

A high gain nonlinear observer: application to the control of an unstable nonlinear process

Silvina I. Biagiola, José L. Figueroa*

Departamento de Ingeniería Eléctrica y de Computadoras, Av. Alem 1253, Universidad Nacional del Sur, 8000 Bahía Blanca, Argentina

Received 9 October 2002; received in revised form 27 February 2004; accepted 8 March 2004

Available online 21 April 2004

Abstract

State estimation has become an important area of research in the field of process engineering. This is because there are many applications that demand the knowledge of many of the state variables, if not all of them. Among others, the implementation of nonlinear control methods as well as monitoring some relevant process variables can be mentioned. The purpose of this paper is to introduce a nonlinear high gain observer in order to estimate the whole process state variables. Whenever some construction conditions hold, it is possible to obtain estimates that converge asymptotically to the actual values. Moreover, this estimator has robust performance in the presence of model uncertainty and measurement noise. A quantitative analysis is developed to measure the observer robustness. Though the estimated states can be used for many purposes, in this work we aim at using the estimates for output regulation. For this goal, a nonlinear controller based on exact linearization is designed. As a particular application, we consider the open-loop unstable jacketed exothermic chemical reactor. This CSTR is widely recognized as a difficult problem for the purpose of control. In order to achieve the control goal, a simple algorithm lying on exact linearization principle is considered. Finally, computer simulations are developed for showing the performance of the proposed nonlinear observer (NO). The performance of the observer when used for control purpose was also evaluated.

© 2004 Elsevier Ltd. All rights reserved.

Keywords: Estimation; Nonlinear observers; Robustness; Process control; CSTR

1. Introduction

With the purpose of process monitoring, control and optimization, the knowledge of some physical state variables of the process is demanded. For instance, there exist many process control strategies, in which the information about the internal state of the process is necessary to calculate the control input. Consequently, the presence of unknown state variables becomes a difficulty which can be overcome with the inclusion of an appropriate state estimator (Gattu & Zafiriou, 1992; Nagrath, Prasad, & Bequette, 2002).

Therefore, the development of suitable algorithms to perform the estimation has captured the attention of many researchers. In this sense, several techniques have been introduced to estimate state variables from the available measurements, usually related to meaningful physico-chemical

variables. There exist many possible kinds of estimators to be used depending on the mathematical structure of the process model and the information available (Gauthier, Hammouri, & Othman, 1992; Soroush, 1997).

In spite of the fact that theories and applications for linear systems are well developed, the highly nonlinear nature of many chemical processes has given rise to nonlinear observers (NO). These observers are designed in such a way that they can cope with the intrinsic nonlinearities of the process dynamics. However, the construction of NO still provides an open research field because the advance in the area of NO often faces many typical obstacles such as very restrictive conditions to be satisfied, uncertainty in the performance and robustness and/or unsatisfactory estimates in the presence of noisy measurements.

A detailed discussion on the current available state estimation techniques applicable to a broad class of nonlinear systems, is provided by Mouyon (1997). Another comprehensive evaluation of various NO was presented by Wang, Peng, and Huang (1997). In a recent paper, Dochain (2003) gives an overview of some state and parameters

* Corresponding author. Tel.: +54-291-4595153; fax: +54-291-4595154.

E-mail address: figueroa@uns.edu.ar (J.L. Figueroa).

Nomenclature

q	reactor feed flow rate
V	reactor volume
x_{1f}	dimensionless reactor feed concentration
x_{2f}	dimensionless reactor feed temperature
x_{3f}	dimensionless cooling-jacket feed temperature

Greek letters

β	dimensionless heat of reaction
δ	dimensionless heat-transfer coefficient
δ_1	reactor to cooling-jacket volume ratio
δ_2	reactor to cooling-jacket density heat capacity ratio
ϕ	nominal Damköhler number based on the reaction feed
γ	dimensionless activation energy
κ	dimensionless Arrhenius reaction rate nonlinearity
τ	dimensionless time

estimation approaches available for chemical and biochemical processes.

With respect to the nonlinear estimation techniques performed up to now, the extended Kalman filter (EKF) is one of the most (if not the most) widely diffused observer among other nonlinear observers based on linearization techniques (Stephanopoulos & San, 1984; Tadayyon & Rohani, 2001). The main drawback of these techniques consists in the difficulties to determine a priori its convergence and speed of convergence. In 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 (Ljung, 1979).

A method based on extended linearization has also been developed to carry out state estimation (Baumann & Rugh, 1986). 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 (Canudas de Wit & Slotine, 1991; Slotine, Hedrick, & Misawa, 1987; Wang et al., 1997). 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.

Taking into account the characteristics of the observers above discussed, the objective of this work is to present a

nonlinear efficient state estimator for later multi-purpose applications. From the construction perspective, the observer herein proposed can be considered as a Luenberger-like observer (Kailath, 1980). Many observers of this type has been dealt with in the literature, specially concerning electrical, mechanical or robotics applications. For instance, trajectory tracking using nonlinear reduced-order observers was applied to a robot arm and to a neural network (García & D'Attellis, 1995). In the field of chemical processes, the work by Gauthier et al. (1992) is considered a relevant contribution in the field of high-gain observers. They proposed a design method that involves finding a symmetric positive definite matrix which is the stationary solution of a set of differential equations. Kazantzis, Kravaris, and Wright (2000) used a nonlinear observer for monitoring autonomous processes. The design methodology involved the solution of partial differential equations. An important feature is that no robustness evaluation of the estimators was accomplished in those works. In a recent contribution, Aguilar, Martínez-Guerra, and Poznyak (2002) introduced a modified Luenberger-like observer specifically dedicated to the estimation of reaction heat in continuous chemical reactors. The estimator design does not include the whole process dynamics, hence a large gain is required so that the estimation error reaches the vicinity of zero.

The approach herein proposed guarantees the estimation error converges towards zero whenever the observer gain is adequately chosen. The estimation procedure is oriented to those nonlinear control methods that require the knowledge of the internal state of the process. The observer implementation is simple and it requires small computational effort. Another advantageous feature of this NO is that it shows robust performance in the presence of noisy measurements and model uncertainty. A bound for the estimation error is deduced as a measure for quantifying the observer robustness. Additionally, the proposed observer is compared with two other widely diffused techniques: the EKF and a sliding nonlinear observer.

In particular, the state estimation methodology is here focused to the control of a jacketed CSTR. This kind of reactors are highly nonlinear, and are known to be an interesting challenge to be overcome by any new estimation and/or control technique.

It must be highlighted that this type of reactors present interesting operational problems due to complex open-loop behavior such as input and output multiplicities, ignition/extinction behavior, parameter sensitivity and even nonlinear oscillations (Russo & Bequette, 1995, references therein). These characteristics explain the need for and the difficulty of feedback control system design. Additionally, it is often desirable to operate CSTRs under open-loop unstable conditions. This is because the reaction rate may yield good productivity while the reactor temperature is still low enough to prevent side reactions or catalyst degradation. Therefore, if any state feedback strategy is applied for controlling the CSTR, it will demand

an accurate determination of the internal state of the process.

In this work, an exact linearization based controller is used for the nonlinear CSTR regulation. This design technique has been extensively treated in the literature. There are many works dealing with the exact linearization technique to control nonlinear processes. Kravaris and Chung (1987), treated the globally linearizing control approach using concepts from differential geometry. Henson and Seborg (1990), presented two different approaches for input/output (I/O) linearization of general nonlinear processes. However, these works, as well as many others dealing with this approach (Daoutidis & Kravaris, 1989), considered that the internal state of the process is known, and available to be used in the I/O strategy. Pröll and Karim (1994) applied both exact linearization and I/O linearization to the control of a bioreactor. They discussed the issue of invertability and tested the approach performance for parameters uncertainties. However, they remained two issues opened for further study: state estimation and the influence of dynamics uncertainties. Viel, Busvelle, and Gauthier (1995) used I/O linearization for stabilizing polymerization reactors. They combined the control technique with a nonlinear Kalman-like state observer.

The work is organized as follows. In Section 2, a Luenberger-like nonlinear observer (LNO) is proposed and two other known observers are described. In Section 3, the controller synthesis is dealt with. The comparison between the observers performance is presented via simulation in Section 4, as well as the proposed observer/controller behavior. Finally, in Section 5, the conclusions are presented.

2. Nonlinear full-order observer designs

The objective of this section is to introduce an observer for estimating the whole state vector. To attend to the jacketed CSTR process, in which the reaction is typically followed up by temperature measurements and the control action usually consists in following a desired temperature profile, the following nonlinear single input/single output (SISO) general model is proposed for the process:

$$\dot{x} = f(x) + g(x)u \quad (1)$$

$$y = h(x) \quad (2)$$

where the vector x ($x \in \mathcal{R}^n$) stands for the state variables and the input u ($u \in \mathcal{R}$) represents the manipulated variable to accomplish the temperature control. The measured output is represented by vector y ($y \in \mathcal{R}$).

In order to perform the estimation, a Luenberger-like observer is developed and proposed for nonlinear state estimation. Its stability and robustness properties are presented. Then, for comparison purpose, two different known observers are briefly described: the EKF and a sliding observer.

2.1. Luenberger-like nonlinear observer (LNO)

To perform the state estimation of the process given by Eqs. (1) and (2), the following LNO is developed:

$$\dot{\hat{x}} = f(\hat{x}) + g(\hat{x})u + \mathcal{O}^{-1}(\hat{x})K_{\text{LNO}}(y - h(\hat{x})) \quad (3)$$

The system in Eq. (3) is a nonlinear observer for the state vector x . Note that the error, calculated as the difference between the measured output y and its evaluation on the estimated states $h(\hat{x})$, is used to improve the estimation and works as a correction factor. The product $\mathcal{O}^{-1}(\hat{x})K_{\text{LNO}}$ is the nonlinear gain of the observer, where K_{LNO} is a matrix of constants to be designed and \mathcal{O} is the Jacobian of the vector $\Phi(x)$. This vector $\Phi(x)$ is defined as

$$\Phi(x) = \begin{bmatrix} h(x) \\ L_f h(x) \\ \vdots \\ L_f^{n-1} h(x) \end{bmatrix} \quad (4)$$

where $L_f h(x)$ represents the Lie derivative of $h(x)$ in the direction of $f(x)$ (Isidori, 1995). Hence, the following equalities behave:

$$L_f h(x) = \frac{\partial h(x)}{\partial x} f(x) \quad (5)$$

$$L_f^j h(x) = \frac{\partial L_f^{j-1} h(x)}{\partial x} f(x) \quad (6)$$

The vector Φ constitutes a nonlinear change of coordinates. The objective is to transform the original process representation to obtain a transformed one in order to make easier the observer design. The transformed model of the process contains known parameters A and C (see Appendix A) that are inserted into the following Lyapunov equation to design the observer gain K_{LNO} :

$$(A - K_{\text{LNO}}C)^T P + P(A - K_{\text{LNO}}C) = -Q \quad (7)$$

where P and Q are positive definite matrix that must satisfy Eq. (7). Additionally, the following constraint must be satisfied:

$$-q_m + 2p_M(L_\gamma + L_\omega U) < 0 \quad (8)$$

with p_M and q_m the maximum and minimum eigenvalues of P and Q , respectively. L_γ and L_ω are Lipschitz constants of the process (see Appendix A). Hence, the dynamics of the estimation error e_x , defined as $e_x = x - \hat{x}$, will be stable. Provided that \mathcal{O} is invertible, that U is a bound for the input u and given the initial condition $\hat{x}(0)$, the following property behaves for any $\alpha > 0$:

$$\|e_x(t)\| \leq \delta e^{-\alpha t} \|e_x(0)\| \quad (9)$$

with $\delta > 0$. Consequently, the norm of the estimation error goes to zero as $t \rightarrow \infty$. Then, the convergence of the algorithm is guaranteed.

