

Modeling and On-line State Estimation of an Ethanol Production Bioprocess

Monica Roman

Department of Automatic Control, University of Craiova, Craiova, Romania
monica@automation.ucv.ro

Abstract—This paper deals with the pseudo bond graph modeling and the design of an asymptotic state observer for an ethanol production bioprocess. The bond graph model of the process is obtained by developing a set of rules, starting from the reactions schemes and taking into account the biochemical phenomena. Then, the unavailable states of the bioprocess are reconstituted from the measurable states by using an asymptotic observer, which is designed without the knowledge of the kinetics being necessary. Several numerical simulations are conducted in order to test the performance of the observer.

Keywords-modeling; bond graphs; bioinformatics; nonlinear systems; observers

1. Introduction

The development of control strategies for biochemical processes is difficult because of the complexity of these processes. These difficulties occur from the presence of living organisms, the high complexity of the metabolic reactions, as well as the high complexity of the interactions between the microorganisms. For these reasons it is necessary to obtain dynamical models with high level of accuracy for their control.

As modeling technique, the bond graph method [1], [2], [3], [4] is used in this work. By its large applicability, this approach represents an important tool in engineering design and operation for chemical based processes [5], [6].

In bioindustry, numerous practical applications are characterized by the lack of on-line measurements. Often, only a part of the concentrations of the components involved are measurable on-line. In such cases, an alternative is the use of state observers. An important difficulty when applying state observers to bioprocesses is related to the uncertainty of models describing their dynamics.

Presently two classes of state observers for bioprocesses can be found in the literature [7], [8]. The first class of observers, including Luenberger and Kalman observers, are based on a perfect knowledge of the model structure. A disadvantage of these observers is that the uncertainty in the model parameters can generate large bias in the estimation of unmeasured states. A second class of observers, called asymptotic observers, is based on the idea that the uncertainty in process models lies in the process kinetics models. The design of these observers is based on mass and energy balances without the knowledge of the process kinetics being necessary.

The paper is organized as follows. In Section II, the pseudo bond graph model of the ethanol production process is developed. Then, Section III deals with the design of an asymptotic observer for this nonlinear bioprocess. In Section IV, several simulations are performed in order to test the behavior of the model and the performance of the proposed observer. Finally, in Section V concluding remarks and further research directions are discussed.

2. Modeling of Ethanol Production Bioprocess

The ethanol production bioprocess is widely used in industry [9], [10]. The ethanol fermentation by using glucose as substrate is characterized by a metabolic pathway described by the following reaction scheme [10]:



where S is the substrate, X is the biomass, E is the ethanol, C is the carbon dioxide, and ϕ is the reaction rate. k_1, k_2, k_3 are the yield coefficients.

From the reaction scheme (1), and considering the mass transfer through the continuous bioreactor, using the modeling procedure [11], the pseudo bond graph model of the bioprocess is achieved. This model is presented in Fig. 1.

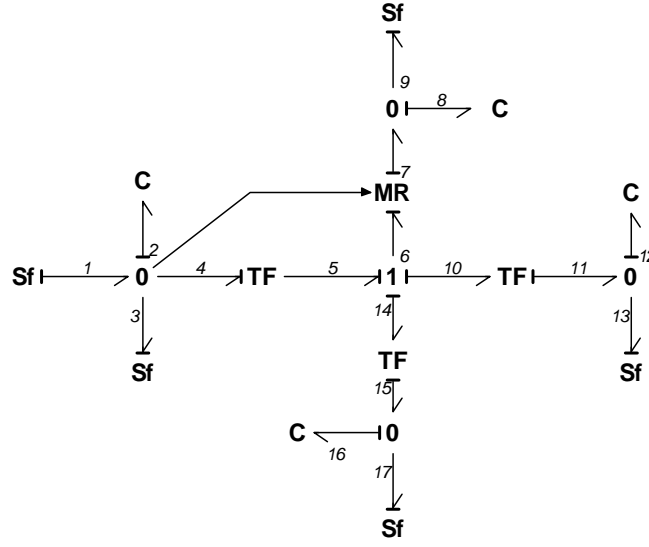


Figure 1. Pseudo bond graph model of ethanol production bioprocess.

