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State estimation in batch processes using a nonlinear observer

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Abstract

This paper deals with the problem of nonlinear states estimation in batch chemical processes. It presents a reduced-order nonlinear observer approach to perform the estimation. The proposed method allows adjustment of the speed of convergence towards zero of the estimation error. The stability properties of the model-based observer are analytically treated in order to show the conditions under which exponential convergence can be achieved. In addition, the performance of the proposed observer is evaluated on batch processes.

Keywords: Nonlinear observer; Nonlinear dynamics; Chemical processes

1. Introduction

In order to control or monitor many technological processes, the problem of states estimation constitutes a strategic topic. With the goal of process control and optimization, the knowledge of some physical state variables provides useful information. This is the case of many widely diffused process control strategies. Therefore, the presence of unknown states becomes a difficulty which can be solved by means of the inclusion of an appropriate state estimator. For this reason, many researchers have focused their attention on the development of suitable algorithms to perform the estimation. In this sense, several techniques have been introduced to estimate state variables from the available measurements, usually related to meaningful physico-chemical variables. From the obtainable information about the process, there exist many possible kinds of estimators to be used depending on the mathematical structure of the process model [1–3].

Notwithstanding the fact that theories and applications for linear systems are well developed, the highly nonlinear essence of many processes has given rise to the development of nonlinear observers. These observers are designed in such a way that they can cope with the intrinsic nonlinearities. However, the construction of nonlinear observers still provides an open research field because the advance in this area often faces many typical obstacles. Among others, the main barriers are the very restrictive conditions to be satisfied, uncertainty in the performance and robustness and/or poor estimation results in the presence of noisy sensors [4].

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As regards the nonlinear estimation techniques developed up to now, the Extended Kalman Filter (EKF) is one of the most widely diffused observers among other nonlinear ones based on linearization techniques [5–7]. In the EKF approach, a Riccati equation must be solved to obtain the estimator gain. Although the EKF could be a good selection to satisfy the trade-off between the measurement noise and the input uncertainty when the assumptions are satisfied, in many cases it can fail. Since the noise model is often unknown, it must be assumed. In such a case, wrong noise assumptions could lead to biased estimates or even diverge.

A method based on extended linearization has also been developed to carry out state estimation [8]. The procedure is based on linearizing with respect to a fixed operating point, and involves finding a function of the output in order to keep the system poles invariant in the vicinity of the mentioned point. Hence, the design procedure is subject to very tight conditions, and even when the output function is found (which is not an easy task) only local performance is ensured.

Another estimation approach includes the sliding observers [9,3]. The design procedure consists in determining a switching gain. One restrictive aspect is that the outputs must lie on specified sliding surfaces to achieve the estimation. Moreover, performance is rarely guaranteed, specially when the outputs are corrupted with noise.

Other procedures for observer construction make use of transformed canonical forms in order to design the estimator gain. In [10], Gauthier et al. proposed a simple observer for input affine systems, whose design involves solving a Riccati equation.

A detailed discussion on many of the available state estimation techniques applicable to a broad class of nonlinear systems, is provided by [2]. Another comprehensive evaluation of various nonlinear observers was presented by Wang et al. [3].

Other developments on state estimation include the recent works by Sundarapandian [20,21]. In [20], he presented a geometric study of the local observer design and established a connection between the design for forced and autonomous systems. In a later contribution [21], he extended the previous results to tackle the problem of global observer design under some stability assumptions. Both approaches include full-order observers, i.e. the whole state vector was estimated. Other proposals present nonlinear receding-horizon observers. In this approach, the observer design is based on the minimization of the distance between the observability map evaluated on the actual states and their estimates (see for instance, [22–24]).

Taking into account the characteristics of the observers discussed above, the objective of this work is to present a nonlinear efficient state estimator for later multi-purpose applications related to batch processes. Batch processes have turned out to be very important during the last decades. One of the main reasons for this is the structural changes in the industry due to the trend towards producing small amounts of assorted products with a high added value. In monitoring and controlling this kind of chemical processes, on-line information about the internal state of the system is very important. Moreover, due to their batch nature, the estimated variables must converge to their actual values in a relative short time. From this point of view, the proposed observer may be useful for control and optimization, as well as for efficient and reliable process-monitoring schemes. The estimation approach herein introduced extends to nonlinear autonomous systems the technique independently developed by Gopinath [11] and Cumming [12] for linear reduced-order observer design.

The proposed observer guarantees that the estimation error exponentially converges towards zero whenever the observer gain is adequately chosen. The observer implementation is simple and it requires small computational effort. Provided observability is achieved, the design approach can be applied for any general type of nonlinear batch-processes models, because no fixed model structure is required. An advantageous feature of the proposed nonlinear observer is that it shows robust performance.

The work is organized as follows. In Section 2, the estimation problem is discussed and the observer design procedure is developed. The evaluation of the observer performance under both model and measurement uncertainties is presented in Section 3 and in this section the proposed observer behaviour is compared with a full order observer and an Extended Kalman Filter. Finally, in Section 4 the conclusions are drawn.

2. Nonlinear observer design approach

A lot of batch processes can be modelled as follows:

$$\dot{x} = F(x) \tag{1}$$

$$y = H(x) \tag{2}$$

where $x \in R^n$ is the state vector and $y \in R^p$ is the vector of measured variables. When full order observers are constructed, all states are estimated from the information provided by the measured variables [10]. In this case, an n-order dynamical system, named the observer, is used for processing the measured signal so that a vector of order n, representing the estimated states, is obtained. However, in many cases the order of the observer can be reduced by using adequately the information provided by the measured variables. In the following, a method to construct a reduced order observer is developed.

