Modelling and Nonlinear Estimation Strategies for an Ethanol Production Bioprocess

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Abstract: This paper deals with the pseudo bond graph modelling 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. Finally, a nonlinear estimation strategy is developed for the identification of unknown kinetics of the bioprocess, by using an observer based estimator. Several numerical simulations are conducted in order to test the performance of the proposed estimation algorithms.

Keywords: 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 modelling technique, the bond graph method (Karnopp et al., 1990, Thoma, 1990, Gawthrop and Smith, 1996, Dauphin-Tanguy, 2000) is used in this work. By its large applicability, this approach represents an important tool in engineering design and operation for chemical based processes (Thoma and Ould Bouamama, 2000, Couenne et al., 2006).

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 (Bastin and Dochain, 1990, Dochain et al., 2001). 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.

One of most important issues concerning the design of controllers for bioprocesses is the estimation of kinetic rates (the so-called kinetics of the bioprocess). Regarding the kinetics estimation, an early approach was based on Kalman filter which leads to complex nonlinear algorithms. A well-known technique is the approach based on adaptive systems theory, which consists in the estimation of unmeasured states with asymptotic observers, and after that, the measurements and the state estimates are used for on-line estimation of kinetics. Such kind of algorithm is, for example, the estimator based on state observer (observer based estimator – OBE) (Bastin and Dochain, 1990, Dochain, 2008).

This paper, which is an extended work of Roman (2011), is organized as follows. In Section 2, the pseudo bond graph model of the ethanol production process is developed. Then, Section 3 deals with the design of an asymptotic observer for this nonlinear bioprocess. In Section 4, the design and the implementation of an observer based estimator for the specific growth rate of the bioprocess is addressed. The kinetics estimation strategy uses both the measurable states and the estimates provided by the asymptotic observer. Several simulations are performed in Section 5 in order to test the behaviour of the model and the performance of the proposed nonlinear estimation strategies. Finally, in Section 6 concluding remarks and further research directions are discussed.

2. MODELLING OF ETHANOL PRODUCTION BIOPROCESS

The ethanol production bioprocess is widely used in industry (Novak et al., 1981, Ferreira, 1995). The ethanol fermentation by using glucose as substrate is characterized by a metabolic pathway described by the following reaction scheme (Ferreira, 1995):

$$k_1 S \xrightarrow{\varphi} X + k_2 E + k_3 C \tag{1}$$

where S is the substrate, X is the biomass, E is the ethanol, C is the carbon dioxide, and φ is the reaction rate. In the reaction scheme (1), k_1, k_2 and k_3 are the so-called yield coefficients of the process.

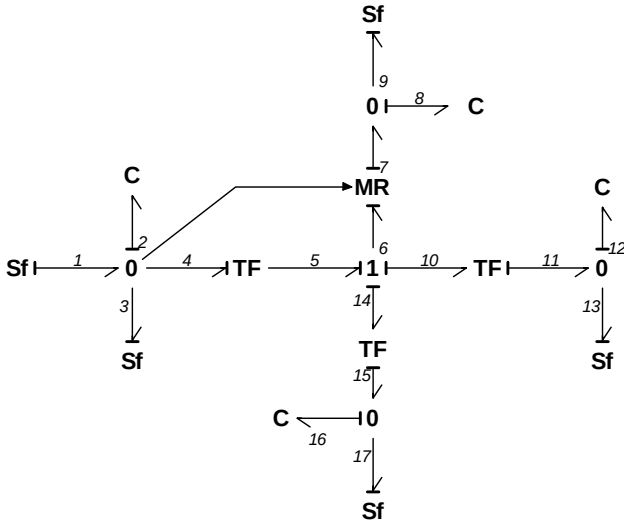

Fig. 1. Pseudo bond graph model of ethanol production bioprocess.

From the reaction scheme (1), considering the mass transfer through the continuous bioreactor, using the modelling procedure (Roman et al., 2010), the pseudo bond graph model of the bioprocess is achieved. This is presented in Fig. 1.