A detailed demonstration based on Lyapunov arguments is presented in Appendix A where the observer convergence and its relationship with the gain selection are dealt with. In addition, in Appendix A we present an extension of the proposed LNO for single input/multiple output (SIMO) nonlinear systems represented by the more general model: $\dot{x} = f(x) + g(x, u)$, $y = h(x)$.

Provided certain stability hypotheses are held, the observer brings an on-line estimation of the whole process state. It can be easily implemented and it only uses the information brought by the output measurements. Moreover, the observer is built using the whole process model, and this nonlinear procedure avoids losing information about the dynamics as well as simplifications, order reduction, or the frequently used linearization methods.

To evaluate the robustness properties of the LNO, a dedicated study is performed. As regards state and parameter estimation in chemical and biochemical processes, Dochain (2003) introduces a weak point related to the theory of the EKO and the nonlinear observers. These observers are commonly used assuming perfect knowledge of the process and that it is difficult to develop error bounds in the presence of large uncertainty in the parameters. To tackle this point, a quantitative analysis for the proposed LNO is herein developed.

Let us consider the model of the process dynamics contains a certain degree of uncertainty, such that it can be written as follows:

$$\begin{aligned} \dot{x} &= f(x) + \Delta_f(x) + [g(x) + \Delta_g(x)]u \\ y &= h(x) \end{aligned} \quad (10)$$

where $\Delta_f(x)$ and $\Delta_g(x)$ stand for the unknown dynamics.

It can be demonstrated that if the LNO is built using only the known model dynamics, and provided some conditions hold, then the following time function is a bound for the estimation error (see Appendix A):

$$\|e_x\| \leq C_1 e^{\theta t} \|e_x(0)\| + \frac{C_2}{\theta} (e^{\theta t} - 1) \quad (11)$$

where C_1 and C_2 are positive constants and θ is a negative constant derived from the observer gain design. Hence, a bound for the estimation error e_x has been deduced for processes with dynamics uncertainty. This bound implies that the norm of the estimation error decays with time as fast as the value θ allows it. From the theoretical perspective, the stationary error can be zero if θ tends to ∞ . However, taking into account practical aspects (as shown later), this design parameter must take a limited value.

Now, another robustness analysis is considered. We study the case where the available measured outputs to perform the estimation differ from the real outputs. Assume that a LNO is designed for the process given by Eqs. (1) and (2) and that the following measured outputs (y_m) are used to accomplish the estimation:

$$y_m = y + \Delta_h \quad (12)$$

Therefore, there is a mismatch between the real output vector y and the measured one (y_m). Then, to construct the observer, the following correction term is proposed:

$$\mathcal{O}^{-1}(\hat{x}) K_{LNO} (y_m - \hat{y}) \quad (13)$$

After some calculations, it can be shown that the following expression is a bound for the estimation error (see Appendix A):

$$\|e_x\| \leq C_1 e^{\theta t} \|e_x(0)\| + \frac{C_3 \|K_{LNO} \Delta_h\|}{\theta} (e^{\theta t} - 1) \quad (14)$$

with C_1 and C_3 constants. Eq. (14) implies that there is a trade-off between the speed of convergence and the ultimate bound. To increase θ in order to augment the speed of convergence involves an increment of $\|K_{LNO} \Delta_h\|$. The results in Eqs. (11)–(14) explain some observations based on simulations reported in many works (Gauthier et al., 1992; Kazantzis et al., 2000). These observations connect the observer gain value and the remaining estimation error when there exists dynamics uncertainty as well as the deteriorating performance with the observer gain increment in the presence of noisy outputs.

2.2. Extended Kalman filter (EKF)

The EKF has been widely used to deal with processes that include high nonlinearities. The derivation of this approach can be found in Jazwinski (1970).

Given the process model (1) and (2) and the initial values $\hat{x}(0|0)$, $P(0|0)$, Q and R , where the symbol ($\hat{\cdot}$) stands for the estimated variables, then the predicted state \hat{x} and weighting matrix P are computed at the instant $k + 1$ by performing the integration of the following equations:

$$\dot{\hat{x}} = f(\hat{x}) + g(\hat{x})u \quad (15)$$

$$\dot{P} = [f_x(\hat{x}) + g_x(\hat{x})u] P + P [f_x(\hat{x}) + g_x(\hat{x})u]^T + Q \quad (16)$$

where k is the number of iterations the algorithm has already been accomplished; f_x and g_x are the Jacobian matrices of f and g on x . This is an improved version of the EKF with respect to the most diffused approach in which both the predicted states and the covariance matrix are calculated using the linearized model (Bastin & Dochain, 1990; Tadayyon & Rohani, 2001).

It must be noticed that for the Kalman filter as a linear unbiased minimum variance estimator, the parameters P , R and Q are the covariance matrices of the estimation, the white noise sequences in the measurements and the states, respectively. However, when used in the EKF, they lost their original meaning and turn out to be only tuning parameters. However, the speed of estimation convergence is strongly influenced by the initial value of matrix P . Since this value is unknown, it must be guessed in order to start the EKF algorithm.

In a second step, the filter gain is calculated as follows:

$$K_{\text{EKF}}(k+1) = P(k+1|k)h_x^T(\hat{x}(k+1|k)) \times [h_x P(k+1|k)h_x^T + R]^{-1} \quad (17)$$

with h_x , the Jacobian matrix of h on x .

Afterwards, the measurement $y(k+1)$ is processed:

$$\hat{x}(k+1|k+1) = \hat{x}(k+1|k) + K_{\text{EKF}}(k+1) \times [y(k+1) - h(\hat{x}(k+1|k))] \quad (18)$$

and then, the new weighting matrix is computed:

$$P(k+1|k+1) = [I - K_{\text{EKF}}(k+1)h_x]P(k+1|k) \times [I - K_{\text{EKF}}(k+1)h_x^T] + K_{\text{EKF}}(k+1)RK_{\text{EKF}}^T(k+1) \quad (19)$$

Then, the counter k is incremented in one and the algorithm is executed again. Further constructive aspects of the EKF can be found in Jazwinski (1970).

In the following, another nonlinear estimation technique is described. It is based on sliding modes principle.

2.3. Sliding nonlinear observer (SNO)

For the purpose of comparison with the proposed LNO, a nonlinear sliding observer is considered. This kind of observers has already been reported in the literature (Canudas de Wit & Slotine, 1991; Slotine et al., 1987; Walcott & Zak, 1987).

To construct a SNO for the process represented by Eqs. (1) and (2), it is necessary to devise a correction function Ψ so that (Wang et al., 1997):

$$\dot{\hat{x}} = f(\hat{x}) + g(\hat{x})u + \Psi(y - \hat{y}) \quad (20)$$

$$\hat{y} = h(\hat{x}) \quad (21)$$

Provided the Jacobian matrix of $h(x)$ exists and it is of full rank in any subset of \mathcal{R}^n , the representation given by Eqs. (1) and (2) can be transformed to obtain:

$$\dot{z} = f^*(z, u) \quad (22)$$

$$y = Cz \quad (23)$$

where $C = [I_p \ 0]$. For design purposes, vector z is partitioned into:

$$z = \begin{bmatrix} z_m \\ z_{um} \end{bmatrix} \quad (24)$$

where $z_m = y$. Hence, the observer in the transformed variables can be stated as follows:

$$\dot{\hat{z}} = f^*(\hat{z}, u) + K_{\text{SNO}}(t)\sigma \quad (25)$$

where $K_{\text{SNO}}(t)$ is a time-varying matrix. This gain is the observer parameter to be designed. Wang et al. (1997) determine K_{SNO} to keep the dynamics poles of $z_{um} - \hat{z}_{um}$ invariant at certain constant values in order to achieve a desired

performance. The vector σ contains the typical switching elements included in sliding structures:

$$\sigma = \begin{bmatrix} \text{sign}(y_1 - \hat{z}_1) \\ \text{sign}(y_2 - \hat{z}_2) \\ \vdots \\ \text{sign}(y_p - \hat{z}_p) \end{bmatrix} \quad (26)$$

where

$$\text{sign}(y) = \begin{cases} 1, & y > 0 \\ -1, & y < 0 \end{cases} \quad (27)$$

If the new state variables z are obtained through the same nonlinear transform as the one in Eq. (4), it can be straightforwardly shown that the system (22) and (23) coincides with the one given by (A.3) and (A.4), which was obtained to construct the LNO. Therefore, the estimation algorithm in original coordinates can be written as follows:

$$\dot{\hat{x}} = f(\hat{x}) + g(\hat{x})u + \mathcal{O}^{-1}(\hat{x})K_{\text{SNO}}(t)\text{sign}(y - h(\hat{x})) \quad (28)$$

where the correction term $\Psi(y - \hat{y})$ in (20) satisfies:

$$\Psi(y - \hat{y}) = \mathcal{O}^{-1}(\hat{x})K_{\text{SNO}}(t)\sigma \quad (29)$$

Once the internal state of the system can be observed, an appropriate control technique based on state knowledge can be performed to achieve a desired trajectory for the temperature inside the reactor. Therefore, we now turn to devise the control strategy.

3. Controller design

Although in many applications in the field of nonlinear processes the control problem is solved via Taylor linearization techniques, it is possible to achieve an improved control performance from an exploitation of the nonlinear model structure using nonlinear control design.

The objective is to control a scalar output variable which is a measured function of the state variables. Then, the goal is to track a reference output signal denoted $y^*(t)$.

