

# Optimization of the Interval Approach for *Chlorella vulgaris* Biomass Estimation

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**Abstract**— As a result of different environmental issues, especially global warming and the greenhouse effect, biotechnology using microalgae has become a very promising alternative for carbon dioxide mitigation. Indeed, these unicellular microorganisms reduce efficiently carbon dioxide emissions through their photosynthetic activity. In order to maximize the efficacy of this biological process, one of the challenges is the efficient on-line estimation of the microalgae biomass for control strategies. In this context, several studies have established the performance and robustness of the interval observer for biomass estimation. This paper proposes a method of optimization of the gains tuning of the interval observer for the biomass concentration of *Chlorella vulgaris* culture in a continuous photobioreactor, using Total Inorganic Carbon measurements. This study provides two procedures for choosing the gains of the estimation strategy under a specific operating condition. The optimization methodology is validated by numerical simulations in the presence of uncertain model parameters and noisy measurements.

## I. INTRODUCTION

As a consequence of global warming and the greenhouse effect, research on CO<sub>2</sub> mitigation technologies have been investigated in order to reduce carbon dioxide emission into the atmosphere [1]. Biological carbon dioxide sequestration has recently become a very attractive proposal allowing biotransformation of carbon dioxide into biomass and other high value molecules through photosynthesis [1]. Among these biological processes, culture of microalgae has received renewed attention as an effective method for CO<sub>2</sub> bio-fixation. These photosynthetic microorganisms are able to assimilate carbon dioxide and bicarbonate ions as source of inorganic carbon to produce a storable form of renewable energy, biomass. The major advantages of using microalgae for this purpose are a high photosynthetic efficiency and a fast growth rate; additionally the possibility of controlling the growth conditions in “photobioreactors” is very attractive [2]. These unicellular microorganisms present higher CO<sub>2</sub> fixation abilities than higher plants [1] [3]. Thus, using microalgae biotechnology for CO<sub>2</sub> sequestration purposes is believed to be a globally significant and

economically viable environmental technology.

The optimization of this biological process is related to the characteristics of the culture system design, the selection of appropriate microalgae and the operating conditions. Several authors have been interested in the selection of microalgae species with high CO<sub>2</sub> fixation ability [4-5]. Indeed, *Chlorella* species are considered very promising candidates for CO<sub>2</sub> fixation, converting significant levels of carbon dioxide in the airstream of photobioreactors into biomass. In this context, *Chlorella sp.* is one of the most studied algae for bio-fixation of carbon dioxide [6]. In the same way, the implication of the green unicellular species *Chlorella vulgaris* for the CO<sub>2</sub> sequestration technology has been highlighted [6-7].

A fundamental step for the implementation of an effective control strategy is based on choosing a reliable model that can effectively describe the biochemical dynamics of microalgae growth. Numerical models have been used for predicting microalgae growth rate and cellular concentration in a given environment. This mathematical equation highlights the influence of light intensity [8], and/or carbon source for growth [9]. Another important step for control purposes is the estimation methods required to overcome the lack of physical sensors. The cellular concentration (or biomass) is an important parameter for CO<sub>2</sub> bio-fixation by microalgae. Thus, designing a robust biomass observer against model and kinetic parameter uncertainty represents a real challenge in bio-processes. Several studies have tackled biomass estimation through the extended Kalman filter [10] and the asymptotic estimator methods [11]. However, several research works have focused on the efficiency of a new estimation approach for microalgal cultures based on the interval analysis method [12-13]. In fact, it allows reconstruction of a guaranteed interval of the unmeasured state from the knowledge of the interval-bounded initial condition, model parameters and on-line available measurements. In the same way, the interval observer can provide upper and lower bounds of the state trajectory from the measurements of total inorganic carbon concentration and environmental parameters such as pH, temperature, light intensity, dilution rate and partial pressure of CO<sub>2</sub>. In this regard, the aim of this study is to improve the interval estimation of *Chlorella vulgaris* biomass through optimization of the estimator gains.