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 *S*, *X*, *E*, and *C* in the bioreactor are represented by bonds 2, 8, 12, and 16 and they are modelled using modulated capacitive elements C. The constitutive equations of C-elements have the following form:

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

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

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

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

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 (L).

Mass flows of the component entering the reaction is modelled using a flow source element Sf_1, and the quantities of the components exiting from the reaction are modelled using also flow source elements Sf represented by bonds 3, 9, 13, and 17; the constitutive equations of these elements are as follows: $f_3 = Sf_3 e_3$, $f_9 = Sf_9 e_9$, $f_{13} = Sf_{13} e_{13}$, $f_{17} = Sf_{17} e_{17}$, 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 modelling of the reaction rate, a modulated two-port R-element, $MR_{6,7}$, was used. 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:

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

$$V\dot{X} = -F_0 X + \varphi V , \tag{7}$$

$$V\dot{E} = -F_0 E + k_2 \varphi V , \tag{8}$$

$$V\dot{C} = -F_0 C + k_3 \varphi V . \tag{9}$$

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:

$$\dot{S} = D S_{in} - D S - k_1 \varphi , \tag{10}$$

$$\dot{X} = -D X + \varphi , \tag{11}$$

$$\dot{E} = -D E + k_2 \varphi , \tag{12}$$

$$\dot{C} = -D C + k_3 \varphi . \tag{13}$$

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

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

Remark 1. The reaction kinetics $\varphi(\xi)$ is nonlinear and incompletely known in most cases. However, it can be modelled as $\varphi(\xi) = \mu(\xi)X$, where μ is the so-called specific growth rate, which can be expressed as Monod law (Bastin and Dochain, 1990):

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

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

3. A STATE ASYMPTOTIC OBSERVER FOR THE ETHANOL PRODUCTION BIOPROCESS

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 (Bastin and Dochain, 1990) will be considered:

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

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 (Bastin and Dochain, 1990, Dochain, 2008). 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 (Bastin and Dochain, 1990) 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 (Bastin and Dochain, 1990, Dochain and Vanrolleghem, 2001), 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 (Selişteanu et al., 2007).

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 $\dim(\xi_a) = rank(K_a) = rank(K)$. Then a linear change of coordinates can be defined as follows:

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

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

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

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:

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

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):

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

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 (Bastin and Dochain, 1990, Dochain and Vanrolleghem, 2001).

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:

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

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 (Bastin and Dochain, 1990, Dochain and Vanrolleghem, 2001).

Remark 2. 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.

In the following, 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:

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

where CTR is the carbon dioxide transfer rate.

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

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

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

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

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. DESIGN OF THE KINETICS ESTIMATION STRATEGY

The most difficult task for the construction of the dynamical model (14) is the modelling of reaction kinetics. Generally speaking, the form of kinetics is complex, nonlinear and in many cases unknown. A common assumption is that a reaction can take place only if all reactants are presented in the bioreactor. Therefore, the reaction rates are necessarily to be zero whenever the concentration of one of the reactants is zero. Thus, the reaction rate can be expressed as $\varphi(\xi) = H(\xi)\mu(\xi, t)$, where $\mu(\xi, t)$ is the specific growth rate. For the ethanol production bioprocess, $H(\xi) = \xi_1 = X$. Then the model (14) becomes:

$$\dot{\xi} = KH(\xi)\mu(\xi, t) - D\xi + F - Q. \quad (27)$$

For the specific growth rate $\mu(\xi, t)$ there exist different models, like Monod's law or Haldane kinetic model (Dochain, 2008, Roman, 2011). However, in practice, the analytical models of the specific growth rate $\mu(t)$ are difficult to obtain. Therefore, this uncertain rate needs to be on-line estimated. If we consider that the specific growth rate is an unknown time varying kinetic parameter $\rho(t) = \mu(t)$, then the model (27) can be written as:

$$\dot{\xi} = KH(\xi)\rho(t) - D\xi + F - Q \quad (28)$$

The design of the on-line kinetics estimation strategy will be done considering that the model of bioprocess fulfils next hypotheses (Bastin and Dochain, 1990, Marino and Tomei, 1995):

H1. All state variables are measurable in real-time (otherwise, the asymptotic state observer provided in Section III will be used);

H2. The vector of feed rates, the dilution rate and the carbon dioxide transfer rate are measurable;

H3. The matrix of yields coefficients K is known.

