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Use of state estimation for inferential nonlinear MPC: a case study

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Abstract

Model predictive control (MPC) has become very popular in process industry and academia because it is an optimizing control technique which can handle hard constraints as well as time delays and mild nonlinearities. Linear MPC may control nonlinear processes by obtaining a linearized model of the plant, however, this approach is only valid in a limited region. In the presence of marked nonlinearities, a substantial improvement can be achieved by using the whole knowledge of the process dynamics.

The use of a nonlinear model for MPC involves the knowledge of the complete state vector and the most significative perturbations in order to obtain the best performance. However, this information may not be directly available through measurement. In this paper, we propose the use of a nonlinear estimator to update the state vector and to infer the unmeasured perturbations.

All the development herein presented is in the context of the control of an open-loop unstable nonlinear reactor with a measurement delay in the controlled variable.

Keywords: Nonlinear model predictive control; State estimation; Inferential control

1. Introduction

Most control applications involve hard constraints on controls and states, however, there is a shortage of design procedures to deal with such constraints. To cope with this fact, model predictive control (MPC) has emerged and now it is widely adopted. It is a well-known result that MPC has often shown to provide improved performance than conventional feedback control schemes, specially in the presence of restrictions related to valve sizes and actuator dynamics. The use of MPC in the chemical engineering field started in the process industries, which is not a common fact among other control techniques. This situation is basically due to flexible constraint-handling capabilities of MPC as well as its robustness properties [1]. The essential feature of MPC is the employment of an explicit model to predict the effect of future control actions on the outputs. This capacity for prediction allows solving optimal control problems on-line, where a specified objective function is minimized over a future horizon. As regards linear plant 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 [2]. 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 shown superior performance, particularly for applications where varying operating conditions over nonlinear regions are expected [3–5]. In this article we will use a first principle nonlinear model to predict the behavior of the process. In the approach herein followed, the knowledge of the complete state vector and the most relevant perturbations is crucial in order to obtain good performance of the control strategy.

Because 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. 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 by Ricker [6]. He used linear, time-invariant

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state-space models and applied state estimation theory. Sistu and Bequette [7] addressed many important issues in nonlinear predictive control of chemical processes. They treated the selection of initial state conditions as a very important fact, especially under plant/model mismatch. To cope with this issue they introduced a nonlinear programming-based process identification scheme.

The inclusion of a state observer is an interesting alternative for estimating state variables, particularly when many of them are unmeasurable. 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 basically limited to the use of Kalman filters [8]. A particular drawback in using the Kalman filter for nonlinear control purposes is the linear nature of the estimator. Gattu and Zafiriou [9] introduced state estimation into nonlinear quadratic dynamic matrix control (NLQDMC). They used a steady-state Kalman filter which is based on a locally linearized model and it must be redesigned at each time step. Additionally, the assumptions on the state noise can lead to significant biases in the state estimates, limiting its applicability and performance. Moreover, 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.

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 [10]. These observers are designed in such a way that they can cope with the intrinsic nonlinearities and can be useful, for example, for on-line estimation in chemical processes [11,12].

In this work, we present a nonlinear efficient state estimator to provide to the nonlinear model predictive controller (NMPC) the estimated value of the internal state and the most significative disturbances of the process. The observer implementation is simple and it requires small computational effort.

The observer/controller design can be applied for a general type of nonlinear process models. In this paper we present the approach in the form of a case study: the control of an open-loop unstable reactor. It must be highlighted that this process has been widely studied because it is highly nonlinear, and it is known to be an interesting challenge to overcome by any new control technique proposal due to the following features:

- The controlled output is measured with a significant delay.
- The process includes a crucial perturbation which is unmeasurable.
- The process is highly nonlinear at the operating point and close to an unstable region.

The work is organized as follows. The reactor is presented in Section 2. In Section 3 the observer design procedure is dealt with. The controller synthesis is developed in Section 4. The results are presented via simulation in Section 5. Finally, in Section 6, the conclusions are drawn.

2. Problem statement: the stirred-tank reactor (CSTR)

The simulated continuous stirred-tank reactor (CSTR) process consists of an irreversible, exothermic reaction (A → B), in a constant volume reactor cooled by a single coolant stream q_c. The whole process can be modeled by the following equations [16]:

$$\dot{C} = \frac{q}{V}[C_f - C] - k_0 C \exp\left(\frac{-E}{RT}\right) \tag{1}$$

$$\dot{T} = \frac{q}{V}(T_0 - T) - \frac{k_0\,\Delta H}{\rho C_p} C \exp\left(\frac{-E}{RT}\right) + \frac{\rho_c C_{pc}}{\rho C_p V} q_c \left[1 - \exp\left(-\frac{hA}{q_c \rho_c C_{pc}}\right)\right](T_{c0} - T) \tag{2}$$

The state variables C and T stand for the reactant concentration and the reactor temperature, respectively. The symbol q_c represents coolant flow rate and the other symbols are constant parameters whose values are defined in Table 1.

An important fact regarding the implementation of the control action is the existence of a time delay ($t_d = 0.5$ min) in the concentration measurement, hence $C_{meas}(t) = C(t - t_d)$. The objective is to control the concentration C by manipulating the coolant flow rate q_c.

The disturbances are the unmeasured feed concentration C_f and the measured coolant temperature T_{c0}. This model is a modified version of the first tank of a two-tank CSTR example by Henson and Seborg [13]. However, in the original model the time delay was zero, which was a simplification for control purposes.