The paper is organized as follows: the first section introduces the mathematical growth model for *Chlorella*

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*vulgaris* and its kinetic expression. The second section is devoted to describing the general structure of the proposed interval observer and the optimization approach of the observer gains. Several simulations are presented in the third section to validate this optimization methodology for biomass estimation against the uncertainty of model parameters. Concluding remarks are stated in the last section.

## II. MICROALGAL BIOREACTOR MODEL

The following section provides details of the governing equations and growth model parameters of *Chlorella vulgaris*. To accurately describe the growth behavior of this green microalga in a photobioreactor, a specific model based on the one proposed by Nouals, cited in [9] [14], by neglecting the substrate inhibition term, implies the association of the Monod model for the light effect and the Contois model for limitation effect by a substrate as the total inorganic carbon [9] [11]. The dynamics of the bioreactor is described by a set of two differential equations. Units of all parameters are given in the Table I.

Biomass evolution is obtained by a standard mass balance in the photobioreactor assuming perfectly-stirred conditions under continuous mode (CSTR):

$$\frac{dX}{dt} = \mu X - DX \quad (1)$$

where  $\mu$  is the specific growth rate of algae,  $X$  is the cellular concentration (biomass in billion cells per liter) in the photobioreactor and  $D$  is the dilution rate, i.e. the ratio of the flow rate of medium to culture volume in the photobioreactor.

Total Inorganic Carbon ( $TIC$  in mole per liter) is the sum of carbon dioxide ( $CO_2$ ), bicarbonate ( $HCO_3^-$ ) and carbonate ion ( $CO_3^{2-}$ ) species in the medium. The predominance of one form is dictated by the  $pH$  of the culture. The dynamics behavior of  $TIC$  consumption is obtained by a mass balance for a CSTR:

$$\frac{d[TIC]}{dt} = -\mu \frac{X}{Y} - D[TIC] + k_L a ([CO_2]^* - [CO_2]) \quad (2)$$

where  $Y$  and  $k_L a$  are the biomass conversion yield which represents the amount of biomass produced to the amount of total inorganic carbon consumed and the gas-liquid transfer coefficient of carbon dioxide, respectively.

The equilibrium carbon dioxide concentration is defined as:

$$[CO_2]^* = \frac{P_{CO_2}}{H} \quad (3)$$

where  $P_{CO_2}$  and  $H$  represent the partial pressure of carbon dioxide (0.05 atm under our experimental conditions) and Henry's constant for carbon dioxide for Bristol 3 N medium at 25°C (29 atm.L.mole<sup>-1</sup>), respectively. Furthermore, the carbon dioxide concentration in the culture is calculated by the following expression:

$$[CO_2] = \frac{[TIC]}{1 + \frac{K_1}{[H^+]} + \frac{K_1 \cdot K_2}{[H^+]^2}} \quad (4)$$

where  $K_1$  ( $pK_1 = 6.35$  at 25°C) and  $K_2$  ( $pK_2 = 10.3$  at 25°C) are the dissociation constants of the chemical equilibriums between ( $CO_2/HCO_3^-$ ) and ( $HCO_3^-/CO_3^{2-}$ ) respectively. Concentration of hydrogen ions in the culture is given by:

$$[H^+] = 10^{-pH} \quad (5)$$

The following model presents the specific growth rate for *Chlorella vulgaris* as a function of light intensity limitation and substrate limitation effect (see [9] for more details):

$$\mu = \mu_{\max} \cdot \left( \frac{E}{K_E + E} \right) \cdot \left( \frac{[TIC]}{K_{CL} \cdot X + [TIC]} \right) \quad (6)$$

where  $\mu_{\max}$ ,  $K_E$  and  $K_{CL}$  are the maximal specific growth rate, the half saturation constant for light intensity available per cell (denoted by  $E$ ) and the half saturation constant for TIC, respectively. These model parameters were identified and validated, through Matlab<sup>TM</sup> environment, with experimental data of *Chlorella vulgaris* cultures operating in batch and continuous [9].

The light intensity accessible per cell is described as following:

$$E = \frac{(I_{in} - I_{out}) A_r}{V \cdot X} \quad (7)$$

where  $I_{in}$ ,  $I_{out}$  and  $A_r$  are the incident, outgoing light intensity and the bioreactor illuminated area, respectively.