To design an exact linearization controller involves finding a nonlinear transform Ω Khalil (1996):

$$\Omega(x) = \begin{bmatrix} l(x) \\ L_f l(x) \\ \vdots \\ L_f^{n-1} l(x) \end{bmatrix} \quad (30)$$

where $l(x)$ is a function of the states. Hence, a vector ζ is defined such that:

$$\zeta = \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \vdots \\ \zeta_n \end{bmatrix} = \Omega(x) \quad (31)$$

Provided an appropriate transform $\Omega(x)$ is chosen, the new representation in ζ coordinates can be written:

$$\begin{aligned}\dot{\zeta}_1 &= \zeta_2 \\ \dot{\zeta}_2 &= \zeta_3 \\ \dots &= \dots \\ \dot{\zeta}_{n-1} &= \zeta_n \\ \dot{\zeta}_n &= \beta(\zeta) + \alpha(\zeta)u\end{aligned}\quad (32)$$

where

$$\alpha(\zeta) = L_g L_f^{n-1} l(\Omega^{-1}(\zeta)) \quad (33)$$

$$\beta(\zeta) = L_f^n l(\Omega^{-1}(\zeta)) \quad (34)$$

If the nonlinear expression $\beta(\zeta) + \alpha(\zeta) u$ is denoted v , with v the new control input, the system given by Eq. (32) turns into a linear controllable form.

It must be pointed out that: if $l(x)$ verifies relative degree n with respect to the control input u and $\Omega(x)$ is a diffeomorphic transform, hence sufficiency conditions are attained to guarantee the nonlinear system in original coordinates is controllable. Note that $l(x)$ is an appropriate function of the states which has to be chosen. However, there is no information a priori about how this function is. Any selection of $l(x)$ will be appropriate if it allows obtaining a diffeomorphic transform $\Omega(x)$. In many low-order systems, the selection of $l(x)$ can be easily guessed. However, for high-order systems, this selection is rarely a trivial task. In such cases, a solver for partial differential equations (PDEs) can be useful to find $l(x)$ (Kazantzis et al., 2000). The theoretical approach as well as many solved examples on this matter are dealt with by Khalil (1996).

Whenever the hypothesis are hold, it is possible to find a control input v (and then, u) such that the output y reaches the desired trajectory y^* .

The basis of the control action herein proposed is to find a control law v which consists of a linear function of $(\zeta_1, \dots, \zeta_n, y^*)$ such that the tracking error $(y^* - y)$ is governed by a prespecified stable linear differential equation. The design parameters are the roots of the Laplace transform of that linear differential equation. Those eigenvalues (i.e. the roots) must be chosen to achieve a stable closed loop system.

4. Application to a continuous stirred tank reactor (CSTR)

The performances of the proposed estimation algorithms will be compared and illustrated through the application to a jacketed tank reactor. The constructive features of the reactor are depicted in Fig. 1.

The mathematical model of the CSTR, where an exothermic irreversible first-order reaction takes place, has been constructed using three nonlinear ordinary differential equations. The material and energy balances based on the assumptions of constant volume inside the reactor, perfect

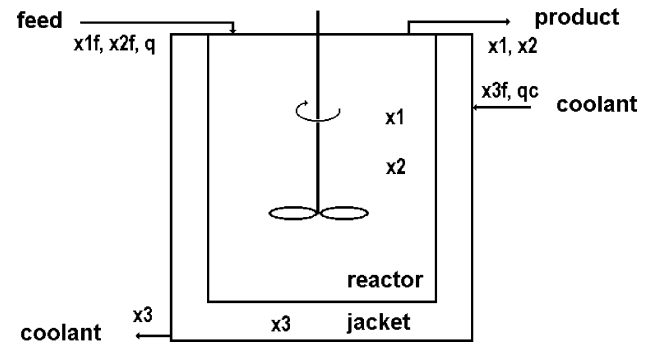


Fig. 1. Scheme of jacketed CSTR.

mixing and constant physical parameters allow to obtain the dynamical model. The differential equations can be written in a dimensionless form as follows (Russo and Bequette, 1995):

$$\frac{dx_1}{d\tau} = q(x_{1f} - x_1) - \phi x_1 \kappa(x_2) \quad (35)$$

$$\frac{dx_2}{d\tau} = q(x_{2f} - x_2) - \delta(x_2 - x_3) - \beta \phi x_1 \kappa(x_2) \quad (36)$$

$$\frac{dx_3}{d\tau} = \delta_1 [q_c(x_{3f} - x_3) + \delta \delta_2 (x_2 - x_3)] \quad (37)$$

with κ :

$$\kappa(x_2) = e^{x_2/(1+x_2/\gamma)} \quad (38)$$

The state variables x_1 , x_2 and x_3 stand for the dimensionless reactant concentration, the reactor temperature and the cooling jacket temperature. The symbol q_c represents the cooling jacket flow rate and the other symbols represent constant parameters whose values are defined in Table 1. These values were taken from Nagrath et al. (2002). Russo and Bequette (1995) reported that this set of parameters cause a particular operation of the reactor given by ignition/extinction behavior. The process dynamics is nonlinear due to the Arrhenius rate expression which describes the dependence of the reaction rate constant (κ) on the temperature (x_2). That is why the CSTR exhibits an open-loop unstable performance as well as

Table 1
CSTR model parameters

Parameter	Value
ϕ	0.072
β	8.0
δ	0.3
γ	20
q	1.0
δ_1	10
δ_2	1.0
x_{1f}	1.0
x_{2f}	0.0
x_{3f}	-1.0

operational and control problems. Moreover, it shows multiplicity behavior with respect to the jacket temperature and jacket flow rate (Nagrath et al., 2002). The CSTR modeled by Eqs. (35) and (37) behaves as an open-loop unstable system if the temperature inside the reactor is between 1.5 and 3.0. However, from an economical point of view, it is often desirable to operate the reactor inside this region. Hence, the selected control strategy must allow to operate the process in the required point. The control objective is to make the dimensionless temperature inside the reactor (x_2) follow a desired trajectory. Both temperatures x_2 and x_3 are measured. In this work, we propose a control technique based on exact linearization as described in Section 3, which demands the knowledge of the internal state of the process. To cope with this, an appropriate state observer must be connected with the controller. Therefore, the observers performance is first analyzed.

In order to evaluate the observers behavior in the more realistic situation in which neither x_{3f} nor q are measured, the observer structures were slightly modified. Both x_{3f} and q can be considered the main disturbances of the process. Note that in the presence of unmeasured disturbances, all the observers can be “extended” to perform the disturbances estimation together with the states estimation. In such a way, the observers append modeled disturbances as augmented states to the original system model. Then, the following observer structure is obtained:

$$\dot{\hat{x}}_{\text{ext}} = f_{\text{ext}}(\hat{x}_{\text{ext}}) + g(\hat{x}_{\text{ext}})u + \text{Corr} \quad (39)$$

$$\hat{y} = h(\hat{x}_{\text{ext}}) \quad (40)$$

with

$$\hat{x}_{\text{ext}} = \begin{bmatrix} \hat{x} \\ \hat{x}_{3f} \\ \hat{q} \end{bmatrix} \quad (41)$$

and

$$f_{\text{ext}} = \begin{bmatrix} f(\hat{x}_{\text{ext}}) \\ 0 \\ 0 \end{bmatrix} \quad (42)$$

The presence of the two zeros in f_{ext} involves that the dynamics model for the disturbances is assumed negligible. Note that Corr is the correction term designed according to each observer, as described in Section 2.

To evaluate and to compare the observers performance, the system was first simulated assuming x_{3f} and q as constant parameters (see Table 1). The process was excited through a constant input signal $q_c = 0.5$ (the jacket flow rate). This variable would be later used as the manipulated variable for control purposes.

The states initial conditions were set to: $x_1(0) = 0.58$, $x_2(0) = 2.67$, $x_3(0) = 0.12$, $\hat{x}_1(0) = 0.80$, $x_1(0)$, $\hat{x}_2(0) = x_2(0)$, $\hat{x}_3(0) = x_3(0)$, $\hat{x}_{3f} = -1$, $\hat{q} = 1$.

The estimation results obtained are depicted in Figs. 2–4. Although the whole state vector was estimated, only the unmeasured state (x_1) was plotted together with the disturbances actual and estimated values. The three observers structures presented in Section 2 were used. For that

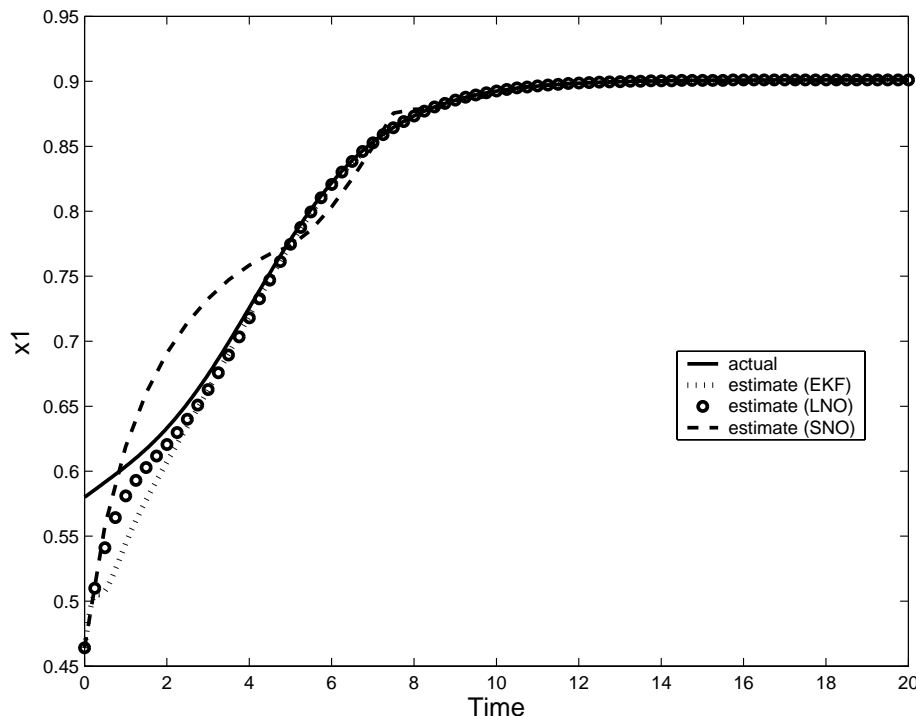


Fig. 2. Concentration inside the reactor.