The process dynamics are nonlinear because the reaction rate is governed by the Arrhenius law. That is why the CSTR exhibits some operational and control problems. The steady-state values for C versus the input q_c are plotted in Fig. 1 which shows the reactor presents multiplicity with respect to the coolant flow rate. The CSTR modeled by Eqs. (1) and (2) behaves as an open-loop unstable system if the concentration inside the reactor is between 0.14 and 0.92. In particular, the point A ($q_c \approx 111.85\,\mathrm{l\,min^{-1}}$) in Fig. 1, is a Hopf bifurcation point. In our application, one of the objectives is to operate

Table 1
Process parameters

Parameter	Value
Process flow rate, q ($\mathrm{l\,min^{-1}}$)	100
Feed concentration, C_f ($\mathrm{mol\,l^{-1}}$)	1
Feed temperature, T_0 (K)	350
Inlet coolant temperature, T_{c0} (K)	350
CSTR volume, V (l)	100
Heat transfer term, hA ($\mathrm{cal\,min^{-1}\,K^{-1}}$)	7×10^5
Reaction rate constant, k_0 ($\mathrm{min^{-1}}$)	7.2×10^{10}
Activation energy term, E/R (K)	10^4
Heat of reaction, ΔH ($\mathrm{cal\,mol^{-1}}$)	-2×10^5
Liquid densities, ρ, ρ_c ($\mathrm{g\,l^{-1}}$)	10^3
Specific heats, C_p, C_{pc} ($\mathrm{cal\,g^{-1}\,K^{-1}}$)	1

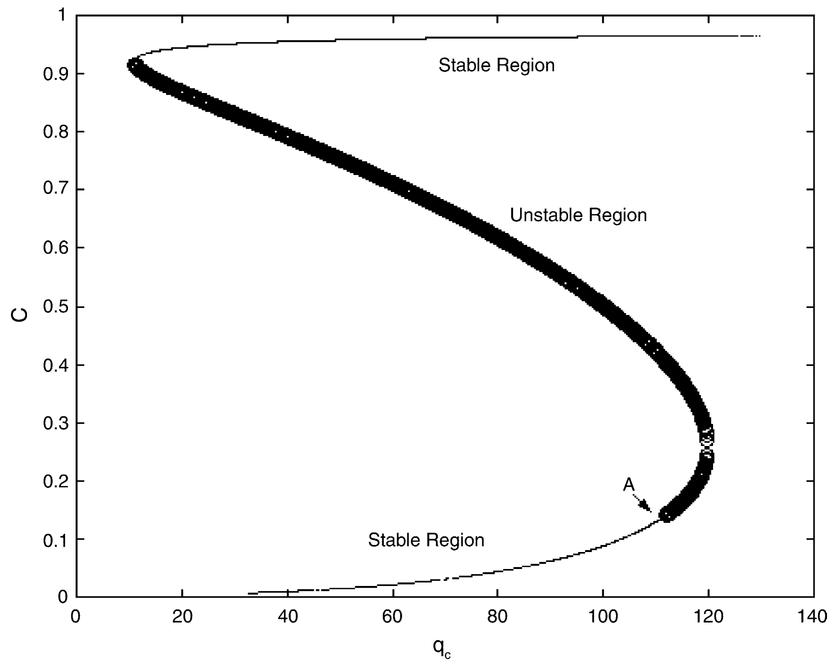

Fig. 1. Steady-state values (C vs. q_c).

the process at constant concentration $C = 0.1\,\mathrm{mol\,l^{-1}}$, which implies that $q_c = 103.41\,\mathrm{l\,min^{-1}}$.

Posed in these terms, the use of this model for nonlinear MPC presents two main difficulties:

- Due to the high nonlinearity (and the nearness to the unstable operation region), it is necessary to know precisely the process state and the perturbations values.
- The measurement delay of the controlled variable limits the performance achievable by the control algorithm.

To overcome these obstacles, the proposed control strategy includes the design of an observer to infer the values of the product concentration and the feed concentration. In the next section, we describe this observer.

3. Nonlinear estimation

The objective of this section is to design an observer for estimating the unmeasured states to be used in the control calculation. Let us consider that the nonlinear model for the process is given by

$$\dot{x} = f(x, u), \qquad y = h(x) \tag{3}$$

where the vector $x \in \Re^n$ stands for the state vector and the input $u \in \Re$ represents the manipulated variable to accomplish the control objective and $y \in \Re$ is the system's output.

3.1. Model reformulation

The objective is to estimate only those states that cannot be measured. Then, a suitable reformulation of the system (3) is posed as follows:

$$\dot{x}_u = F_u(x_u, \bar{x}_u, u), \qquad \dot{\bar{x}}_u = \bar{F}_u(x_u, \bar{x}_u, u),$$
$$y = H(x_u, \bar{x}_u)$$

where x_u stands for the unmeasured states in vector x, and the rest of the states are symbolized as $\bar{x}_u$. Provided that $\bar{x}_u$ can be written as

$$\bar{x}_u = \bar{H}(x_u, y)$$

then

$$\dot{y} = \frac{\partial H}{\partial x_u} F_u + \frac{\partial H}{\partial \bar{x}_u} \bar{F}_u \triangleq \Psi(x_u, \bar{H}(x_u, y), u) \triangleq g_0(x_u, y, u),$$

$$\dot{x}_u = F_u(x_u, \bar{H}(x_u, y), u) \triangleq g_x(x_u, y, u)$$

Therefore, the system can be rewritten as follows:

$$\dot{x}_u = g_x(x_u, y, u) \tag{4}$$

$$\dot{y} = g_0(x_u, y, u) \tag{5}$$

The construction of the nonlinear observer herein proposed makes use of a change of coordinates, which has been frequently used in the design of high gain nonlinear observers [14,15]. Then, the following transform is introduced:

$$\begin{aligned} z_1 &\triangleq g_0(x_u, y, u) \\ z_2 &\triangleq g_1(x_u, y, u) \\ &\vdots \\ z_{n-1} &\triangleq g_{n-2}(x_u, y, u) \end{aligned} \tag{6}$$

This transform can be expressed in brief as $z = \gamma(x_\mathrm{u}, y, u) = [g_0\ g_1 \cdots g_{n-2}]^\mathrm{T}$; $z \in \Re^{n-1}$.

The dynamics in the z-domain are given by:

$$\begin{aligned}
\dot{y} &\stackrel{\triangle}{=} z_1 = g_0(x_\mathrm{u}, y, u)\\
\dot{z}_1 &= \left[\frac{\partial g_0}{\partial x_\mathrm{u}} g_x(x_\mathrm{u}, y, u) + \frac{\partial g_0}{\partial y} g_0(x_\mathrm{u}, y, u) + \frac{\partial g_0}{\partial u}\dot{u}\right]\\
&\stackrel{\triangle}{=} g_1(x_\mathrm{u}, y, u) + \rho_1(x_\mathrm{u}, y, u) + \varphi_1(x_\mathrm{u}, y, u)\dot{u}\\
\dot{z}_2 &= \left[\frac{\partial g_1}{\partial x_\mathrm{u}} g_x(x_\mathrm{u}, y, u) + \frac{\partial g_1}{\partial y} g_0(x_\mathrm{u}, y, u) + \frac{\partial g_1}{\partial u}\dot{u}\right]\\
&\stackrel{\triangle}{=} g_2(x_\mathrm{u}, y, u) + \rho_2(x_\mathrm{u}, y, u) + \varphi_2(x_\mathrm{u}, y, u)\dot{u}\\
&\vdots\\
\dot{z}_{n-1} &= \left[\frac{\partial g_{n-2}}{\partial x_\mathrm{u}} g_x(x_\mathrm{u}, y, u) + \frac{\partial g_{n-2}}{\partial y} g_0(x_\mathrm{u}, y, u) + \frac{\partial g_{n-2}}{\partial u}\dot{u}\right]\\
\dot{z}_{n-1} &\stackrel{\triangle}{=} g_{n-1}(x_\mathrm{u}, y, u) + \rho_{n-1}(x_\mathrm{u}, y, u) + \varphi_{n-1}(x_\mathrm{u}, y, u)\dot{u}
\end{aligned} \tag{7}$$