The fundamental idea behind the design of an estimator based on a state observer technique is to use a state observer, not for the state estimation, but in order to provide the information needed for updating the estimates of the kinetic parameters. The nonlinear estimation algorithm for the ethanol production bioprocess (28) can be written as (Bastin and Dochain, 1990, Marino and Tomei, 1995, Selişteanu et al., 2010):

$$\dot{\xi}_{est} = KH(\xi)\hat{\rho}(t) - D\xi + F - Q - \Psi(\xi - \xi_{est}) \quad (29)$$

$$\dot{\hat{\rho}} = [KH(\xi)]^T \Theta(\xi - \xi_{est}) \quad (30)$$

In (29) and (30), $\hat{\rho}$ is the on-line estimate of the unknown parameter (in fact, the unknown kinetics – the specific growth rate). The first equation of this algorithm is a state observer, used for updating the estimate $\hat{\rho}$, and not for

state estimation. The update is generated by the estimation error $e = (\xi - \xi_{est})$, where ξ_{est} is the on-line estimation of the state vector (provided by the OBE; it is not the estimated state vector from Section 3). The error $\rho - \hat{\rho}$ is directly reflected by the estimation error e. The matrix Ψ is a gain matrix. In the second equation of the algorithm, the injection matrix Θ is chosen such that the matrix $\Psi^T\Theta + \Theta\Psi$ is negative defined, with $\dim(\Psi) = \dim(\Theta) = 4 \times 4$. The design parameters of the estimator (29), (30) are the matrices Ψ and Θ. The choice of these matrices must be done such that the algorithm to be stable and convergent. The properties of stability and convergence for this estimator have been discussed at length in (Bastin and Dochain, 1990, Marino and Tomei, 1995). A typical choice for the matrices Ψ and Θ is of diagonal form:

$$\Psi = \underset{i=1,\ldots,4}{diag}\{-\psi_i\}, \Theta = \underset{j=1,\ldots,4}{diag}\{\theta_j\}, \quad \psi_i, \theta_j \in \Re_+ \quad (31)$$

After some straightforward calculation, by using (28) and (29)-(31), the detailed equations of the on-line estimator based on state observer for the unknown specific rates are obtained as follows:

$$\begin{aligned}
\dot{\xi}_{1est} &= \dot{X}_{est} = \hat{X}\hat{\rho} - D\hat{X} + \psi_1(\hat{X} - X_{est}) \\
\dot{\xi}_{2est} &= \dot{S}_{est} = -k_1\hat{X}\hat{\rho} - DS + \psi_2(S - S_{est}) \\
\dot{\xi}_{3est} &= \dot{E}_{est} = k_2\hat{X}\hat{\rho} - DE + \psi_3(E - E_{est}) \\
\dot{\xi}_{4est} &= \dot{C}_{est} = k_3\hat{X}\hat{\rho} - D\hat{C} - CTR + \psi_4(\hat{C} - C_{est}) \\
\dot{\hat{\rho}} &= \dot{\hat{\mu}} = \hat{X}\theta_1(\hat{X} - X_{est}) - k_1\hat{X}\theta_2(S - S_{est}) + \\
&\quad k_2\hat{X}\theta_3(E - E_{est}) + k_3\hat{X}\theta_4(\hat{C} - C_{est})
\end{aligned} \quad (32)$$

Remark 3. The observer-based estimator (32) uses the measurements of substrate and ethanol concentrations, and the estimates of biomass and carbon dioxide concentrations $\hat{X}$ and $\hat{C}$ provided by the asymptotic observer (26), respectively. Thus, the nonlinear estimation strategy consists in a two-step procedure: first, the necessary state variables are estimated, and then these estimates are used for the implementation of the OBE for the unknown kinetics.

