

# Application of Structured Population Balance Model for the Numerical Simulation of a Continuous Photobioreactor

Pietro Altimari\*, Francesca Pagnanelli, Luigi Toro

Dipartimento di Chimica, Università "Sapienza" di Roma, Piazzale Aldo Moro 5, 00185 Roma  
 pietro.altimari@uniroma1.it

The application of a structured population balance model to the numerical simulation of microalgal growth in a continuous photobioreactor is discussed. The analysis is focused on the interplay between microalgal metabolism and photobioreactor operation. The proposed model is structured to describe the evolution of mass distribution among different stages of the cell division cycle. Numerical results provide indications about the impact of the implemented nutrient supply strategy on biomass productivity. These information are of relevance in applications where nutrient deprivation is imposed to enhance the production of prescribed products.

## 1. Introduction

Microalgae offer the potential to convert inexpensive resources (sunlight, water and carbon dioxide) into products of significant industrial interest as, for example, dyes, fatty acids, medicine and healthy food (Trabucco et al., 2011). Considerable attention has also been attracted by these microorganisms in the context of renewable energy. Microalgae can indeed accumulate lipids with chemical composition similar to that of vegetable oil employed for biodiesel production, and can attain growth rate per unit area larger than that of any terrestrial plant (Chisti, 2007).

As photosynthetic microorganisms, microalgae can use light to generate the energy needed to metabolic activities. Numerous studies have in this respect focused on the research of reactor solutions ensuring uniform light distribution within the culture. In this framework, mathematical models providing a detailed description of light propagation in photobioreactors have been presented (Perner-Nochta and Posten, 2007). Owing to the lack of reliable kinetic models, a reduced number of studies have in contrast addressed the prediction of biomass productivity, nutrient and metabolite concentration. Moreover, only few attempts have been made to integrate a description of the microalgal metabolism in the formulation of a photobioreactor mathematical model (Concas et al., 2010). Most of the proposed models are based on the assumption that individual cells have the same mass and composition. This assumption rules out the possibility to accurately describe the interaction between cell metabolism and external environmental factors. It is on the other hand known that any individual cell develops through a cycle of events preceding mitosis (cell division) (Pascual and Caswell, 1997). Environmental factors (nutrient concentration and light) control the progression through the cell cycle. In particular, experiments have demonstrated that nutrient deprivation can block the progression through particular stages of the cycle leading to cell synchronization (Massie et al., 2010). In this latter condition, cells divide at the same time and a large growth in the cell number is found within a short time interval. Also, it must be taken into account that nutrient uptake is arrested during particular stages of the cycle. The response to nutrient deprivation can therefore be very different depending on the position of the cell within the cycle (Bernard, 2011).

The description of the cell cycle can be integrated into the mathematical model of a photobioreactor by recourse to an age structured population balance model (Pascual and Caswell, 1997). It can be assumed in this framework that microorganism proceed at velocity depending on nutrient availability through an initial age interval while metabolic activities are carried out irrespective of nutrient concentration following a prescribed age. This assumption, commonly referred to as transition point hypothesis, has been found effective in qualitatively describing the synchronization induced in microalgal cultures by nutrient

deprivation. Age structured balance models are however of difficult quantitative validation as it is complex or even impossible to track experimentally the age of individual microorganisms. Also, the microalgal growth rate is in general depending on the microalgal mass rather than age.

In this contribution, numerical simulations of the mathematical model of a photobioreactor are performed to analyze the influence of the nutrient concentration and light intensity on biomass productivity. A structured population balance model is coupled to reactor mass balance differential equations to describe the mass distribution of individual microorganisms among the different stages of the cell cycle. Mass and age are therefore employed as internal variables to describe the status of any microorganism. This enables structuring the cell cycle into resource dependent and resource independent phases while allowing for the application of mass depending growth rate expressions. The possibility to reproduce the evolution of mass distribution among different stages of the cell cycle can also be exploited for the experimental validation of the model. The population balance model is therefore formulated in such a way that nutrient uptake is arrested during an isolated phase of the cycle. Replication is also accounted through recourse to a probability division function. Numerical results provide indications about the impact of the implemented nutrient supply strategy on biomass productivity. These information are of practical relevance in applications where nutrient deprivation is imposed to enhance the production of prescribed products.