where

$$\frac{\partial g_{j-1}}{\partial x_\mathrm{u}} g_x = g_j, \qquad \frac{\partial g_{j-1}}{\partial y} g_0 = \rho_j, \qquad \frac{\partial g_{j-1}}{\partial u} = \varphi_j, \qquad j = 1, \ldots, n$$

If $\partial\gamma/\partial x_\mathrm{u}$ is not singular in (x_u, y, u), then there exists γ^i such that $x_\mathrm{u} = \gamma^i(z, y, u)$ is the function which allows calculating x_u from z, y and u. Therefore, the process model in the z-domain is:

$$\dot{z} = Az + \rho(z, y, u) + \varphi(z, y, u)\dot{u} \tag{8}$$

with $z \in \Re^{n-1}$, $\rho = [\rho_1 \cdots \rho_{n-1}]^\mathrm{T}|_{x_\mathrm{u}=\gamma^i(z,y,u)}$, $\varphi = [\varphi_1 \cdots \varphi_{n-1}]^\mathrm{T}|_{x_\mathrm{u}=\gamma^i(z,y,u)}$ and $A \in \Re^{(n-1)\times(n-1)}$:

$$A = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0\\ 0 & 0 & 1 & \cdots & 0\\ \vdots & \ddots & \ddots & \ddots & \vdots\\ 0 & \cdots & \cdots & \cdots & 1\\ 0 & \cdots & \cdots & \cdots & 0 \end{bmatrix}$$

3.2. Observer

The following observer is proposed to estimate the state vector in the transform domain z:

$$\dot{\hat{z}} = A\hat{z} + \rho(\hat{z}, y, u) + K[\dot{y} - \hat{z}_1], \qquad \nu \stackrel{\triangle}{=} \hat{z} - Ky \tag{9}$$

Then,

$$\begin{aligned}\dot{\nu} = \dot{\hat{z}} - K\dot{y}, \qquad \dot{\nu} &= A(\nu + Ky) + \rho(\nu + Ky, y, u)\\ &\quad - K(\nu_1 + k_1 y)\end{aligned} \tag{10}$$

with k_1 the first element of vector K.

Note that in the proposed observer, the constant K vector is the unique parameter to be designed. This parameter has to be calculated for guaranteeing the estimation error convergence. However, the observer is implemented through Eq. (10) to diminish the influence of measurement noise on the estimates.

3.3. Convergence of estimation error

Although the observer is implemented by using Eq. (10), Eq. (9) can be used to design K:

$$\begin{aligned}\dot{z} &= Az + \rho(z, y, u) + \varphi(z, y, u)\dot{u},\\ \dot{\hat{z}} &= A\hat{z} + \rho(\hat{z}, y, u) + KC(z - \hat{z})\end{aligned} \tag{11}$$

Let $e \stackrel{\triangle}{=} z - \hat{z}$ be the estimation error in z coordinates, then

$$\dot{e} \stackrel{\triangle}{=} \dot{z} - \dot{\hat{z}} = A_\mathrm{c} e + \Delta\rho + \varphi(z, y, u)\dot{u} \tag{12}$$

with $C = [10 \cdots 0]$, $\Delta\rho =^{\triangle} \rho(z, y, u) - \rho(\hat{z}, y, u)$ and $A_\mathrm{c} = (A - KC)$. To accomplish the observer's stability analysis, the dynamics of the error $e(t)$ in Eq. (12) is evaluated. In this way, a connection between the design parameter K and the stability of the estimation algorithm is obtained. A detailed description of the analysis procedure is provided in Appendix A. It should be noted that if the transformed system in Eq. (8) does not depend on $\dot{u}$ (that indeed occurs in many systems), then the estimation error converges asymptotically towards zero as $t \to \infty$. Otherwise, there is an ultimate bound which can become smaller by changing the design parameter K (see Appendix A).

3.4. Application to the CSTR

The state observer developed above is dedicated to the estimation of the internal state of the open-loop unstable CSTR. We know from the description in Section 2, that the temperature T inside the reactor is measured on-line, but the measurement of C is significantly delayed. Moreover, the system is perturbed by the unknown inlet concentration C_f. Therefore, the goal is to obtain an on-line estimation of C and C_f based on the measured variable T. To accomplish the estimation, the state vector is expanded to include the disturbance C_f. Then, the estimated vector is $x_\mathrm{u} = [\,C\ C_\mathrm{f}\,]$. Under the assumption that there is no information about the dynamics of C_f, then it is assumed slowly varying (i.e. $\dot{C}_\mathrm{f} = 0$).

