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Robust state estimation for repetitive operating mode process: Application to sequencing batch reactors

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Abstract

The issue of this paper is related with the on-line state estimation of a class of sequencing batch reactors (SBR). This operating mode of SBR can be analyzed as a repetitive process, where some operating conditions changes from one batch to other, which leads to nominal model degradation of the plant and consequently a bad estimation performance when standard observers are employed. To avoid the problems above mentioned it is proposed a finite time convergence observer with a fractional power of the time estimation error plus a discrete integral-type contribution of the discrete estimation error in order to reach finite time convergence and compensate the modeling error which arises when each batch is processed. The proposed observer is applied to a class of simple bioreactor model experimentally corroborated, where numerical simulations show the satisfactory performance of the proposed methodology in comparison with standard nonlinear Luenberger observers. Mathematical proof of the convergence of the proposed observer is addressed.

Keywords: State estimation; Hybrid observer; Repetitive process; Batch bioreactor

1. Introduction

The estimators or observers for states and uncertainties can play a key role during the early detection of hazardous and unsafe operating conditions and process control. Following this spirit, several researches have been focused in the proposition of estimation methodologies for states variables and uncertainties present in industrial processes.

As is well known, one of the first state observers employed in industrial operation is the extended Kalman filters, because of their easy implementation and capabilities to deal with errors in the modeling and the measurements in its structure. Nonetheless, this design is based on linearized approaches of the nonlinear system, where robustness and asymptotic convergence properties are difficult to prove [1]. Recently Aguilar et al. [2,3] propose state observers for chemical reactors with uncertain kinetics, however all these approaches provide an asymptotic convergence of the observers.

However for batch processing mode the state observers needs to converge in a finite time, because only a time period is available to conduce the process to satisfactory performance, in comparison with the continuous process mode where a time operating restriction is not enough important. In contrast, for observing purposes, convergence in finite time is an attractive feature which is very important for industrial applications which operate under fast dynamic conditions and time processing restriction. Finite time observer design has been presented in several papers, for example, in Ref. [4] a finite time observer design for linear systems is developed, where the convergence time can be assigned independently of the observer eigenvalues. Other approach considers a class of nonlinear systems which can be transformed on Brunovsky form to construct finite time observers under the frame of sliding theory with application to synchronization of chaotic systems [5]. Generally finite time controllers and observers have been applied to robot manipulators [6,7], secure data transmission [5,8] but the process control and estimation applications are up-to-date very few. As far as we know, the application of finite time observers to repetitive process are not enough studied. The main problem with the design of a state observer for repetitive process is related with the hybrid observer structure that must be considered in

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the sense that the proposed observers must to converge in the finite time when each batch is processed and besides with the number of batch processes, in other words, the observer must contain a continuous (in time) and discrete (in batches number) contributions.

2. Mathematical assumptions

The mathematical model above presented can be represented as nonlinear plant, with linear output which can be described by the following lumped parameter model:

$$\begin{aligned}\dot{X}_j(t) &= \Phi_j(X_j(t), U(t)) + \Delta\Phi(j)\\ Y_j(t) &= h(X_j(t)) = CX_j(t)\end{aligned} \tag{1}$$

Here, $X \in \Re^n$ is the vector of states; $U \in \Re^r$ is the vector control input; $Y \in \Re^m$ is the system output; $\Phi_j(\circ) : \Re^{n+r} \to \Re^n$ is a nonlinear vector field; $\Delta\Phi(j)$ is the modeling error which arises from each batch to other, $j = 1, 2, \ldots, p$ is related with the batch number, note that the modeling error can be considered as a constant disturbance when the corresponding batch is performed in time and it only changes with the batch number, moreover $\Delta\Phi(j) = 0$ for $j = 1$, i.e. the first batch processed is completely described by the nominal mathematical model. Now, consider the following assumptions:

A1. The system given by Eq. (1) is locally uniformly observable, since for all $x \in \Re^n$ and $u \in \Re^r$,

$$\text{rank}\left\{\frac{\partial}{\partial x}\zeta\right\} = n$$

Here ζ is the observability vector function defined as $\zeta = (\mathrm{d}L_\mathrm{f}^0 h_1, \ldots, \mathrm{d}L_\mathrm{f}^0 h_m, \ldots, \mathrm{d}L_\mathrm{f}^1 h_1, \ldots, \mathrm{d}L_\mathrm{f}^1 h_m, \ldots, \mathrm{d}L_\mathrm{f}^{n-1} h_1, \ldots, \mathrm{d}L_\mathrm{f}^{n-1} h_m)^\mathrm{T}$, being $L_\mathrm{f}^d h_s$ ($s = 1, 2, \ldots, m$) the d-order Lie derivatives.