The rest of the paper is structured as follows. In section 2, the adopted mathematical model is described. In section 3, results of numerical simulation of proposed model are presented. Final remarks end the paper.

## 2. Mathematical model

We consider a continuous stirred tank photobioreactor for microalgal growth. The analysis is focused on the interaction between cell cycle and reactor operation. The main issue to be addressed in this context is the existence of a stage during which progression through the cycle is possible regardless nutrient availability. Age structured population balance models can be used for this purpose (Pascual and Caswell, 1997). This approach is however of difficult experimental validation and does not account for the influence of cell mass on the velocity of progression through the cycle. It is for example unlikely that new born cells can undergo division without experiencing a preliminary growth. The use of cell mass alone as internal variable would rule out on the other hand the possibility to define a stage independent of nutrients availability. In absence of nutrients, cell growth is indeed invariably arrested.

In the following, a structured population balance model is coupled to the reactor mass balance differential equations to describe the evolution of mass distribution of microorganisms among different stages of the division cycle. Both mass and age are employed to define the cell status. The concentration of nitrates, phosphates and dissolved oxygen are therefore computed along with the distribution of microorganisms in the mass-age space. Equations governing the dynamics of nutrient concentrations can be written as follows:

$$\frac{dC_j}{dt} = -Dil(C_{j,in} - C_j) - \frac{1}{Y_{Xj}} \int_0^{\infty} \int_0^{\infty} r(m, I, C_j, C_{O_2}) \Phi(m, p) dm dp \quad (1)$$

$$j = NO_3^-, H_2PO_4^-$$

$$\frac{dC_{O_2}}{dt} = -Dil(C_{O_2,in} - C_j) - \frac{1}{Y_{XO_2}} \int_0^{\infty} \int_0^{\infty} r(I, C_j, C_{O_2}) \Phi(m, p) m dm dp \quad (2)$$

where  $r(I, C_j, C_{O_2})$  is the specific growth rate,  $m$  and  $p$  are the mass and age of a microorganism respectively,  $\Phi(m, p) dm dp$  is the number of microalgae with  $(m, p) \in [m - dm, m + dm] \times [p - dp, p + dp]$ ,  $C_j$  is the concentration of the species  $j$ ,  $I$  is the light intensity,  $Y_{Xj}$  is the ratio of the weight of produced biomass to the weight of the consumed nutrient  $j$ ,  $Dil$  is the reactor dilution. The following expression is adopted for the growth velocity:

$$\frac{dm}{dt} = r(I, C_j, C_{O_2}) m = \mu_{max} \frac{I^n}{I_K^n + I^n} \prod_{i=1}^2 \frac{C_j}{K_j + C_j} \left( 1 - \frac{C_{O_2}}{C_{O_2,max}} \right) \cdot m \quad (3)$$

To incorporate the transition point hypothesis, we divide the cell cycle into a resource dependent and a

resource independent segment. It is assumed that the maturation velocity  $dp/dt$  is depending on the concentration of nutrients when  $m \in [0, m_c]$  while  $dp/dt$  is constant beyond the transition point  $m_c$ . The following dependence is in particular adopted:

$$\frac{dp}{dt} = r(I, C_j, C_{O_2}) \cdot p_{ref} \quad m \in [0, m_c] \quad (4)$$

$$\frac{dp}{dt} = \mu_{max} \cdot p_{ref} \quad m > m_c \quad (5)$$

The population balance governing the evolution of the distribution function  $\Phi(m, p, t)$  can in this framework structured as follows:

$$\frac{\partial \Phi}{\partial t} = - \frac{\partial r m \Phi}{\partial m} - \frac{\partial r p_{ref} \Phi}{\partial m} - Dil \Phi - \Gamma(m, p, C_j, C_{O_2}) \Phi \quad m \in [0, m_c] \quad (6)$$

$$\frac{\partial \Phi}{\partial t} = - \frac{\partial r m \Phi}{\partial m} - \frac{\partial \mu_{max} p_{ref} \Phi}{\partial p} - Dil \Phi - \Gamma(m, p, C_j, C_{O_2}) \Phi \quad m > m_c \quad (7)$$

where  $\Gamma(m, p, C_j, C_{O_2})$  denotes the division rate. The following expression is employed for this function:

$$\Gamma(m, p, C_j, C_{O_2}) = \frac{dm}{dt} \frac{\delta_1(m)}{1 - \int_0^m \delta_1(s) ds} + \frac{dp}{dt} \frac{\delta_2(p)}{1 - \int_0^m \delta_2(s) ds} \quad (8)$$

$\delta_1$  and  $\delta_2$  are the probability density functions for mass and age at division. Normal distributions are used to describe these two latter functions. It should be noted that with the illustrated modelling approach, microorganisms characterized by mass larger than  $m_c$  can increase their age even in absence of nutrients. This allows microorganisms with mass larger than  $m_c$  to undergo division irrespective of nutrients availability.

The model is completed by formulating the following boundary condition to Eq (6)-Eq (7):

$$\Phi(0, p, t) = 0 \quad (9)$$

$$\frac{dp}{dt} \Phi(m, 0, t) = 2 \int_0^{\infty} \Gamma(m, p, C_j, C_{O_2}) \Phi(m, p, t) dp \quad (10)$$

Eq (8) expresses the impossibility to have microorganisms with mass equal to zero while boundary condition Eq (10) describes cell replication. Once the distribution function is computed, the biomass concentration can be evaluated as follows:

$$C_X = \int_0^{\infty} \int_0^{\infty} \Phi(m, p) m dm dp \quad (11)$$

The average light intensity  $I$  within the culture is computed as follows:

$$I(t) = \frac{I_0(t)}{L_{eq} K_a C_X} \cdot [1 - \exp(-L_{eq} K_a C_X)] \quad (12)$$

where  $L_{eq}$  is the length of the light path and is related to the reactor diameter (Molina Grima et al., 2001). The described model was reduced by finite difference techniques (Mantzaris et al., 2001) to a system of ordinary differential equations and numerically integrated. Parameter values adopted in the numerical simulation are reported in Table 1. Data related to the normal distribution functions employed to describe

cell division have been selected based on the indications of (Pascual and Caswell, 1997; Concas et al., 2010) and references therein.

Table 1: Model parameters

$\mu_{\max}$	$2.06\text{E-}05\text{ s}^{-1}$	$K_a$	$0.15\text{ m}^2\text{ g}^{-1}$
$I_K$	$160\text{ }\mu\text{E m}^{-2}\text{ s}^{-1}$	$C_{O2\max}$	$47.9\text{ g m}^3$
$I_0$	$160\text{ }\mu\text{E m}^{-2}\text{ s}^{-1}$	$Y_{X/1}$	2.7
$n$	1.5	$Y_{X/2}$	41
$K_1$	$5.314\text{ g m}^{-3}$	$Y_{X/O2}$	0.5
$K_2$	$0.028\text{ g m}^{-3}$	$p_{ref}$	1 day
$K_{eq}$	$1.6\text{E-}03\text{ m}$	$m_c$	$6\cdot 10^{-10}\text{ g}$

### 3. Results

To analyze the interaction between microalgal metabolism and photobioreactor operation, numerical simulation of the formulated mathematical model was performed in the assumption of batch operation, that is  $Dil = 0$ . The initial distribution  $\Phi(m, p, 0)$  was assumed to be normal. The predicted evolution of the distribution function is illustrated in Figure 1.