The outgoing light intensity can be calculated by an analytical expression as a function of biomass and the incident light intensity according to the following relation (see [14] for more details):

$$I_{out} = C_1 \cdot I_{in} \cdot X^{C_2} \quad (8)$$

with  $C_1$  and  $C_2$  constants depending essentially on the reactor geometry.

This work proposes a robust interval observer of biomass estimation from  $TIC$  measurements and with the model parameter uncertainty. The main goal is the accurate choice of the observer gains in order to optimize the biomass estimation of *Chlorella vulgaris*.

## III. DESIGN OF THE INTERVAL OBSERVER

### A. Estimation methodology

In this section, a robust interval observer for biomass estimation will be proposed using the model structure shown in Section II. This approach is based on the interval analysis, i.e. reconstruction of an upper and lower bound of the missing state. In this direction, the developments below are an extension of the application and results obtained in [13]. The design of this observer is based on the properties of the monotone dynamical systems [15], i.e. the missing state must be bounded by a solution of dynamical systems that fulfills the condition of "cooperative systems". This



Through the condition on the observer gains cited previously (13), the system (15) is cooperative and the positive error is bounded by:

$$0 \leq e^+(t) \leq e^{++}(t) \quad \forall t$$

where  $e^{++}(t)$  is the solution of the system:

$$\dot{e}^{++} = J^{++} e^{++} + \Lambda(X, \mu_{\max}^+) \quad (18)$$

with the initialization step given by:

$$e^{++}(0) = e^+(0)$$

The term  $\Lambda$  remains bounded as follows:

$$\Lambda \leq \begin{pmatrix} 0 \\ \mu_{\max}^+ \cdot \frac{k_L a \cdot Y \cdot [CO_2]^*}{D} \end{pmatrix} \quad (19)$$

The stability of the error is guaranteed if the matrix  $J^{++}$  is Hurwitz, leading to the following conditions:

$$\begin{cases} \text{Trac}(J^{++}) = -2D - \frac{g_1^+}{Y} - \alpha \cdot k_L a + \mu_{\max}^+ + \frac{g_2^+}{Y} < 0 \\ \text{Det}(J^{++}) = \left( \left( -D - \frac{g_1^+}{Y} - \alpha \cdot k_L a \right) \left( \mu_{\max}^+ - D + \frac{g_2^+}{Y} \right) \right) \\ \quad - \left( -\frac{g_2^+}{Y} \left( \alpha \cdot k_L a + \frac{g_1^+}{Y} \right) \right) > 0 \end{cases} \quad (20)$$

Thus, the stability of the error dynamics is fulfilled as long as the condition of cooperativity (13) and stability (20) on the observer gains are satisfied:

$$\begin{cases} g_1^+ \geq -\alpha \cdot Y \cdot k_L a \\ g_2^+ < \min \left[ \begin{array}{l} 0 \\ g_1^+ + Y \cdot (2D + \alpha \cdot k_L a - \mu_{\max}^+) \\ \left( \frac{D \cdot Y + g_1^+ + \alpha \cdot k_L a \cdot Y}{D} \right) (D - \mu_{\max}^+) \end{array} \right] \end{cases} \quad (21)$$

The interval observer design (14) allows reconstructing a stable and guaranteed interval of the biomass through the estimation of lower and upper bounds, described by:

$$\begin{cases} X^-(t) \leq X(t) \leq X^+(t), \quad \forall t \geq 0 \\ \text{and } X^+(t) - X^-(t) \text{ stable} \end{cases} \quad (22)$$

Moreover, from (18) and (19), an upper bound for the biomass estimation error can be derived as follows:

$$e_X(\infty) \leq -(J^{++})^{-1} \cdot \begin{pmatrix} 0 \\ \mu_{\max}^+ \cdot \frac{k_L a \cdot Y \cdot [CO_2]^*}{D} \end{pmatrix} \quad (23)$$

### B. Gain design and optimization approach

The objective of this part is to optimize the interval approach of biomass estimation of *Chlorella vulgaris* through an optimized choice of observer gains  $g_1$  and  $g_2$ .