The directions of the half arrows in the bond graph correspond to the progress of the reactions, going out from the component S towards X , E , and C . In bond graph terms, the mass balances of the components involved in the bioreactor are represented by four 0-junctions: $0_{1,2,3,4}$ (mass balance for S), $0_{7,8,9}$ (mass balance for X), $0_{11,12,13}$ (mass balance for E), and $0_{15,16,17}$ (mass balance for C).

The accumulations of species S , X , E , and C in the bioreactor are represented by bonds 2, 8, 12, and 16 and they are modeled using modulated capacitive elements C . The constitutive equations of C -elements are obtained using constitutive relations of 0-junction, and they have the following form:

$$e_2 = \frac{1}{C_2} q_2 = \frac{1}{C_2} \int (f_1 - f_3 - f_4) dt, \quad (2)$$

$$e_8 = \frac{1}{C_8} q_8 = \frac{1}{C_8} \int (f_7 - f_9) dt, \quad (3)$$

$$e_{12} = \frac{1}{C_{12}} q_{12} = \frac{1}{C_{12}} \int (f_{11} - f_{13}) dt, \quad (4)$$

$$e_{16} = \frac{1}{C_{16}} q_{16} = \frac{1}{C_{16}} \int (f_{15} - f_{17}) dt, \quad (5)$$

where C_2 , C_8 , C_{12} , and C_{16} are the parameters of C -elements:

$$C_2 = C_8 = C_{12} = C_{16} = V,$$

with V being the bioreactor volume (1).

Mass flows of the component entering the reaction is modeled using a flow source element Sf_1 , and the quantities of the components exiting from the reaction are modeled using also flow source elements Sf represented by bonds 3, 9, 13, and 17; the constitutive equations of these elements are:

$$\begin{aligned} f_3 &= Sf_3 e_3, \quad f_9 = Sf_9 e_9, \\ f_{13} &= Sf_{13} e_{13}, \quad f_{17} = Sf_{17} e_{17}, \end{aligned}$$

where Sf_3 , Sf_9 , Sf_{13} , and Sf_{17} are the parameters of Sf -elements:

$$Sf_3 = Sf_9 = Sf_{17} = F_0,$$

where F_0 is the output rate (L/h).

The transformer elements $TF_{4,5}$, $TF_{10,11}$, $TF_{14,15}$ were introduced to model the yield coefficients $k_i, i = \overline{1,3}$.

For the modeling of the reaction rate we used a modulated two-port R-element, $MR_{6,7}$. From the constitutive relation of the 1-junction element, we obtain $1_{5,6,10,14}$, where the constitutive relations of MR element imply that $f_6 = \mu e_8 V$; μ is the specific growth rate, $\varphi = \mu e_8$.

The signification of bond graph elements is as follows: e_2 is the substrate concentration S (mmole/L), e_8 - the biomass concentration X (mmole/L), and e_{12} - the ethanol concentration E (mmole/L), and e_{16} is the concentration of carbon dioxide (mmole/L); $f_1 = F_{in} S_{in}$ where F_{in} is the input feed rate (L/h), S_{in} is the influent substrate concentration (mmole/L). Taking into account all these aspects, from (2)-(5) we will obtain the dynamical model of the ethanol production bioprocess:

$$V\dot{S} = F_{in} S_{in} - F_0 S - k_1 \varphi V, \quad (6)$$

$$V\dot{X} = -F_0 X + \varphi V, \quad (7)$$

$$V\dot{E} = -F_0 E + k_2 \varphi V, \quad (8)$$

$$V\dot{C} = -F_0 C + k_3 \varphi V. \quad (9)$$

Taking into account that $F_{in} = F_0$, and the dilution rate $D = \frac{F_{in}}{V} = \frac{1}{t_r}$, with t_r - medium residence time, the above equations become:

$$\dot{S} = DS_{in} - DS - k_1 \varphi, \quad (10)$$

$$\dot{X} = -DX + \varphi, \quad (11)$$

$$\dot{E} = -D_0 E + k_2 \varphi, \quad (12)$$

$$\dot{C} = -F_0 C + k_3 \varphi. \quad (13)$$

Using the following notations: $\xi = [X \ S \ E \ C]^T$, $K = [1 \ -k_1 \ k_2 \ k_3]^T$, $F = [0 \ DS_{in} \ 0 \ 0]^T$, and $Q = [0 \ 0 \ 0 \ 0]^T$, the equations (10)-(13) can be written in the following dynamical state-space form:

$$\dot{\xi} = K \cdot \varphi(\xi) - D\xi + F - Q. \quad (14)$$

The reaction kinetics $\varphi(\xi)$ is nonlinear and incompletely known in most cases. However, it can be modeled as: $\varphi(\xi) = \mu(\xi)X$, where μ is the so-called specific growth rate, which can be expressed as Monod law [7]:

$$\mu(S) = \mu^* S / (K_m + S),$$

where μ^* is the maximum specific rate and K_m is the Michaelis-Menten constant.