The task is to design an observer to estimate the vector of state variables **X**, considering that **Y** is measured on-line and **U** is known at each time interval.

3. Estimation methodology

Proposition 1. *The following dynamic system is a finite time observer for system* (1):

$$\dot{\hat{X}}_j(t) = \Phi_j(\hat{X}_j(t), U(t)) - K_\mathrm{ct}(|Y_j(t) - C\hat{X}_j(t)|^{1/q}) + K_\mathrm{d}\sum_{j=1}^{p}(Y_j(t = T) - C\hat{X}_j(t = T)) \tag{2}$$

where K_ct and K_d are the observer gains and $q \in Z^+$, $q > 1$ considering q an odd number and T is the batch processing time.

3.1. Sketch of proof of Proposition 1

Defining the estimation error as $\xi(t, j) = X_j(t) - \hat{X}_j(t)$ and resting the Eq. (1) minus the Eq. (2) can be constructed the estimation error's dynamics as follows:

$$\dot{\xi} = \Phi_j(X_j(t), U(t)) - \Phi_j(\hat{X}_j(t), U(t)) + K_\mathrm{ct}|Y_j(t) - C\hat{X}_j(t)|^{1/q} + \Delta\Phi(j) - K_\mathrm{d}\sum_{j=1}^{p}(Y_j(t = T) - C\hat{X}_j(t = T)) \tag{3}$$

Note that the dynamic of the estimation error depends on two variables, time (t) and the batch number (j), i.e. $\dot{\xi} = \dot{\xi}(t, j)$, now considering the structure of Eq. (3) the right side of the equation can be separated into two functions, one of them time dependent, and the other depends on the batch number j such that $\dot{\xi} = f_1(t) + f_2(j)$, this structure allows to separated the convergence analysis on both two estimation errors such that $\dot{\xi} = \dot{e}_1 + \dot{e}_2$ where we define:

$$\dot{e}_1 = f_1(t) = \Phi_j(X_j(t), U(t)) - \Phi_j(\hat{X}_j(t), U(t)) + K_\mathrm{ct}|Y_j(t) - C\hat{X}_j(t)|^{1/q}$$

and

$$\dot{e}_2 = f_2(j) = \Delta\Phi(j) - K_\mathrm{d}\sum_{j=1}^{p}(Y_j(t = T) - C\hat{X}_j(t = T))$$

3.1.1. Convergence analysis of the continuous time finite observer contribution

In this section it is analyzed the convergence characteristics of the time depending terms of the estimation error, to show the observer's convergence properties in the time domain, in accordance with the following equation:

$$\dot{e}_1 = \Phi_j(X_j(t), U(t)) - \Phi_j(\hat{X}_j(t), U(t)) + K_\mathrm{ct}|Y_j(t) - C\hat{X}_j(t)|^{1/q} \tag{4}$$

note that the time varying terms contains a fraction order power contribution of the absolute value of the named measurement error $(Y_j(t) - C\hat{X}_j(t))$ this kind of contribution can lead to reach a finite convergence, such that considering $\dot{e}_\mathrm{d} = K_\mathrm{ct}|e_\mathrm{d}|^{1/q}$ as the desired trajectory it reach finite time stabilization, in accordance with Ref. [9].