5. SIMULATION RESULTS AND DISCUSSIONS

Several simulations were performed to validate the nonlinear bond graph model and to test the proposed estimation strategies. 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 (Ferreira, 1995):

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

In the following, three 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 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 carbon dioxide concentration and its estimate are presented. It can be observed the good behaviour of the asymptotic observer.

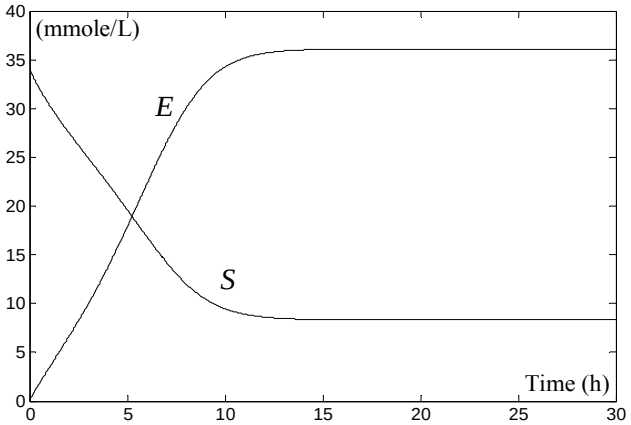

Fig. 2. Evolution of substrate and ethanol concentrations (case (i)).

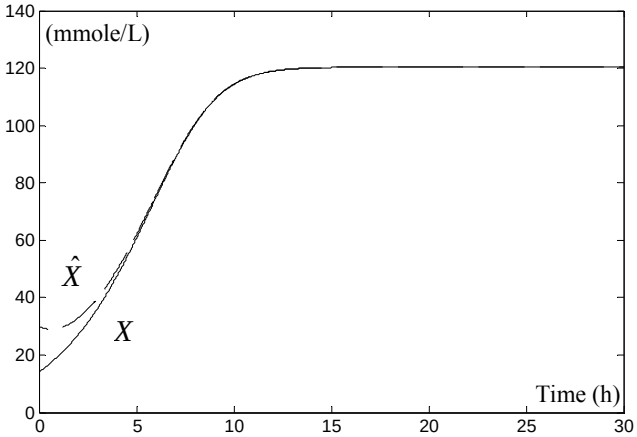

Fig. 3. Time profiles of biomass concentration and its estimate – free-noise data (i).

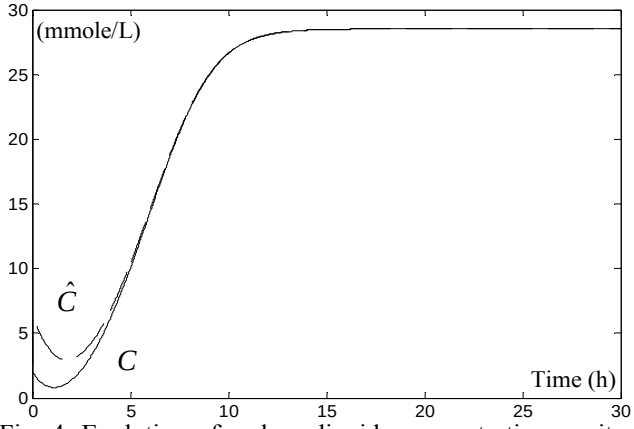

Fig. 4. Evolution of carbon dioxide concentration vs. its estimate (i).

(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 4 hours.