3. Design of the State Asymptotic Observer

A common problem of the ethanol production bioprocesses is the absence of cheap and reliable sensors capable of providing direct, on-line measurements of biological variables. This fact can produce serious

problems when some control laws are implemented. In most cases, the substrate and ethanol concentrations may be the only measurements which are available on-line. In this case, the unmeasured variables (i.e. biomass and dissolved oxygen concentrations) can be estimated by using an appropriate state observer.

In order to design a state observer for the ethanol production process, the general class of observers for bioprocesses of the form (14), developed in [7] will be considered:

$$\dot{\hat{\xi}} = K\varphi(\hat{\xi}) - D\hat{\xi} + F - Q + \Omega(\hat{\xi})(\zeta_1 - \hat{\zeta}_1), \quad (15)$$

where $\hat{\xi}$ is the estimated state vector, $\Omega(\hat{\xi})$ is a gain matrix, and ζ_1 is the vector of measurable state variables: $\zeta_1 = L\xi$, L – a selection matrix. The design of observer lies in the choice of the gain matrix.

Based on the general form (15), the so-called exponential observers (Luenberger or Kalman observers) can be designed for the bioprocess if the reaction rate $\varphi(\xi)$ is completely known [7], [8]. However, the reaction rates are usually incompletely known; therefore it is not always possible to design and to use such observers. For the ethanol production bioprocess, by inspecting the observability matrix [7] and after some straightforward calculation, the conclusion is that an exponential observer (such as the extended Luenberger or Kalman observers) cannot be derived.

Then, another possibility is to use an asymptotic observer [7], [8], which can be designed even without knowledge of kinetic reaction. The design is based on some useful changes of coordinates, which lead to a submodel of (14) which is independent of the kinetics. To obtain the change of coordinates, a partition of state vector ξ in two parts is considered [12].

This partition denoted (ξ_a, ξ_b) induces partitions of the yield matrix K : (K_a, K_b) , also of the rate vectors F and Q : (F_a, F_b) , (Q_a, Q_b) accordingly. We will chose a state partition such that the submatrix K_a is full rank and $\dim(\xi_a) = \text{rank}(K_a) = \text{rank}(K)$. Then a linear change of coordinates can be defined as follows:

$$z = G\xi_a + \xi_b, \quad (16)$$

with z an auxiliary state vector and G the solution of the matrix equation $GK_a + K_b = 0$. In the new coordinates, the model (14) can be rewritten as

$$\begin{aligned} \dot{\xi}_a &= K_a \varphi(\xi_a, z - G\xi_a) - D\xi_a + F_a - Q_a, \\ \dot{z} &= -Dz + G(F_a - Q_a) + F_b - Q_b. \end{aligned} \quad (17)$$

Then, it results that the dynamics of the auxiliary state variables is independent of the reaction kinetics. Now z can be rewritten as a linear combination of the vectors of measured states ζ_1 and unmeasured states ζ_2 :

$$z = G_1\zeta_1 + G_2\zeta_2, \quad (18)$$

with G_1 and G_2 well defined matrices. If the matrix G_2 is left invertible, the asymptotic observer equations for (14) derive from the structure of equations (17) and (18):

$$\begin{aligned} \dot{\hat{z}} &= -D\hat{z} + G(F_a - Q_a) + F_b - Q_b, \\ \hat{\zeta}_2 &= G_2^+(\hat{z} - G_1\zeta_1), \end{aligned} \quad (19)$$

where $G_2^+ = (G_2^T G_2)^{-1} G_2^T$.

The asymptotic observer is indeed independent of the kinetics. The asymptotic observer (19) has good convergence and stability performance [7], [8].