The state vector x is subdivided into two parts, x_R and $\bar{x}_R$, so that $x = \begin{bmatrix} x_R^T & \bar{x}_R^T \end{bmatrix}^T$, where $x_R \in R^m$ and $\bar{x}_R \in R^p$, with $m+p=n$. It must be remarked that the partition x_R includes all the unmeasured states to be estimated. Therefore, Eqs. (1) and (2) can be rewritten in the following way:

$$\dot{x}_R = F_R(x_R, \bar{x}_R) \tag{3}$$

$$\dot{\bar{x}}_R = \bar{F}_R(x_R, \bar{x}_R) \tag{4}$$

$$y = H(x_R, \bar{x}_R). \tag{5}$$

By assuming that the Implicit Function Theorem is satisfied by (5), there exists a function $\tilde{H}$ so that:

$$\bar{x}_R = \tilde{H}(x_R, y). \tag{6}$$

Note that

$$\dot{y} = \frac{\partial H}{\partial x_R} F_R + \frac{\partial H}{\partial \bar{x}_R} \bar{F}_R \triangleq \psi(x_R, \bar{x}_R). \tag{7}$$

Thus, by using Eqs. (3), (6) and (7), the following formulation is achieved:

$$\dot{x}_R = F_R(x_R, \tilde{H}(x_R, y)) \tag{8}$$

$$\dot{y} = \psi(x_R, \tilde{H}(x_R, y)). \tag{9}$$

By denoting $f(x_R, y) = F_R(x_R, \tilde{H}(x_R, y))$ and $g(x_R, y) = \psi(x_R, \tilde{H}(x_R, y))$, Eqs. (8) and (9) can be rewritten as:

$$\dot{x}_R = f(x_R, y) \tag{10}$$

$$\dot{y} = g(x_R, y) \tag{11}$$

where y and $g(.)$ are equal to $[y_1 \dots y_p]^T$ and $[g_1(.) \dots g_p(.)]^T$, respectively. When a full order observer is used, both vectors (x_R and y) are estimated so that the observer order is $m+p$ [10]. Nevertheless, it must be remarked that since the vector y is measured, it does not need to be estimated. In this case, an m-order observer can be constructed. This kind of observer is named the reduced-order observer. In what follows, a method for constructing an estimator for the vector x_R is proposed.

Without loss of generality, it can be assumed that $m \geq p$. A nonlinear transformation from x_R and y can be considered. In order to obtain the observer, the following nonlinear transformation is considered:

$$z = [z_1 \dots z_m]^T \triangleq \gamma^T = [\gamma_1(x_R, y) \dots \gamma_m(x_R, y)]^T \in R^m \tag{12}$$

where z are the state variables in the new coordinates. Therefore, the following transformed system is obtained:

$$\dot{y}_1 = g_1(x_R, y) = \gamma_1(x_R, y) \triangleq z_1 \tag{13}$$

$$\dot{z}_1 = \frac{\partial \gamma_1}{\partial x_R} f + \frac{\partial \gamma_1}{\partial y} g = \gamma_2(x_R, y) \triangleq z_2 \tag{14}$$

$$\dot{z}_2 = \frac{\partial \gamma_2}{\partial x_R} f + \frac{\partial \gamma_2}{\partial y} g = \gamma_3(x_R, y) \triangleq z_3 \tag{15}$$

$$\vdots$$

$$\dot{z}_{l_1-1} = \frac{\partial \gamma_{l_1-1}}{\partial x_R} f + \frac{\partial \gamma_{l_1-1}}{\partial y} g = \gamma_{l_1}(x_R, y) \triangleq z_{l_1} \tag{16}$$

$$\dot{z}_{l_1} = \frac{\partial \gamma_{l_1}}{\partial x_R} f + \frac{\partial \gamma_{l_1}}{\partial y} g \triangleq \sigma_1(x_R, y) \tag{17}$$

$$\dot{y}_2 = g_2(x_R, y) = \gamma_{l_1+1}(x_R, y) \triangleq z_{l_1+1} \tag{18}$$

$$\dot{z}_{l_1+1} = \frac{\partial \gamma_{l_1+1}}{\partial x_R} f + \frac{\partial \gamma_{l_1+1}}{\partial y} g = \gamma_{l_1+2}(x_R, y) \triangleq z_{l_1+2} \tag{19}$$

$$\vdots$$

$$\dot{z}_{l_1+l_2-1} = \frac{\partial \gamma_{l_1+l_2-1}}{\partial x_R} f + \frac{\partial \gamma_{l_1+l_2-1}}{\partial y} g = \gamma_{l_1+l_2}(x_R, y) = z_{l_1+l_2} \tag{20}$$

$$\dot{z}_{l_1+l_2} = \frac{\partial \gamma_{l_1+l_2}}{\partial x_R} f + \frac{\partial \gamma_{l_1+l_2}}{\partial y} g \triangleq \sigma_2(x_R, y) \tag{21}$$

$$\vdots$$

$$\dot{y}_p = g_p(x_R, y) = \gamma_{l_1+\cdots+l_{p-1}+1}(x_R, y) \triangleq z_{l_1+\cdots+l_{p-1}+1} \tag{22}$$

$$\dot{z}_{l_1+\cdots+l_{p-1}+1} = \frac{\partial \gamma_{l_1+\cdots+l_{p-1}+1}}{\partial x_R} f + \frac{\partial \gamma_{l_1+\cdots+l_{p-1}+1}}{\partial y} g = \gamma_{l_1+\cdots+l_{p-1}+2}(x_R, y) = \triangleq z_{l_1+\cdots+l_{p-1}+2} \tag{23}$$

$$\vdots$$

$$\dot{z}_{l_1+\cdots+l_p-1} = \frac{\partial \gamma_{l_1+\cdots+l_p-1}}{\partial x_R} f + \frac{\partial \gamma_{l_1+\cdots+l_p-1}}{\partial y} g = \gamma_{l_1+\cdots+l_p} \triangleq z_{l_1+\cdots+l_p} \tag{24}$$

$$\dot{z}_{l_1+\cdots+l_p} = \frac{\partial \gamma_{l_1+\cdots+l_p}}{\partial x_R} f + \frac{\partial \gamma_{l_1+\cdots+l_p}}{\partial y} g \triangleq \sigma_p(x_R, y) \tag{25}$$

where $\sum_{k=1}^{p} l_k = m$. Assuming that $\frac{\partial \gamma}{\partial x_R}$ is not singular in (x_R, y) there exists $x_R = \tilde{\gamma}(z, y)$, which means that the vector x_R (i.e. in original coordinates) can be calculated from the knowledge of vectors z and y, using the function $\tilde{\gamma}$. In new coordinates, the model given by (10) and (11) becomes:

$$\dot{z} = Az + \rho(z, y) \tag{26}$$

$$\dot{y} = Cz \tag{27}$$

where

$$\rho(z, y) = \left[0 \cdots \sigma_1(x_R, y) \quad 0 \cdots \sigma_2(x_R, y) \cdots \quad \sigma_p(x_R, y)\right]^{\mathrm{T}} |_{(x_R = \tilde{\gamma}(z,y))}.$$

