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Application of state estimation based NMPC to an unstable nonlinear process

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Abstract

Model predictive control (MPC) has become very popular both in process industry and academia due to its effectiveness in dealing with nonlinear, multivariable and/or hard-constrained plants.

Although linear MPC can be applied for controlling nonlinear processes by obtaining a linearized model of the plant, this is only valid in a limited region. Therefore, a substantial improvement can be achieved by using the whole knowledge of the process dynamics, specially in the presence of marked nonlinearities. This effect can be strong if the process to control is open-loop unstable.

The purpose of this paper is to introduce a nonlinear model predictive controller (NMPC) based on nonlinear state estimation, in order to exploit the knowledge of the nonlinear dynamics and to avoid modeling simplifications or linearization.

A state-space formulation is proposed to achieve the control objective. To update the optimization involved in NMPC strategy, state estimation based on the measured outputs is proposed.

As a particular application, we consider an 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 NMPController coupled with a state observer are designed. The observer is also used to estimate some unmeasured disturbances. Finally, computer simulations are developed for showing the performance of both the nonlinear observer and the control strategy.

Keywords: Observers; State estimation; Model predictive control; CSTR; Process control

1. Introduction

A typical feature of chemical process control is the existence of various operative constraints due to economic or safety concerns as well as restrictions related to valve sizes and actuator dynamics. Consequently, all these issues limit the expected performance of the controlled system. To cope with this fact, many techniques such as model predictive control (MPC) have emerged. It is a well-known result that MPC has often shown to provide improved performance than conventional feedback control schemes. The use of MPC in the chemical engineering field started in the process industries, which is not a common fact among other control techniques (Ogunnaike and Ray, 1994). This fact is basically due to flexible constraint-handling capabilities of MPC as well as its robustness properties (Bemporad and Morari, 1999).

The name MPC arises from the intention of using an explicit model of the process to be controlled which is used to predict the future output behavior. This capacity of prediction allows solving optimal control problems on line, where tracking error, i.e. the difference between the predicted output and the desired reference, is minimized over a future horizon. As regards linear plants control, superior behavior has been achieved using MPC in the case of non-minimum phase processes or systems with input constraints where future set points are known, as well as for stabilizing unstable linear plants (Eaton and Rawlings, 1992).

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Moreover, this control scheme has also proven to be useful for regulating many nonlinear plants. Many recent attempts to include nonlinear models in MPC have exhibited an improved performance, particularly for those applications where varying operating conditions over nonlinear regions are expected (García et al., 1989; Pröll and Karim, 1994).

The inherent feature of MPC is the reiterated optimization of an open-loop performance objective over the prediction horizon. There are many methods available in order to update the optimization problem. For instance, the reset of the model's initial conditions, estimation of model's parameters and/or states or inference of output disturbances can be performed (Eaton and Rawlings, 1992).

The advantages of employing state estimation instead of the frequently used approach of the additive output disturbance (commonly used in dynamic matrix control), have been shown in the works by Ricker (Ricker, 1990; Lee and Ricker, 1994). He used linear, time-invariant state-space models and applied state estimation theory. Sistu and Bequette (1991) addressed many important issues in nonlinear predictive control of chemical processes. They treated the selection of initial state conditions as a very important fact, specially under plant/model mismatch. To cope with this issue they introduced a nonlinear programming-based process identification scheme. An interesting alternative for estimating state variables, particularly when many or all of them are unmeasurable, is to use an state observer. The use of state observers based on measured outputs has already been considered for solving state space formulations of MPC problems. However, those approaches are limited to the use of Kalman filters (Li et al., 1989; Gattu and Zafiriou, 1992; Nagrath et al., 2002). A particular drawback in using this estimator for nonlinear control purposes is the linear nature of the estimator. This problem is magnified when the process to be controlled is unstable. In this case, any mismatch between real and estimated states could deteriorate the closed-loop performance or even drive the process to instability.

In spite of 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. Depending on 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 (Wang et al., 1997). In this sense, the standard 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 and San, 1984; Tadayyon and Rohani, 2001). For instance, Lee and Ricker (1994) proposed a state observer based MPC strategy using successive linearization. They derived a recursive EKF-type state estimator, providing the minimum-variance state estimates. The linear approximations of state/measurement equations are calculated at each sampling time. The main drawback of the traditional EKF approach consists in the difficulties to determine a priori its convergence and speed of convergence. 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 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 and 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. 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 nonlinear observers was presented by Wang et al. (1997).

In this paper, we show how to combine state estimation with NMPC to both satisfy the manipulated variable constraints and to provide the desired output value, even in the presence of unmeasured disturbances. Therefore, nonlinear state estimators are introduced to provide the NMPController the estimated value of the internal state of a nonlinear unstable process. We present two alternatives to state estimation: the EKF and a nonlinear high gain observer. Both of them are tested for extended estimation when unmeasured disturbances have to be estimated for control purposes.

In particular, both the state estimation methodologies and the NMPC technique are 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 overcome by any new 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 and Bequette, 1995 and 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. Another important example of a practical reactor operated at an open-loop unstable steady state is the styrene polymerization reactor dealt with in the work by Prasad et al. (2002). The reasons why polymerization processes present challenging control applications are therein addressed. Particularly, as polymer properties are generally not measurable on-line model based approaches are used for control purposes. Moreover, the inclusion of an estimator is required to handle state variable and parameter estimation.

The previous reasons evidence why CSTRs are known as an interesting barrier to be overcome by any new control technique proposal.

The work is organized as follows. The controller synthesis is developed in Section 2. In Section 3, the observers design procedure are dealt with. The evaluation of the observer-based controller performance is presented via simulation in Section 4. Finally, in Section 5, the conclusions are presented.

2. Nonlinear model-predictive controller

When applying MPC, the controller is designed in order to generate a manipulated variable profile to optimize some open-loop performance objective on a time interval p known as prediction horizon. The feedback loop is incorporated because the measurement is used to update the optimization problem for the next time step.

One of the main advantages of MPC is its capability for handling control problems where off-line computation of the control law is complicated or even impossible. Moreover, MPC is one of the scarce methods suitable for controlling hardly constrained plants. In MPC strategy, the current control action arises from the solution of an on-line, finite horizon open-loop optimal control problem. This problem is solved at each sampling instant, using the current state of the plant as the initial state. Once the optimization is performed, an optimal control sequence is obtained and only the first control in the sequence is implemented on the plant.

