Monitoring of a class of partially known bioreactor models employing a bounded error estimator

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Abstract— **The problem of monitoring in a common class of partially known bioreactor models is addressed. A reduced order observer namely bounded error estimator is proposed. The biomass is estimated by means of substrate concentration measurements. The estimation methodology is based on a suitable change of variable which allows generating artificial variables to infer the remaining mass concentrations constructing a differential-algebraic structure. The proposed methodology is applied to a class of Haldane unstructured kinetic model with success. Stability analysis in a Lyapunov sense for the estimation error is performed. Some remarks about the convergence characteristics of the proposed estimator are given and numerical simulations show its satisfactory performance. Finally, a high gain observer is presented: the convergence is possible only when the model is perfectly known.**

Keywords: Observability, nonlinear systems, Lyapunov stability, state observers.

I. INTRODUCTION

Operating a bioreactor is not a simple task, as during a bioreacting process, variables such as concentrations are generally determined by off-line laboratory analysis, making this set of variables of limited use for control purposes and on-line monitoring. However, these variables can be on-line estimated using *soft sensors*.

Over the last few years, the importance of on-line monitoring of biotechnological processes has increased. A first step to efficient bioreactor operation is the adequate implementation of online measurements of essential variables such as substrate and biomass concentrations. Advantages of continuous monitoring of key variables include gaining knowledge about the state of the process and the possibility of detecting and isolating abnormal process developments at early stages. This reduces process costs, contributes to process safety and helps in trouble-shooting and process accommodation. The main problem in fermentation monitoring and control is the fact that process variables usually cannot be measured on-line. Monitoring and controlling these processes can therefore be difficult because only indirect measurements are available online, while calculated values may be rather uncertain. This can be due to uncertainty with respect to the equations used, measurement errors or both. For automatic control this may have serious consequences, especially as the actual variables of interest often cannot be directly controlled and related variables are controlled instead. In fermentation processes, on-line and off-line measurements are the main source of information about the state of the process. In combination with model-based calculations, they are used to produce estimations for monitoring purposes as well as for automatic and manual process control (Bastin and Dochain, 1990), (Masoud, 1997).

Observation schemes are widely used for reconstructing states of dynamical systems (Aguilar-López et. al, 2006). Most of the contributions are related to asymptotic observers for monitoring, fault detections and control issues whereas the real necessities of industrial plants are related to a fast response of the monitoring and regulation methodologies.

Special attention was given to filtering techniques, namely extended Kalman filter, adaptive observers, and artificial neural networks (ANN), (Dávila and Fridman, 2005), (Hu and Wang, 2002), (Levant, 2001), however for these techniques the right tuning of the estimators gains is difficult. It is shown that software based state estimation is a powerful technique that can be successfully used to enhance automatic control performance of biological systems as well as in system monitoring and on-line optimization.

In this paper we consider the growth rate partially known. Following this idea, the necessity to adapt an observation scheme to the available knowledge of the growth rate immediately arises. The main contribution in this work is to show a state estimator which is a simplified version of the methodology given by (Lemesle and Gouzé, 2005) where a simple linear change of variable given in a natural manner allows to develop a differential-algebraic state estimator. Results show an adequate performance of the considered methodology. The technique is not the same as (Alvarez-Ramirez et. al, 1999) since we do not have derivators. The proposed estimation methodology is applied to a kind of unstructured kinetic model: the Haldane model, which is considered for biological process with substrate inhibition. The above mentioned kinetic model is applied to a class of continuous stirred bioreactors.

In what follows, the statement of the problem is presented; an observability condition is given in the differential-algebraic setting. In section III, the bounded error estimator is designed. Section IV shows a high gain observer as a comparison with the proposed methodology. Finally, we give some concluding remarks.

II. Problem Statement

A. The model

Consider the following nonlinear system

$$\begin{aligned} \dot{x} &= f(x,u) \\ y &= h(x) \end{aligned} \tag{1}$$

where $x \in R^n$, $u \in R^m$, $m \le n$, $y \in R^p$.