From the comparison of (26) and (27) with Eqs. (13) and (25), the following assignment is obtained:

$$A = \begin{bmatrix} A_1 & 0 & 0 \\ \vdots & \ddots & \vdots \\ 0 & A_k & 0 \\ \vdots & \ddots & \vdots \\ 0 & 0 & A_p \end{bmatrix} \tag{28}$$

where A_k is a matrix of dimension $l_k \times l_k$, with $k = 1, \ldots, p$, given by

$$A_k = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & 1 \\ 0 & \cdots & \cdots & \cdots & 0 \end{bmatrix} \tag{29}$$

and C is a matrix of dimension $p \times m$ given by

$$C = \begin{bmatrix} C_1^1 \\ C_2^{l_1+1} \\ \vdots \\ C_i^j \\ \vdots \\ C_p^{l_1+\cdots+l_{p-1}+1} \end{bmatrix} \tag{30}$$

where C_i^j, with $j = 1, \ldots, \sum_{k=1}^{(j-1)} l_k + 1$, is a row vector with 1 in the position j and zero otherwise. Under this construction, the pair (C, A) is observable.

Theorem. *Considering the nonlinear system given by (26) and (27) and assuming that $\rho(z, y)$ is Lipschitz in z with a Lipschitz constant L, the following system:*

$$\dot{\hat{z}} = A\hat{z} + \rho(\hat{z}, y) + G(\dot{y} - C\hat{z}) \tag{31}$$

where $(\hat{\ })$ stands for estimated variables, with G a constant matrix, is an observer with exponential speed of convergence, if there exist P and Q positive definite matrices satisfying

$$(A - GC)^{\mathrm{T}} P + P(A - GC) = -Q \tag{32}$$

and

$$-\lambda_Q^{\min} + 2\lambda_P^{\max} L < 0 \tag{33}$$

where $\lambda_Q^{\min}$ is the minimum eigenvalue of matrix Q, $\lambda_P^{\max}$ is the maximum eigenvalue of matrix P.

Proof. See Appendix.

Note that the correction term $G(\dot{y} - C\hat{z})$ in Eq. (31) uses the time derivative of the measured variables. Because the measured variables can be contaminated with noise, it is preferred to avoid differentiating them. For this reason, the observer equations are modified introducing the change of variables given by:

$$\nu = \hat{z} - Gy. \tag{34}$$

In this way, $\hat{z}$ is calculated as:

$$\dot{\nu} = A\hat{z} + \rho(\hat{z}, y) - GC\hat{z} \tag{35}$$

$$\hat{z} = \nu + Gy. \tag{36}$$

After $\hat{z}$ has been calculated, the estimated variables in original coordinates ($\hat{x}_R$) are obtained using the function $\tilde{\gamma}$:

$$\hat{x}_R = \tilde{\gamma}(\hat{z}, y). \tag{37}$$

Eqs. (35)–(37) are used to obtain estimates of x_R variables provided that vector y is measured. When it is possible to select the P, Q and G matrices in (32) in order to satisfy the constraint given by (33), the estimation error ($e = x_R - \hat{x}_R$) converges to zero in an exponential way.

Table 1
Parameters of the bioprocess model

Parameter	Value
μ_0	0.0967
K_s	0.4076
k_1	0.2102
K_f	1.6717×10^{-5}
β_1	0.1112
β_2	1.6655

3. Application to bioprocesses

3.1. Batch bioreactor

In order to illustrate the observer design when two outputs are measured and two variables are estimated, a batch bioprocess is dealt with. In the field of bioprocesses, state estimation appears as the backbone in both monitoring and control. This fact is basically connected with the lack of cheap and reliable instrumentation to measure on-line the main variables of the process. That is why many researchers have focused their attention on suitable algorithms to perform the estimation [13–16].

In this section, simulation results on a *Thiobacillus ferrooxidans* batch culture are presented. The bacterium *T. ferrooxidans* is one of the most important biological lixiviants with reference to oxidation of ferrous and sulfide minerals [17]. Because the measurement of biomass concentration (x) inside the reactor is particularly troublesome, the estimation of that variable becomes necessary. The reaction performed by the bacteria consists in the oxidation of Fe^{+2} into Fe^{+3}, which are referred to as the substrate (s) and the product (p), respectively.

Because the measurements of pH and the concentration rate s/p are provided on-line by standard sensors [16], we propose to estimate both biomass and substrate concentration in order to know all the state variables of the process.

In [18], Kumar and Gandhi reported a complete mathematical model to describe the dynamics of the bioleaching process performed by *T. ferrooxidans*. Under certain culture conditions, the cell death can be neglected and the following model is valid:

$$\dot{x}(t) = \mu(t)x(t) \tag{38}$$

$$\dot{s}(t) = -k_1\mu(t)x(t) \tag{39}$$

$$\dot{p}(t) = -\dot{s}(t) - K_f p(t)10^{\mathrm{pH}(t)} \tag{40}$$

$$\dot{\mathrm{pH}}(t) = -\beta_1\dot{s}(t) - \beta_2 K_f p(t)10^{\mathrm{pH}(t)} \tag{41}$$

where the specific growth rate μ is assumed to be Monod:

$$\mu = \frac{\mu_0 s(t)}{K_s + s(t)}. \tag{42}$$

The process parameters are: μ_0, K_s, k_1, K_f, β_1, β_2. Their values were reported in [18], and are shown in Table 1. The measurements are s/p and pH. Defining a new variable $r = s/p$, the system (38)–(41) is easily modified to obtain the description given by Eqs. (10) and (11).

$$\dot{x} = \mu x \tag{43}$$

$$\dot{s} = -k_1\mu x \tag{44}$$

$$\dot{r} = -k_1\mu x(r + r^2)\frac{1}{s} + K_f r 10^{\mathrm{pH}} \tag{45}$$

$$\dot{\mathrm{pH}} = \beta_1 k_1 \mu x - \beta_2 K_f \frac{s}{r} 10^{\mathrm{pH}} \tag{46}$$

with

$$x_R = \begin{bmatrix} x & s \end{bmatrix}^{\mathrm{T}} \quad \text{and} \quad y = \begin{bmatrix} r & \mathrm{pH} \end{bmatrix}^{\mathrm{T}}. \tag{47}$$