When the yield matrix has full rank, another useful asymptotic observer can be obtained. Thus, the state vector can be partitioned directly in measured states ζ_1 and unmeasured states ζ_2 , and correspondingly partitions (K_1, K_2) , (F_1, F_2) , (Q_1, Q_2) . Then a linear coordinate transformation which uses the entire vector of measured states can be written:

$$z = \Gamma \zeta_1 + \zeta_2. \quad (20)$$

The matrix Γ can be obtained from the equation $\Gamma K_1 + K_2 = 0$, i.e. $\Gamma = -K_2 K_1^+$, with $K_1^+ = (K_1^T K_1)^{-1} K_1^T$. By using the state transformation (20), the initial system (14) can be written as:

$$\begin{aligned} \dot{\zeta}_1 &= K_1 \varphi(\zeta_1, z - \Gamma \zeta_1) - D \zeta_1 + F_1 - Q_1, \\ \dot{z} &= -Dz + \Gamma(F_1 - Q_1) + F_2 - Q_2. \end{aligned} \quad (21)$$

Then, the asymptotic observer is obtained as follows:

$$\begin{aligned} \dot{\hat{z}} &= -D\hat{z} + \Gamma(F_1 - Q_1) + F_2 - Q_2, \\ \hat{\zeta}_2 &= \hat{z} - \Gamma \zeta_1. \end{aligned} \quad (22)$$

The asymptotic observer (22) is independent of the kinetics and has good convergence and stability performance [7], [8].

Because the yield matrix of the ethanol production bioprocess (10)-(13) is full rank (in fact, in this particular case we have a yield vector), the asymptotic observer (22) can be designed and implemented.

Thus, taking into account that the substrate and ethanol concentrations are on-line measured and the biomass and dissolved oxygen concentrations should be estimated, we will use the next partitions of the state vector, yield vector and of the rate vectors:

$$\begin{aligned} \zeta_1 &= [S \ E]^T = [\xi_2 \ \xi_3]^T, \zeta_2 = [X \ C]^T = [\xi_1 \ \xi_4]^T, \\ K_1 &= [-k_1 \ k_2]^T, K_2 = [1 \ k_3]^T, \\ F_1 &= [DS_{in} \ 0]^T, F_2 = [0 \ 0]^T, \\ Q_1 &= [0 \ 0]^T, Q_2 = [0 \ -CTR]^T. \end{aligned} \quad (23)$$

Then, a linear coordinate transformation of the form (20) is used, with the matrix Γ given by:

$$\Gamma = [\gamma_{ij}]_{i,j=1,2} = \begin{bmatrix} k_1/(k_1^2 + k_2^2) & -k_2/(k_1^2 + k_2^2) \\ k_1 k_3/(k_1^2 + k_2^2) & -k_2 k_3/(k_1^2 + k_2^2) \end{bmatrix}. \quad (24)$$

The auxiliary state variables obtained from (20), (24) are:

$$z_1 = \gamma_{11} \xi_2 + \gamma_{12} \xi_3 + \xi_1, \quad z_2 = \gamma_{21} \xi_2 + \gamma_{22} \xi_3 + \xi_4. \quad (25)$$

Then, the detailed equations of the asymptotic observer are obtained as:

$$\begin{aligned} \begin{bmatrix} \dot{\hat{z}}_1 \\ \dot{\hat{z}}_2 \end{bmatrix} &= -D \begin{bmatrix} \hat{z}_1 \\ \hat{z}_2 \end{bmatrix} + \begin{bmatrix} \gamma_{11} & \gamma_{12} \\ \gamma_{21} & \gamma_{22} \end{bmatrix} \begin{bmatrix} DS_{in} \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ -CTR \end{bmatrix} \\ \begin{bmatrix} \hat{X} \\ \hat{C} \end{bmatrix} &= \begin{bmatrix} \hat{\xi}_1 \\ \hat{\xi}_4 \end{bmatrix} = \begin{bmatrix} \hat{z}_1 - \gamma_{11} \xi_2 - \gamma_{12} \xi_3 \\ \hat{z}_2 - \gamma_{21} \xi_2 - \gamma_{22} \xi_3 \end{bmatrix} \end{aligned} \quad (26)$$

The asymptotic observer (26) allows the on-line reconstruction of the unmeasured concentrations by using the available measurements, without the use of the reaction kinetics.