Let us recall the classical observer definition. An observer for system (1) is a dynamical system $\dot{\hat{x}} = \hat{f}(\hat{x},u,y)$, whose task is state estimation. Usually is required at least that $\|\hat{x}-x\| \to 0$ as $t \to \infty$. Although in some cases, exponentially convergence is also required (Gauthier et al., 1992).

Definition 1: an estimator is said to be bounded if the estimation error ($\|\hat{x}-x\|$) belongs to an open ball with radius proportional to some value that depends on its estimation error.

In all paper, we will consider a class of bioreactor model. The simplified Haldane model taken from (Vargas et al., 2000), is describe by

$$\frac{dS}{dt} = D(S_{in}-S) - \mu(S)\frac{X}{Y_{S/X}} + k_d X \tag{2a}$$

$$\frac{dX}{dt} = -DX + \mu(S)X - k_d X \tag{2b}$$

where $\mu(S) = \mu_{\max} S / (\delta + S + S^2/\phi)$ is the specific growth rate and $\mu_{\max}$ is the maximum growth rate.

We assume that $\mu(S)$ is partially known, which is common in biology (Gouzé and Lemesle, 2001). Generally, $\mu(S)$ is between two bounds meaning that we know a function $\hat{\mu}(S)$ such that $|\mu(S)-\hat{\mu}(S)| < a$, where $a \in R^+$, and $\mu(0) = \hat{\mu}(0) = 0$. We introduce an important lemma about lower bounded properties of $\mu(S)$.

Lema 1 (Hadj-Sadok, 1999): there exists a constant $\varepsilon \in R$, such that $S(0) > \varepsilon$ implies $S(t) > \varepsilon$ for all t. Thus, for any smooth function $\mu(S)$, $\mu(S(t)) > \mu(\varepsilon)$ for all t.

From lemma 1, we could always choose ε such that $\hat{\mu}(S(t)) > \hat{\mu}(\varepsilon) = r$, where $r \in R^+$.

The state variables S, X are substrate and biomass concentrations, respectively, $D = q/V$ is the dilution rate with V the volume of the bioreactor and q the constant flow passing through the bioreactor, S_{in} is the input substrate concentration, $Y_{S/X}$ is the corresponding yield coefficient. Let us notice that the inputs $D = u$ and S_{in} are fixed. Moreover, we assume that the measured output is,

$$y = S \tag{3}$$

B. Algebraic Observability Condition (AOC)

Before proposing the bounded error estimator, a definition concerning on *algebraic observability condition* is given, for more details see (Diop and Martínez-Guerra, 2001).

Definition 2: consider the system described by (1), where $x = (x_1 \quad x_2 \quad \dots \quad x_n)^T$. A state x_i, $i = \{1, 2, \cdots, n\}$, is said to be algebraically observable with respect to $\{u, y\}$ if it satisfies a differential polynomial in terms of u, y and some of their time derivatives, i. e., $P(x_i, u, \dot{u}, \dots, y, \dot{y}, \dots) = 0$, $i = \{1, 2, \cdots, n\}$.

Replacing $y = S$ into equation (2a), the algebraic observability condition for Haldane model is calculated as follows,

$$\dot{y} - u(S_{in}-y) + \left(\frac{\mu_{\max}\phi\, y}{\delta\phi + \phi\, y + y^2} \frac{1}{Y_{S/X}} - k_d \right) X = 0 \tag{4}$$

From equation (4), it is clear that the state variable X satisfies the AOC thus, X is algebraically observable.

III. BOUNDED ERROR ESTIMATOR

A. Estimator design

In what follows, the corresponding estimated concentration is denoted by ^, and we assume that S is measured exactly, i.e., $S = \hat{S}$. Then, we only reconstruct the biomass variable X.

