in the middle of the 12 hours daylight period. This phenomenon is caused by the excess of incident light that occurs around noon. During the 12 hours of darkness (night time) there is no cell growth, since the microalgae requires light to grow.

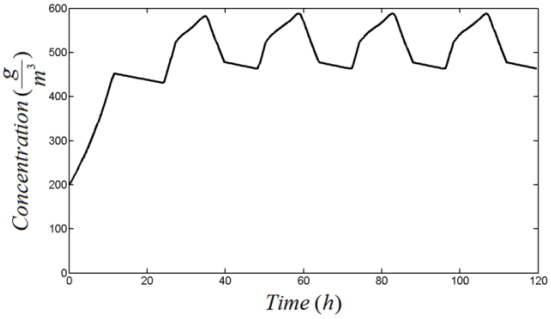

Figure 3. Biomass concentration versus simulation time for semi-continuous cultivation.

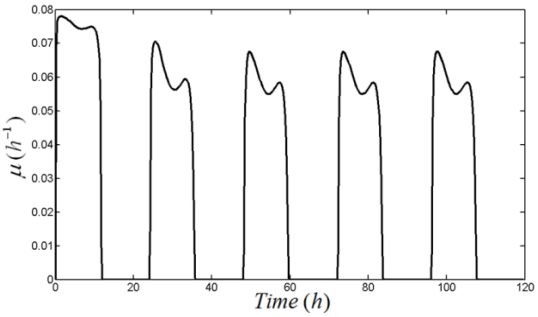

Figure 4. Specific growth rate versus simulation time for semi-continuous cultivation.

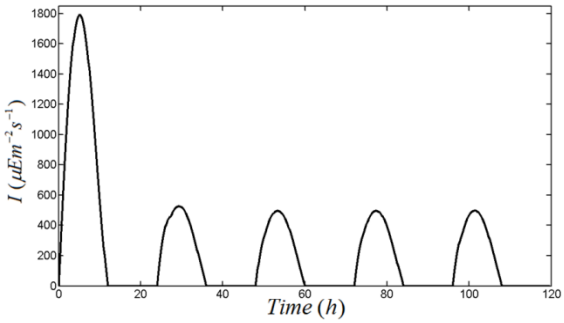

Figure 5. Mean light intensity within the photobioreactor pipes versus simulation time for semi-continuous cultivation.

CONCLUSION

This paper presented a mathematical model of a photobioreactor for cultivating microalgae with the objective of studying the microalgae growth as a function of temperature and average intensity of light inside the photobioreactor tubes. Simulation results showed that the highest biomass production was reached at a temperature of $294\ K$, showing that the model is capable of capturing growth inhibition as a function of temperature. It is also important to highlight that the photoinhibition phenomenon due to the excess of sunlight was properly reproduced by the proposed mathematical formulation. Another important innovation of this study is the fact that the current computational model could simulate the complete daily cycle, i.e., 24 h (day and night).

The method proved to capture the actual expected microalgae growth trends as a function of several parameters. The results show that there are opportunities for optimization of photobioreactor design and operating conditions that could lead to high yields of biomass production.

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