For simplicity and to achieve better convergence properties, we choose a suitable transform to eliminate in Eq. (8) the dependence on $\dot{u}$:

$$\begin{aligned}
z_1 &= \frac{q}{V}(T_0 - T) - \frac{k_0\,\Delta H}{\rho C_p} C\,\mathrm{e}^{-E/RT},\\
z_2 &= \left(-\frac{q}{V} - \frac{k_0\,\Delta H}{\rho C_p} C \frac{E}{RT^2}\,\mathrm{e}^{-E/RT}\right)\\
&\quad \times \left[\frac{q}{V}(T_0 - T) - \frac{k_0\,\Delta H}{\rho C_p} C\,\mathrm{e}^{-E/RT}\right]\\
&\quad - \frac{k_0\,\Delta H}{\rho C_p}\dot{C}\,\mathrm{e}^{-E/RT}
\end{aligned}$$

This selection coincides with the expressions of $\dot{T}$ and $\ddot{T}$ without including the terms that contain the input q_c. Then, the original states can be recovered from the transformed ones as follows:

$$C = \frac{e^{E/RT}}{\beta_1}(\alpha_1 T - \alpha_1 T_f + z_1),$$
$$C_f = -\frac{e^{E/RT}}{\alpha_1\beta_1}\left[(\alpha_1 T - \alpha_1 T_f + z_1)\left(-\alpha_1 - k_0\, e^{-E/RT} + \frac{E z_1}{RT^2}\right) - \alpha_1 z_1 - z_2\right]$$

with $\alpha_1 = q/V$ and $\beta_1 = -\Delta H k_0/\rho C_p$. In this way, a stable reduced-order observer (i.e., only unmeasured variables are estimated) is applied for the nonlinear system to attain on-line estimation of the unmeasured process state and perturbation. Note that nonlinear observers such as the ones introduced in [14,15]are not suitable for this application. Because there is only one measured state and two variables to estimate, those full-order observers (i.e., both measured and unmeasured vectors are estimated) would not satisfy the requirement due to the observability constraint. Moreover, the reduced-order observer like the one developed in [15] cannot estimate both C and C_f, and other reduced-order techniques such as the ones introduced in [12,11] would involve tedious calculation and the convergence of the estimation error towards zero cannot be achieved.

Note that the observer herein introduced can be easily implemented and it is only based on the temperature measurement. 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.

Once the internal state of the system and perturbation can be observed, the nonlinear model predictive control technique based on state knowledge can be performed to achieve the desired control goal. This will be studied in the next section.

4. 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. In the 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 [17], 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 through 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 outputs deviations from their setpoints. This information is obtained for calculating the future manipulated variables.

The sequence of steps to follow in order to achieve the control action can be described as follows. First of all, the nonlinear original model of states x, the output y and control input u is the one given by Eq. (3):

$$\dot{x} = f(x, u), \qquad y = h(x)$$

The Euler discretization of this system gives:

$$x((k+1)\,\Delta t) = F(x(k\,\Delta t), u(k\,\Delta t)),$$
$$y(k\,\Delta t) = h(x(k\,\Delta t))$$

where Δt is the sampling time. For brevity, the model can be written as follows:

$$x(k+1) = F(x(k), u(k)), \qquad y(k) = h(x(k)) \tag{13}$$

The optimization problem for the typical NMPC formulation is [19]:

$$\min_{u(k|k),u(k+1|k),\ldots,u(k+M-1|k)} J = \phi[y(k+P|k)] + \sum_{j=0}^{P-1} L[y(k+j|k), u(k+j|k), \Delta u(k+j|k)], \tag{14}$$

where $u(k+1|k)$ is the input $u(k+1)$ calculated from information available at time k, $y(k+1|k)$ the output $y(k+1)$ calculated from information available at time k, $\Delta u(k+j|k) = u(k+j|k) - u(k+j-1|k)$, M the control horizon, P 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:

$$\begin{aligned} L = {} & [y(k+j|k) - y_s(k)]^T Q[y(k+j|k) - y_s(k)] \\ & + [u(k+j|k) - u_s(k)]^T R[u(k+j|k) - u_s(k)] \\ & + \Delta u(k+j|k)^T S\, \Delta u(k+j|k) \end{aligned} \tag{15}$$

$$\phi = [y(k+P|k) - y_s(k)]^T Q[y(k+P|k) - y_s(k)], \tag{16}$$

where $u_s(k)$ and $y_s(k)$ are steady-state targets for u and y, respectively. Q is a symmetric positive semi-definite penalty matrix on the states, R a symmetric positive definite penalty matrix on the inputs, and S a symmetric positive semi-definite

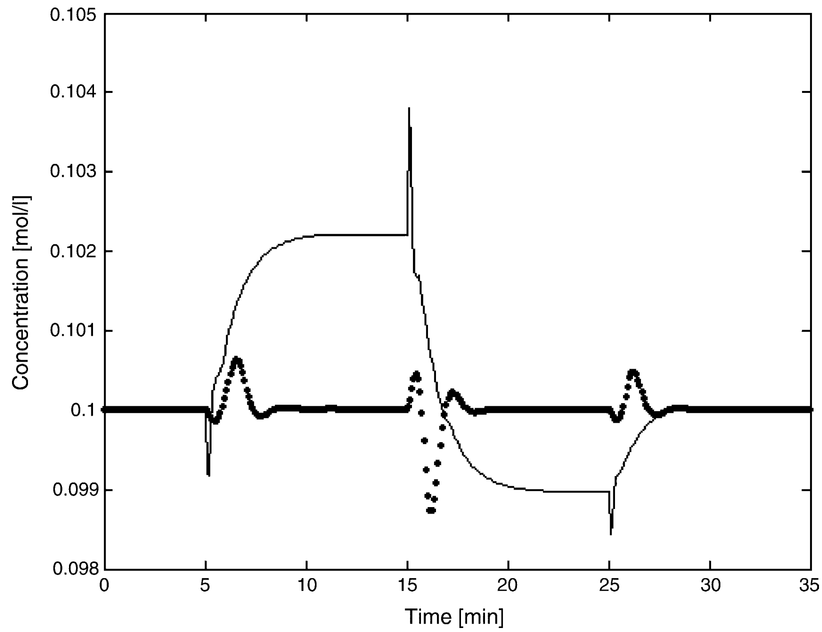

Fig. 2. Regulation results. NMPC based on RLS (full line) and NMPC based on NO (dotted line).

penalty matrix on the rate of change in the inputs. The principal controller tuning parameters are M, P, Q, R, S and the sample period Δt. It is important to note that this objective function is the most used in the literature, however, some authors use a more general approach and replace the output vector $y(k+j|k)$ by the state vector $x(k+j|k)$. This equivalent formulation has the drawback that in some applications the reference value for the states are not available (see example section).