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 exact nonlinear model structure using nonlinear control techniques. In NMPC the model of the process is formulated in the form of nonlinear differential equations. This control strategy involves a computation at each sampling time in order to predict the values of future outputs and the minimization of output deviations from their setpoints. This information is obtained for calculating the future manipulated variables.

The sequence of steps to be followed in order to achieve the control action can be described as follows. First of all, the nonlinear original single input/multiple output (SIMO) model is

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

$$y = h(x), \tag{2}$$

where the vector x ($x \in \Re^n$) stands for the state variables and the input u ($u \in \Re$) represents the manipulated variable to accomplish the control goal. The measured outputs are represented by vector y ($y \in \Re^l$). A discretized representation of system (1)–(2) can be written in the following form:

$$\begin{aligned} x_{k+1} &= F(x_k) + G(x_k)u_k, \\ y_k &= h(x_k). \end{aligned} \tag{3}$$

The optimization problem for the prototypical NMPC formulation is (Meadows and Rawlings, 1997)

$$\begin{aligned} &\min_{u(k|k),u(k+1|k),\ldots,u(k+m-1|k)} J \\ &\quad = \phi[x(k+p|k)] + \sum_{j=0}^{p-1} L[x(k+j|k), \\ &\qquad u(k+j|k), \Delta u(k+j|k)], \end{aligned} \tag{4}$$

where $u(k+1|k)$ is the input $u(k+1)$ calculated from information available at time k, $x(k+1|k)$ is the state $x(k+1)$ calculated from information available at time k, $\Delta u(k+j|k) = u(k+j|k) - u(k+j-1|k)$, m is the control horizon, p is the prediction horizon and ϕ and L are (possibly) nonlinear functions of their arguments. The optimization problem is solved subject to the constraints discussed below. The functions ϕ and L can be chosen to satisfy a wide variety of objectives. In many applications, it is meaningful to consider quadratic functions of the following form:

$$\begin{aligned} L = &[x(k+j|k) - x_s(k)]^{\mathrm{T}} Q [x(k+j|k) - x_s(k)] \\ &+ [u(k+j|k) - u_s(k)]^{\mathrm{T}} R [u(k+j|k) - u_s(k)] \\ &+ \Delta u(k+j|k)^{\mathrm{T}} S \Delta u(k+j|k), \end{aligned} \tag{5}$$

$$\phi = [x(k+p|k) - x_s(k)]^{\mathrm{T}} Q [x(k+p|k) - x_s(k)], \tag{6}$$

where $u_s(k)$ and $x_s(k)$ are steady-state targets for u and x, respectively. Q is a symmetric positive semi-definite penalty matrix on the states, R is a symmetric positive definite penalty matrix on the inputs, and S is a symmetric positive semi-definite penalty matrix on the rate of change in the inputs. The main tuning parameters of the controller are m, p, Q, R, S and the sample period Δt.

The predicted states are obtained from the nonlinear model given by Eq. (3). Successive iterations of the model equations yield:

$$\begin{aligned} x(k+1|k) &= F(x(k|k)) + G(x(k|k))u(k|k) \\ &\equiv G_1(x(k), u(k|k)), \\ x(k+2|k) &= G_1(x(k+1|k), u(k+1|k)) \\ &= G_1((x(k), u(k|k)), u(k+1|k)) \\ &\equiv G_2(x(k), u(k|k), u(k+1|k)) \\ &\;\;\vdots \\ x(k+j|k) &= G_j(x(k), u(k|k), \\ &\qquad u(k+1|k), \ldots, u(k+j-1|k)), \end{aligned}$$

where $x(k|k) = x(k)$ is a vector of current state variables. The control horizon m is less than the prediction horizon p, then, the output predictions are generated by setting inputs beyond the control horizon equal to the last computed value: $u(k+j|k) = u(k+m-1|k)$, $m \leqslant j \leqslant p$. Note that the prediction

$y(k+j|k)$ depends on the current state variables, as well as the calculated input sequence. Therefore, NMPC requires measurements or estimates of the state variables. This is discussed in more detail below.

Solution of the NMPC problem yields the input sequence: $u(k|k), u(k+1|k), \ldots, u(k+m-1|k)$. Only the first input vector in the sequence is actually implemented: $u(k) = u(k|k)$. Then, the prediction horizon is moved forward one time step, and the problem is solved using new process measurements. This receding horizon formulation yields improved closed-loop performance in the presence of unmeasured disturbances and modeling errors.

An important characteristic of process control problems is the presence of constraints on input, state and output variables. Input constraints arise due to actuator limitations such as saturation and rate-of-change restrictions. State and output constraints are usually associated with operational limitations such as equipment specifications and safety considerations. These constraints can be posed as

$$\begin{aligned}
&u^L \leqslant u(k+j|k) \leqslant u^U, \quad 0 \leqslant j \leqslant m-1\\
&\Delta u^L \leqslant \Delta u(k+j|k) \leqslant \Delta u^U, \quad 0 \leqslant j \leqslant m-1\\
&x^L \leqslant x(k+j|k) \leqslant x^U, \quad 1 \leqslant j \leqslant p-1\\
&y^L \leqslant y(k+j|k) \leqslant y^U, \quad 1 \leqslant j \leqslant p-1
\end{aligned}$$

where the superscripts L and U stand for the admissible lower and upper bounds for the variables.

Therefore, the model is used to predict the system response and, consequently, to optimize it subject to constraints on input, output and state variables.

From the explanation above, it is clear that some information about the state vector is demanded. However, the whole state vector is hardly ever available through measurement. In order to provide variables estimates, based on the available measured outputs, a suitable state observer will be incorporated. Then, the information brought by the observer can be used to obtain corrected values for the initial states even when they are measured. This is because a suitable estimator with good stability properties can improve the values provided by noisy sensors. Moreover, the advantage of introducing an appropriate observer is that the internal state estimation will be more reliable than the one obtained by running the open-loop model (specially in the presence of dynamics uncertainty or in the present case of unstable systems). Therefore, we now turn to the observer design problem.

3. Nonlinear full-order observers

The objective of this section is to introduce an observer for estimating the whole state vector. In order to perform the estimation, two different observers are developed. First of all, a modified version of the widely diffused EKF is proposed.

3.1. EKF

It is a well-known fact that when the mathematical model of the process includes high nonlinearities, the performance of the standard linear Kalman filter deteriorates. In such cases, it may be suitable to apply the extended version of the Kalman filter in order to deal with the process nonlinearities. The derivation of this approach can be found in Jazwinski (1970).