Now, consider the following assumption:

A2. The function $\Phi(\circ)$ complies with Lipschitz condition with respect to $X_j(t)$, i.e. $|\Phi_j(X_j(t), U) - \Phi_j(\hat{X}_j(t), U)| \le L|X_j(t) - \hat{X}_j(t)|$; $L > 0$; and uniformly bounded on U therefore taking the norm of Eq. (4) it can be expressed as:

$$|\dot{e}_1| \le L|X_j(t) - \hat{X}_j(t)| + K_\mathrm{ct}C^{1/q}|X_j(t) - \hat{X}_j(t)|^{1/q} \tag{5}$$

Note that inequality (5) is a Bernoulli-type ordinary differential inequation, such that for its solution it is possible to define the following change of variable for each scalar component of the vector e_1, we define:

$$\Gamma_i = e_{1,i}^{(1-1/q)}, \quad i = 1, \ldots, n \quad \text{with} \quad e_{1,i} \ne 0 \tag{6}$$

Expressing the time domain estimation error in the new variable ($e_{1,i} = \Gamma_i e_{1,i}^{1/q}$), it is possible to find its dynamics as it is shown by Eq. (7).

$$\dot{e}_{1,i} = \left(\frac{q}{q-1}\right) \dot{\Gamma}_i e_{1,i}^{1/q} \tag{7}$$

Combining Eqs. (5)–(7) the following equation is generated:

$$\left|\left(\frac{q}{q-1}\right) \dot{\Gamma}_i e_{1,i}^{1/q}\right| \leq L_i |\Gamma_i e_{1,i}^{1/q}| + k_i |e_{1,i}^{1/q}| \tag{8}$$

where k_i is the scalar entry of the matrix product $K_{ct}C^{1/q}$. Finally, it is possible to find the quota for the variable norm (inequality (9)). Note that the below expression is a first order differential inequality.

$$|\dot{\Gamma}_i| \leq L_i \left|\left(\frac{q-1}{q}\right) \Gamma_i\right| + \left(\frac{q-1}{q}\right) k_i \tag{9}$$

Before to continue with the analysis, the following comments are done:

$$\begin{aligned} & e_{1,i} = 0 \Rightarrow \Gamma_i = 0 \\ & e_{1,i} \neq 0 \Rightarrow \Gamma_i \neq 0, \quad \text{i.e.} \\ & \left.\begin{cases} e_{1,i} > 0 \\ e_{1,i} < 0, q \text{ odd} \end{cases}\right\} \Rightarrow \Gamma_i > 0 \\ & q > 1 \Rightarrow \left(\frac{q-1}{q}\right) > 0 \end{aligned} \tag{10}$$

A3. Consider $e_{1,i} \neq 0$ and $q \in Z^+$, q odd, $(q-1)/q > 0$.

Now applying the relationship $|x| = \text{sign}(x)x$ and performing algebraic manipulations onto inequality (9), the following is obtained:

$$\text{sign}(\dot{\Gamma}_i)\dot{\Gamma}_i \leq L_i \left(\frac{q-1}{q}\right) \text{sign}(\Gamma_i)\Gamma_i + k_i \frac{q-1}{q} \tag{11}$$

Now, it is possible to find some relationships among the variable Γ_i and the sign of its dynamics then by assuming A3, we obtain the general solution of inequality (11) for $t_0 = 0$:

$$\begin{aligned} \Gamma_i(t) \leq & \exp\left(-\frac{L_i((q-1)/q)\,\text{sign}(\Gamma_i)}{\text{sign}(\dot{\Gamma}_i)} t\right) \\ & \times \int_0^t \exp\left[\frac{L_i((q-1)/q)\,\text{sign}(\Gamma_i)}{\text{sign}(\dot{\Gamma}_i)} \tau\right] \left[\frac{((q-1)/q)k_i}{\text{sign}(\dot{\Gamma}_i)}\right] \text{d}\tau \\ & + \Gamma_i(t_0) \exp\left[-\frac{L_i((q-1)/q)\,\text{sign}(\Gamma_i)}{\text{sign}(\dot{\Gamma}_i)} t\right] \\ & \text{if } \text{sign}(\dot{\Gamma}_i) > 0 \end{aligned} \tag{12}$$