Consider the Haldane's model given by system (2), and make the change of variable

$$z = X + k\,S \tag{5}$$

where $k \in R$ is fixed.

The dynamics of z is,

$$\dot{z} = -\left[D + k_d - k\,k_d + \left(\frac{k}{Y_{S/X}} - 1 \right) \mu(S) \right] z + + (1-k) k\,k_d S + \left(\frac{k}{Y_{S/X}} - 1 \right) k\,\mu(S) S + k\,D\,S_{in} \quad (6)$$

Proposition 1: if we choose the estimator's gain such that $Y_{S/X} < k \leq 1 + D / k_d$ and $|\mu(S) - \hat{\mu}(S)| < a$, $a \in R^+$. Then, the system (7) is a bounded error estimator of (6).

$$\dot{\hat{z}} = -\left[D + k_d - k\,k_d + \left(\frac{k}{Y_{S/X}} - 1 \right) \hat{\mu}(S) \right] \hat{z} + + (1-k) k\,k_d S + \left(\frac{k}{Y_{S/X}} - 1 \right) k\,\hat{\mu}(S) S + k\,D\,S_{in} \quad (7)$$

For the proof, define the estimation error,

$$e = z - \hat{z} \quad (8)$$

Then, using equations (6) and (7) the estimation error dynamic is obtained as

$$\dot{e} = -\left[D + k_d - k\,k_d + \left(\frac{k}{Y_{S/X}} - 1 \right) \hat{\mu}(S) \right] e + + \left(\frac{k}{Y_{S/X}} - 1 \right) [\mu(S) - \hat{\mu}(S)] k\,S - \left(\frac{k}{Y_{S/X}} - 1 \right) [\mu(S) - \hat{\mu}(S)] z \quad (9)$$

To analyze the stability of equation (9) we consider the following Lyapunov function candidate

$$V = \frac{1}{2} e^2 \quad (10)$$

The time derivative of equation (10) is

$$\dot{V} = e\,\dot{e} \quad (11)$$

Replacing (9) into (11) yields

$$\dot{V} = -\left[D + k_d - k\,k_d + \left(\frac{k}{Y_{S/X}} - 1 \right) \hat{\mu}(S) \right] e^2 + + \left(\frac{k}{Y_{S/X}} - 1 \right) [\mu(S) - \hat{\mu}(S)] k\,S\,e - \left(\frac{k}{Y_{S/X}} - 1 \right) [\mu(S) - \hat{\mu}(S)] z\,e \quad (12)$$

Equation (12) is written alternatively as

$$\dot{V} = -\left[D + k_d - k\,k_d + \left(\frac{k}{Y_{S/X}} - 1 \right) \hat{\mu}(S) \right] e^2 - - \left(\frac{k}{Y_{S/X}} - 1 \right) [\mu(S) - \hat{\mu}(S)] X\,e \quad (13)$$

Now, from lemma 1 and taking into account that $Y_{S/X} < k \leq 1 + D / k_d$, $|\mu(S) - \hat{\mu}(S)| < a$, and X is bounded, equation (13) leads to,

$$\dot{V} \leq -\left[D + k_d - kk_d + \left(\frac{k}{Y_{S/X}} - 1 \right) r \right] e^2 + \left(\frac{k}{Y_{S/X}} - 1 \right) aX_{\max} |e| = -\lambda\,e^2 + w|e|$$

where,

$$\lambda = D + k_d - kk_d + \left(\frac{k}{Y_{S/X}} - 1 \right) r \text{ and } w = \left(\frac{k}{Y_{S/X}} - 1 \right) aX_{\max}$$