The nonlinear transformation is given by:

$$z_1 = g_1(x, s, r, \text{pH}) = -k_1\mu x(r + r^2)\frac{1}{s} + K_f r 10^{\text{pH}} \tag{48}$$

$$z_2 = g_2(x, s, r, \text{pH}) = \beta_1 k_1 \mu x - \beta_2 K_f \left(\frac{s}{r}\right) 10^{\text{pH}}. \tag{49}$$

Therefore, biomass (x) and substrate (s) estimates can be obtained by using the following observer:

$$\dot{\nu}_1 = \sigma_1(\hat{x}, \hat{s}, r, \text{pH}) - g_{11}\dot{\hat{r}} - g_{12}\dot{\hat{\text{pH}}} \tag{50}$$

$$\dot{\nu}_2 = \sigma_2(\hat{x}, \hat{s}, r, \text{pH}) - g_{21}\dot{\hat{r}} - g_{22}\dot{\hat{\text{pH}}} \tag{51}$$

where $g_{11}, g_{12}, g_{21}, g_{22}$ are the elements of the observer matrix gain G, and:

$$\dot{\hat{r}} = -k_1\hat{\mu}\hat{x}(r + r^2)\frac{1}{\hat{s}} + K_f r 10^{\text{pH}} \tag{52}$$

$$\dot{\hat{\text{pH}}} = \beta_1 k_1 \hat{\mu}\hat{x} - \beta_2 K_f \left(\frac{\hat{s}}{r}\right) 10^{\text{pH}} \tag{53}$$

$$\hat{z}_1 = \nu_1 + g_{11} r + g_{12}\text{pH} \tag{54}$$

$$\hat{z}_2 = \nu_2 + g_{21} r + g_{22}\text{pH} \tag{55}$$

$$\hat{x} = \frac{1}{\beta_1}\left(\hat{z}_2 + \beta_2 K_f \left(\frac{\hat{s}}{r}\right) 10^{\text{pH}}\right)\frac{K_s + \hat{s}}{k_1\mu_m\hat{s}} \tag{56}$$

$$\hat{s} = \frac{-\hat{z}_2(r + r^2)}{\beta_1\left(\hat{z}_1 - K_f r 10^{\text{pH}}\right) + \beta_2(1 + r)K_f 10^{\text{pH}}}. \tag{57}$$

Taking into account that $r = s/p$, the estimated product is calculated as $\hat{p} = \frac{\hat{s}}{r}$. The observer performance was tested by simulation. Two different values for G, with:

$$G = \begin{bmatrix} g_{11} & 0 \\ 0 & g_{22} \end{bmatrix}$$

were selected. Both of them satisfy the condition given by (76)

$$G_1 = \begin{bmatrix} 0.5 & 0 \\ 0 & 0.5 \end{bmatrix}, \qquad G_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{58}$$

In both cases initial conditions of the bioprocess and estimated variables were: $x(0) = 3.4$ mg/l, $p(0) = 0.213$ g/l, $s(0) = 8.05$ g/l, $\text{pH}(0) = 1.92$, $\hat{x}(0) = 4$ mg/l and $\hat{s}(0) = 6$ g/l. The performance of the observer is illustrated in Figs. 1–8. Figs. 1–3 show actual state variables and estimated ones (estimated biomass, estimated substrate and estimated product) when the observer gain is given by $G = G_1$. The estimation results achieved with $G = G_2$ are depicted in Figs. 5–7. Figs. 4 and 8 show the estimation errors for $G = G_1$ and $G = G_2$, respectively. In both cases, the results exhibit good convergence properties of the estimated variables to the actual ones. The speed of convergence can be modified by changing the values of g_{11} and g_{22}. If g_{11} and g_{22} are increased, a higher speed of convergence is achieved.

3.2. *Observer performance under uncertainties*

The bioreactor example is continued by analysing the performance under uncertainties. In this way, it will be possible to establish the main advantages of the proposed reduced order observer.

However, in order to simplify the analysis and to concentrate the attention on the observer properties, it is assumed that the substrate (s) measurement is provided. Then, the problem of estimating biomass (x) from substrate measurement under model and measurements uncertainties is tackled. Taking into account the new problem

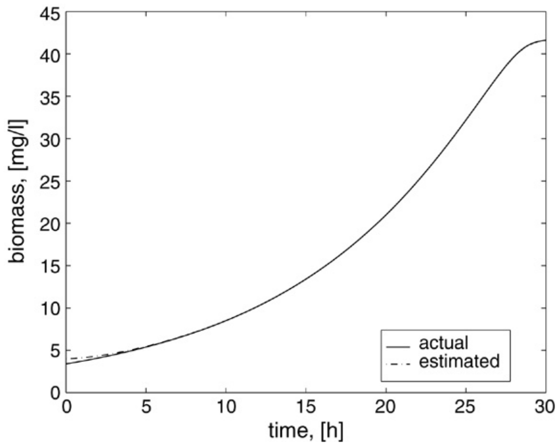

Fig. 1. Biomass (full line) and estimated biomass (dashed line) ($G = G_1$).

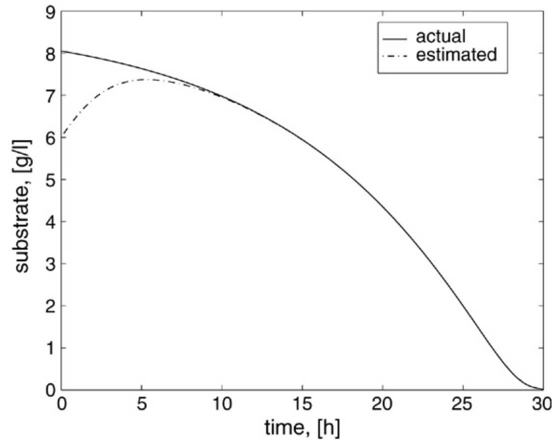

Fig. 2. Substrate (full line) and estimated substrate (dashed line) ($G = G_1$).