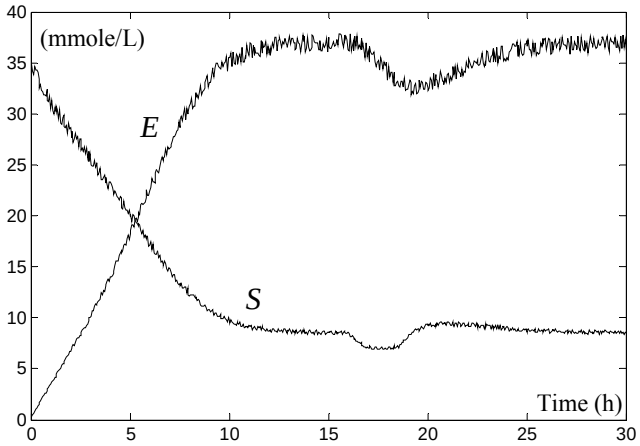

Fig. 5. Profiles of noisy measurements of substrate and ethanol concentrations (case (ii)).

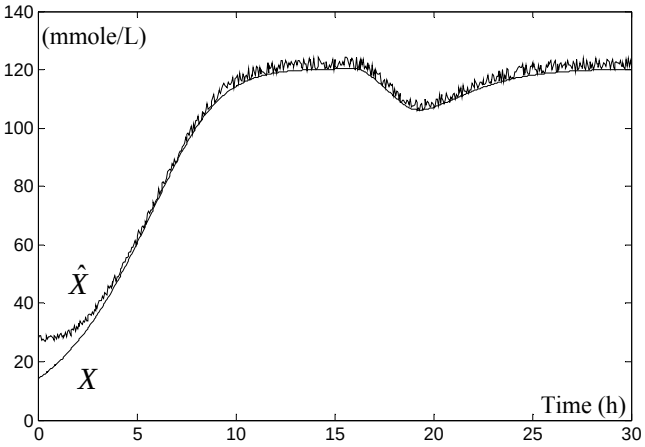

Fig. 6. Evolution of biomass concentration vs. its estimate – noisy data and parametric disturbance (ii).

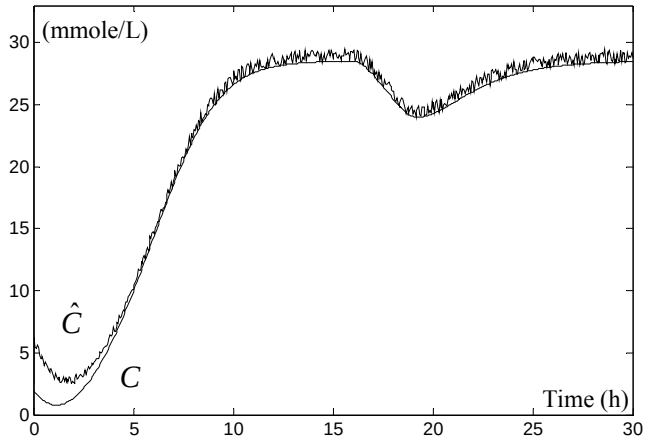

Fig. 7. Carbon dioxide concentrations and its estimate – noisy data and parametric disturbance (ii).

In Fig. 5, the noisy measurements of substrate and ethanol concentrations are presented. Figures 6 and 7 depict the profiles of estimates and "true" concentrations when noisy data are used and the parametric disturbance occurs.

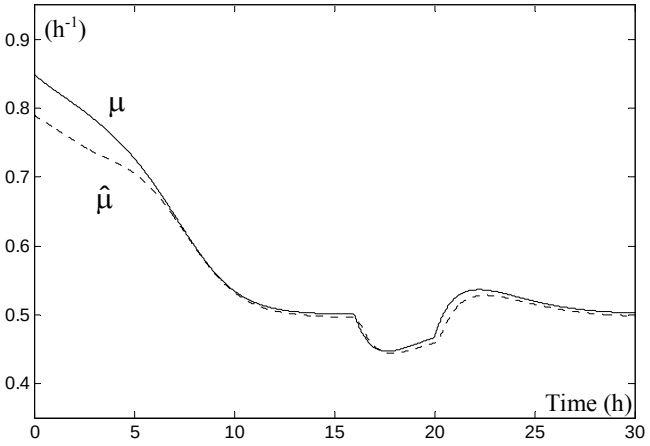

Fig. 8. Specific growth rate versus its estimate provided by OBE – free noise data and parametric disturbance (iii).