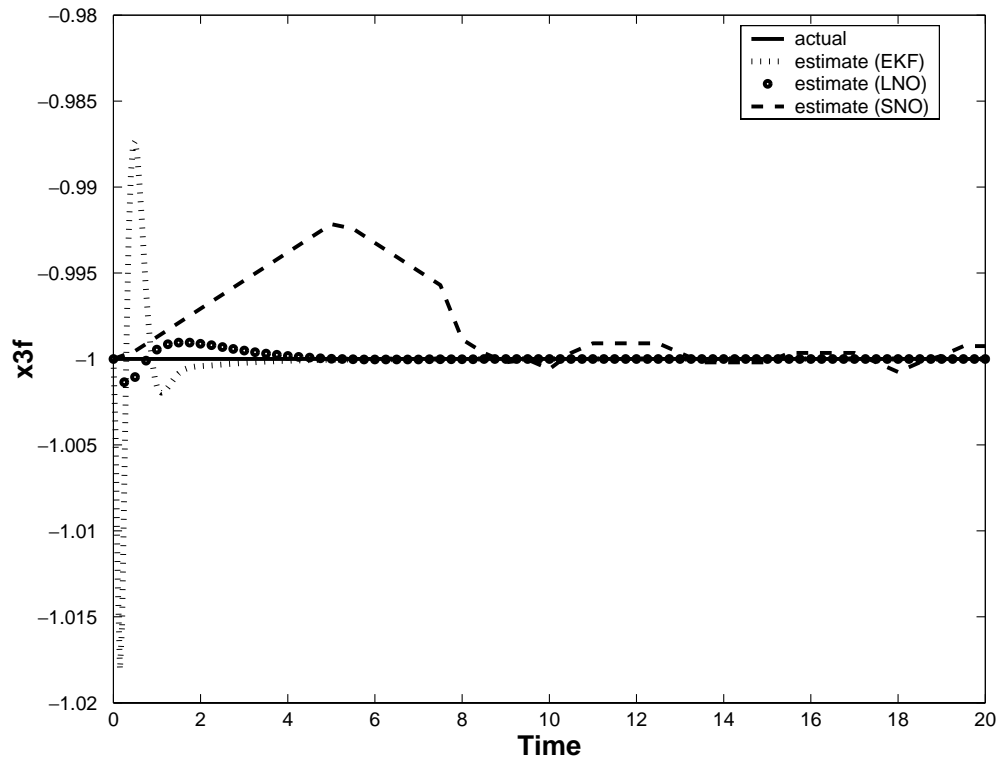


Fig. 3. Jacket feed temperature.

purpose, the EKF parameters were set to the following values:

$$R = \begin{bmatrix} 0.001 & 0 \\ 0 & 0.001 \end{bmatrix}, \quad Q = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.01 & 0 \\ 0 & 0 & 0 & 0 & 0.01 \end{bmatrix},$$

$$P(0|0) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The initial value of P as well as the values of R and Q , are the EKF parameters. In practice, these values can be obtained from previously available plant data. However, when more accurate parameters are required to achieve optimal state estimation or if no real data are available, the appropriate values of these parameters are set using a trial and error approach (Tadayyon and Rohani, 2001). In the CSTR application, the previous values were respectively chosen for R , Q and $P(0|0)$, as they provided better estimation results than other tested values.

For the Luenberger-like observer, the gain K_{LNO} was set to

$$K_{LNO} = \begin{bmatrix} 6.5199 & 0.1829 \\ 6.9024 & 0.2193 \\ 0.6253 & 0.0201 \\ 0.1679 & 0.6551 \\ 0.0168 & 0.0630 \end{bmatrix}$$

to fix the poles of the pair (A, C) to $\{-0.025, -0.025, -0.625, -0.250, -6.250\}$ (see Appendix A). The SNO time-varying gain was calculated in order to obtain time-invariant poles equal to: $\{-0.02, -0.02, -0.03, -0.03, -0.60\}$.

In order to test the behavior of the proposed LNO in the presence of model uncertainty, several estimations were performed. For this purpose, it was considered a mismatch between the real dimensionless activation energy (γ) and its value in the model. It is already known that the activation energy is a difficult parameter to identify. For instance, Henson and Seborg (1990) considered in their article a mismatch of 2%. Because this parameter is in the exponential expression for the reaction rate, the uncertainty is magnified. In this work, a difference up to 25% between the real parameter and its value in the model was considered.

Fig. 5 shows the observer performance attained in the presence of parameter mismatch. The error bound is given by the complete Eq. (11), and it goes to a

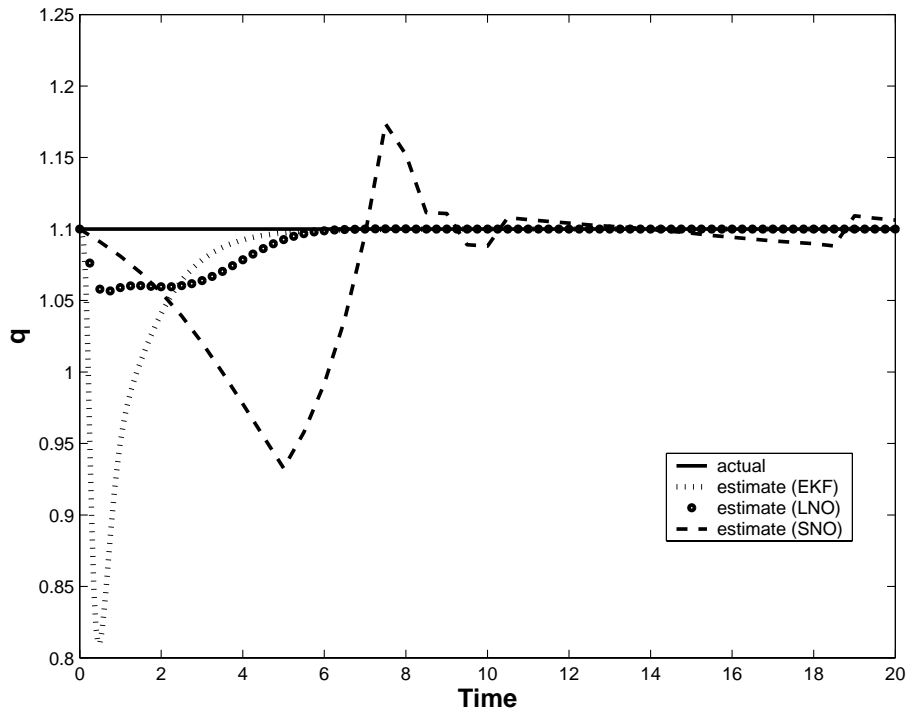


Fig. 4. Reactor feed flow rate.

finite non-zero value as $t \rightarrow \infty$ (see dash-dotted line in Fig. 5). The initial conditions to start the estimation were randomly generated subject to the following constraints: $\hat{x}_1(0) \in [0.8x_1(0), 1.2x_1(0)]$, $\hat{x}_2(0) \in [0.95x_2(0), 1.05x_2(0)]$, $\hat{x}_3(0) \in [0.95x_3(0), 1.05x_3(0)]$,

$\hat{x}_{3f}(0) \in [0.8x_{3f}(0), 1.2x_{3f}(0)]$, $\hat{q}(0) \in [0.95q(0), 1.05q(0)]$. The full-line curves in Fig. 5 show the different observer realizations. On the hand, the full-line curves in Fig. 6 shows the different observer realizations when no parameter uncertainty exists. Then, the error bound is given

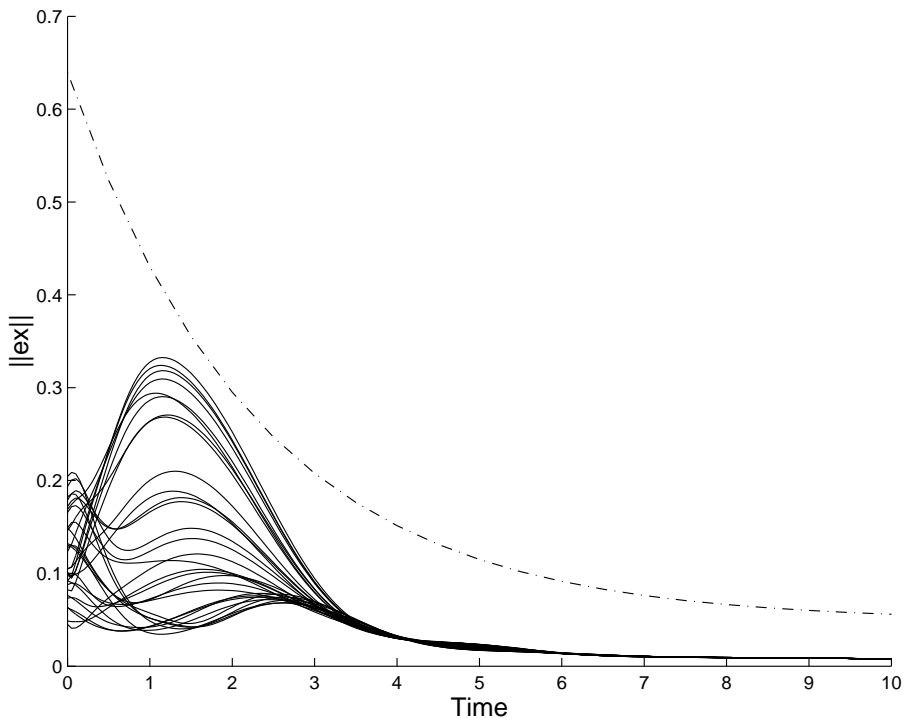


Fig. 5. Estimation error (under dynamics uncertainty): observer realizations (—) and calculated bound (- -).

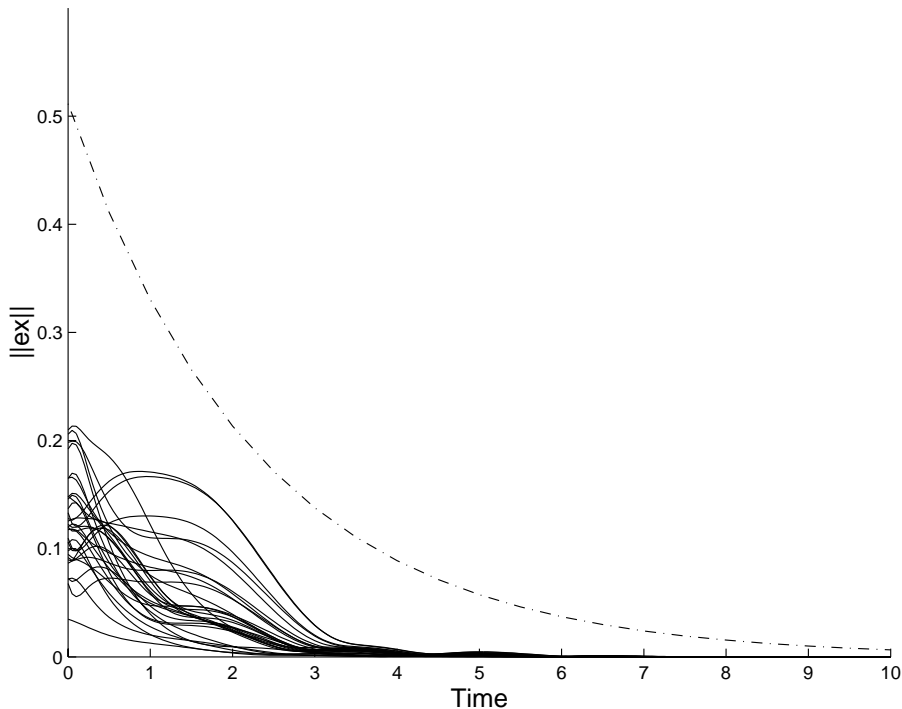


Fig. 6. Estimation error (without dynamics uncertainty): observer realizations (—) and calculated bound (-.-).

by the first term in the expression (11), and it goes to zero as $t \rightarrow \infty$ (see dash-dotted line).