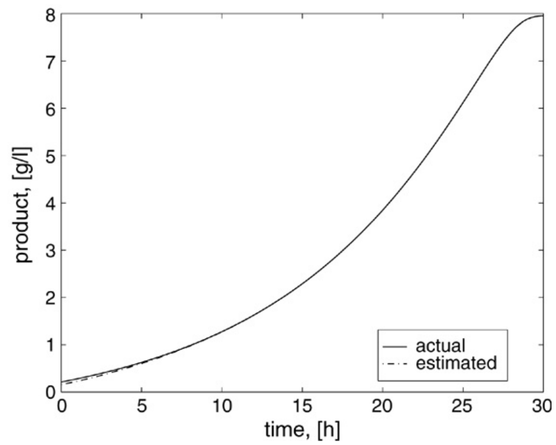

Fig. 3. Product (full line) and estimated product (dashed line) ($G = G_1$).

formulation (substrate measurement), the model to be considered for biomass estimation is reduced to:

$$\dot{x}(t) = \mu(t)x \quad (59)$$

$$\dot{s}(t) = -k_1\mu(t)x. \quad (60)$$

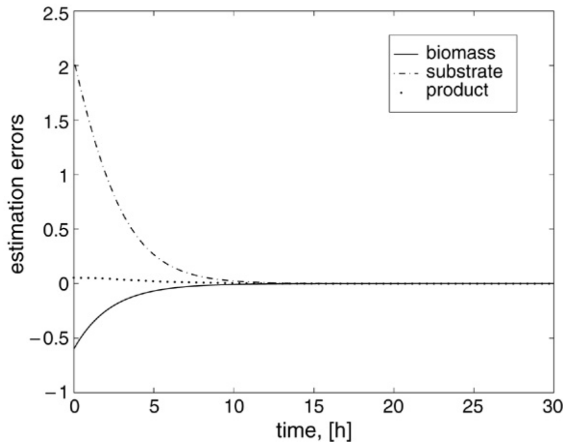

Fig. 4. Estimation errors: biomass (full line), substrate (dashed line), product (dash–dotted line) ($G = G_1$).

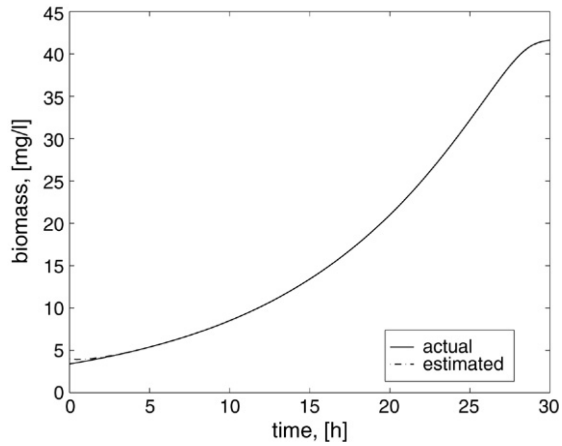

Fig. 5. Biomass (full line) and estimated biomass (dashed line) ($G = G_2$).

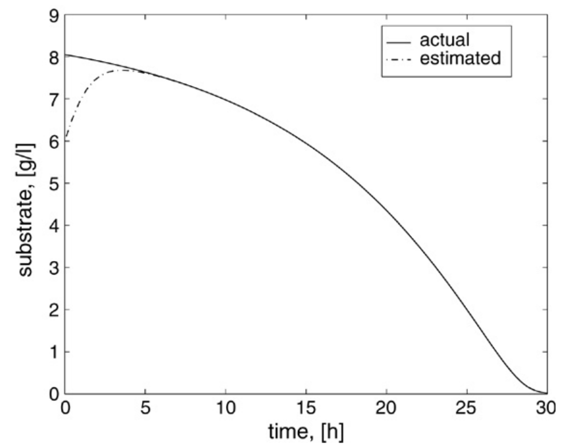

Fig. 6. Substrate (full line) and estimated substrate (dashed line) ($G = G_2$).

The specific growth rate (μ) will be approximated by a Monod description (see Eq. (42)). k_1 is the substrate/biomass yield and it is constant.

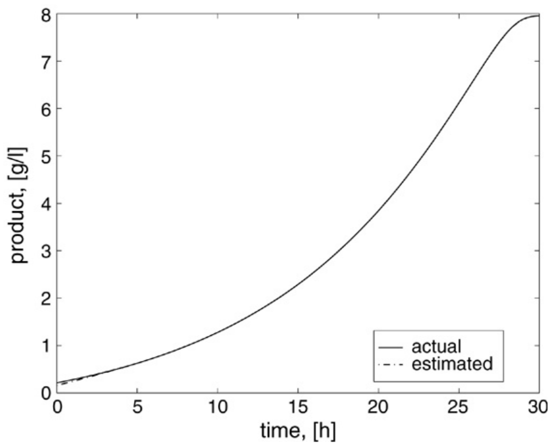

Fig. 7. Product (full line) and estimated product (dashed line) ($G = G_2$).

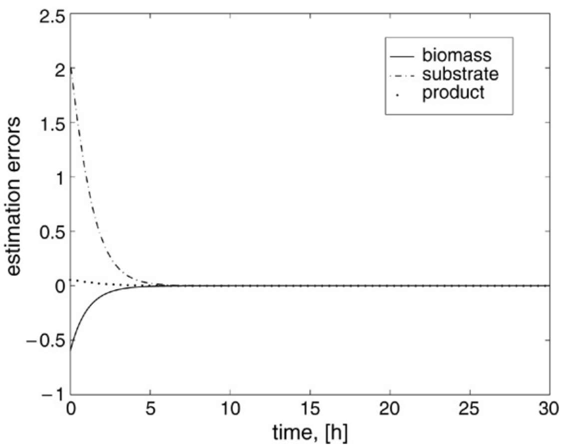

Fig. 8. Estimation errors: biomass (full line), substrate (dashed line), product (dash–dotted line) ($G = G_2$).

The performance of the reduced order observer herein proposed will be compared with a nonlinear full order observer and an EKF. These estimators are chosen for the comparison for two reasons. On one hand, full order observers are generally used and reduced versions are discarded because only robustness against output noise is considered. On the other hand, the EKF is a widely diffused technique and consequently, it is a well-known estimation method for many users.