Thus, in order to ensure the exponential convergence of

this observer,  $g_1$  and  $g_2$  must be tuned in order to fulfill the cooperative condition and to minimize the guaranteed interval between the upper and lower bounds. This technique considers that the error dynamics applied to the two states  $(Z, X)$  is governed by a second order system. In the same way, the aim is to set the convergence dynamics across the tuning of eigenvalues of the Jacobian matrix (17).

Consequently, calculating the characteristic polynomial of  $J^{++}$ , the tuning of the interval observer gain  $g_1$  and  $g_2$  is performed by the following equation:

$$\begin{cases} g_1^+ = -Y \cdot \frac{D^2 + \omega_0^2 - 2\xi \cdot D \cdot \omega_0}{\mu_{\max}^+} - Y \cdot \alpha \cdot k_L a \\ g_2^+ = Y \cdot \left( 2D - \mu_{\max}^+ - 2\omega_0 \cdot \xi + \alpha \cdot k_L a + \frac{g_1^+}{Y} \right) \end{cases} \quad (24)$$

where  $\omega_0$  and  $\xi$  represent the natural frequency and damping coefficient of the second order system, respectively.

From (21) and (24), the cooperativity condition on  $g_1$  gives conditions on values of  $\omega_0$  and  $\xi$ :

$$\begin{cases} \xi > 1 \\ \xi \cdot D - D \cdot \sqrt{\xi^2 - 1} \leq \omega_0 \leq \xi \cdot D + D \cdot \sqrt{\xi^2 - 1} \end{cases} \quad (25)$$

It can be noticed from (25) that the natural frequency has a minimum bound equal to the dilution rate  $D$ . Thus, the observer convergence speed is limited by the value of the dilution rate. Consequently, eigenvalues of the error dynamics are chosen so that the estimation error behavior has good convergence properties.

Another way to tune the observer's convergence consists in choosing its gains  $(g_1, g_2)$  so that the estimation error respects a given accuracy. Indeed, (23) gives an upper bound on the biomass steady state error. Thus, estimator gains are determined by minimizing this steady state error under constraints that the system is cooperative and the error dynamics is stable:

$$\min_{g_1, g_2} -(J^{++})^{-1} \cdot \begin{pmatrix} 0 \\ \mu_{\max}^+ \cdot \frac{k_L a \cdot Y \cdot [CO_2]^*}{D} \end{pmatrix} \quad (26)$$

s.t. (21)

However, the solution of problem (26) is to set  $g_2 \rightarrow -\infty$ . To fix a finite value of  $g_2$ , one can either choose a desired error value and solve (25) so that the criterion is equal to this value; or deal simultaneously with the observer's convergence and the steady state error value. In the next section, this optimization problem is solved so that a given steady error value is guaranteed.

### C. Estimator robustness w.r.t. model uncertainties

Previously, only uncertainties in growth rate parameters were considered. However, other parameters can affect the estimator efficiency, namely the biomass conversion yield  $Y$  and the gas-liquid transfer coefficient of carbon dioxide  $k_L a$ .

Estimator dynamics equations (14) were modified in order

to introduce lower and upper bounds of these parameters, leading to similar error dynamics as (17).

In this case, the bound of the steady state error (23) depends on the difference of the upper and lower bounds of  $k_L a$  and  $Y$ . The minimum value reached by the new steady state error bound could not be decreased as desired and depends on the culture conditions and on the model accuracy. For instance, in case of  $k_L a$  mismatch only, the upper bound of biomass steady state estimation error tends to a nonzero value, leading to the following relationship:

$$e_X(\infty) \leq Y \cdot \frac{k_L a^+ - k_L a^-}{D} \cdot [CO_2]^* \quad (27)$$

Thus, depending on  $k_L a^+ - k_L a^-$ ,  $Y$  and  $D$ , the estimator gains could be optimized if the desired error is bigger than the limit given in (27). A similar result has been found for biomass conversion yield  $Y$ . In the general case, this error cannot be reduced as desired since this upper bound is fixed by culture conditions. In the next section, this phenomenon will be highlighted by simulation results.