To test the observers performance in other disadvantageous conditions, additional simulations were carried out based on noise corrupted measurements. Figs. 7–9

show the estimation results obtained in this case. For this purpose, the outputs x_2 and x_3 were corrupted with uniformly distributed white noise signals. Then, it was assumed that zero-mean noise signals were respectively added to the nominal outputs. The noise signals amplitudes

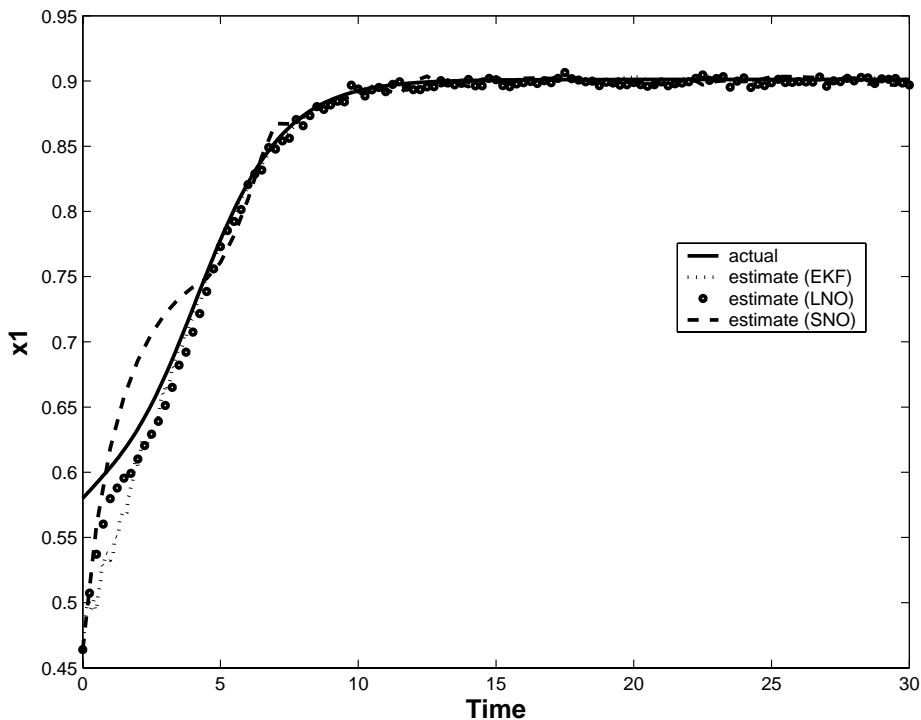


Fig. 7. Reactant concentration inside the reactor.

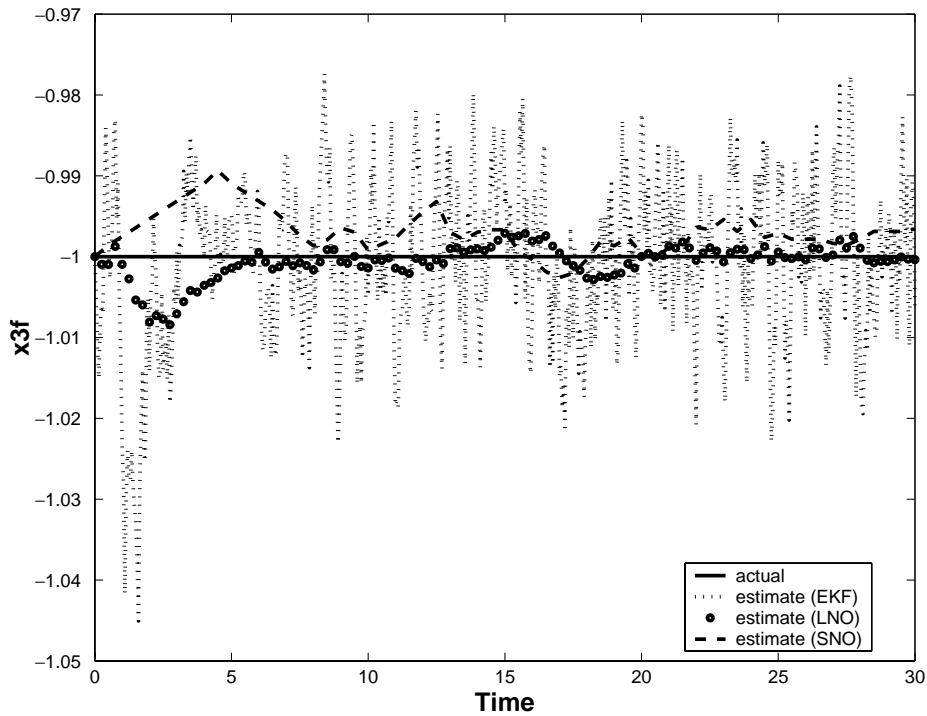


Fig. 8. Cooling-jacket feed temperature.

varied between -5 and $+5\%$ of the nominal outputs values.

Additionally, other simulations were performed to evaluate the observers responses for time-varying x_{3f} and q . The

results are shown in Figs. 10–13. The peaking phenomenon that appears in the EKF simulations is due to the presence of significant overshoots in the estimated variables. As was previously mentioned, the design parameters of the EKF are

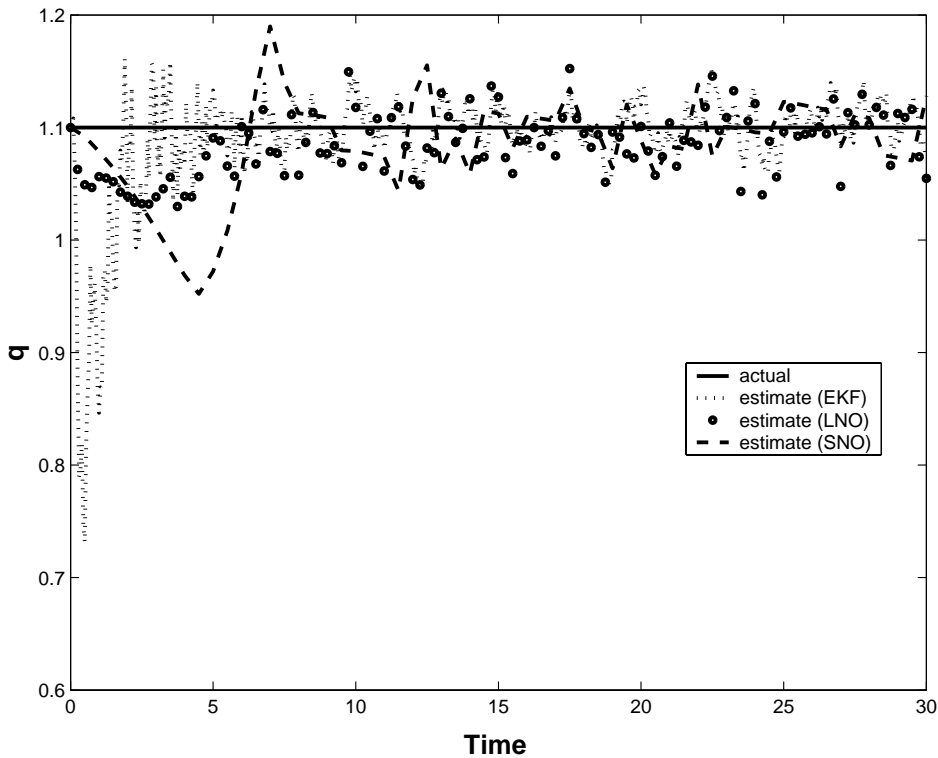


Fig. 9. Reactor feed flow rate.

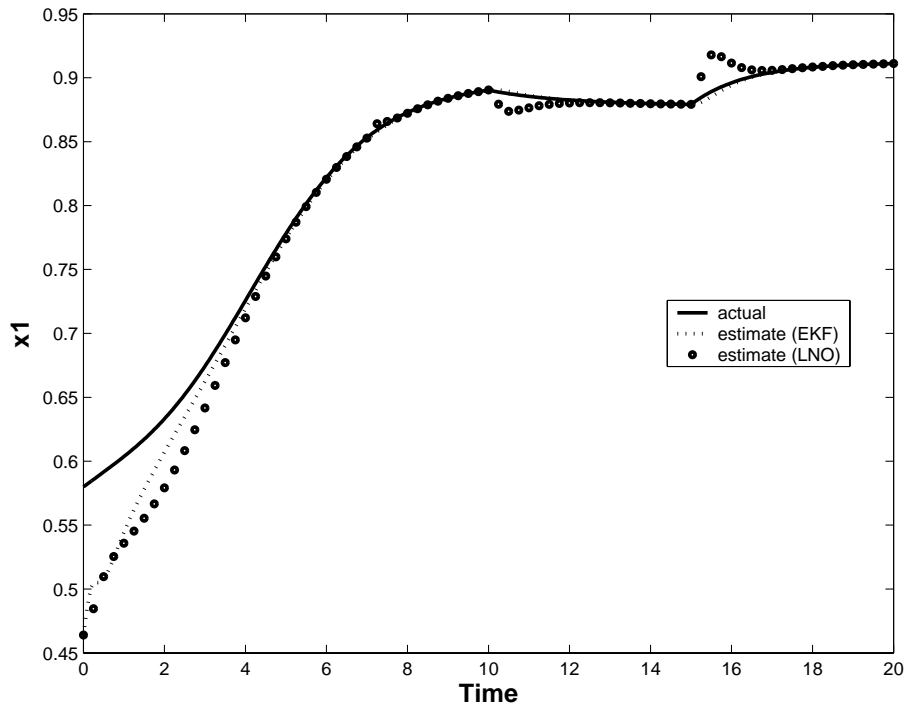


Fig. 10. Concentration inside the reactor.

just tuning values to be guessed. This is because when the filter is applied to a nonlinear deterministic problem, the parameters lose the original meaning they had in the linear KF. The KF has been used for estimation in jacketed CSTR (Nagrath et al., 2002) and a linearized model valid

for the operation point was considered. However, the EKF is preferred to the KF when used for estimation in nonlinear processes, especially when used in a wide operation region. With respect to the LNO estimation results shown in Figs. 10 and 12, the peaks are more severe than those