4. Simulation Results

Several simulations were performed to validate the nonlinear bond graph model and to test the proposed asymptotic observer. The ethanol production process has been simulated by numerical integration of equations (10)-(13) obtained via bond graph approach, by using the next bioprocess parameters [10]:

$$\mu^* = 1.1h^{-1}, K_m = 10mmole/L, k_1 = 0.18, k_2 = 0.3, \\ k_3 = 0.32, S_{in} = mmole/L, CTR = 5mmole/Lh, D = 0.5h^{-1}.$$

Two simulation scenarios were considered:

(i) First, the asymptotic observer (26) was implemented for the bioprocess (10)-(13) with Monod form of the specific growth rate, in “ideal” conditions, supposing that no parametric disturbances occur and that free-noise the on-line measurements are available. Fig. 2 shows the evolution of the substrate and ethanol concentrations. Fig. 3 depicts the estimated biomass concentration versus the “true” profile, while in Fig. 4 the dissolved oxygen concentration and its estimate are presented. It can be observed the good behavior of the asymptotic observer.

(ii) The next simulation was conducted in more realistic conditions. Thus, the on-line measurements of substrate and ethanol concentrations are vitiated with an additive Gaussian noise of 5% from their nominal value. Furthermore, a parametric disturbance of the influent substrate is considered. This disturbance is of 20% of its nominal value and occurs for an interval of 2.5 hours. In Fig. 5, the noisy measurements of substrate and ethanol concentrations are presented.

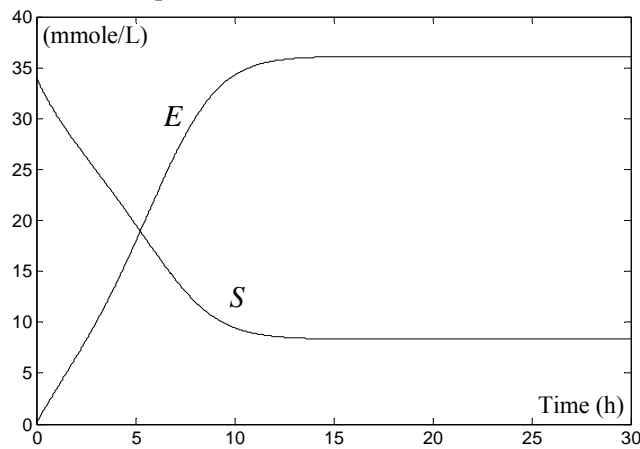


Figure 2. Evolution of substrate and ethanol concentrations (case (i)).

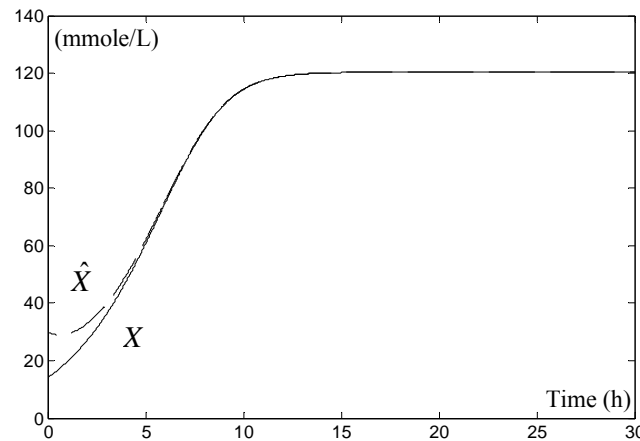


Figure 3. Time profiles of biomass concentration and its estimate – free-noise data (i).

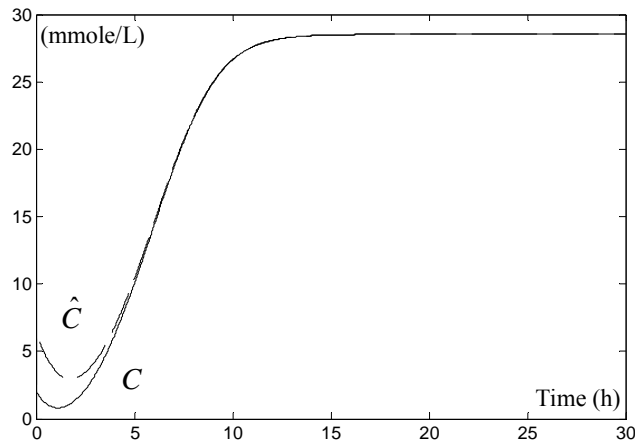


Figure 4. Evolution of dissolved oxygen concentrations vs. its estimate (i).