After algebraic manipulations of Eq. (12) the following inequality is obtained:

$$\begin{aligned} \Gamma_i(t) \leq & L_i^{-1} \frac{k_i}{\text{sign}(\Gamma_i)} \left[1 - \exp\left[-\frac{L_i((q-1)/q)\,\text{sign}(\Gamma_i)}{\text{sign}(\dot{\Gamma}_i)} t\right]\right] \\ & + \Gamma_i(t_0) \exp\left[-\frac{L_i((q-1)/q)\,\text{sign}(\Gamma_i)}{\text{sign}(\dot{\Gamma}_i)} t\right] \end{aligned} \tag{13}$$

If $\text{sign}(\Gamma_i)/\text{sign}(\dot{\Gamma}_i) > 0$ and t is large enough and considering (10) then:

$$0 \leq \Gamma_i(t) \leq L_i^{-1} \frac{k_i}{\text{sign}(\Gamma_i)} \tag{14}$$

If k_i is *small* enough $\Gamma_i(t) \to \varepsilon_i$ with $\varepsilon_i > 0$ as small as be desired. Furthermore $e_{1,i} = \sqrt[q-1]{\Gamma_i^q}$, then $e_{1,i} = \sqrt[q-1]{\varepsilon_i^q}$, we choose $\bar{e} = \max_i e_{1,i}$ and $\bar{\varepsilon} = \max_i \varepsilon_i$. It can be concluded that the maximum of the time domain estimation error belongs to the open ball with ratio proportional to $\sqrt[q-1]{(L_i^{-1}(k_i/\text{sign}(\Gamma_i)))^q}$.

3.1.1.1. Observer convergence time. In order to determine the convergence time of the proposed observer, let us consider Eq. (13). As it can be seen the second term of the right side of the above equation is time dependent, at steady-state condition this term must exhibit a numerical value close to zero (Eq. (15)).

$$\Gamma_i(t_0) \exp\left[\frac{L_i((q-1)/q)\,\text{sign}(\Gamma_i)}{\text{sign}(\dot{\Gamma}_i)} t\right]_{t=t_{tf}} = \tilde{\varepsilon}_i \approx 0 \tag{15}$$

Here, τ is the convergence time of the observer to the open ball $\bar{e} \in B_{\bar{\varepsilon}}(0)$; after algebraic manipulations, the following equation for the convergence time is calculated as:

$$\begin{aligned} & t_{FT} = \max_i t_{FT,i} \quad \text{with} \quad t_{FT,i} = Ln \tilde{\varepsilon}_i^{\eta} \\ & \text{where} \quad \eta = -\frac{q}{L_i(q-1)} \frac{\text{sign}(\dot{\Gamma}_i)}{\text{sign}(\Gamma_i)} \end{aligned} \tag{16}$$

3.1.2. Convergence analysis of the discrete observer contribution

For the corresponding stability analysis for the discrete contribution of the proposed observer, let us consider the below equation, presented in Section 3.1, which consider the batch number evolution of the estimation: $\dot{e}_2 = \Delta\Phi(j) - K_d \sum_{j=1}^{p} (Y_j(t=T) - C\hat{X}_j(t=T))$. Now given the discrete nature of this estimation error the corresponding difference equation is as follows:

$$e_{2,j+1} = e_{2,j}(j) + \left(\Delta\Phi(j) - K_d C \sum_{j=1}^{p} e_{2,j}(j)\right) \tag{17}$$

Now, the above equation can be expressed as:

$$\begin{aligned} & e_{2,j+1} = e_{2,j}(j) + \Delta\Phi(j) - K_d C e_{3,j}(j) \\ & e_{3,j+1} = e_{3,j}(j) + e_{2,j}(j) \end{aligned}$$

Or in vector notation:

$$e_{j+1} = A_\pi e_j + \Theta_j(j) \tag{18}$$

where

$$e_{j+1} = \begin{bmatrix} e_{2,j+1} \\ e_{3,j+1} \end{bmatrix}; \qquad A_\pi = \begin{bmatrix} 1-\pi & -K_d C \\ 1 & 1-\pi \end{bmatrix};$$

$$\Theta_j = \begin{bmatrix} \Delta\Phi + \pi e_{2,j} \\ \pi e_{3,j} \end{bmatrix}$$

$\pi > 1$ is a stabilizing parameter [10] and A_π is a Hurwitz stable matrix with an adequate choosing of the observer gains K_d and π, note that the observer gain K_d provide stability to the observer, because it compensate the nonlinear term related with the error modeling $\Delta\Phi$, which arises with the number of the batch evolution.