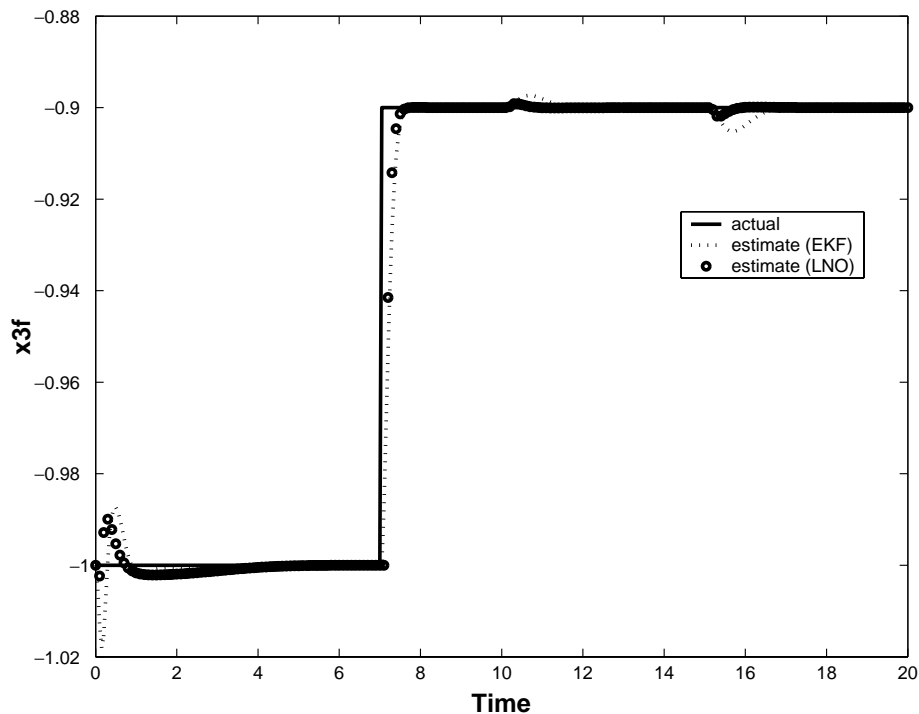


Fig. 11. Cooling-jacket feed temperature.

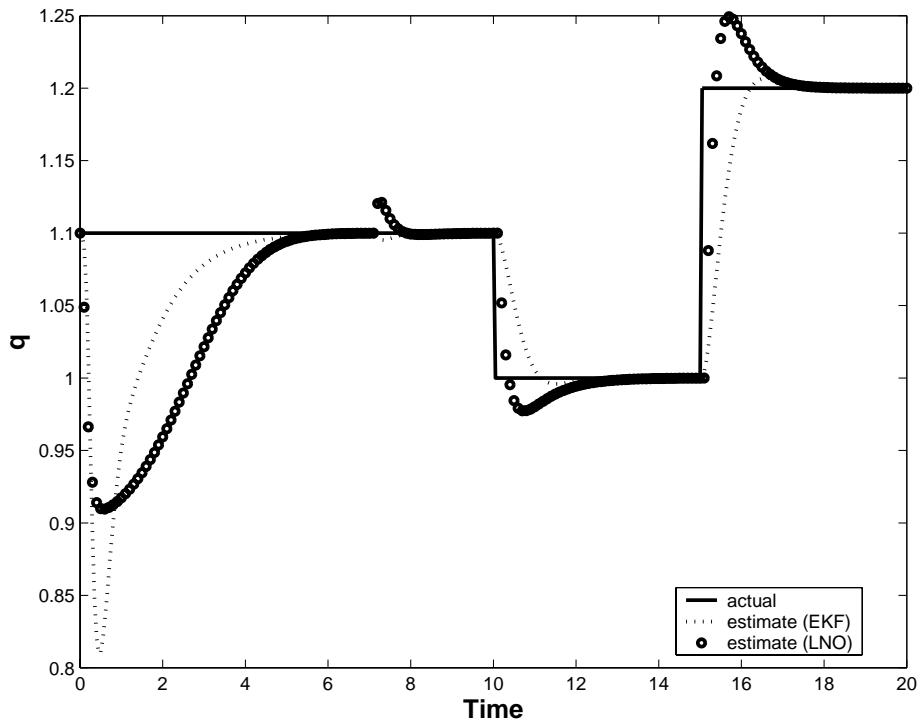


Fig. 12. Reactor feed flow rate.

generated by the EKF. In this case, three unmeasured variables must be estimated and only two measured variables are available. For this reason, the estimation can give rise to a phenomenon known as peaking. This happens when some of the estimated states increase/decrease to a certain value

and then decrease/increase with a variable magnitude. The peaks amplitude and their extinction speed depend on the nature of the system nonlinearity, the initial estimation errors, as well as on the magnitude of the observer gain. The peaking phenomenon plays an important role in the stabilization

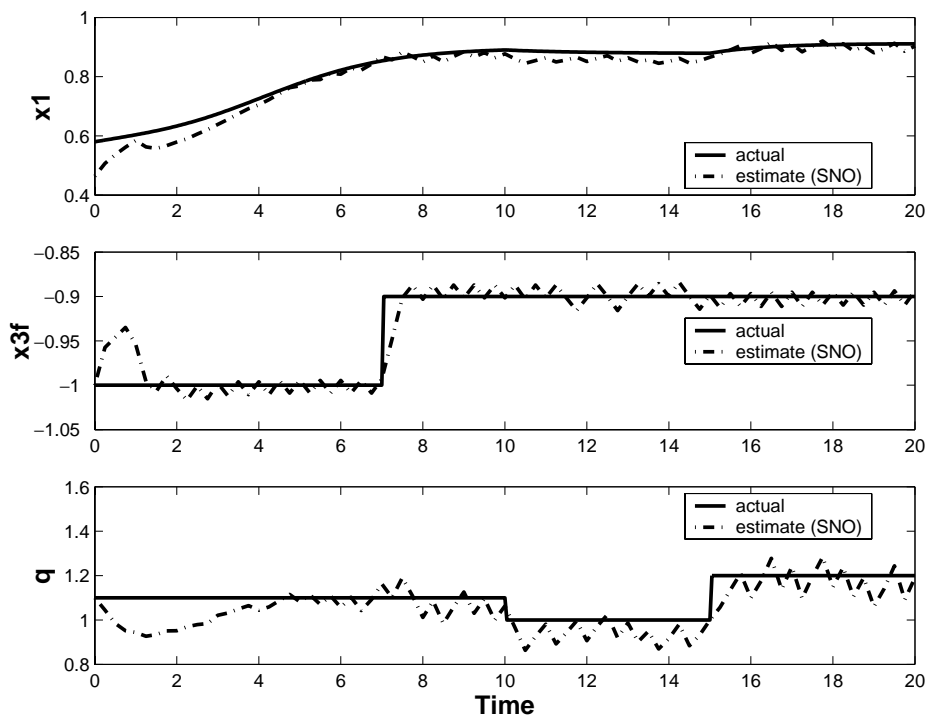


Fig. 13. Reactant concentration, cooling-jacket feed temperature and reactor feed flow rate.

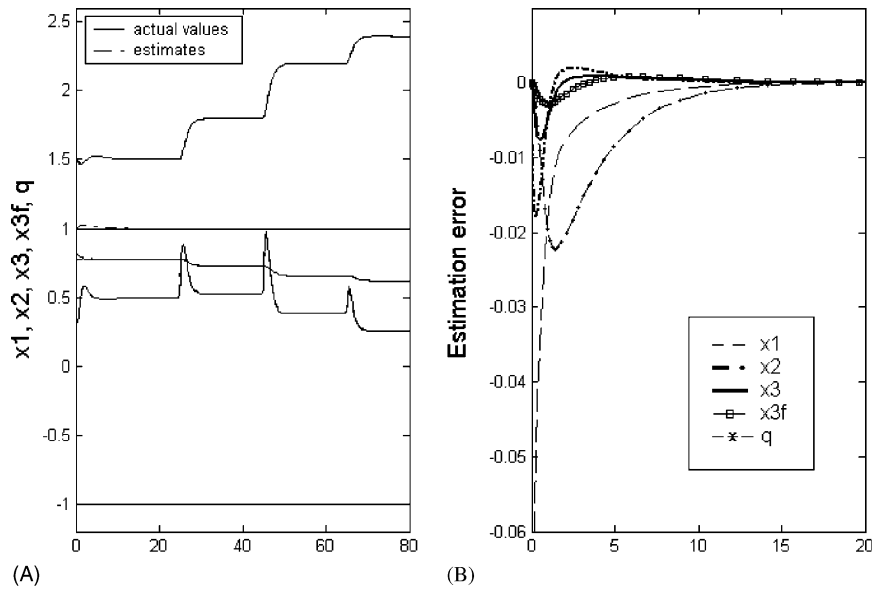


Fig. 14. States and parameters estimation: (A) estimates curves; (B) error curves.

of nonlinear systems (Sepulchre, 1997; Sussmann & Kokotovic, 1991).

As regards the sliding observer, the results show there is a certain time interval before the estimates start to reach the actual variable. Besides that, the high switching gain originates a chattering phenomenon usually associated to sliding estimation methods. Although the estimation results obtained with the SNO may be acceptable for many purposes,

they can be inappropriate when used to calculate the required control action. Particularly, if we want to determine on-line the necessary control input some difficulties may arise because the estimates are not derivable with respect to time.

The estimation results show the advantageous behavior of the LNO with respect to the other approaches. Additionally, the LNO exhibits a satisfactory performance when used with

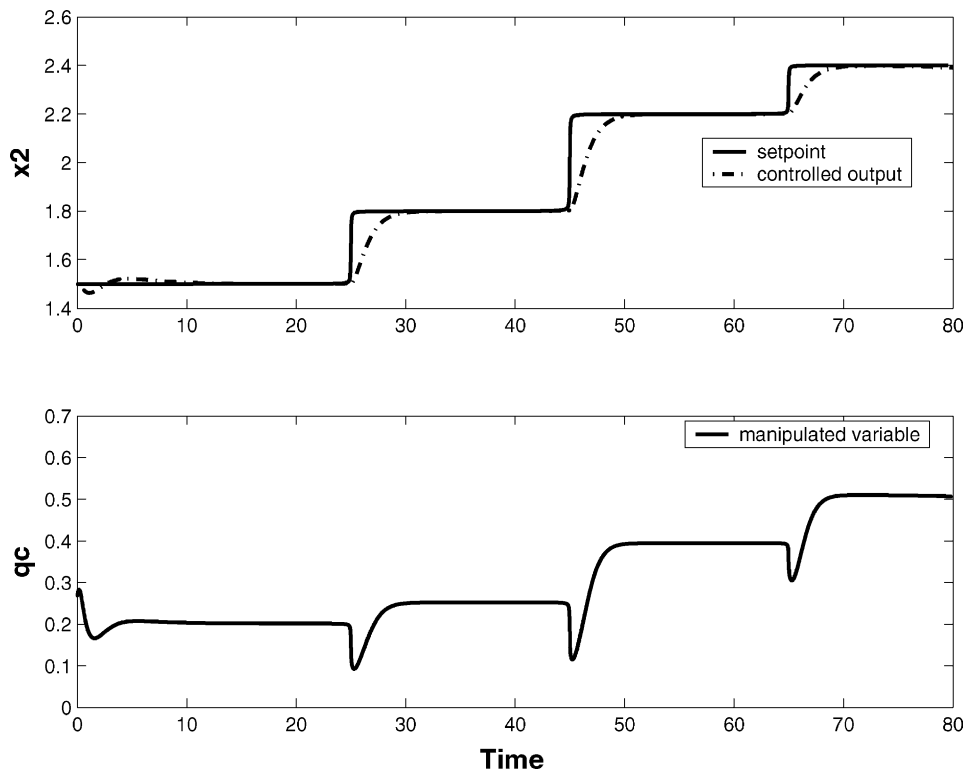


Fig. 15. Controlled temperature and control input.

noisy measurements. While the LNO estimates show the noise has been partially filtered by the observer, the EKF estimates evidence that the measurements noise is amplified by the observer.