3.2.1. Extended Kalman filter

In the EKF approach, a Riccati equation must be solved to obtain the estimator gain. This approach assumes the knowledge of the noise model in order to obtain the optimum estimated value. However, that model is frequently unknown and it must be assumed. Hence, wrong noise assumptions could lead to biased estimates or even diverge.

For the bioreactor application, the EKF estimator can be written as:

$$\begin{bmatrix} \dot{\hat{x}} \\ \dot{\hat{s}} \end{bmatrix} = \begin{bmatrix} \hat{\mu}\hat{x} \\ -k_1\hat{\mu}\hat{x} \end{bmatrix} + K(s - \hat{s}) \tag{61}$$

where $\hat{\mu} = \mu_0\hat{s}/(K_s + \hat{s})$. The time-varying EKF gain is calculated as:

$$K = PH'R^{-1} \tag{62}$$

$$\dot{P} = FP + PF' + Q - KRK' \tag{63}$$

$$F = \begin{bmatrix} \hat{\mu} & \hat{x}\dfrac{\partial \hat{\mu}}{\partial \hat{s}} \\ -k_1\hat{\mu} & -k_1\hat{x}\dfrac{\partial \hat{\mu}}{\partial \hat{s}} \end{bmatrix} \tag{64}$$

$$H = \begin{bmatrix} 0 & 1 \end{bmatrix} \tag{65}$$

with $\frac{\partial \hat{\mu}}{\partial \hat{s}} = \mu_0/(K_s + \hat{s}) - \mu_0\hat{s}/(K_s + \hat{s})^2$.

3.2.2. Full order nonlinear observer (FOO)

In the FOO algorithm, the correction term gain is nonlinear and it is related to the Jacobian of the nonlinear observability matrix. Its design is based on a nonlinear change of coordinates such that the dynamical algorithm equations can be expressed in either original coordinates or transformed ones. Then, nonlinear transformation is inverted for obtaining the estimates in original coordinates.

When the full order nonlinear observer is implemented to the batch bioreactor, the following algorithm is obtained:

$$\dot{\hat{z}}_1 = \hat{z}_2 + G_1(s - \hat{z}_1) \tag{66}$$

$$\dot{\hat{z}}_2 = \sigma(\hat{x}, \hat{z}_1) + G_2(s - \hat{z}_1) \tag{67}$$

$$\hat{x} = \hat{z}_2/(-k_1\hat{\mu}) \tag{68}$$

$$\hat{s} = \hat{z}_1 \tag{69}$$

where

$$\sigma(\hat{x}, \hat{z}_1) = -k_1\left[\frac{\partial \hat{\mu}}{\partial \hat{z}_1}(-k_1\hat{\mu}\hat{x}^2) + \hat{\mu}^2\hat{x}\right]$$

with $\hat{\mu} = \mu_0\hat{z}_1/(K_s + \hat{z}_1)$.

3.2.3. Reduced order nonlinear observer (ROO)

As proposed, it is reasonable to think that measured variables do not need to be estimated. For this reason, the proposed ROO can be used. Then, as the substrate is measured, it does not need to be estimated. Therefore, a reduced order observer is constructed for estimating biomass exclusively. The ROO algorithm is as follows:

$$\dot{\nu} = \rho(\hat{x}, s) - G\hat{z} \tag{70}$$

$$\hat{z} = \nu + Gs \tag{71}$$

$$\hat{x} = \frac{\hat{z}}{-k_1\mu} \tag{72}$$

where

$$\rho(\hat{x}, s) = -k_1\left[\frac{\partial \mu}{\partial s}(-k_1\mu\hat{x}^2) + \mu^2\hat{x}\right].$$

3.2.4. A comparative performance analysis

A comparative performance analysis of the three estimators is accomplished on the basis of the batch process above. The proposed observer (ROO) behaviour in the presence of uncertainties is compared with a FOO and an EKF. It must be highlighted that in this comparison the uncertainties are assumed unknown. Generally, the EKF gain is adjusted by using information on the uncertainties (for instance, noise covariance matrices). However, in our case that is not possible, since the uncertainties parameters are assumed unknown. For this reason, the EKF gain is set such that the EKF dynamic performance coincides with the ROO's in the nominal case (i.e. when uncertainties do not exist). For this purpose, the EKF parameters (Q and R) are set as follows. Q is chosen equal to zero and R is set to let the EKF achieve the desired speed of convergence. In this way, the observers perform similarly in absence of uncertainties. It is important to remark that under the above assumptions observers gains have to be kept fixed for all tests.

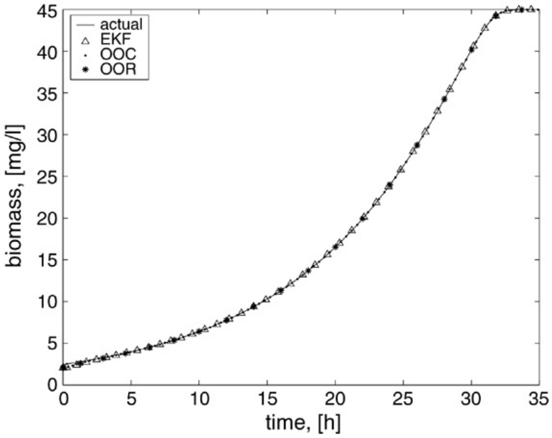

Fig. 9. Estimation for nominal model (case I).

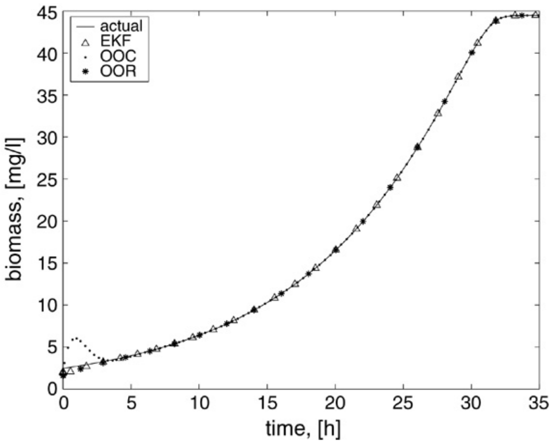

Fig. 10. Estimation for nominal model (case II).