Considering the following discrete Lyapunov equation, where $P = P^T > 0$:

$$V_j = e_j^T P e_j \tag{19}$$

Such that the corresponding discrete dynamic is given by the following difference equation:

$$V_{j+1} - V_j = 2e_j^T P(A_\pi e_j + \Theta_j) \tag{20}$$

In accordance with assumption A2:

$$|\Theta_j| \le D|M_j(X_j - \hat{X}_j)| = D|M_j e_j| \tag{21}$$

where D is the corresponding Lipschitz constant and M_j is a symmetric definite positive matrix playing role of a normalizing matrix (since different components of the state variables may have a different physical nature).

Substituting:

$$V_{j+1} - V_j \le 2|e_j^T|P(A_\pi + DM_j)|e_j| \tag{22}$$

Considering with an appropriate choosing of the observer gain K_d we have that: $A_\pi + D|M_j|$ is a definite negative matrix.

Note that the above equation can be employed for observer's tuning purposes, therefore:

$$V_{j+1} - V_j \le 2|e_j^T|P(A_\pi + D|M_j|)|e_j| < 0 \tag{23}$$

Which proof that the discrete contribution of the observer, asymptotically converges.

4. Batch reactor modeling

As is well known the modeling of biological systems, in particular for bioreacting process is a hard task because the parameters related are time-variant and highly nonlinear functions of the system's states, process and environmental conditions. In particular sequencing batch wastewater bioreactors where the organic matter to be degraded (substrate measured as chemical oxygen demand) changes continuously its composition, the sludge inoculated (biomass measured as volatile suspended solids) is not well characterized and the process variables do not follow an exact operation policy, made that the right simulation, monitoring and control be very difficult tasks for the high varying parameters model and operating conditions.

In particular, we develop a simple nominal mathematical model of a batch wastewater bioreactor to be employed as nominal plant for the design of the proposed state estimation methodology, this model is based on mass balance for substrate and biomass concentration, which are the most important variables that describes the dynamics of the biological phase of the bioreactor. Substrate concentration is considered as the measured variable considering that it measured as COD is routinely made in industrial operation [11]. Naturally most complex model containing a large system of nonlinear ordinary differential equations (ODEs) have been studied and reported in the open literature [12] and could be employed in this work, but for illustration simplicity a two states model is employed.

4.1. Experimental

Bench-scale bioreactor was utilized. These units are made of Plexiglas with a volume capacity of 15 l. The air was supplied using air diffusers stone in the reactor bottom to keep the dissolved oxygen (DO) concentration at values higher than 2.0 mg/l. The bubbles produced during the aeration kept the contents of the bioreactor well mixed and homogeneous. Municipal wastewater was utilized for the experiments. Start-up was performed with wastewater and inoculated with biological sludge. Samples were taken out from the wastewater reservoir. Chemical oxygen demand (COD) and the volatile suspended solids (SSV) were determined in each sample employing the methodology proposed in Ref. [13]. The mean of three analyses for concentrations evaluations were taken, in order to obtain the results reported as below.

4.2. Modeling

As usual, it is considered a continuous version of the bioreactor in order to obtain the bio-kinetic coefficients [14]:

For the reaction rate of substrate consumption:

$$r_s = \frac{\mu_{max}}{Y_d}\frac{X_1 X_2}{K_s + X_2} = \frac{X_{2o} - X_2}{\theta} \tag{24}$$

Linearizing equation (a) and taking the inverse, Eq. (25) is obtained.

$$\frac{X_1\theta}{X_{2o} - X_2} = \frac{Y_d K_s}{\mu_{max}}\frac{1}{X_2} + \frac{Y_d}{\mu_{max}} \tag{25}$$

K_s was obtained by plotting $X_1\theta/(X_{2o} - X_2)$ versus $1/X_2$.