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

$$\dot{\hat{x}} = f(\hat{x}) + g(\hat{x})u, \tag{7}$$

$$\dot{P}_K = [f_x(\hat{x}) + g_x(\hat{x})u]\, P_K + P_K\, [f_x(\hat{x}) + g_x(\hat{x})u]^{\mathrm{T}} + Q_K \tag{8}$$

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 $\hat{x}$. Note that this particular approach of the EKF uses the knowledge of the nonlinear model to update the state of the process. 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 and Dochain, 1990; Tadayyon and Rohani, 2001).

It must be noticed that for the Kalman filter as a linear unbiased minimum variance estimator, the parameters P_K, R_K and Q_K have all physical meaning. Particularly, P_K is the estimation covariance matrix, R_K is the covariance matrix of the white noise sequences in the measurements and Q_K is the covariance matrix of the white noise sequences in the states. However, when used in the EKF, they lost their original meaning and turn out to be only tuning parameters. Nevertheless, the speed of estimation convergence is strongly influenced by the initial value of matrix P_K. 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:

$$\begin{aligned}K_{EKF}(k+1) = {} & P_K(k+1|k)h_x^{\mathrm{T}}(\hat{x}(k+1|k))\\ & \times[h_x P_K(k+1|k)h_x^{\mathrm{T}} + R_K]^{-1},\end{aligned} \tag{9}$$

with h_x, the Jacobian matrix of h on x.

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

$$\begin{aligned}\hat{x}(k+1|k+1) = {} & \hat{x}(k+1|k) + K_{EKF}(k+1)\\ & \times[y(k+1) - h(\hat{x}(k+1|k))]\end{aligned} \tag{10}$$

and then, the new weighting matrix is computed:

$$\begin{aligned}&P_K(k+1|k+1)\\ &\quad = [I - K_{EKF}(k+1)h_x]P_K(k+1|k)\\ &\qquad \times[I - K_{EKF}(k+1)h_x^{\mathrm{T}}]\\ &\qquad + K_{EKF}(k+1)R_K K_{EKF}^{\mathrm{T}}(k+1).\end{aligned} \tag{11}$$

Then, the counter k is incremented in one and the algorithm is executed again.

The EKF algorithm is an approximation of the original linear Kalman filter to deal with nonlinear processes. It is important to note that when linearization techniques are applied, convergence and speed of convergence are local properties, i.e. the estimation error can converge in a given time interval and diverge in another one.

Another alternative to carry out the state estimation in this type of systems is to implement an observer based on a nonlinear design criterion to cope with the information brought by the process model.

3.2. Luenberger-like nonlinear observer (LNO)

Different approaches to the nonlinear observer problem have been used. One of the classical solutions consists in the design of a high gain observer. This method is useful when there exists a coordinates change that transforms the system in a canonical form of uniform observability with respect to the inputs (Gauthier et al., 1992; Ciccarella et al., 1993; García et al., 2000; Aguilar et al., 2002). This is the type of design approach herein followed. A high gain observer is introduced to perform the estimation, and its exponential convergence in the absence of noise is established (see Appendix).

To perform the state estimation of the process given by Eqs. (1)–(2), the following Luenberger-like nonlinear observer (LNO) is developed:

$$\dot{\hat{x}} = f(\hat{x}) + g(\hat{x})u + \mathcal{O}^{-1}(\hat{x})K_{LNO}(y - h(\hat{x})). \tag{12}$$

The system in Eq. (12) 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 $\mathcal{O}^{-1}(\hat{x})K_{LNO}$ is the nonlinear gain of the observer, where K_{LNO} is a vector of constants to be designed and $\mathcal{O}$ is the Jacobian of the vector $\Phi(x)$. This vector $\Phi(x)$ is defined as:

$$\Phi(x) = \begin{bmatrix} h(x) \\ L_f h(x) \\ \vdots \\ L_f^{n-1} h(x) \end{bmatrix}, \tag{13}$$

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:

$$L_f h(x) = \frac{\partial h(x)}{\partial x} f(x), \tag{14}$$

$$L_f^j h(x) = \frac{\partial L_f^{j-1} h(x)}{\partial x} f(x). \tag{15}$$

The vector Φ constitutes a nonlinear change of coordinates and it is used to design K_{LNO} such that the dynamics of the estimation error $\tilde{x}$, defined as $\tilde{x} = x - \hat{x}$, is stable. Provided that $\mathcal{O}$ is invertible, and that the input u is bounded (see Appendix), given the initial condition $\hat{x}(0)$, the following property behaves for any $\alpha > 0$:

$$\|\tilde{x}(t)\| \leqslant \zeta e^{-\alpha t} \|\tilde{x}(0)\|, \tag{16}$$

with $\zeta > 0$. The gain K_{LNO} must be appropriately chosen to guarantee stability. A detailed demonstration based on Lyapunov arguments is presented in the appendix where the observer convergence and its relationship with the gain selection are dealt with.

Therefore, a stable observer has been developed for the nonlinear system (1)–(2). Provided the stability hypotheses are held, the observer brings an on-line estimation of the whole process state. The observer can be easily implemented and it only uses the information brought by the output measurements. Moreover, the observer was 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.

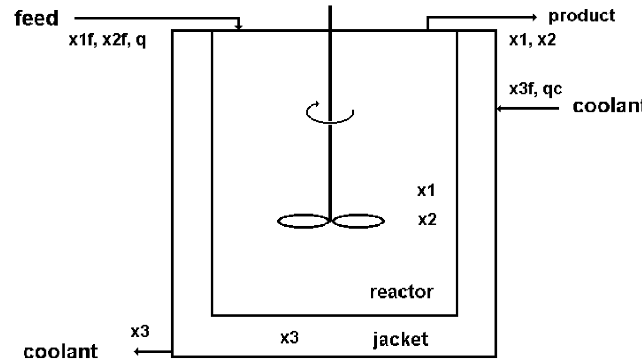

Fig. 1. Scheme of jacketed CSTR.