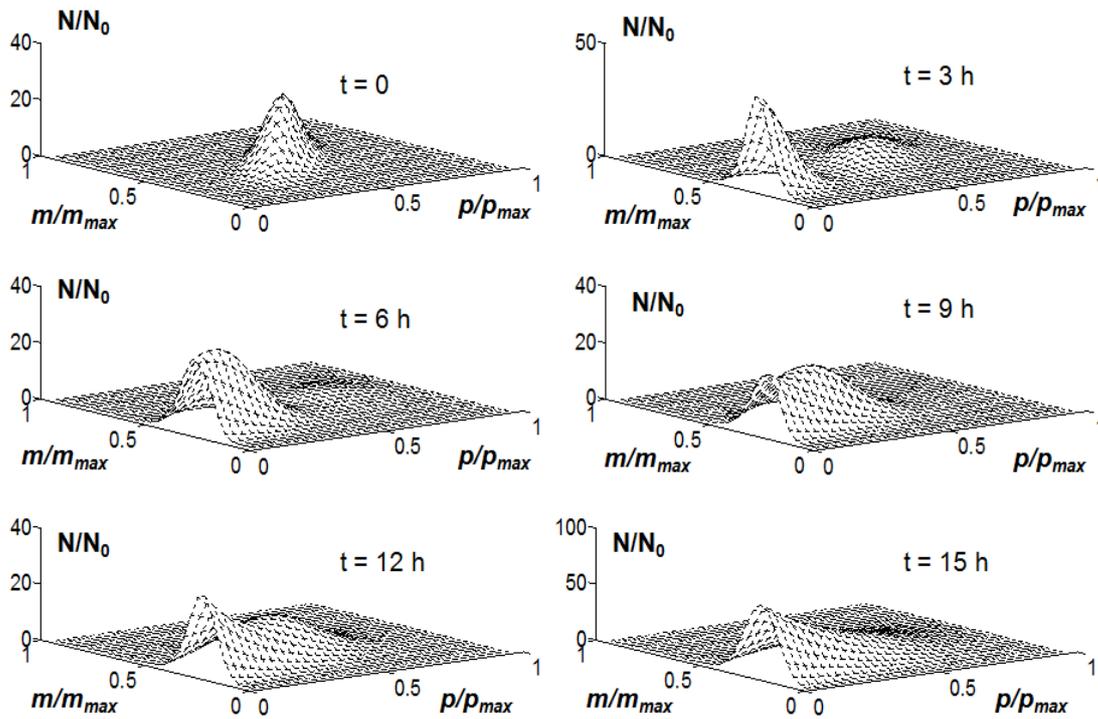


Figure 1: Evolution of the cell distribution function during batch operation. Age and mass values are scaled by two reference values  $m_{\max}$  and  $p_{\max}$  respectively ( $m_{\max} = 10^{-9}\text{ g}$ ;  $p_{\max} = 2\text{ days}$ ).

Surface diagrams of the distribution function  $\Phi(m, p, t)$  at successive time instants are displayed. Cell division initially determines a rapid increase in the fraction of microorganisms at low maturation and mass values. A moving front is then formed as new born cells grow and increase their age. A bimodal distribution is consequently found following an initial transient. New born microorganisms then increase their mass and move in direction of the transition point  $m_c$ . The progressive depletion of nutrients arrests the progression of microalgae through the cycle.

The evolution of the concentration of biomass and nutrients corresponding to the discussed numerical simulation is reported in Figure 2. It is apparent that the arrest of biomass growth is determined by the depletion of nitrates.