The right-hand side of the foregoing inequality is not negative since near the origin, the positive linear term $w|e|$ dominates the negative quadratic term $-\lambda\,e^2$. However, $\dot{V}$ is negative outside the set $\{|e| \leq w/\lambda\}$. Let c, ε be some upper bounds for $V(e)$. With $c > w^2/2\lambda^2$, solutions starting in the set $\{V(e) \leq c\}$ will remain therein for all time because $\dot{V}$ is negative on the boundary $V = c$. Hence, the solutions of equation (9) are uniformly bounded (Khalil, 2002). Moreover, if $(w^2/2\lambda^2) < \varepsilon < c$, then $\dot{V}$ will be negative in the set $\{\varepsilon \leq V \leq c\}$, which shows that, in this set V will decrease monotonically until the solutions enters the set $\{V \leq \varepsilon\}$. From that time on, the solution cannot leave the set $\{V \leq \varepsilon\}$ since $\dot{V}$ is negative on the boundary $V = \varepsilon$. According to (Khalil, 2002), the solution is uniformly ultimately bounded with the ultimate bound $|e| \leq \sqrt{2\varepsilon}$. For instance, defining c and ε as follows

$$c = \left(\frac{k}{Y_{S/X}} \frac{aX_{\max}}{\lambda} \right)^2, \quad \varepsilon = \left(k \frac{aX_{\max}}{\lambda} \right)^2$$

the ultimate bound is, $|e| \leq \sqrt{2}\,k \frac{aX_{\max}}{\lambda}$

Corollary 1: if the growth rate is perfectly known, i. e., $\mu(S) = \hat{\mu}(S)$, and we choose the estimator's gain such that

$Y_{S/X} < k \le 1 + D/k_d$. Then, the system (14) is an asymptotic estimator of (6).

$$\dot{\hat{z}} = -\left[D + k_d - k\,k_d + \left(\frac{k}{Y_{S/X}} - 1 \right) \mu(S) \right] \hat{z} +$$
$$+ (1-k) k\,k_d S + \left(\frac{k}{Y_{S/X}} - 1 \right) k\,\mu(S) S + k\,D\,S_{in} \quad (14)$$

Indeed, the dynamics of the error in this case is

$$\dot{e} = -\left[D + k_d - k\,k_d + \left(\frac{k}{Y_{S/X}} - 1 \right) \mu(S) \right] e$$

and the corresponding time derivative of Lyapunov function candidate (10) is

$$\dot{V} = -\left[D + k_d - k\,k_d + \left(\frac{k}{Y_{S/X}} - 1 \right) \mu(S) \right] e^2 < 0$$

Moreover, X can be reconstructed considering

$$\hat{X} = \hat{z} - k\,S \quad (15)$$

B. Numerical simulations

For all simulations in this paper we take $S_{in} = 50$, $D = 0.1$, $Y_{S/X} = 0.9$, $k_d = 0.01$ and the initial conditions $S(0) = 60$, $X(0) = 40$, $\hat{X}(0) = 30$, $\hat{z}(0) = 90$, with appropriate units. The estimator's gain is $k = 1$. The growth rates are chosen as

$$\mu(S) = \frac{S}{140 + S + S^2/81.25} \text{ and } \hat{\mu}(S) = \frac{0.8\,S}{140 + S + S^2/81.25}$$

when the model is well known for the asymptotic estimator and when the model is partially known for the bounded error estimator, respectively. The simulations results were carried out with the help of Matlab 7.1 Software with Simulink 6.3 as the toolbox.

The performance index of the corresponding estimation process is calculated as (Martínez-Guerra, et. al, 2000)

$$J = \frac{1}{t + 0.001} \int_0^t \| e(\tau) \|^2 \, d\tau \quad (16)$$

where $e(t)$ is the corresponding state estimation error (the difference between the actual observed signal and its estimate).

First, in figure 1 we show the simulation results for the bounded error estimator given by proposition 1, and the corresponding results for the asymptotic estimator given by corollary 1 (without any noise in the system output). Furthermore, in figure 2 is shown the effect of noise in the estimation process. A white noise is added in the measurement ($\sigma = 0.1$, $\pm 10\%$ around the current value of the measured output). We can observe that the bounded error estimator is robust against noisy measurement. Finally, in figure 3 is illustrated the performance index given by (16) for the corresponding estimation process. It should be noted that the quadratic estimation error (performance index) is bounded on average and has a tendency to decrease.