The predicted output is obtained from the nonlinear model given by Eq. (13). Successive iterations of the model equations yield

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

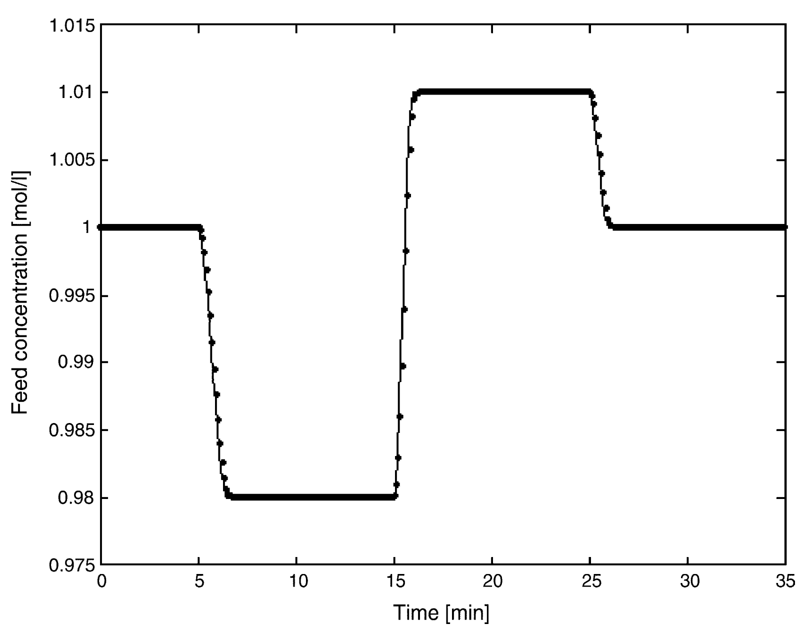

Fig. 3. Observer-based NMPC regulation.

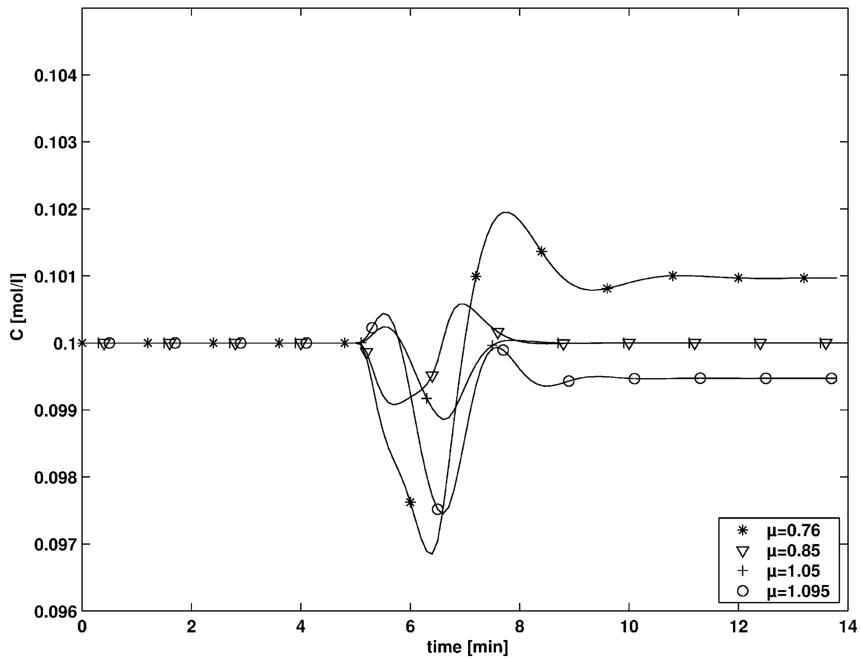

Fig. 4. Influence of the disturbance on the controller's performance.

where $x(k|k) = x(k)$ is a vector of current state variables. The control horizon M should be less than the prediction horizon P. Then, the output prediction is generated by setting inputs beyond the control horizon equal to the last computed value: $u(k + j|k) = u(k + M - 1|k)$, $M \leq j \leq P$. 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.

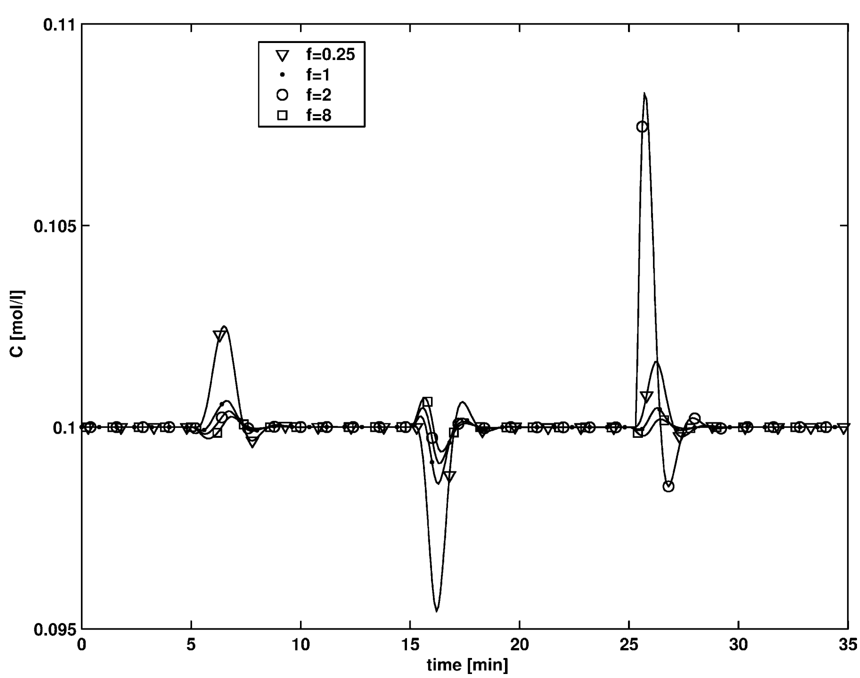

Fig. 5. Influence of the observer's gain.