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

4.1. Process description

The performance 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 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

Table 1
CSTR model parameters

Dimensionless parameter	Value
ϕ	0.072
β	8.0
δ	0.3
γ	20
q	1.0
$\delta 1$	10
$\delta 2$	1.0
x_{1f}	1.0
x_{2f}	0.0
x_{3f}	−1.0

Bequette, 1995):

$$\frac{dx_1}{d\tau}=q(x_{1f}-x_1)-\phi x_1\kappa(x_2), \tag{17}$$

$$\frac{dx_2}{d\tau}=q(x_{2f}-x_2)-\delta(x_2-x_3)-\beta\phi x_1\kappa(x_2), \tag{18}$$

$$\frac{dx_3}{d\tau}=\delta_1[q_c(x_{3f}-x_3)+\delta\delta_2(x_2-x_3)], \tag{19}$$

with κ:

$$\kappa(x_2)=e^{x_2/(1+x_2/\gamma)}. \tag{20}$$

The state variables x_1, x_2 and x_3 stand for the dimensionless reactant concentration, the reactor temperature and the cooling jacket temperature, respectively. The symbol q_c represents the cooling jacket flow rate (manipulated variable) 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 operational and control problems. Fig. 2 shows the plot of the steady state values for x_2 (denoted as x_2^{ss}) versus the input q_c. The other states are related with these values by the following expressions:

$$x_1^{ss}=\frac{qx_{1f}}{q+\phi\kappa(x_2^{ss})}, \tag{21}$$

$$x_3^{ss}=\frac{q_cx_{3f}+\delta\delta_2x_2^{ss}}{q_c+\delta\delta_2}. \tag{22}$$

As shown in Fig. 2, the reactor presents multiplicity behavior with respect to the jacket temperature and jacket flow rate (Nagrath et al., 2002). The CSTR modeled by Eqs. (17)–(19) 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 NMPC technique, which demands the knowledge of the internal state of the process. It must be pointed out that MPC combined with a Kalman filter, has already been used for temperature control in a CSTR (Nagrath et al., 2002). Although it proved to work for regulation purposes (i.e. to set x_2 to a fixed value), it is not valid for tracking objectives. This is because the Kalman filter is based on a linearization around a fixed point and it hardly works when trying to follow the unstable open-loop steady-state region.

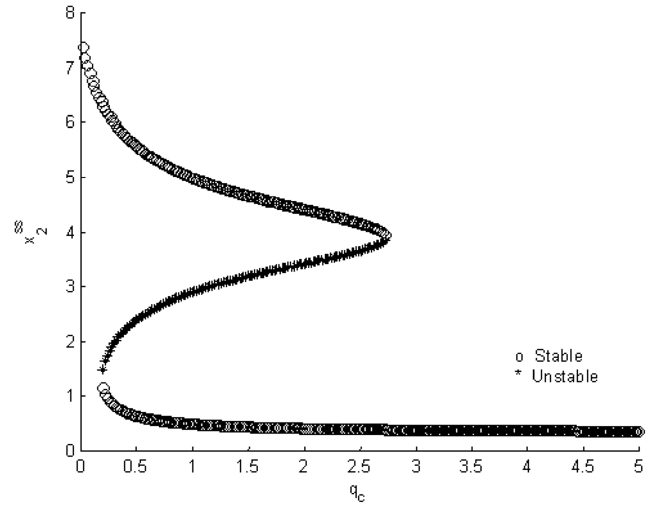

Fig. 2. Steady state points for the jacketed CSTR.

4.2. Model predictive control

The flow q_c is the manipulated variable and its optimal value is calculated at each sampling instant using NMPC methodology. For this application the sample time, prediction horizon and the control horizon were $\Delta t = 0.05$ min, $p=20$ and $m=5$, respectively. The values selected for the weights in the objective function used for the optimization along the finite horizon were $Q=\text{diag}\{0, 10^4, 0\}$, $R=5$ and $S=0$. Because real control valves have a limited rangeability, there are extreme admissible values for the manipulated variable. In this case: $0\leqslant q_c\leqslant 2$ for $0\leqslant j\leqslant m$. Under the previous conditions the optimal control sequence was calculated under the assumption of complete measurability of the states. Figs. 3 and 4 show the plots for setpoint tracking and disturbance rejection. The considered perturbations are $x_{3f}=-0.9$ for $t>1$, $x_{1f}=1.01$ for $t>15$ and $q=0.99$ for $6\leqslant t\leqslant 10$. In Fig. 4, two different cases are considered: measured perturbation and unknown perturbation. From this plot it is clear that to obtain good control performance is very important the knowledge about the perturbation. Then, the structure of the states observer is slightly modified to estimate the perturbations.

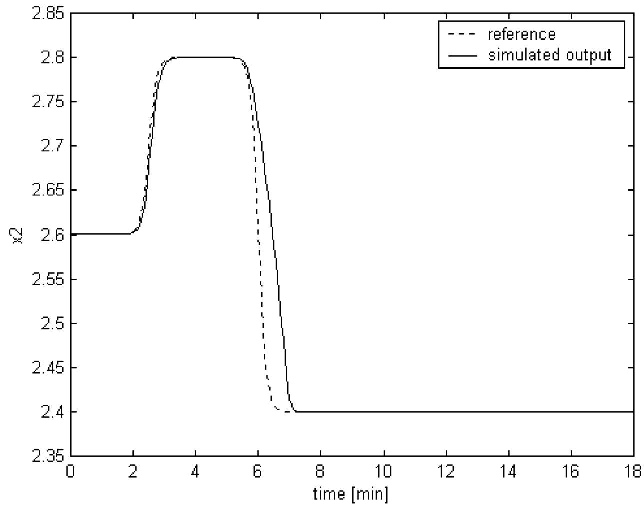

Fig. 3. Process output for reference tracking based on measured states.

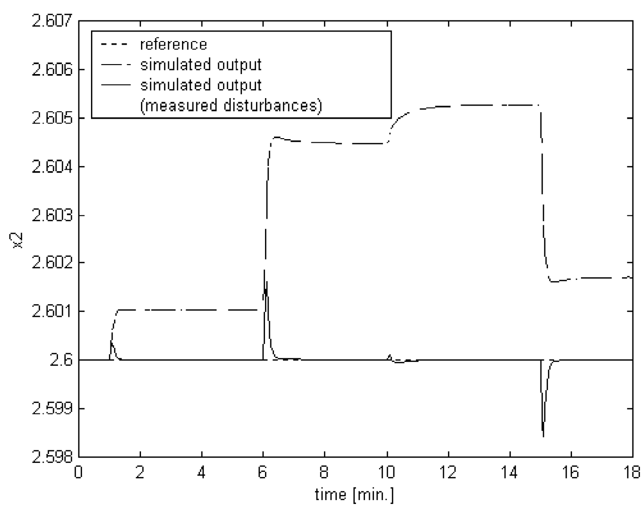

Fig. 4. Process output for disturbance rejection based on measured states.