The Y_d value was obtained, independently, measuring the slope of Eq. (26).

$$\frac{1}{\theta} = Y_d\frac{r_s}{X_1} - k_d \tag{26}$$

where X_1 and X_2 are the biomass and substrate concentration, respectively, Y_d the yield coefficient and θ is the dilution rate.

Using this value μ_{max} was calculated from Eq. (24).

Now, the mathematical model described below is related to the biological phase of a class of wastewater batch bioreactor, which will be the case study. It consists of mass balances for the biomass (X_1, Eq. (27)) and substrate (X_2, Eq. (28)) concentrations, which are represented by a set of two nonlinear ODEs:

$$\dot{X}_1 = \mu(X_2)X_1 \tag{27}$$

$$\dot{X}_2 = -\mu(X_2)\frac{X_1}{Y_d} \tag{28}$$

$$Y = X_2 \tag{29}$$

As it is commonly considered, the yield coefficient depends on the substrate concentration in a linear way (Eq. (29)) and the specific growth rate in accordance with a Monod's model.

$$Y_d = 0.01 + 0.03X_2 \tag{30}$$

$$\mu(X_2) = \frac{0.3X_2}{1.75 + X_2} \tag{31}$$

5. Numerical experiments

In order to show the performance of the proposed estimation methodology, the mathematical model above presented, was simulated in a sequencing mode operation. Were simulated a sequence of 10 processed batches, changing the initial condition of the ODE between each processed batch and adding a modeling error to the kinetic terms, both via random generator number, considering ±10% for the initial conditions for substrate and biomass concentrations and ±5% on the kinetic term, the nominal initial condition for biomass and substrate concentration in the bioreactor are 2 and 20 g/l, respectively. The proposed observer was implemented and a standard nonlinear Luenberger observer was implemented for comparison purposes. As usual, the substrate concentration is considered as the corresponding measured output, such that the biomass concentration is the task of the estimation methodology. The observer gain of the fractional order contribution is considered of $K_{ct} = [0.1\ \ 2.5]\,\mathrm{h}^{-1}$ and the corresponding gain of the integral-type contribution is $K_d = [0.01\ \ 0.225]\,\mathrm{h}^{-1}$, the gain of

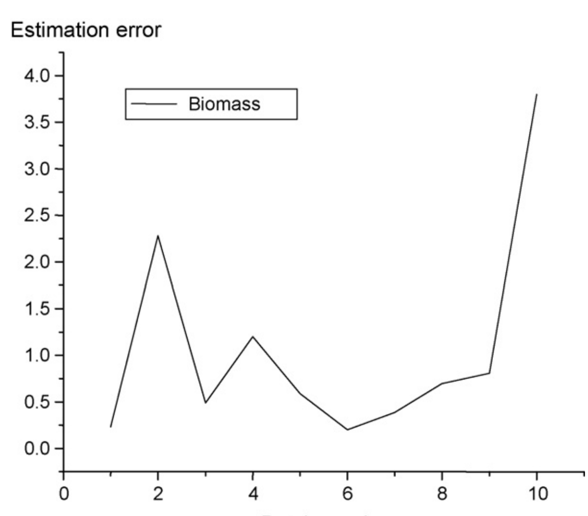

Fig. 1. Discrete estimation error for biomass concentration using a nonlinear Luenberger observer.

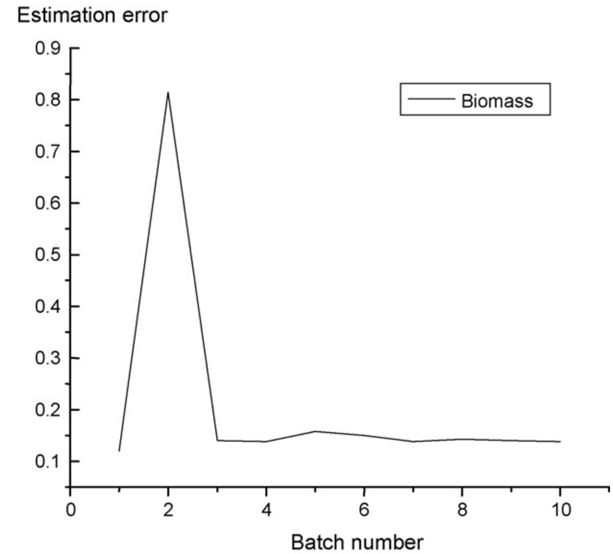

Fig. 2. Discrete estimation error for biomass concentration using the proposed observer.