The LNO exhibits good convergence properties, i.e. the estimates rapidly reach the actual values. Moreover, it has the convenient feature that the gain can be easily designed in order to let the observer achieve a certain speed of convergence. The assignment of arbitrarily chosen eigenvalues for the pair (A, C) is a fast manner to obtain K_{LNO} , however, a stability analysis must be accomplished such as the sufficient condition of Eq. (A.14).

To continue with the control objective, states and disturbances were estimated and the estimates were on-line used to calculate the control input q_c . The estimation results are shown in Fig. 14. The states initial conditions were set to: $x_1(0) = 0.7748$, $x_2(0) = 1.5000$, $x_3(0) = 0.4952$, $\hat{x}_1(0) = 1.10$, $\hat{x}_1(0) = x_1(0)$, $\hat{x}_2(0) = x_2(0)$, $\hat{x}_3(0) = x_3(0)$, $\hat{x}_{3f} = -1$, $\hat{q} = 1$.

In order to propose a candidate function $l(x)$ to obtain the transform $\Omega(x)$ to achieve exact linearization, it must be taken into account that $l(x)$ must satisfy the following condition:

$$\frac{\partial l(x)}{\partial x} (g(x) \quad [f, g]_{(x)}) = [0 \quad 0] \quad (43)$$

where $[f, g]_{(x)}$ is defined as $(\partial g(x)/\partial x)f(x) - (\partial f(x)/\partial x)g(x)$. It can be straightforwardly verified that if any of the outputs (x_2 or x_3) is selected as a candidate for $l(x)$, the condition (43) does not hold. Therefore, the system is not input/output linearizable. However, replacing $l(x)$ by x_1 allows to obtain a diffeomorphic transform Ω which shows the system is input/states linearizable.

The necessary control law q_c to track the desired temperature trajectory is:

$$q_c(t) = \frac{1}{\delta\delta_1(\hat{x}_{3f} - \hat{x}_3)} \left[\left(\hat{q} + \delta - \beta\phi\hat{x}_1 \frac{d\kappa(\hat{x}_2)}{dt} - \lambda_1 \right) \times \frac{d\hat{x}_2}{dt} - \lambda_2(\hat{x}_2 - x_2^*) - \beta\phi \frac{d\hat{x}_1}{dt} \kappa(\hat{x}_2) - \delta^2\delta_1\delta_2(\hat{x}_2 - \hat{x}_3) \right] \quad (44)$$

The coefficients λ_i are chosen to achieve a stable model for the tracking error dynamics. Particularly, $\lambda_1 = 2.5$ and $\lambda_2 = 1.5$ were selected to fix the eigenvalues of the error dynamics to -1 and -1.5 . The tracking error is given by $x_2^*(t) - x_2(t)$, where $x_2^*(t)$ is the desired trajectory for the temperature inside the reactor and $x_2(t)$ is the controlled output.

Fig. 15 shows the measured temperature and the reference trajectory. The manipulated signal $q_c(t)$ is also depicted in Fig. 15. From the results, it can be seen that the proposed observer/controller structure shows good performance in achieving the output regulation. It is remarked that although other control techniques have been reported in the literature to stabilize the CSTR in a desired operation point,

the feedback controller herein introduced shows a satisfactory behavior to achieve reference tracking. In this way, many different points of the open-loop unstable region are reached.

5. Conclusions

In the present work, the problem of state variables estimation has been tackled. In particular, the analysis has been focused on the estimation of the states and time varying parameters in an open-loop unstable CSTR. In order to perform the estimation, we proposed a high-gain full order observer that robustly estimates the whole state vector and the varying parameters based on the available measurements. The stability properties of the estimator were developed. Provided model uncertainty does not exist, the estimation error converges towards zero. However, if there is a mismatch between the real process dynamics and the model used, the error norm converges to a finite bounded value. A similar behavior takes place if there is a bounded difference between the available measured outputs and the real ones. Moreover, the observer design was used in a control strategy to track a desired reference for the temperature inside the reactor. The controller has been developed following the principle of input/states exact linearization and the conditions which demands the knowledge of the internal state of the system and disturbances. Because there were some unmeasured variables, the problem was overcome by incorporating the extended observer to the control structure.

Finally, computer simulations were developed to illustrate the performance of the nonlinear observer. Good agreement between the actual and estimated states was attained, as well as a successful behavior of the whole observer/controller structure.

Acknowledgements

This work was financially supported by the National Council of Scientific and Technological Research (CONICET) and by the Universidad Nacional del Sur.

Appendix A

The design parameter K_{LNO} must be selected in order to guarantee the estimation algorithm convergence. The LNO herein proposed is constructed using a change of coordinates (Ciccarella, Dalla Mora, & Germani, 1993; García, Troparevsky, & Mancilla Aguilar, 2000). The change of coordinates selected in this work is the one given by Eq. (4), which transforms the original system by defining the following transform variable z :

$$z = \Phi(x) \quad (A.1)$$

and

$$x = \Phi^{-1}(z) \quad (\text{A.2})$$

which constitutes a change of coordinates in \mathcal{R}^n . Therefore, the original system given by Eqs. (1) and (2) can be rewritten in the new coordinates as follows:

$$\dot{z} = Az + BL_f^n h(\Phi^{-1}(z)) + L_g \Phi(\Phi^{-1}(z))u \quad (\text{A.3})$$

$$y = Cz \quad (\text{A.4})$$

with

$$A = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & & & & \vdots \\ 0 & 0 & \cdots & 0 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}, \quad (\text{A.5})$$

$$C = [1 \quad 0 \quad \cdots \quad 0]$$

and

$$L_g \Phi(\cdot)u = \begin{bmatrix} L_g h(x) \\ L_g L_f h(x) \\ \vdots \\ L_g L_f^{n-1} h(x) \end{bmatrix} u \quad (\text{A.6})$$

Then, the following observer in the z -domain is proposed:

$$\begin{aligned} \dot{\hat{z}} &= (A - K_{LNO}C)\hat{z} + K_{LNO}y + BL_f^n h(\Phi^{-1}(\hat{z})) \\ &\quad + L_g \Phi(\Phi^{-1}(\hat{z}))u \end{aligned} \quad (\text{A.7})$$

The time derivative of the estimation error ($z - \hat{z}$) can be written as follows:

$$\begin{aligned} \dot{e}_z &= \dot{z} - \dot{\hat{z}} = (A - K_{LNO}C)e_z + B[L_f^n h(\Phi^{-1}(z)) \\ &\quad - L_f^n h(\Phi^{-1}(\hat{z}))] + [L_g \Phi(\Phi^{-1}(z)) \\ &\quad - L_g \Phi(\Phi^{-1}(\hat{z}))]u \end{aligned} \quad (\text{A.8})$$

To select the constant vector gain K_{LNO} , the following Lyapunov candidate function is chosen:

$$V = e_z^T P e_z \quad (\text{A.9})$$

with P a positive definite matrix. Then,

$$\dot{V} = \dot{e}_z^T P e_z + e_z^T P \dot{e}_z \quad (\text{A.10})$$

$$\begin{aligned} \dot{V} &= e_z^T [(A - K_{LNO}C)^T P + P(A - K_{LNO}C)]e_z \\ &\quad + 2(\gamma - \hat{\gamma})^T P e_z + 2(\omega - \hat{\omega})^T P e_z u \end{aligned} \quad (\text{A.11})$$

where $\gamma(\cdot)$ and $\omega(\cdot)$ stand for $L_f^n h(\Phi^{-1}(\cdot))$ and $L_g \Phi(\Phi^{-1}(\cdot))$, respectively. Now, provided that P and a positive definite matrix Q satisfy the Eq. (7):

$$(A - K_{LNO}C)^T P + P(A - K_{LNO}C) = -Q \quad (\text{A.12})$$

and let q_m and p_M be the minimum and the maximum eigenvalues of Q and P , respectively. Under the assumptions that:

$$\begin{aligned} \|u\| &\leq U \\ \|\gamma - \hat{\gamma}\| &\leq L_\gamma \|z - \hat{z}\| \\ \|\omega - \hat{\omega}\| &\leq L_\omega \|z - \hat{z}\| \end{aligned} \quad (\text{A.13})$$

where L_γ and L_ω are the Lipschitz constants of the respective functions and provided the previous conditions behave, the following inequality can be obtained:

$$\dot{V} \leq (-q_m + 2p_M(L_\gamma + L_\omega U))\|e_z\|^2 \quad (\text{A.14})$$

If the gain K_{LNO} is selected such that p_M and q_m satisfy Eq. (8):

$$-q_m + 2p_M(L_\gamma + L_\omega U) < 0$$

then, \dot{V} turns out to be negative and the norm of the estimation error goes to zero as $t \rightarrow \infty$. Hence, the convergence of the algorithm is guaranteed. If the transform $\Phi(x)$ is nonsingular and Φ^{-1} is uniformly Lipschitz, then revisiting Eqs. (A.1) and (A.2) the condition given by Eq. (9) is obtained.

It must be remarked that Eq. (A.14) sets a sufficient condition to guarantee stability. However, in some cases it may result rather conservative. That is why in many applications good estimation performance could be achieved even when the gain K_{LNO} does not satisfy Eq. (A.14).