Case I. In a first step, the nominal process is considered to carry on the estimation. The parameters of the nominal plant are: $k_1 = 0.21$; $\mu_0 = 0.1$; $K_s = 0.4$, and the initial values for biomass and substrate concentration are $x(0) = 2.465$ mg/l and $s(0) = 8.93$ g/l, respectively. The initial estimation conditions are set to $\hat{x}(0) = 2.054$ mg/l, $\hat{s}(0) = s(0)$, which are maintained for the three observers, which are tuned as follows. The EKF parameters are set to $Q = 0_{2\times 2}$ and $R = 0.01$; the FOO gains are $G_1 = G_2 = 2$ and the ROO gain is $G = 0.7$. These parameters are kept for all the simulations herein. The simulation results in Fig. 9 show that all the algorithms have a similar performance, and good convergence properties under nominal conditions.

Case II. In a second step, the previous simulation is repeated, but now the initial value for substrate is also assumed uncertain $\hat{s}(0) = 1.02\, s(0)$. Simulation results are shown in Fig. 10. Under these conditions, a typical dynamics behaviour of the full order observers is exhibited. The peaking phenomenon appears at the estimation beginning.

Case III. Now, parameter uncertainty is considered. A mismatch in the parameter k_1 is included, by introducing the value $1.1k_1$ in the plant model assumed in the observer design. Initial biomass and substrate values are set as in Case I (and they are kept invariant from now on). The estimation results are shown in Fig. 11. Under these conditions, there is an offset in the estimates. All observers evidence an analogous behaviour, and they cannot reject the parameter uncertainty.

Case IV. Another situation of parameter uncertainty is evaluated. In this case, a mismatch in the parameter μ_0 is considered by introducing the value $1.1\mu_0$ in the plant model used for the observer design. Simulation results are depicted in Fig. 12. Again, it appears an offset in the estimates. However, for this parameter uncertainty the EKF performance surpasses the ones of the other observers.

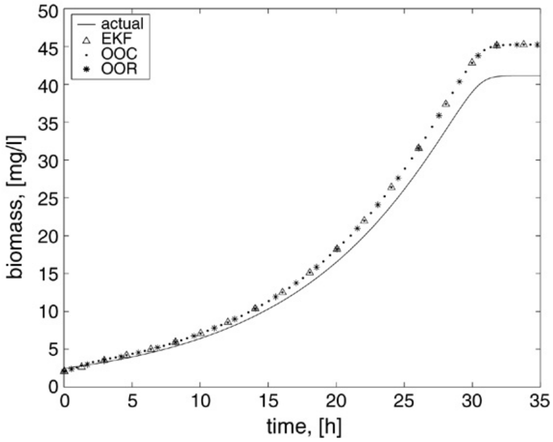

Fig. 11. Estimation under parameter uncertainty (case III).

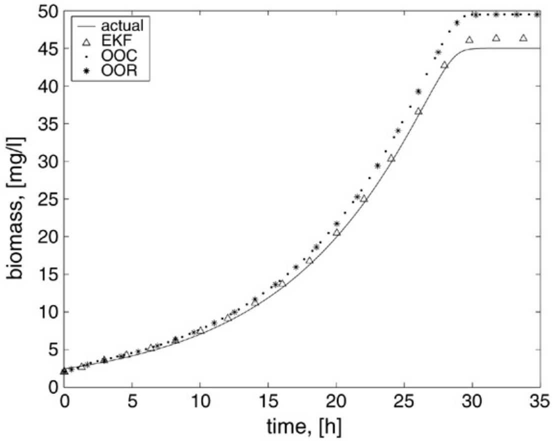

Fig. 12. Estimation under parameter uncertainty (case IV).

Case V. A different situation of uncertainty is proposed. In this case, dynamics uncertainty is included by considering an additional term in the nominal model of the process. A biomass extinction term due to mortality has been reported in various bioprocess [18], usually generated by the product poisoning effect. However, this phenomenon is usually unmodelled, and the mismatch between the real process and its model can be significant. To accomplish the estimation under this situation, a mortality term $\mu_d\,[k_p\,(s(0) - s(t))]^2 x$ with $\mu_d = 0.01$, and $k_p = 0.8$ is included [18]. The results are shown in Fig. 13. The observers behaviour evidences an offset. However, the EKF performance is significantly worse than the FOO and the ROO performances. Note that at $t = 35$ h the EKF estimation error is approximately 600%.

Case VI. Finally, estimation under both dynamics uncertainty and noisy measurement is evaluated. As in the previous case, the term due to mortality is considered for the real process. Additionally, the problem of biomass estimation based on substrate noisy measurement is tackled. For this purpose, an additive noise signal is generated. A zero mean white noise with variance 0.01 is coloured through a linear dynamics whose time constant is 0.1. The results are shown in Fig. 14. The observers performance show a trade-off between uncertainty and noise rejection. It can be noted that the EKF estimator exhibits a significant error.

It should be pointed out that an improvement of the performance of each observer (i.e. EKF, FOO and ROO) would be expected if the estimated vector were extended. This is the basis of the strategy usually referred to as "dynamics extension" which has been widely used in many previous works on this matter (see for instance [25–28]). Note that to accomplish this extension a model for the dynamics is needed (for instance, constant parameters can be assumed). In such cases the estimation error is subject to the accuracy of the extended dynamics model. However, the spirit of

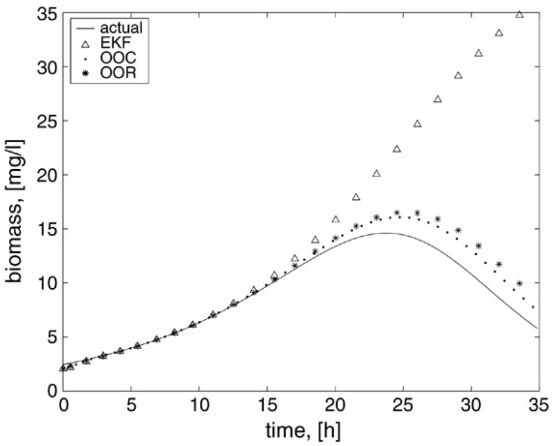

Fig. 13. Estimation under dynamics uncertainty (case V).