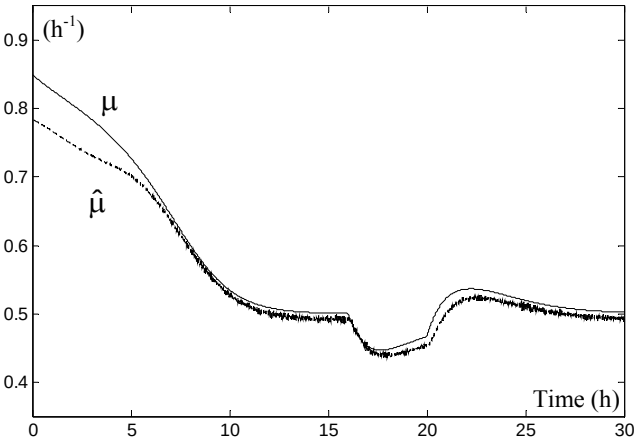

Fig. 9. Specific growth rate versus its estimate provided by OBE – noisy data and parametric disturbance (iii).

It can be observed that the asymptotic observer has a good behaviour, despite the action of these perturbations. The estimates are influenced by the noisy measurements, but the convergence and stability of the algorithm are kept.

(iii) In this simulation scenario, the nonlinear OBE (32) was implemented in the same realistic conditions as in previous case. In order to study the performance of this observer, the results are compared with data generated from simulation of the process model (14). The specific growth rate for this simulation is of the Monod form given in the Remark 1 – this kinetic expression is introduced only for simulation; therefore this model is not used in the process of the observer design. The main goal of the OBE was to reconstitute the time evolution of the specific growth rate. The values of the tuning parameters were set to $\psi_i = 10, i = 1...4$, and $\theta_i = 2, i = 1,...,4$. Fig. 8 shows the time profiles of the specific growth rate and of its estimate (free noise measurements), and Fig. 9 depicts the same evolution but for noisy data of substrate and

ethanol concentrations. It can be seen from this time evolution diagrams that the on-line nonlinear estimator provides good estimates for the unknown kinetics of the bioprocess.

Also, it can be noticed that the measurement noise induces some noisy estimates of the kinetics, but the noise effect is limited. This effect can be reduced for lower values of tuning parameters. The problem for a large value of these parameters is that the observer becomes noise sensitive. The value of the tuning parameter is therefore a compromise between a good estimation and the noise rejection.

6. CONCLUSION

This work approached the pseudo bond graph modelling 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 and an observer based estimator for the kinetics. 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.

In order to overcome problems such as the modelling uncertainties and the lack of on-line measurements for the ethanol production process, two nonlinear estimation strategies were designed for the estimation of state variables and imprecisely known kinetic rate inside the bioprocess.

Because the classical exponential observes cannot be applied on this kind of bioprocesses, an asymptotic observer was designed for the biomass and carbon dioxide concentrations. The design was achieved without the use of the process kinetics. Also, an observer based estimator was implemented to provide the information needed for updating the estimates of the unknown specific growth rate. The advantages of the OBE are simplicity of design, good convergence and stability properties. On the other hand, the big number of tuning parameters can be considered as a drawback of this strategy.

The numerical simulations showed that the proposed estimation algorithms can cope with parametric disturbances and noisy data. The obtained results are quite encouraging from simulation point of view. The proposed observers can be used for the design of advanced control strategies for the ethanol production bioprocess.

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