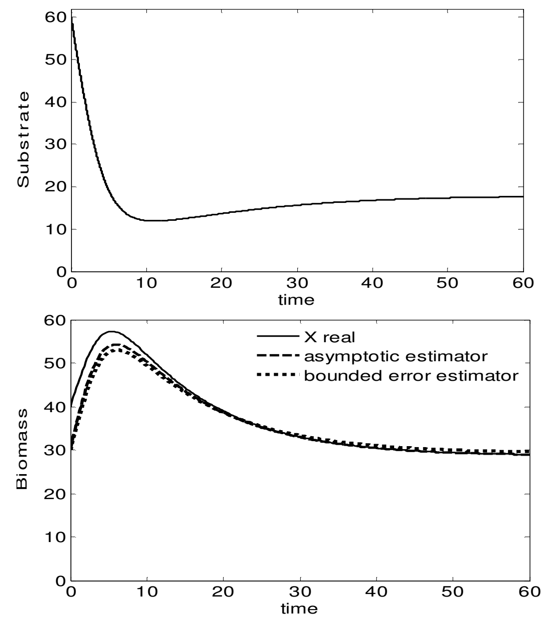


Figure 1. State Variables.

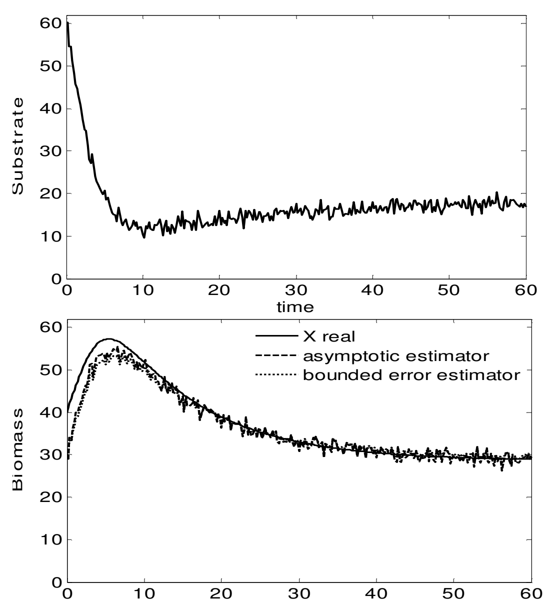
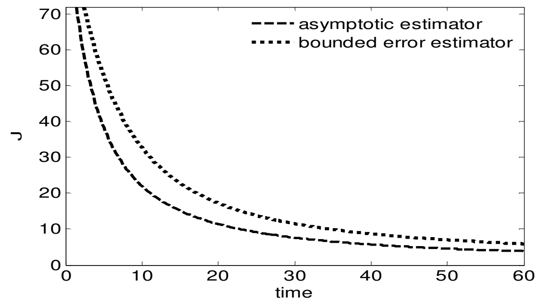
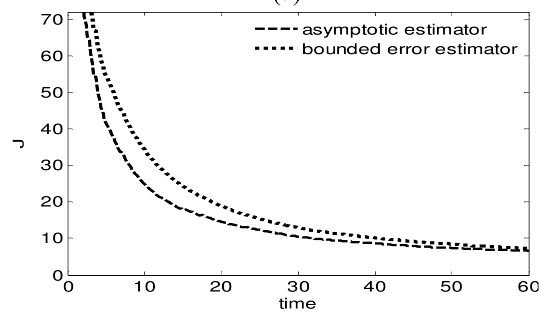


Figure 2. State Variables (with noise in the system output).



(a)



(b)

Figure 3. Quadratic estimation error. (a) Without any noise, (b) with white noise; in the system output.