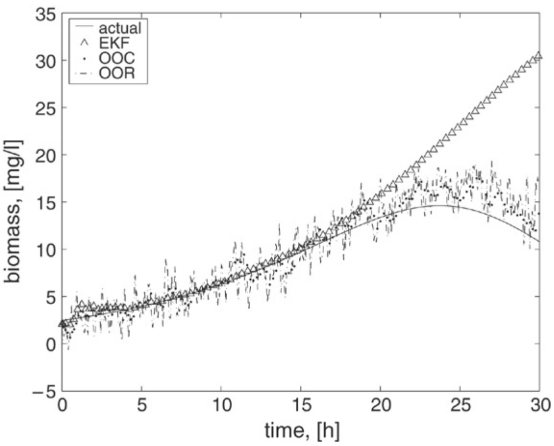

Fig. 14. Estimation under dynamics uncertainty and noisy measurement (case VI).

the example herein developed is to compare the three observers under the same situation. Therefore, the additional estimation of unknown parameters and/or dynamics is omitted in all the cases (i.e. for the three observers).

3.2.5. Comments on estimators performance

Roughly speaking, it is possible to remark that when the gain in the correction term is increased, the transient convergence can be deteriorated if the peaking phenomenon appears in FOO. From this point of view, ROO arises as a better option. However, the ROO estimator could be noisier than the FOO. In addition, it is possible to note that EKF is not always the best option, since it is designed by assuming a given noise model. When the uncertainty model substantially differs from the assumed noise model, EKF performance could be very poor. This is the case of the unmodelled death phenomenon in the analysed bioreactor.

Then, it is possible to argue that the proposed reduced order observer should be the best choice for improving the transient performance (peaking phenomenon is reduced) and for rejecting dynamics uncertainties, when their models do not adjust to the EKF assumptions.

4. Conclusions

A nonlinear reduced order observer for estimating states variables in batch processes has been introduced. Convergence of the estimated states to the true ones is obtained if there exists the non-singular transformation $\gamma(x, y)$ and the condition given by (77) is satisfied. The observer implementation is simple and it requires small computational effort. The design approach can be applied for any general type of nonlinear batch processes models, because no fixed model structure is required. Furthermore, according to the proposed design framework, it is possible to develop a reduced-order estimation, i.e. only the unmeasured state variables are estimated, using the information provided by the measured outputs of the process. The potential use of the nonlinear observer was illustrated by state estimation in a batch bioprocess. Simulation results showed the good performance that can be achieved with the proposed method. In addition, robustness aspects of the proposed observer were analysed and its performance was compared with a full-order observer and an EKF.

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Appendix

The proof is based on the Lyapunov method [19]. Let e_z be the estimation error (i.e. $e_z = z - \hat{z}$). Consider the candidate Lyapunov function $V = e_z^{\mathrm{T}} P e_z$, with P a positive definite matrix. Therefore, the V derivative with respect to time is

$$\begin{aligned}\dot{V} &= \dot{e}_z^{\mathrm{T}} P e_z + e_z^{\mathrm{T}} P \dot{e}_z \\ &= e_z^{\mathrm{T}} \left[(A - GC)^{\mathrm{T}} P + P(A - GC) \right] e_z + 2 e_z^{\mathrm{T}} P[\rho(z, y) - \rho(\hat{z}, y)]. \end{aligned} \tag{73}$$

Note that the pair (A, C) is observable. As a consequence, there exists a positive definite matrix Q and a matrix G so that:

$$(A - GC)^{\mathrm{T}} P + P(A - GC) = -Q \tag{74}$$

can be solved. By using (74), Eq. (73) becomes:

$$\dot{V} = -e_z^{\mathrm{T}} Q e_z + 2 e_z^{\mathrm{T}} P[\rho(z, y) - \rho(\hat{z}, y)]. \tag{75}$$

Provided that $\rho(z, y)$ is Lipschitz in z, with constant L (i.e. $\|\rho(z, y) - \rho(\hat{z}, y)\| \leq L\|e_z\|$), the $\dot{V}$ can be bounded as follows:

$$\dot{V} \leq (-\lambda_Q^{\min} + 2\lambda_P^{\max} L)\|e_z\|^2 \tag{76}$$

where $\lambda_Q^{\min}$ is the minimum eigenvalue of Q and $\lambda_P^{\max}$ is the maximum eigenvalue of P. Then, if

$$-\lambda_Q^{\min} + 2\lambda_P^{\max} L < 0, \tag{77}$$

the estimation error converges exponentially to zero since:

$$\dot{V} \leq \frac{(-\lambda_Q^{\min} + 2\lambda_P^{\max} L)}{\lambda_P^{\min}} V \tag{78}$$

where $\lambda_P^{\min}$ is the minimum eigenvalue of P. Then

$$V(t) \leq V(0) \mathrm{e}^{\frac{(-\lambda_Q^{\min} + 2\lambda_P^{\max} L)}{\lambda_P^{\min}} t} \tag{79}$$

and the following inequality holds:

$$\lambda_P^{\min} \|e_z\|^2 \leq \lambda_P^{\max} \|e_z(0)\|^2 \, \mathrm{e}^{\frac{(-\lambda_Q^{\min} + 2\lambda_P^{\max} L)}{\lambda_P^{\min}} t} \tag{80}$$

which can be rearranged as follows:

$$\|e_z\| \le \sqrt{\frac{\lambda_P^{\max}}{\lambda_P^{\min}}}\|e_z(0)\|\mathrm{e}^{\frac{(-\lambda_Q^{\min}+2\lambda_P^{\max}L)}{2\lambda_P^{\min}}t}. \tag{81}$$

Note that

$$\|z(0)-\hat{z}(0)\| \le L_\gamma \|x(0)-\hat{x}(0)\| \tag{82}$$

and

$$\|x-\hat{x}\| \le L_{\tilde{\gamma}}\|z-\hat{z}\|. \tag{83}$$

Consequently, a bound for the estimation error in the original coordinates is given by:

$$\|x_R-\hat{x}_R\| \le L_{\tilde{\gamma}}L_\gamma\sqrt{\frac{\lambda_P^{\max}}{\lambda_P^{\min}}}\|x_R(0)-\hat{x}_R(0)\|\,\mathrm{e}^{\frac{(-\lambda_Q^{\min}+2\lambda_P^{\max}L)}{2\lambda_P^{\min}}t}. \tag{84}$$

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