4.3. State observer and perturbation estimation

To cope with the assumption of unmeasured states, an appropriate state observer must be connected with the controller. Therefore, the observers performance is now 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 dealt with in Section 2 can be "extended" to perform the disturbances estimation together with the states estimation. In such a way, the observers append modeled disturbances to the original system's model. In such a way, an augmented states vector is obtained. Then, the following observer structure is obtained:

$$\dot{\hat{x}}_{\text{ext}} = f_{\text{ext}}(\hat{x}_{\text{ext}}) + g(\hat{x}_{\text{ext}})u + \text{Corr}, \tag{23}$$

$$\hat{y} = h(\hat{x}_{\text{ext}}), \tag{24}$$

with

$$\hat{x}_{\text{ext}} = \begin{bmatrix} \hat{x} \\ \hat{x}_{3f} \\ \hat{q} \end{bmatrix} \tag{25}$$

and

$$f_{\text{ext}} = \begin{bmatrix} f(\hat{x}_{\text{ext}}) \\ 0 \\ 0 \end{bmatrix} \tag{26}$$

In this case, the presence of the two zeros in f_{ext} involves that there is no information available on the disturbances dynamics. These zeros would also appear if the disturbances dynamics were assumed negligible. However, the disturbances could be described by any other type of model, such as ramps, sinusoids, etc. or they could be the output of a stochastic process as in the description proposed by Lee and Ricker (1994). In all the alternative cases, an appropriate deterministic or stochastic model should be considered to describe the knowledge about the disturbance dynamics.

Note that Corr is the correction term designed according to each observer. The two observers structures presented in Section 2 were used. For that purpose, the EKF parameters were set to the following values:

$$R_K = \begin{bmatrix} 0.001 & 0 \\ 0 & 0.001 \end{bmatrix}, \quad Q_K = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.01 & 0 \\ 0 & 0 & 0 & 0 & 0.01 \end{bmatrix},$$

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

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

$$K_{LNO} = \begin{bmatrix} 7.4002 & -0.0497 \\ 18.0013 & -0.2402 \\ 14.4019 & -0.2901 \\ -0.0031 & 4.5998 \\ -0.0075 & 5.2795 \end{bmatrix}$$

in order to fix the eigenvalues of $(A + K_{LNO}C)$ to $\{-2.4, -3.0, -2.2, -2.4, -2.0\}$ (see Eq. (34) in the appendix). Note that the gain K_{LNO} must satisfy the stability condition stated by (41). A "practical" way for tuning the LNO consists in selecting the gain by fixing the eigenvalues of $(A + K_{LNO}C)$ (i.e., the linear part of the error dynamics) to the desired values, and then check if (41) holds. Provided the inequality is satisfied, a heuristic tuning has been accomplished and, moreover, it is endorsed by a rigorous stability test.

Simulation results were carried out to compare the performance of various observers. Fig. 5 shows the states estimates and the disturbances estimates obtained with a Kalman filter, a standard EKF, a modified EKF (as described in Section 3.1) and the LNO. The initial conditions were set to:

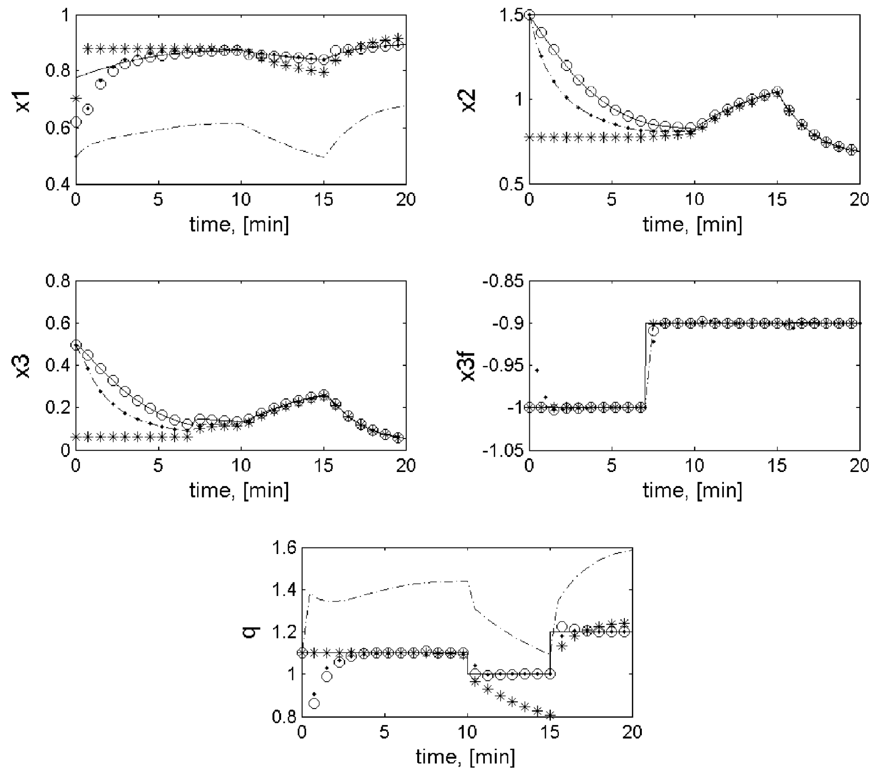

Fig. 5. Observers performance: actual values (-); KF estimates (∗), standard EKF estimates (-.), modified EKF estimates (.) and LNO estimates (o).

$x_1(0) = \hat{x}_1(0) = 0.7748$, $x_2(0) = 1.5000$, $\hat{x}_2(0) = 0.8x_2(0)$, $x_3(0)=\hat{x}_3(0)=0.4952$, $x_{3f}(0)=\hat{x}_{3f}(0)=-1$, $q(0)=\hat{q}(0)=1.1$. The constant input was $q_c = 0.2016$. From the results, the LNO provides good estimates, as well as the modified EKF. The convergence properties of the LNO can be appreciated. On the other hand, both the Kalman filter and the linearized standard EKF show an inefficient behavior.

In the following subsection, some simulation results are developed to test the NMPC and observers performance.