IV. A NOTE ON FULL-ORDER OBSERVERS: THE HIGH GAIN OBSERVER

A. Observer design

Consider that system (1) satisfies the AOC. In this case to estimate the state-space vector x, we can suggest a nonlinear high gain observer (Gauthier et. al, 1992), (Martínez-Guerra et. al, 2000) with the following structure,

$$\dot{\hat{x}} = f(\hat{x},u) + K(y - C\hat{x}) \qquad (17)$$
$$\hat{x} \in R^n , \qquad \hat{x}_0 = \hat{x}(t_0)$$

where the observer's gain matrix is given by,

$$K = S_\theta^{-1} C^T , \qquad S_\theta = \left(\frac{1}{\theta^{i+j-1}} S_{ij} \right)_{i,j=1,\dots,n}$$

and the positive parameter θ determines the desired convergence velocity. Moreover, $S_\theta > 0$, $S_\theta = S_\theta^T$ should be a solution of the algebraic equation,

$$S_\theta \left(E + \frac{\theta}{2} I \right) + \left(E^T + \frac{\theta}{2} I \right) S_\theta = C^T C , \qquad E = \begin{pmatrix} 0 & I_{n-1,n-1} \\ 0 & 0 \end{pmatrix}$$

As shown by (Gauthier et. al, 1992), (Martínez Guerra and de Leon-Morales, 1996), under certain technical a assumptions (Lipschitz conditions for nonlinear functions under consideration) this nonlinear observer has an arbitrary exponential decay for any initial conditions. We obtain the following high order observer for the system (2) applying the observation scheme (17),

$$\dot{\hat{S}} = D\left(S_{in} - \hat{S}\right) - \frac{\mu_{\max} \hat{S}}{\delta + \hat{S} + \hat{S}^2/\phi} \frac{\hat{X}}{Y_{S/X}} + k_d \hat{X} - 2\theta\left(\hat{S} - y\right)$$

$$\dot{\hat{X}} = -D\hat{X} + \frac{\mu_{\max} \hat{S}}{\delta + \hat{S} + \hat{S}^2/\phi} \hat{X} - k_d \hat{X} -$$
$$- \frac{1}{-\mu_{\max} \hat{S} + Y_{S/X} \left(\delta + \hat{S} + \frac{\hat{S}^2}{\phi} \right) k_d} \left\{ 2\theta \frac{\mu_{\max} \hat{X}\left(\delta - S^2/\phi\right)}{\left(\delta + \hat{S} + \hat{S}^2/\phi\right)} + \right.$$
$$\left. + \theta^2 Y_{S/X} \left(\delta + \hat{S} + \hat{S}^2/\phi\right) \right\} \left(\hat{S} - y\right)$$

B. Simulations

In the same way, we show two simulations: when the model is well known and when the model is partially known. The initial conditions for the observer are $\hat{S}(0) = 40$, $\hat{X}(0) = 30$, with appropriate units. The estimator's gain is $\theta = 2$. The simulations results of high gain observer are presented in figure 4 and figure 5. In figure 4, without any noise in the system output, when the model is perfectly known the rate of convergence is fast, on the other hand, when the model is partially known the observer does not reconstruct the state variables. In figure 5, we studied the effect of noise in the measurement (white noise with $\sigma = 0.1$, $\pm 5\%$ around the current value of the measured output), we can see that the high gain observer is very sensitive to the noise in the system output. Figure 6 shows the performance index. It should be noted that this observer only reconstruct the state variables when the model is well known.