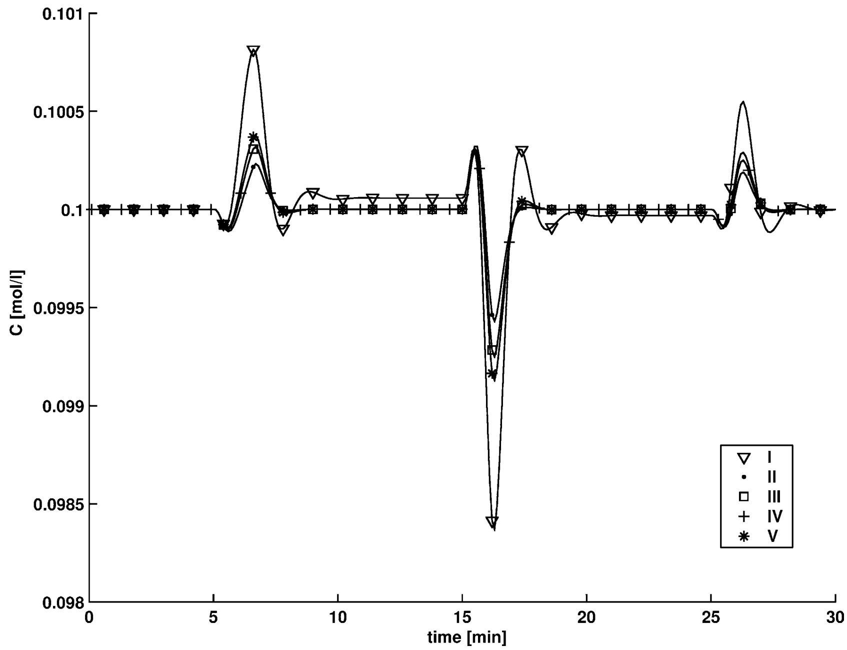

Fig. 6. Influence of the tuning parameters.

An important characteristic of process control problems is the presence of constraints on input, state and output variables. These constraints can be posed as

$$u^{\mathrm{L}} \leq u(k+j|k) \leq u^{\mathrm{U}}, \quad 0 \leq j \leq M-1,$$
$$\Delta u^{\mathrm{L}} \leq \Delta u(k+j|k) \leq \Delta u^{\mathrm{U}}, \quad 0 \leq j \leq M-1,$$
$$x^{\mathrm{L}} \leq x(k+j|k) \leq x^{\mathrm{U}}, \quad 1 \leq j \leq P-1,$$
$$y^{\mathrm{L}} \leq y(k+j|k) \leq y^{\mathrm{U}}, \quad 1 \leq j \leq P-1$$

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 can be found that some information about the state vector may be necessary. However, the whole state vector is hardly ever available through measurement. The simplest method to perform this correction

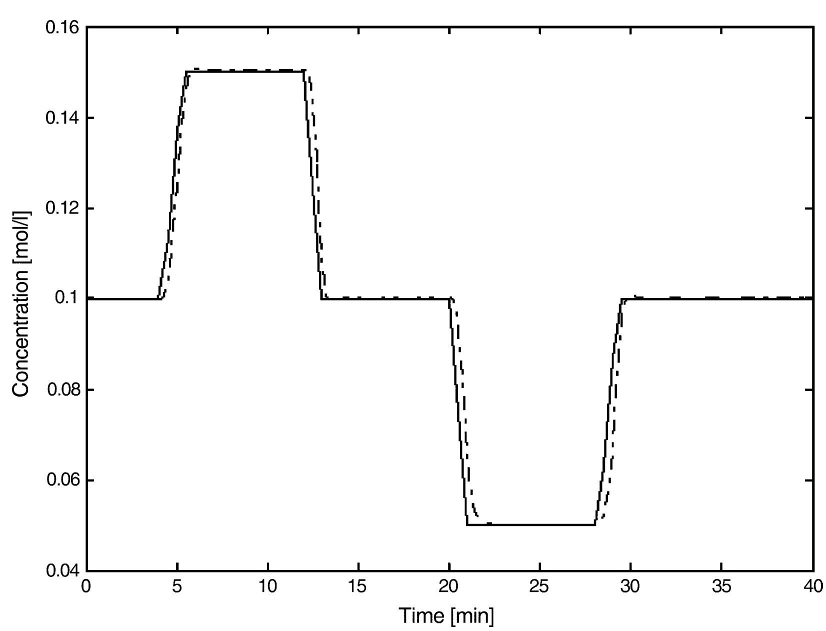

Fig. 7. NMPController/observer tracking.

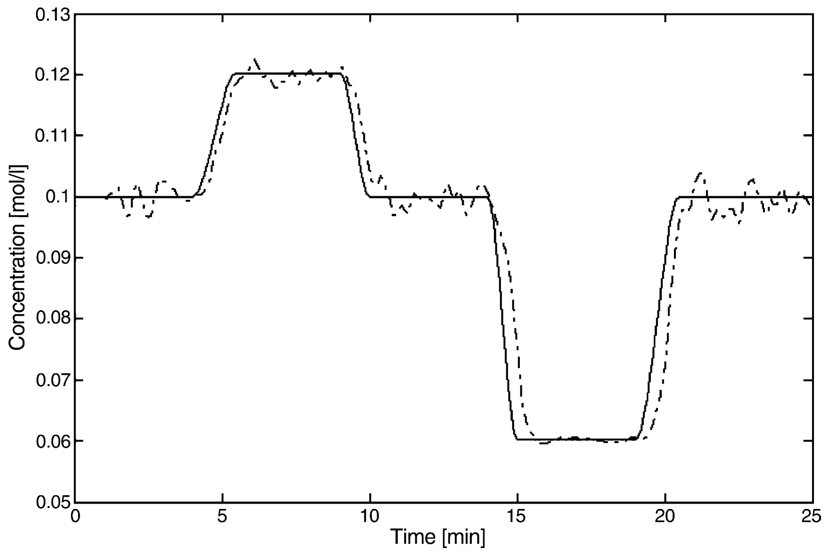

Fig. 8. NMPController/observer tracking based on noisy measurement.

is the use of an additive disturbance estimation $\hat{d}$. This approach is widely used in linear MPC (for example in DMC). The idea is to modify the output description given by Eq. (13) as follows:

$$y(k) = h(x(k)) + \hat{d}(k) \tag{17}$$

with

$$\hat{d}(k) = y_m(k) - y(k|k),$$
$$\hat{d}(k + j) = \hat{d}(k), \quad 1 \leq j \leq P - 1 \tag{18}$$

where the process output measurement $y_m(k)$ as well as the disturbance, are considered constant along the prediction horizon P. In order to provide more adequate variables estimations, based on the available measured outputs, a suitable state observer will be incorporated in this paper. The observer can be used to bring information about the unmeasured variables of the process. The advantage of using a closed-loop observer is that the internal state estimation will be more reliable than the estimation obtained by running the open-loop model (specially in the presence of dynamics uncertainty or in the case of unstable systems).