the standard nonlinear Luenberger observer was chosen as K_{ct}. Figs. 1 and 2 show the performance of the observers in relationship with the processed batch number, i.e. considering the estimation error when $t = T$, as can be seen the nonlinear Luenberger observer presents a growth in the discrete estimation error and the proposed observer tends to compensate the modeling errors and consequently the discrete estimation error decrease with the batch numbers. Figs. 3 and 4 are related with the continuous (time) performance of the biomass in the bioreactor,

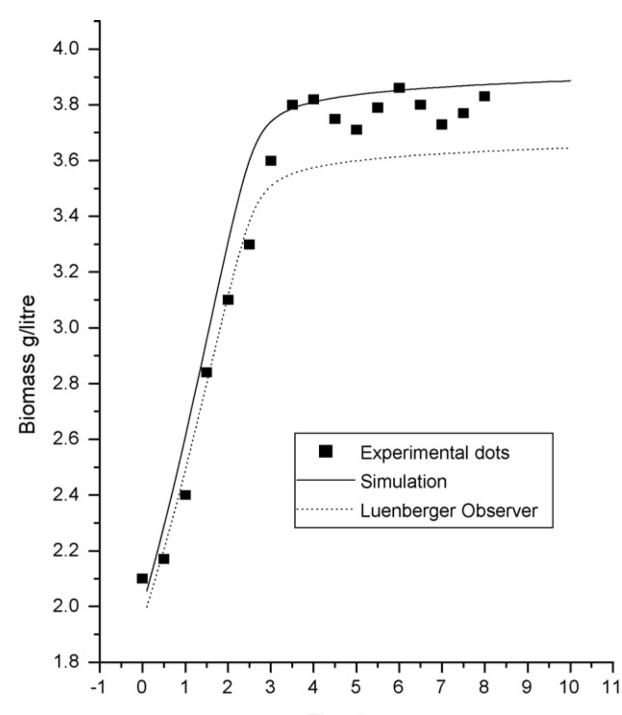

Fig. 3. Biomass concentration estimation in batch number 3 using a nonlinear Luenberger observer.

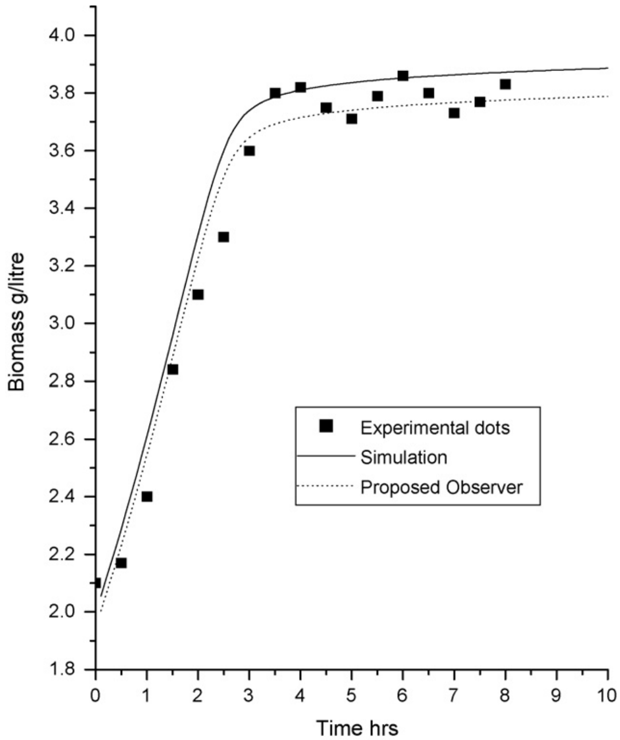

Fig. 4. Biomass concentration estimation in batch number 3 using the proposed observer.

showing the performance on the batch number 4; is observed a faster response of the proposed observer, which is the characteristic desired of the finite time observer, in comparison with the standard observer; note that for this class of process the biomass is the most important state variable to be estimate. In Figs. 5 and 6 is shown the performance of the both two observers, it can be appreciate a similar performance, but consider that the substrate concentration is the measured output, such that the observer only *filter* the corresponding input information. In this particular batch, a comparison of the mathematical model and the corresponding experimental data is made, can be concluded that the model represents satisfactory the process considered here.