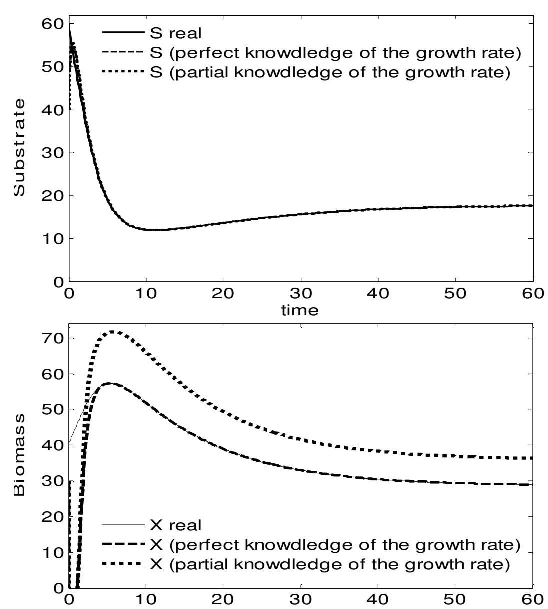


Figure 4. State Variables

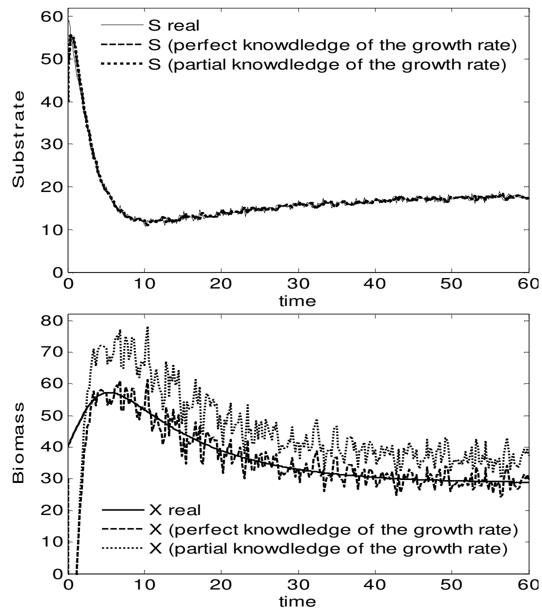
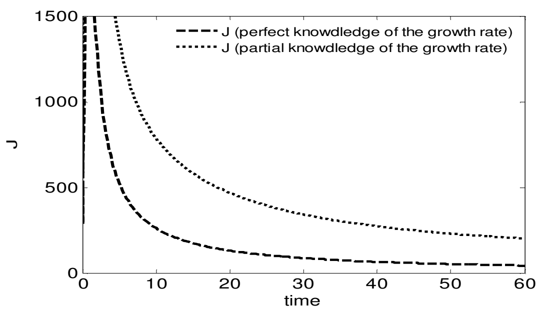
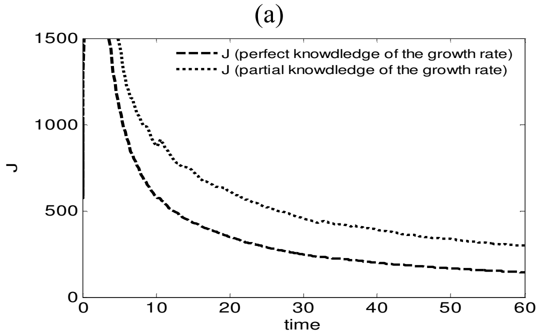


Figure 5. State Variables (with noise in the system output).



(a)



(b)

Figure 6. Quadratic estimation error. (a) Without any noise, (b) with white noise; in the system output.

V. Conclusion

In this paper we have presented a bounded error estimator for bioprocess with unstructured growth models. We have proven the stability of the corresponding estimation error in a Lyapunov sense. By means of a linear change of variable given in a natural manner and with some algebraic manipulations have been constructed the state estimator, which converges to the current states of the reference model given. We have demonstrated that the bounded error estimator under consideration provides good enough state-space estimates which were bounded on average. Moreover, we have constructed a high gain observer in which the convergence is fast only if the model is well known, but does not exists convergence if the model is partially known. Finally, we have presented some simulations to illustrate the effectiveness of the suggested approach, which shows some robustness properties against noisy measurements.

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