4.4. Evaluation of the NMPC/observer performance

Figs. 6 and 7 show the simulation results for a tracking case when the NMPController is used in conjunction with each of the two observers presented in the previous subsection. The output variable x_2 and the manipulated variable q_c are depicted. These plots show that the response using the EKF is slightly faster than the one obtained for the NLO. Additionally, when perturbations take place, the EKF shows a superior disturbance rejection effect (see Figs. 8 and 9). This is due mainly to the fact that the EKF estimates better the perturbation than the NLO.

An additional test was performed moving the operative point along the unstable zone. The results are presented in Figs. 10 and 11. In this case, it is important to note that the delay in the descendent section of the trajectory is due to the saturation of the manipulated variable at the upper bound.

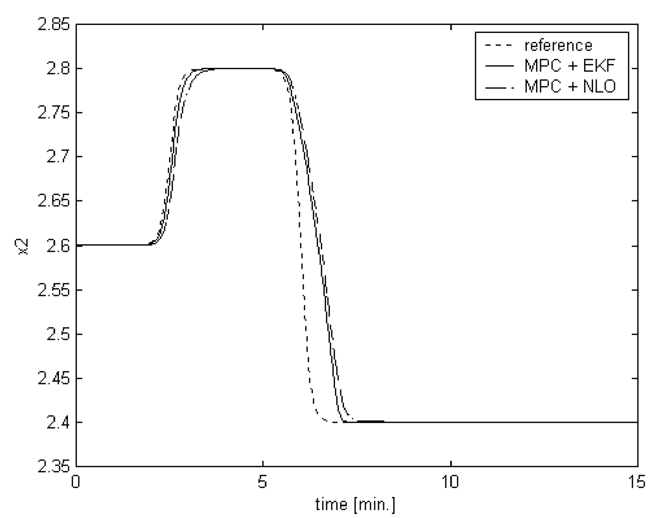

Fig. 6. Process output for reference tracking.

Finally, a simulation including sensor noise is performed to check the robustness of both observers. For this purpose, the outputs x_2 and x_3 were assumed corrupted with uniformly distributed white noise signals. Note that the whole knowledge about R_K and Q_K was used in the EKF tuning, and $P_K(0|0)$ was chosen to provide the best estimation results (after testing other possible initial values). The results are presented in Fig. 12. From these plots it is clear that

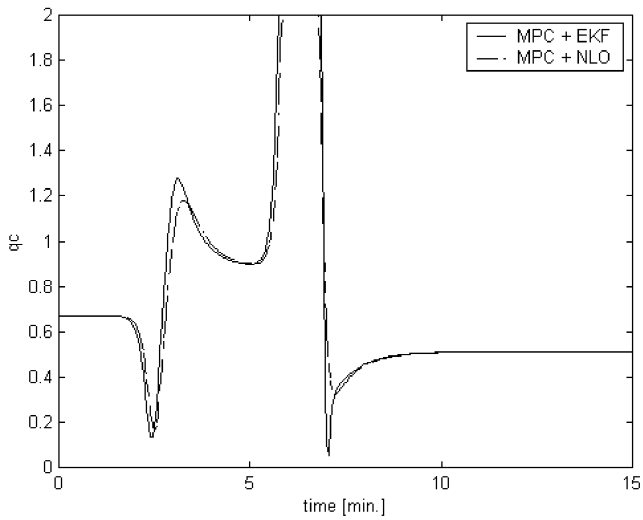

Fig. 7. Manipulated variable for reference tracking.

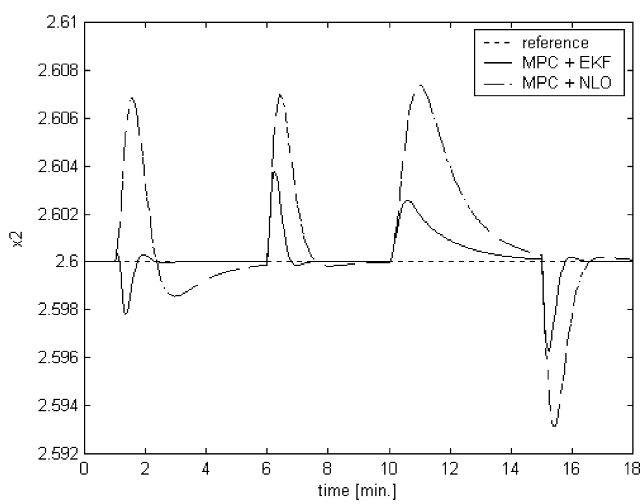

Fig. 8. Process output for disturbance rejection.

the EKF is strongly influenced by the noise. Consequently, if the estimation is based on noisy measurements, the EKF requires a larger control effort than the LNO.

5. Conclusions

In the present work the problem of nonlinear model predictive control for unstable processes has been tackled. In particular, the analysis has been focused on the estimation of the states and time varying parameters in a CSTR. In order to control the process, we proposed a control algorithm that uses all the information available. To perform the estimation, we introduced a high gain full order observer that robustly estimates the whole state vector and the varying parameters based on the available measurements. Additionally, several comparisons with an EKF approach were developed.

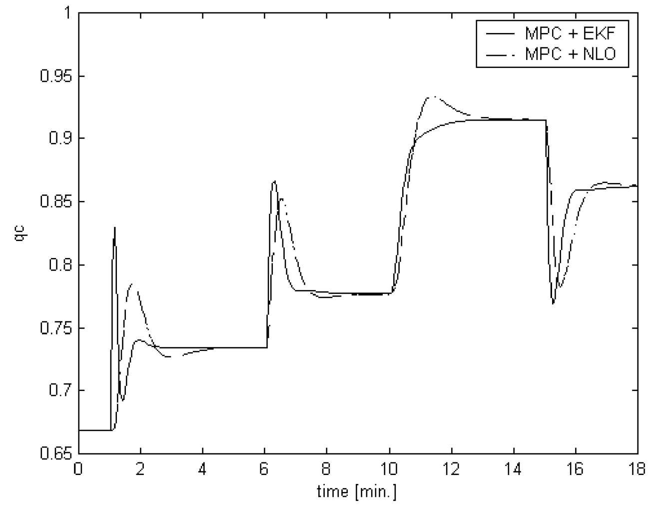

Fig. 9. Manipulated variable for disturbance rejection.