4.1. CSTR control

For the controller design, we use a discrete version of the process model. The objective function to be minimized is

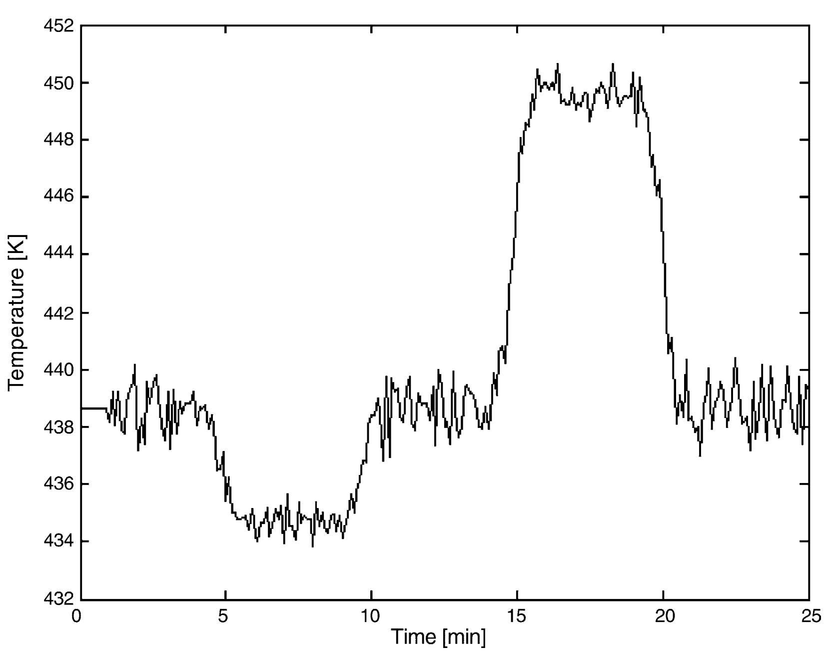

Fig. 9. Temperature (noise-corrupted measurement).

defined as follows:

$$f_{\mathrm{obj}} = Q\sum_{i=1}^{P}[C(\mathrm{i}\Delta t) - C^{\mathrm{sp}}]^2 + R\sum_{i=1}^{M}[q_{\mathrm{c}}(\mathrm{i}\Delta t) - q_{\mathrm{c}}((i-1)\Delta t)]^2 + S\sum_{i=1}^{M}[q_{\mathrm{c}}(\mathrm{i}\Delta t) - q_{\mathrm{c}}(0)]^2$$

where C^{sp} is the set point for the controlled variable, $Q = 8 \times 10^6$, $R = 500$ and $S = 0.005$. The controller parameters were tuned as follows: sample time $\Delta t = 0.1$ min, the prediction horizon $P = 20$ and the control horizon $M = 5$. To ensure small steady-state error the constraint $|C(P\,\Delta t) - C^{\mathrm{ss}}| < \varepsilon$ is imposed to the control problem, where ε is a small positive value. For the implementation of this scheme we consider that the temperature is measured and the disturbance C_{f} is unknown.

5. Simulation results

The developed observer/controller structure was tested for the CSTR regulation purpose. The goal was to keep the concentration inside the CSTR equal to 0.1 mol/l, in the presence of the unmeasured feed concentration disturbance. The good performance achieved by the observer/controller is plotted in Fig. 2 (dotted line). The controller's parameters Q, R and S were set to 8 000 000, 500 and 0.005, respectively, and the observer's gain was set to $K = [\,20\ \ 300\,]^{\mathrm{T}}$. The controller performance based on the nonlinear observer was compared with the results obtained when a recursive least squares (RLS) estimator [18] was added to the NMPController. RLS with directional forgetting together with the improved Euler method had been applied for the same CSTR [16], to estimate the reagent concentration when its measurement is delayed. The same method and settings that in [16] were used in this work. The results are shown in Fig. 2 (full line). The simulation was accomplished setting the forgetting factor to 0.9, the initial parameters vector equal to [1 1 0]. The initial value for the covariance matrix was set to $10^6 I$, with I the identity matrix. Both results depicted in Fig. 2 were obtained for the disturbance variation shown in Fig. 3. From the results, the proposed observer/controller structure evidences good performance to reject the disturbance. This is because the estimation provided by the observer converges to the actual state. On the other hand, the RLS estimation shows an offset when the unmeasured disturbance changes significantly.

To evaluate the observer/controller robustness for regulation purpose in the presence of different feed concentration variations, additional simulations were performed. For this purpose, the same operation point was considered. Fig. 4 shows the system output when the disturbance is increased μ times its nominal value. It was verified that the lower and upper disturbance variations that destabilize the system correspond to $\mu = 0.76$ and $\mu = 1.095$, respectively. Moreover, the controller's sensitiveness to changes in the tuning parameters was tested. First, the influence of the observer's design parameter K on the output was evaluated. For this purpose, the gain K was increased f times the initial value $K = [\,20\ \ 300\,]^{\mathrm{T}}$. The simulation results are depicted in Fig. 5. The closed-loop system shows a stable behavior for f between 0.25 and 8. For comparison purposes, a performance index defined as $I = (1/N)\sum_{k=1}^{N}[C(k) - C^{\mathrm{sp}}]$ (for $N = 351$ samples) was calculated. This index values goes from 5.74×10^{-7} to 1.57×10^{-8} for $f = 0.25$ and $f = 8$, respectively. It was also tested that the controlled system becomes unstable for $f = 23$. Secondly, a test was carried out to evaluate the influence of the controller tuning on the system output. Then, different values were assigned to the objective function parameters while the observer gain remains being $K = [\,20\ \ 300\,]^{\mathrm{T}}$. Table 2 presents the controller performance index I for the different settings of the objective function while Fig. 6 shows some of the outputs. In this way it was tested that the controlled system remains stable for a wide set of tuning parameters around the proposed nominal values.

Table 2
Controller's performance index

Parameters (Q, R, S)	Index, I
8×10^4, 500, 0.005 (case I)	6.2262×10^{-8}
8×10^6, 500, 0.005	1.2093×10^{-8}
8×10^7, 500, 0.005	Unstable
8×10^7, 500, 0.005	Unstable
8×10^6, 50, 0.005	Unstable
8×10^6, 100, 0.005	3.8323×10^{-9}
8×10^6, 250, 0.005 (case II)	7.2508×10^{-9}
8×10^6, 750, 0.005 (case V)	1.6205×10^{-8}
8×10^6, 500, 0.0005	1.2085×10^{-8}
8×10^6, 500, 0.001 (case III)	1.2086×10^{-8}
8×10^6, 500, 0.01 (case IV)	1.2102×10^{-8}
8×10^6, 500, 0.1	Unstable

The results in Fig. 7, show the observer-based controller is also able to track a reference signal. Another test for concentration tracking is shown in Fig. 8. In this case, the information is based on a noise-corrupted temperature measurements. The measured temperature is constructed by adding to the real deterministic process output a white noise signal whose statistics are mean 0.50 and variance 0.34. The temperature inside the reactor is depicted in Fig. 9.