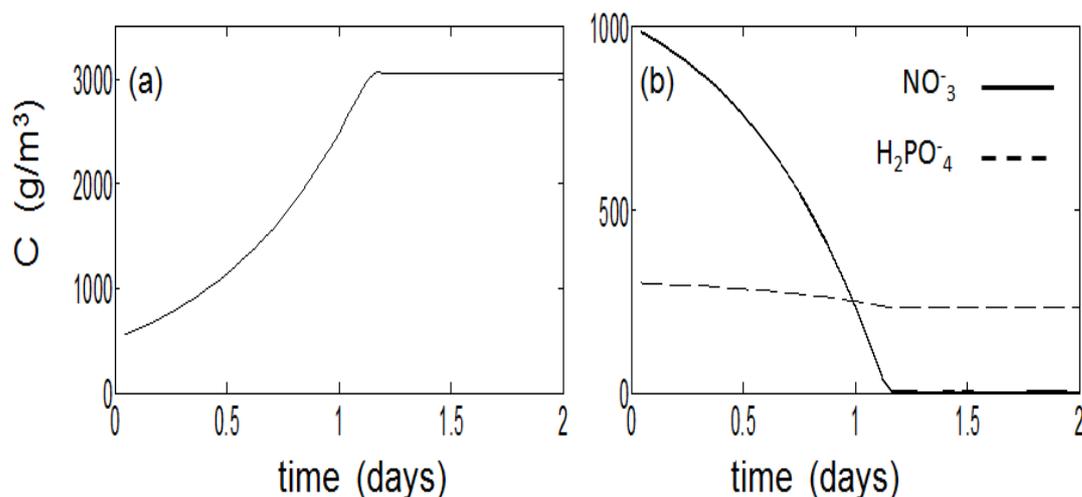


Figure 2: Evolution of biomass and nutrient concentration during batch operation; a) biomass concentration; b) nitrates and phosphates concentrations.

Since nutrient depletion can block microorganisms in the resource dependent segment of the cycle, it is of fundamental importance to evaluate the impact of the nutrient supply strategy on microalgal growth. Typically, microalgae are cultivated through recourse to a fed-batch strategy. With this strategy, the photobioreactor is initially operated in batch till attaining nutrient deprivation conditions. Then, biomass is harvested and fresh nutrients are supplied. It must be remarked that nutrient deprivation conditions are necessary to stimulate the synthesis of important products as, for example, bio-oil or hydrogen. They are in some cases maintained for a prolonged time interval before harvesting biomass and supplying fresh medium. The impact of the period of harvesting and fresh medium supply on microalgal growth must be analyzed to attain optimal productivity values.

Figure 3 illustrates the influence of the time interval between two successive harvesting phases on microalgal growth in fed-batch operation. The evolution of the biomass concentration immediately before harvesting is displayed as the harvesting period  $\Delta t$  is varied. Numerical simulations were performed by instantaneously reducing and increasing respectively biomass and nutrient concentration at harvesting. The ratio of the harvested to the original culture volume was assumed to be equal to 10. Biomass concentration decreases leading to the wash-out of the photobioreactor at harvesting period around 1 day. Under these conditions, harvesting is performed before biomass concentration can attain satisfactory values and a reduction in the amount of collected biomass is progressively found. A gradual increase in the average microalgal growth rate is observed as the harvesting period is increased to 2 days. This latter period enables minimizing the time needed to the reactor to attain regime conditions. The time needed to reach the regime successively increases as larger values are selected for the period of harvesting. This can be explained by taking into account that an exceedingly large period of harvesting increases the time interval during which the culture is left in nutrient deprivation condition and, thus, unable to grow.