Figures 6 and 7 depict the profiles of estimates and “true” concentrations when noisy data are used and the parametric disturbance occurs. It can be observed that the asymptotic observer has a good behavior, despite the action of these perturbations. The estimates are influenced by the noisy measurements, but the convergence and stability of the algorithm are kept.

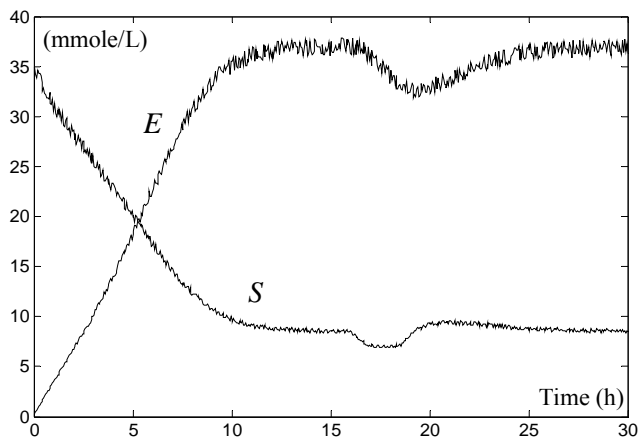


Figure 5. Profiles of noisy measurements of substrate and ethanol concentrations (case (ii)).

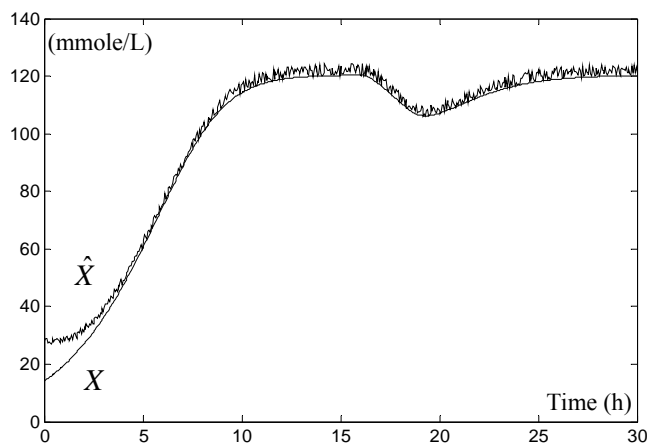


Figure 6. Evolution of biomass concentration vs. its estimate – noisy data and parametric disturbance (ii).

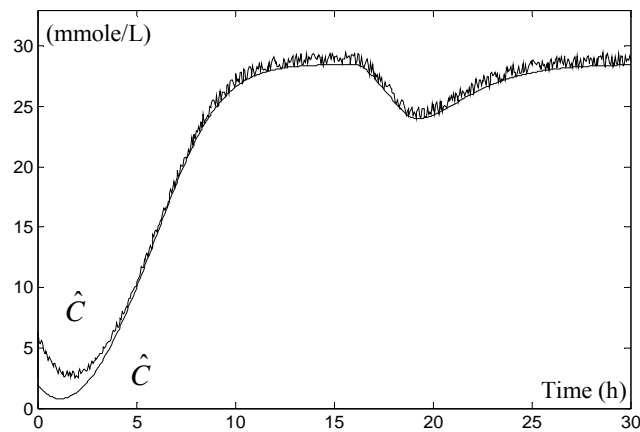


Figure 7. Dissolved oxygen concentrations and its estimate – noisy data and parametric disturbance (ii).

5. Conclusion

This work approached the pseudo bond graph modeling of an ethanol production process carried out inside a continuous bioreactor. The obtained model was used in order to design an asymptotic observer for the unavailable states of this bioprocess.

The bond graph model was obtained in a natural way, starting with reaction scheme and using base elements of bond graph methodology and pseudo bonds. The dynamical nonlinear model obtained using the bond graph approach is equivalent with the dynamical state-space model obtained using classical methods.

Because the classical exponential observers cannot be applied on this kind of bioprocesses, an asymptotic observer was designed for the biomass and dissolved oxygen concentrations. The design was achieved without the use of the process kinetics. The numerical simulations showed that the observer can cope with parametric disturbances and noisy data. The observer can be used for the implementation of advanced control strategies.

6. Acknowledgment

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7. References

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