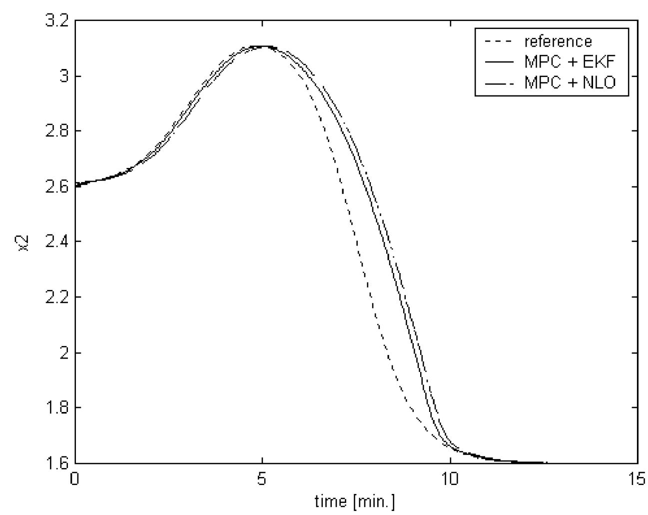

Fig. 10. Process output for a large change in the reference.

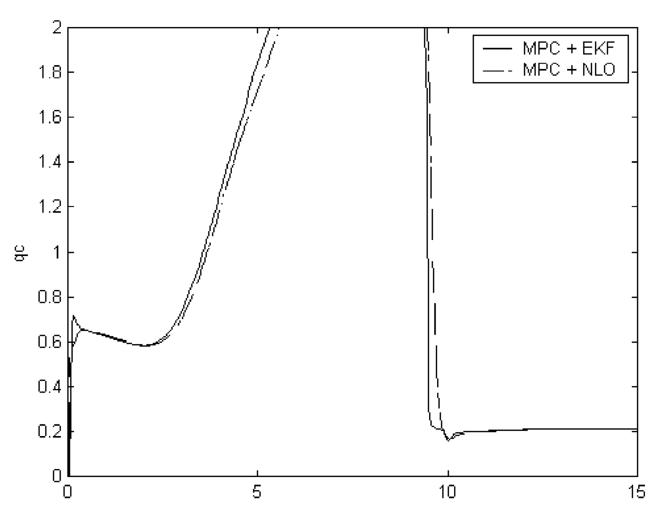

Fig. 11. Manipulated variable for a large change in the reference.

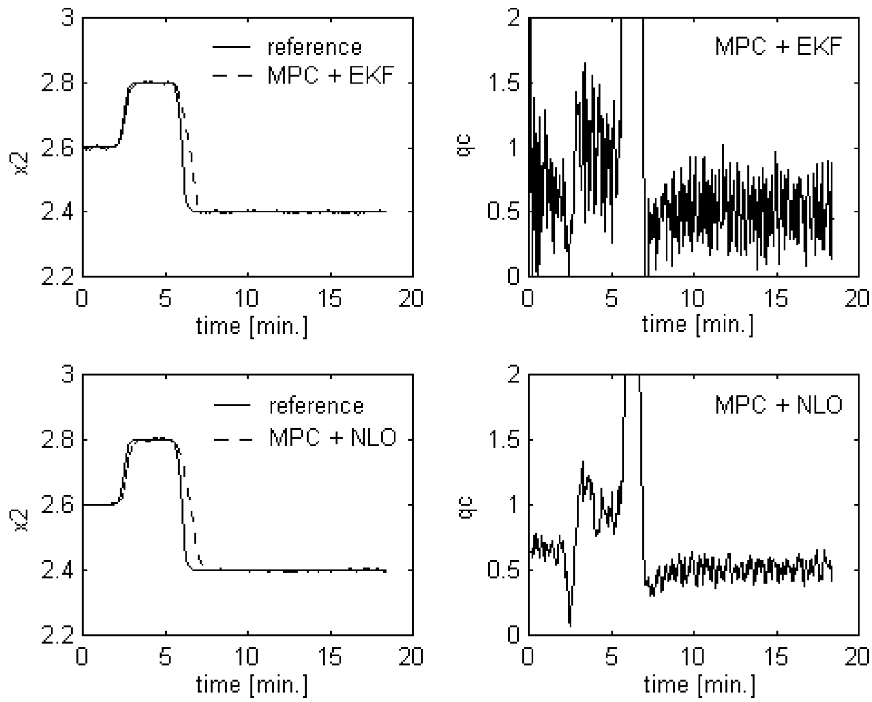

Fig. 12. Controlled and manipulated variables in the presence of noisy measurements.

While the design criterion for the LNO is based on stability properties, the EKF design parameters are 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 Kalman filter (KF).

Finally, computer simulations were developed to illustrate the performance of both the nonlinear observer and the control strategy. A successful behavior of the whole observer/controller structure was attained.

Notation

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

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Appendix

The design parameter K_{LNO} must be selected in order to guarantee the estimation algorithm convergence. The Luenberger-like nonlinear observer herein proposed is constructed using a change of coordinates (Ciccarella et al., 1993; García et al., 2000). The change of coordinates selected in this work is the one given by Eq. (13), which transforms the original system by defining the following transform variable z:

$$z = \Phi(x) \tag{27}$$

and

$$x = \Phi^{-1}(z), \tag{28}$$

which constitutes a change of coordinates in $\Re^n$. Therefore, the original system given by Eqs. (1)–(2) can be rewritten in the new coordinates as follows:

$$\dot{z}=Az + BL_f^n h(\Phi^{-1}(z)) + L_g\Phi(\Phi^{-1}(z))u, \tag{29}$$

$$y=Cz, \tag{30}$$

with

$$A=\begin{bmatrix}0 & 1 & 0 & \cdots & 0\\ 0 & 0 & 1 & \cdots & 0\\ \vdots & & & & \vdots\\ 0 & 0 & \cdots & 0 & 0\end{bmatrix},\quad B=\begin{bmatrix}0\\ \vdots\\ 0\\ 1\end{bmatrix},$$

$$C=[1\quad 0\quad \cdots\quad 0] \tag{31}$$

and

$$Lg\Phi(.)u=\begin{bmatrix}L_g h(x)\\ L_g L_f h(x)\\ \vdots\\ L_g L_f^{n-1} h(x)\end{bmatrix}u. \tag{32}$$

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

$$\dot{\hat{z}}=(A-K_{LNO}C)\hat{z}+K_{LNO}y+BL_f^n h(\Phi^{-1}(\hat{z}))$$
$$+L_g\Phi(\Phi^{-1}(\hat{z}))u. \tag{33}$$