#### IV. NUMERICAL SIMULATION

The validation of this study was provided by numerical simulation based on the model parameters of *Chlorella vulgaris* presented in Table I. An identification and validation phase of the growth model parameters (6) was carried out in the Matlab<sup>TM</sup> environment through a set of batch and continuous cultures of *Chlorella vulgaris* in a photobioreactor of 9.6 L under optimal growth conditions [9]. In the following, 30% mismatch on the growth rate model parameters is considered. Simulations also consider a measurement noise acting on the substrate measurement of zero means and 0.01 standard deviation. The initialization step is given by:

$$X(0) = 20 \cdot 10^9 \text{ cell L}^{-1} \quad TIC(0) = 10^{-3} \text{ mole L}^{-1}$$

with an initialization error of biomass selected to be more or less 20 billion cells per liter.

TABLE I  
GROWTH MODEL AND SIMULATION PARAMETERS FOR *CHLORELLA VULGARIS* IN A PHOTOBIOREACTOR

parameter	Unit	Value
$\mu_{\max}$	$\text{h}^{-1}$	0.08
$K_E$	$\mu\text{E} \cdot \text{s}^{-1} \cdot 10^9 \cdot \text{cell}^{-1}$	0.14
$K_{CL}$	$\text{mole} \cdot 10^9 \cdot \text{cell}^{-1}$	$1.28 \cdot 10^{-5}$
$C_1$		0.49
$C_2$		-0.92
$V$	L	9.6
$A_r$	$\text{m}^2$	0.31
$k_L a$	$\text{h}^{-1}$	1.36
$Y$	$10^9 \text{ cell} \cdot \text{mole TIC}^{-1}$	3555
$H$	$\text{atm} \cdot \text{L} \cdot \text{mole}^{-1}$	29
$D$	$\text{h}^{-1}$	0.01

The main simulation parameters consider a  $90 \mu\text{mole} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$  incident light intensity, a constant  $pH$  value of 6

(experimentally, the  $pH$  is stabilized around this value) and  $P_{CO_2}$  fixed at 0.05 atm. The sampling period is set to 10 minutes.

The major purpose of this study is to enhance the performance of the interval observer previously described, in Section III, through an optimization of the gains design. The performance analysis is evaluated by the monitoring of the biomass evolution and the efficient study of estimation through an optimized, stable and robust guaranteed interval against uncertainties of model parameters.

##### A. Biomass estimation with uncertainties on growth rate parameters

During this part, improving the performance of the interval observer was analyzed through a study of the impact of an optimal choice of the natural frequency of the error dynamics on the efficiency of biomass estimation.

First, the importance of the cooperativity condition is showed in simulation and is illustrated in Fig. 1. Two cases are considered: a first observer which does not respect the cooperativity condition (by setting the damping factor  $\xi = 0.7$ ), and a second one with  $\xi = 2$  which is thus cooperative. The two observers have the same natural frequency satisfying (25). As shown in Fig. 1, the second observer helps to estimate the real biomass concentration, by giving good upper and lower estimation bounds. Conversely, the loss of the cooperativity condition leads to an inversion of these upper and lower bounds. Thus, choosing estimator eigenvalues according to (25) helps to guarantee the cooperativity condition.

Fig. 2 illustrates the influence of the natural frequency on the transient behavior of the interval estimation. Three values of the natural frequency  $\omega_0$  are tested, chosen according to (25) ( $5D$ ,  $10D$  and  $15D$ , denoted respectively as cases 1 to 3 in the figure). It can be noticed that upper and lower estimators converge to the real biomass concentration, despite the growth rate model uncertainties. On the other hand, it can be highlighted that the steady state biomass estimation error depends on the estimator gains chosen.

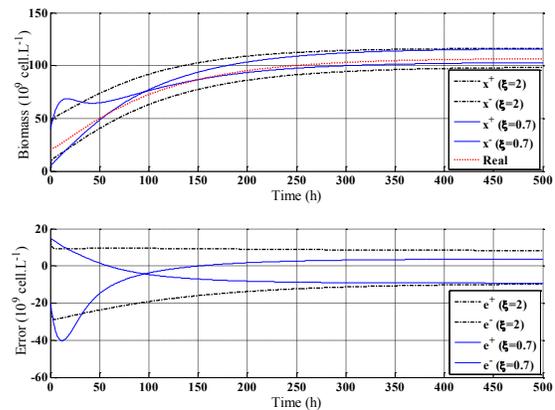


Fig. 1: Observer simulation with 30% model mismatch: influence of damping factor of error dynamics.