These results illustrate the robust performance of the observer-based controller, even when the CSTR is a critical nonlinear process under significant disturbance variation and in the presence of noisy measurements.

6. Conclusions

In this work, the objective was to develop a nonlinear model-based controller using nonlinear state estimation. The purpose was accomplished by incorporating a nonlinear full-order state observer to the existing nonlinear model predictive control theory.

The developed controller results computationally efficient and performs well, even in the case of regulation as well as tracking. Additionally, the controller exhibits good behavior when both the controller and the estimator use noisy measurements.

The simulation results showed good agreement between the actual and estimated states, as well as a successful behavior of the controller/observer structure.

Appendix A

For the stability analysis introduced in Section 3.3, the following function V is proposed:

$$\begin{aligned} V &= e^T P_0 e, \\ \dot{V} &= \dot{e}^T P_0 e + e^T P_0 \dot{e} \\ &= e^T A_c^T P_0 e + \Delta\rho^T P_0 e + \varphi^T \dot{u} P_0 e + e^T P_0 A_c e \\ &\quad + e^T P_0 \Delta\rho + e^T P_0 \varphi \dot{u}, \\ \dot{V} &= e^T (A_c^T P_0 + P_0 A_c) e + 2\Delta\rho^T P_0 e + 2\varphi^T \dot{u} P_0 e \end{aligned} \tag{A.1}$$

with P_0 a positive definite matrix. Due to Eq. (A.1), the following inequalities hold:

$$p_{\min} \|e\|^2 \le V \le p_{\max} \|e\|^2 \tag{A.2}$$

where $p_{\min}$ and $p_{\max}$ are the minimum and maximum eigenvalues of P_0, respectively. Provided that there exist positive values M_0 and L_0 such that $\|\varphi^T \dot{u}\| \le M_0$ and $\|\Delta\rho\| \le L_0 \|e\|$, then

$$\dot{V} \le -q_{\min} \|e\|^2 + 2 p_{\max} L_0 \|e\|^2 + 2 p_{\max} M_0 \|e\| \tag{A.3}$$

where $q_{\min}$ is the minimum eigenvalue of Q_0, with Q_0 a positive definite matrix solution of $(A - KC)^T P_0 + P_0 (A - KC) = -Q_0$. Then:

$$\dot{V} \le (-q_{\min} + 2 p_{\max} L_0) \frac{V}{p_{\min}} + 2 \frac{p_{\max}}{\sqrt{p_{\min}}} M_0 \sqrt{V} \tag{A.4}$$

$$\frac{\dot{V}}{2\sqrt{V}} \le -\sigma \sqrt{V} + \xi \tag{A.5}$$

with $\sigma \triangleq q_{\min} - 2 p_{\max} L_0 / 2 p_{\min}$ and $\xi \triangleq p_{\max} M_0 / \sqrt{p_{\min}} > 0$. If K is chosen to satisfy the inequality $q_{\min} > 2 p_{\max} L_0$, then $\sigma > 0$. From Eq. (A.5):

$$\frac{\mathrm{d}\sqrt{V}}{\mathrm{d}t} \le -\sigma \sqrt{V} + \xi$$

$$\sqrt{V} \le \sqrt{V(0)}\, \mathrm{e}^{-\sigma t} + \int_0^t \mathrm{e}^{-\sigma(t-\tau)} \xi \, \mathrm{d}\tau \tag{A.6}$$

$$\sqrt{V} \le \sqrt{V(0)}\, \mathrm{e}^{-\sigma t} + \xi\, \mathrm{e}^{-\sigma t} \int_0^t \mathrm{e}^{\sigma \tau} \, \mathrm{d}\tau \tag{A.7}$$

$$\sqrt{V} \le \sqrt{V(0)}\, \mathrm{e}^{-\sigma t} + \frac{\xi}{\sigma} [1 - \mathrm{e}^{-\sigma t}] \le \sqrt{V(0)}\, \mathrm{e}^{-\sigma t} + \frac{\xi}{\sigma} \tag{A.8}$$

and taking into account the inequalities in Eq. (A.2):

$$\|e\| \le \mathrm{e}^{-\sigma t} \sqrt{\frac{p_{\max}}{p_{\min}}} \|e(0)\| + \frac{\xi}{\sigma} \tag{A.9}$$

Denoting $\kappa = \sqrt{p_{\max}/p_{\min}}$ and $\lambda = \xi/\sigma$:

$$\|z - \hat{z}\| \le \kappa\, \mathrm{e}^{-\sigma t} \|z(0) - \hat{z(0)}\| + \lambda \tag{A.10}$$

Because

$$x_u - \hat{x}_u = \gamma^i(z, y, u) - \gamma^i(\hat{z}, y, u) \tag{A.11}$$

and

$$\|x_u - \hat{x}_u\| \le L_{\gamma^i} \|z - \hat{z}\| \tag{A.12}$$

with L_{γ^i} a Lipschitz constant for γ^i, and because $\|z - \hat{z}\| \le L_\gamma \|x_u - \hat{x}_u\|$, then

$$\|x_u - \hat{x}_u\| \le L_{\gamma^i} L_\gamma \kappa\, \mathrm{e}^{-\sigma t} \|x_u(0) - \hat{x}_u(0)\| + \lambda \tag{A.13}$$

It should be noted that if the transformed system in Eq. (8) does not depend on $\dot{u}$, then M_0 is zero. Besides, $\lambda = 0$ and then the error $\|x_u - \hat{x}_u\|$ converges asymptotically towards zero as $t \to \infty$. On the other hand, if $\lambda \ne 0$, there is an ultimate bound which can become smaller by changing the design parameter K.

Note that Eq. (A.3) establishes a sufficient condition to guarantee stability. However, in some cases it may be a rather conservative result. As a consequence of this fact, in many applications good estimation performance could be achieved even when Eq. (A.3) is not strictly satisfied.

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