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

$$\dot{e_z}=\dot{z}-\dot{\hat{z}}$$
$$=(A+K_{LNO}C)e_z+B[L_f^n h(\Phi^{-1}(z))-L_f^n h(\Phi^{-1}(\hat{z}))]$$
$$+[L_g\Phi(\Phi^{-1}(z))-L_g\Phi(\Phi^{-1}(\hat{z}))]u. \tag{34}$$

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

$$V=e_z^{\mathrm{T}}P_N e_z \tag{35}$$

with P_N a positive definite matrix. Then,

$$\dot{V}=\dot{e}_z^{\mathrm{T}}P_N e_z+e_z^{\mathrm{T}}P_N\dot{e}_z \tag{36}$$
$$=e_z^{\mathrm{T}}[(A+K_{LNO}C)^{\mathrm{T}}P_N+P_N(A+K_{LNO}C)]e_z$$
$$+2(\gamma-\hat{\gamma})^{\mathrm{T}}P_N e_z+2(\omega-\hat{\omega})^{\mathrm{T}}P_N e_z u \tag{37}$$

where $\gamma(.)$ and $\omega(.)$ stand for $L_f^n h(\Phi^{-1}(.))$ and $L_g\Phi(\Phi^{-1}(.))$, respectively. Now, provided that both P_N and a positive definite matrix Q_N satisfy the following equation:

$$(A+K_{LNO}C)^{\mathrm{T}}P_N+P_N(A+K_{LNO}C)=-Q_N \tag{38}$$

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

$$\|u\|\leqslant U,$$
$$\|\gamma-\hat{\gamma}\|\leqslant L_\gamma\|z-\hat{z}\|,$$
$$\|\omega-\hat{\omega}\|\leqslant L_\omega\|z-\hat{z}\|, \tag{39}$$

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

$$\dot{V}\leqslant(-q_m+2p_M(L_\gamma+L_\omega U))\|e_z\|^2. \tag{40}$$

If the gain K_{LNO} is selected such that p_M and q_m satisfy

$$-q_m+2p_M(L_\gamma+L_\omega U)<0, \tag{41}$$

then, $\dot{V}$ turns out to be negative and the norm of the estimation error goes to zero as $t\to\infty$. Hence, the convergence of the algorithm is guaranteed. If the transform $\Phi(x)$ is nonsingular and Φ^{-1} is uniformly Lipschitz, then revisiting Eqs. (27)–(28) the condition given by Eq. (16) is obtained.

It must be remarked that Eq. (40) 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 can be achieved even when the gain K_{LNO} does not satisfy Eq. (40).

References

Aguilar, R., Martínez-Guerra, R., Pozniak, A., 2002. Reaction heat estimation in continuous chemical reactors using high gain observers. Chemical Engineering Journal 87, 351–356.

Bastin, G., Dochain, D., 1990. On-line Estimation and Adaptive Control of Bioreactors. Elsevier Science Publishers, New York, USA.

Baumann, W.T., Rugh, W.J., 1986. Feedback control of nonlinear systems by extended linearization. IEEE Transactions on Automatic Control AC-31, 40–46.

Bemporad, A., Morari, M., 1990. Robust model predictive control: a survey. Garulli, A., Tesi, A., Vicino, A. (Eds.), Robustness in Identification and Control. Lecture Notes in Control and Information Sciences, vol. 245. Springer, Berlin.

Ciccarella, G., Dalla Mora, M., Germani, A., 1993. A Luenberger-like observer for nonlinear systems. International Journal of Control 57, 537–556.

Eaton, J., Rawlings, J., 1992. Model-predictive control of chemical processes. Chemical Engineering Science 47 (4), 705–711.

García, C., Prett, D., Morari, M., 1989. Model predictive control: theory and practice—a survey. Automatica 25, 335–348.

García, R.A., Troparevsky, M.I., Mancilla Aguilar, J.L., 2000. An observer for nonlinear noisy systems. Latin American Applied Research 30 (2), 87–92.

Gattu, G., Zafiriou, E., 1992. Nonlinear quadratic matrix control with state estimation. Industrial and Engineering Chemistry Research 31, 1096–1104.

Gauthier, J., Hammouri, H., Othman, S., 1992. A simple observer for nonlinear systems. Applications to bioreactors. IEEE Transactions on Automatic Control 37 (6), 875–879.

Isidori, A., 1995. Nonlinear Control Systems. third ed. Springer, London.

Jazwinski, A., 1970. Stochastic Processes and Filtering Theory. Academic Press, New York.

Lee, J., Ricker, N., 1994. Extended Kalman Filter based nonlinear model predictive control. Industrial and Engineering Chemistry Research 33, 1530–1541.

Li, S., Lim, K., Fisher, D., 1989. A state space formulation for model predictive control. A.I.Ch.E. Journal 35 (2), 241–249.

Ljung, L., 1979. Asymptotic behavior of the extended Kalman filter as a parameter estimator for linear systems. IEEE Transactions on Automatic Control AC-24, 36–50.

Meadows, E.S., Rawlings, J.B., 1997. Model predictive control. In: Henson, M.A., Seborg, D.E. (Eds.), Non Linear Process Control. Prentice-Hall, Englewood Cliffs, NJ, p. 233.

Mouyon, Ph., 1997. Tools for nonlinear observer design. 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, 365–378.

Ogunnaike, B., Ray, W., 1994. Process Dynamics Modelling, and Control. Oxford University Press, New York.

Prasad, V., Schley, M., Russo, L.P., Bequette, B.W., 2002. Product property and production rate control of styrene polymerization. Journal of Process Control 12, 353–372.

Pröll, T., Karim, N., 1994. Model-predictive pH control using real-time NARX approach. A.I.Ch.E. Journal 40 (2), 269–282.
Ricker, N., 1990. Model predictive control with state estimation. Industrial and Engineering Chemistry Research 29, 374–382.
Russo, L.P., Bequette, W., 1995. Impact of process design on the multiplicity behavior of a jacketed exothermic CSTR. A.I.Ch.E. Journal 41 (1), 135–147.
Sistu, P., Bequette, B., 1991. Nonlinear predictive control of uncertain processes: application to a CSTR. A.I.Ch.E. Journal 37 (11), 1711–1723.
Stephanopoulos, G., San, K.Y., 1984. Studies on on-line bioreactor identification. Biotechnology and Bioengineering 26, 1176–1188.
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, 255–262.
Wang, G., Peng, S., Huang, H., 1997. A sliding observer for nonlinear process control. Chemical Engineering Science 52 (5), 787–805.