In order to decrease the steady state error, the estimator gains are optimized by solving problem (26). The aim is to ensure a steady state error less than 2 billion cells per liter (i.e. about 2% error).

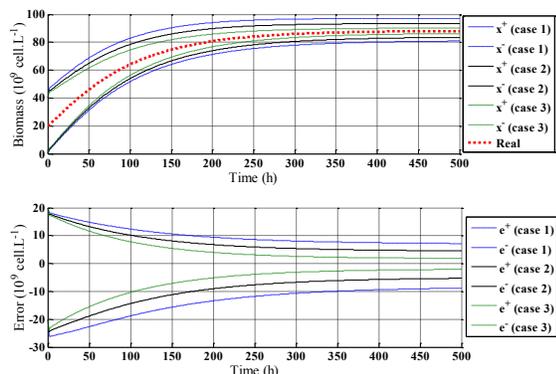


Fig. 2: Observer simulation with 30% model mismatch: influence of natural frequency of error dynamics.

Results with the obtained optimal estimator are shown in Fig. 3, as well as those found in case 3 of Fig. 2. It can be noticed that the optimized estimator presents the best convergence and accuracy properties. In fact, the optimization algorithm decreases the gain  $g_2$  until the desired accuracy is fulfilled.

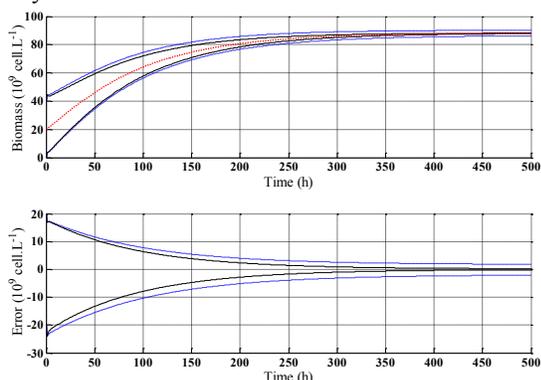


Fig. 3: Biomass estimation and its error: real (dotted red line), imposed eigenvalues (blue dashed line), optimized gains (black full line).

Finally, Fig. 4 illustrates the estimator behavior with both growth rate parameters and  $k_L a$  mismatch about 30% and 10%, respectively, with different initialization errors (resp. 5, 10 and 20.10<sup>9</sup> cells/L). The same final accuracy is reached (about 10 billion cells per liter), and the final value depends only on the accuracy of the  $k_L a$  value and of the dilution rate.

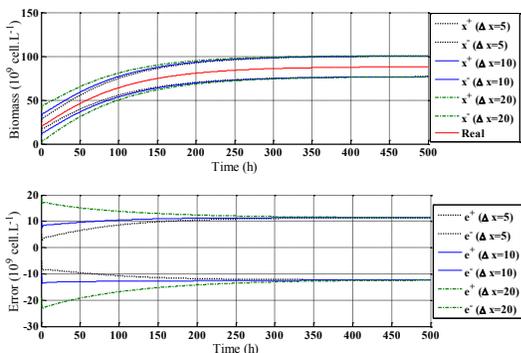


Fig. 4: Biomass estimation and its error: growth rate model parameters and  $k_L a$  mismatch, with different initialization errors.

## V. CONCLUSION

In this paper, an enhancement of the interval observer performance for the biomass *Chlorella vulgaris* estimation

was studied. This optimization approach concerns the design of the observer gain, which can be tuned by choosing error dynamics or by optimizing estimator gains so that a steady state error level is reached. This study showed, through several simulations, that the interval observer is robust against uncertainties of the model parameters, which is not the case of the classical asymptotic observer. Further work will involve the experimental validation of this approach for biomass estimation. It will also examine the improvement of biomass estimation in case of uncertainties on the mass conversion yield  $Y$  and on the gas-liquid mass  $k_L a$  considering other robust estimator structures.

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