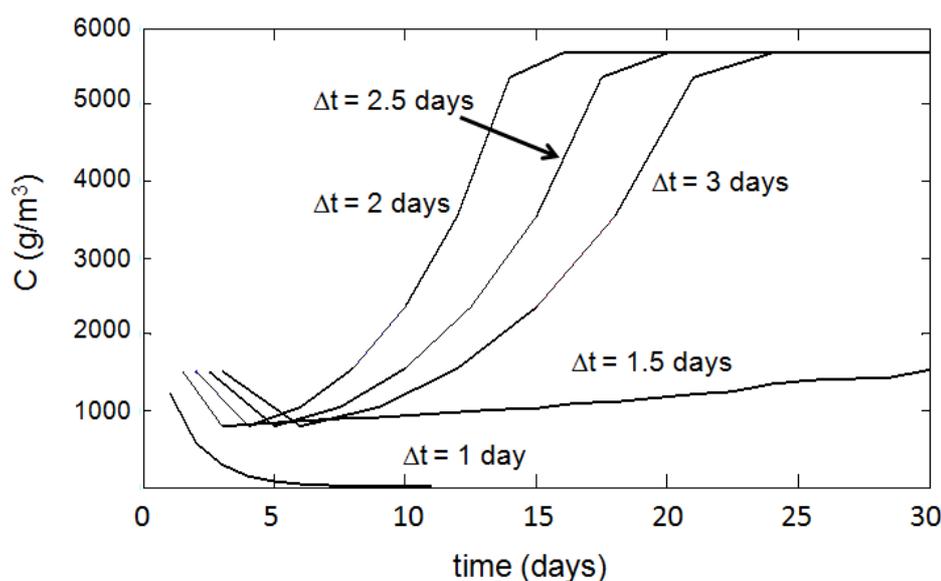


Figure 3: Influence of the harvesting period on microalgal growth in fed-batch operation. Any displayed curve describes the evolution of the biomass concentration predicted immediately before harvesting.

#### 4. Conclusions

The article discussed the application of a structured population balance model to the numerical simulation of microalgal growth in continuous stirred photobioreactor. The analysis was focused on the interaction between microalgal division cycle and photobioreactor operation. From this perspective, the mathematical model was structured so as to allow for the prediction of the mass distribution among different stages of the division cycle. Mass and age were therefore employed as internal variables to describe the status of any microorganism. This enables structuring the cell cycle into resource dependent and resource independent phases while allowing for the application of a mass depending growth rate expression. The possibility to reproduce the evolution of mass distribution among different stages of the cell cycle can also be exploited for the experimental validation of the model. Numerical simulations of the formulated mathematical model were performed to analyze the influence of the nutrient supply strategy on microalgal growth. The illustrated modelling approach can provide valuable insight into the analysis of applications where nutrient deprivation is imposed to stimulate the production of prescribed products.

#### References

- Bernard O., 2011, Hurdles and challenges for modelling and control of microalgae for CO<sub>2</sub> mitigation and biofuel production, *Journal of Process Control* 21, 1378-1389.
- Chisti Y., 2007, Biodiesel from microalgae, *Biotechnol. Adv.* 25, 294-306.
- Concas A., Pisua M., Cao G., 2010, Novel simulation model of the solar collector of BIOCOIL photobioreactors for CO<sub>2</sub> sequestration with microalgae, *Chemical Engineering Journal*. 157, 297-303.
- Mantzaris N.V., Daoutidis P., Sreenc F., 2001, Numerical solution of multi-variable cell population balance models: I. Finite difference methods, *Computers and Chemical Engineering*. 25, 1411-1440.
- Massie T.M., Blasius B., Weithoff G., Gaedke U., Fussmann G.F., 2010, Cycles, phase synchronization, and entrainment in single-species phytoplankton populations, *Proceedings of the National Academy of Sciences*. 107, 4236-4241.
- Molina Grima E., Sevilla J.F., Ación Fernández F.G., Chisti Y., 2001, Tubular photobioreactor design for algal cultures, *J. Biotechnol.* 92,113-135.
- Pascual M., Caswell H., 1997, From the cell cycle to population cycles in phytoplankton-nutrient interactions, *Ecology*. 78, 897-912.
- Perner-Nochta I., Posten C., 2007, Simulations of light intensity variation in photobioreactors *Journal of Biotechnology*. 131, 276-285.
- Trabucco F., Cruz Viggi C., Pagnanelli F., Toro L., 2011, Development of an Integrated Process for Bio-Oil Production from Microalgae, *Chemical Engineering Transactions*, 24, 1237-1241.