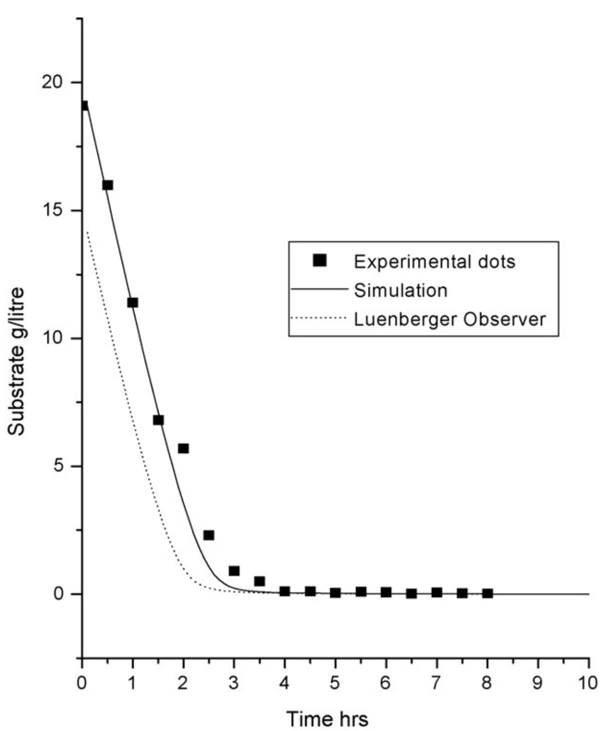

Fig. 5. Substrate concentration estimation in batch number 3 using a nonlinear Luenberger observer.

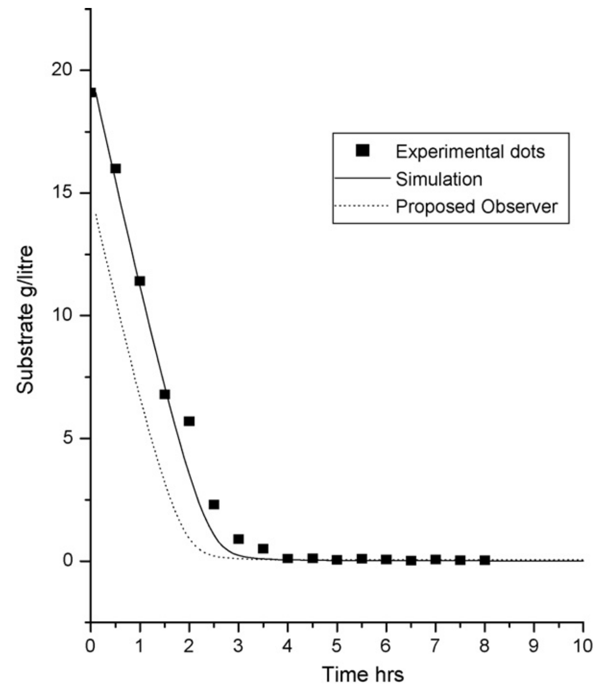

Fig. 6. Substrate concentration estimation in batch number 3 using the proposed observer.

6. Concluding remarks

A hybrid observer, which shows continuous and discrete convergence properties, is designed for a class of repetitive operation mode process; in particular it is applied to sequencing batch reactor (SBR) with an adequate success. The continuous (in time) contribution of the observer posses a finite time convergence properties, as is shown in the mathematical frame of the work under the assumption of the model's nonlinearities are Lipschitz. Related with the discrete observer structure, a discrete integral-type of the corresponding estimation error is considered in order to compensate the modeling error raised between each processed batch, with a good performance in accordance with the theorist frame developed and the simulations realized.

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