To evaluate the robustness properties of the LNO, a quantitative analysis is herein introduced. Let us first consider that in the process model there is some dynamics uncertainty. This situation can be stated as in Eq. (10):

$$\dot{x} = [f(x) + \Delta_f(x)] + [g(x) + \Delta_g(x)]u; \quad y = h(x)$$

where $\Delta_f(x)$ and $\Delta_g(x)$ are the unknown parts of the process dynamics. In order to represent the uncertainty process in the transform domain, let us recall Eq. (A.1). Then,

$$\dot{z} = \frac{\partial \Phi}{\partial x} \dot{x} \quad (\text{A.15})$$

Consequently, the uncertain process can be written as

$$\begin{aligned} \dot{z} &= Az + BL_f^n h(\Phi^{-1}(z)) + L_g \Phi(\Phi^{-1}(z))u \\ &\quad + \delta_1(\Phi^{-1}(z)) + \delta_2(\Phi^{-1}(z))u \end{aligned} \quad (\text{A.16})$$

$$y = Cz \quad (\text{A.17})$$

where $\delta_1 = (\partial \Phi / \partial x) \Delta_f$ and $\delta_2 = (\partial \Phi / \partial x) \Delta_g$. Because the terms δ_1 and δ_2 are not accurately known, the following observer is proposed for the uncertain system:

$$\begin{aligned} \dot{\hat{z}} &= A\hat{z} + BL_f^n h(\Phi^{-1}(\hat{z})) + L_g \Phi(\Phi^{-1}(\hat{z}))u + G(y - \hat{y}) \end{aligned} \quad (\text{A.18})$$

Therefore, the dynamics of the estimation error is given by:

$$\dot{e}_z \triangleq \dot{z} - \dot{\hat{z}} = (A - GC)e_z + (\gamma - \hat{\gamma}) + (\omega - \hat{\omega})u + \delta_1 + \delta_2 u \quad (\text{A.19})$$

In order to find a bound for the estimation error, a function V like the one in Eq. (A.9) is chosen. Then, taking into account that $V \geq p_m \|e_z\|^2$ (with p_m the minimum eigenvalue of P) the following inequality is obtained:

$$\dot{V} \leq \left(-\frac{q_m}{p_m} + 2\frac{PM}{p_m}(L_\gamma + L_\omega U) \right) V + 2p_m(\Delta_1 + \Delta_2 U) \sqrt{\frac{V}{p_m}} \quad (\text{A.20})$$

Let us rename as follows

$$\theta \triangleq -\frac{q_m}{2p_m} + \frac{PM}{p_m}(L_\gamma + L_\omega U)$$

$$\xi \triangleq \frac{PM}{p_m}(\Delta_1 + \Delta_2 U)$$

Then, the following bound for e_z is obtained:

$$\|e_z\| \leq \sqrt{\frac{PM}{p_m}} e^{\theta t} \|e_z(0)\| + \frac{\xi}{\theta} (e^{\theta t} - 1) \quad (\text{A.21})$$

If we recall that

$$\|x - \hat{x}\| = \|\Phi^{-1}(z) - \Phi^{-1}(\hat{z})\| \leq L_\gamma \|z - \hat{z}\|$$

$$\|\Phi(x(0)) - \Phi(\hat{x}(0))\| \leq L_{x0} \|x(0) - \hat{x}(0)\|$$

then, the following expression is obtained:

$$\|e_x\| \leq L_\gamma L_{x0} \sqrt{\frac{PM}{p_m}} e^{\theta t} \|e_x(0)\| + L_\gamma \frac{\xi}{\theta} (e^{\theta t} - 1) \quad (\text{A.22})$$

which can be rewritten as Eq. (11):

$$\|e_x\| \leq C_1 e^{\theta t} \|e_x(0)\| + \frac{C_2}{\theta} (e^{\theta t} - 1)$$

with C_1 and C_2 constants. Hence, a bound for the estimation error e_x has been deduced for processes with dynamics uncertainty.

Now, a different case will be considered. Assume that a LNO is design for the process given by Eqs. (1) and (2). To accomplish the estimation, the available measured outputs (y_m) are:

$$y_m = y + \Delta_h$$

as defined in Eq. (12). Therefore, the observer algorithm in the z -domain can be written as follows:

$$\dot{\hat{z}} = A\hat{z} + \hat{\gamma} + \hat{\omega}u + K_{LNO}(y_m - \hat{y}) \quad (\text{A.23})$$

And the error dynamics is given by

$$\dot{e}_z = (A - K_{LNO}C)e_z + (\gamma - \hat{\gamma}) + (\omega - \hat{\omega})u - K_{LNO}\Delta_h \quad (\text{A.24})$$

Then, after similar calculations than in the previous case, the following bound for the estimation error is obtained:

$$\|e_x\| \leq L_\gamma L_{x0} \sqrt{\frac{PM}{p_m}} e^{\theta t} \|e_x(0)\| + \frac{L_\gamma PM}{\theta p_m} \|K_{LNO}\Delta_h\| (e^{\theta t} - 1) \quad (\text{A.25})$$

which can be written as Eq. (14):

$$\|e_x\| \leq C_1 e^{\theta t} \|e_x(0)\| + \frac{C_3 \|K_{LNO}\Delta_h\|}{\theta} (e^{\theta t} - 1)$$

A.1. The extension of the LNO design for general nonlinear SIMO systems

The LNO design procedure can now be extended for any observable SIMO system represented by the following model:

$$\dot{x} = f(x) + g(x, u) \quad (\text{A.26})$$

$$y = h(x) \quad (\text{A.27})$$

where ($x \in \mathcal{R}^n$), ($u \in \mathcal{R}$) and ($y \in \mathcal{R}^m$).

In such a case, the vector $\Phi(x)$ in Eq. (4) has to be reformulated as follows in order to obtain a change of coordinates for the SIMO system:

$$\Phi(x) = \begin{bmatrix} h_1(x) & L_f^1 h_1(x) & \cdots & L_f^{\rho_1} h_1(x) & h_2(x) & \cdots \\ & L_f^{\rho_2} h_2(x) & \cdots & h_r(x) & \cdots & L_f^{\rho_r} h_r(x) \end{bmatrix}^T$$

where the elements ρ_i are integers that must verify the necessary condition $\sum_{i=1}^r \rho_i = n$ to obtain a diffeomorphic transform $\Phi(x)$. As there exist more than one output, $\Phi(x)$ may be constructed using different outputs selections. If all the m outputs are included in its construction, then $r = m$. However, if only some of the outputs are used, then $r > m$. In this way, the transform $z = \Phi(x)$ is obtained. With this transform and the model given by Eqs. (A.26) and (A.27), the observer can be reformulated.

References

- Aguilar, R., Martínez-Guerra, R., & Poznyak, A. (2002). Reaction heat estimation in continuous chemical reactors using high gain observers. *Chemical Engineering Journal*, 87, 351.
- Bastin, G., & Dochain, D. (1990). *On-line estimation and adaptive control of bioreactors*. New York, USA: Elsevier.
- Baumann, W. T., & Rugh, W. J. (1986). Feedback control of nonlinear systems by extended linearization. *IEEE Transactions on Automatic Control*, AC-31, 40.
- Canudas de Wit, C., & Slotine, J. (1991). Sliding observers for robot manipulators. *Automatica*, 27, 859.
- Ciccarella, G., Dalla Mora, M., & Germani, A. (1993). A Luenberger-like observer for nonlinear systems. *International Journal of Control*, 57, 537.
- Dautodis, P., & Kravaris, C. (1989). Synthesis of feedforward/state feedback controllers for nonlinear processes. *AIChE J.*, 35(10), 1616.

- Dochain, D. (2003). State and parameter estimation in chemical and biochemical processes: a tutorial. *Journal of Process Control*, 13, 801.
- García, R., & D'Attellis, C. (1995). Trajectory tracking in nonlinear systems via nonlinear reduced-order observers. *International Journal of Control*, 62(3), 685.
- García, R. A., Troparevsky, M. I., & Mancilla Aguilar, J. L. (2000). An observer for nonlinear noisy systems. *Latin American Applied Research*, 30 (2), 87.
- Gattu, G., & Zafriou, E. (1992). Nonlinear quadratic matrix control with state estimation. *Industrial Engineering and Chemical Research*, 31, 1096.
- Gauthier, J., Hammouri, H., & Othman, S. (1992). A simple observer for nonlinear systems. Applications to bioreactors. *IEEE Transactions on Automatic Control*, 37(6), 875.
- Henson, M., & Seborg, D. (1990). Input/output linearization of general nonlinear processes. *AIChE Journal*, 36(11), 1753.
- Isidori, A. (1995). *Nonlinear control systems* (3rd ed.). London: Springer-Verlag.
- Jazwinski, A. (1970). *Stochastic processes and filtering theory*. New York: Academic Press.
- Kailath, T. (1980). *Linear systems*. Englewood Cliffs, NJ: Prentice-Hall.
- Kazantzis, N., Kravaris, C., & Wright, R. (2000). Nonlinear observer design for process monitoring. *Industrial Engineering and Chemical Research*, 39, 408.
- Khalil, H. (1996). *Nonlinear systems* (2nd ed.). New Jersey, USA: Prentice-Hall.
- Kravaris, N., & Chung, C. (1987). Nonlinear state feedback synthesis by global input/output linearization. *AIChE Journal*, 33, 592.
- Ljung, L. (1979). Asymptotic behavior of the extended Kalman filter as a parameter estimator for linear systems. *IEEE Transactions on Automatic Control*, AC-24, 36.
- Mouyon, Ph. (1997). Tools for nonlinear observer design. In *Proceedings of the IEEE international symposium on diagnostics and drivers (SDEMPED'97)*, September 1–3, Carry-Le-Rouet, France.
- Nagrath, D., Prasad, V., & Bequette, W. (2002). A model predictive formulation for control of open-loop unstable cascade systems. *Chemical Engineering Science*, 57, 365.
- Pröll, T., & Karim, N. M. (1994). Nonlinear control of a bioreactor model using exact and I/O linearization. *International Journal of Control*, 60(4), 499.
- Russo, L. P., & Bequette, W. (1995). Impact of process design on the multiplicity behavior of a jacketed exothermic CSTR. *AIChE Journal*, 41(1), 135.
- Sepulchre, R. (1997). Slow peaking and low-gain designs for global stabilization of nonlinear systems. In *Proceedings of the 36th conference on decision and control (CDC)*, San Diego, CA, USA, FA01 9:10, pp. 3491–3496.
- Slotine, J., Hedrick, J. K., & Misawa, E. A. (1987). On sliding observers for nonlinear systems. *ASME Journal of Dynamics and System Measurement Control*, 109, 245.
- Soroush, M. (1997). Nonlinear state-observer design with application to reactors. *Chemical Engineering Science*, 52(3), 387.
- Stephanopoulos, G., & San, K. Y. (1984). Studies on On-line Bioreactor Identification. *Biotechnology and Bioengineering*, 26, 1176.
- Sussmann, H., & Kokotovic, P. (1991). The peaking phenomenon and the global stabilization of nonlinear systems. *IEEE Transactions on Automatic Control*, 36(4), 424.
- Tadayyon, A., & Rohani, S. (2001). Extended Kalman filter-based nonlinear model predictive control of a continuous KCl–NaCl crystallizer. *The Canadian Journal of Chemical Engineering*, 79, 255.
- Viel, F., Busvelle, E., & Gauthier, J. P. (1995). Stability of polymerization reactors using I/O linearization and a high-gain observer. *Automatica*, 31(7), 971.
- Walcott, B. L., & Zak, S. H. (1987). State observation of nonlinear uncertain dynamical systems. *IEEE Transactions on Automatic Control*, AC-32, 166.
- Wang, G., Peng, S., & Huang, H. (1997). A sliding observer for nonlinear process control. *Chemical Engineering Science*, 52(5), 787.