8th International IFAC Symposium on
Dynamics and Control of Process Systems
Preprints Vol.1, June 6-8, 2007, Cancún, Mexico

CONSTRUCTIVE MPC OF A CLASS OF EXOTHERMIC CSTRs

José Figueroa[(1)*], Silvina Biagiola[(1)], and Jesús Álvarez[(2)]

(1) Departamento de Ingeniería Eléctrica y de Computadoras, Universidad Nacional del Sur – CONICET, Av. Alem 1253, (8000) Bahía Blanca, ARGENTINA.
(2) Departamento de Ingeniería de Procesos e Hidráulica, Universidad Autónoma Metropolitana, Unidad Iztapalapa, Apartado Postal 55534, 09340 D.F., MEXICO.)
** Corresponding author: e-mail:figueroa@uns.edu.ar ; Fax: +54-291-45955154*

Abstract: In this paper is addressed the problem of controlling a (possible open-loop unstable) CSTR with flow and temperature measurements, with emphasis on the attainment of control robustness, linearity, decentralization, and model independency features. The combination of constructive and MPC ideas yields: (i) an unconstrained controller that is optimal with respect to a meaningful objective function, does not need ~~to~~ the on-line solution of a two-point boundary value problem (TPBVP), and yields the same behavior than the one of a conventional nonlinear MPC, and (ii) a constructive MPC that handles constraints and is simpler and less model dependent than its nonlinear MPC counterpart. The proposed approach is tested with a representative example through simulations.

Keywords: Inventory control, PI, Model-based control, Nonlinear systems, Reactor control, State observers.

1. INTRODUCTION

The control of exothermic reactors has been the subject of extensive research, mainly to their outstanding nonlinearity features such as multiplicity and open-loop instability. The exothermic reactor process has been a benchmark example for almost all control studies (Aris and Amundson, 1958; Cebuhar and Constanza, 1984; Hoo and Kantor, 1985; Álvarez *et al.*, 1989; Álvarez *et al.*, 1984; Viel *et al.*, 1997; Gauthier and Kupka, 2001; Antonelli and Astolfi, 2003; Biagiola and Figueroa, 2004). In industrial practice, these reactors are controlled with PI cascade linear control, and possibly feed dosage manipulation according to supervisory control.

The Model Predictive Control (MPC) strategy constitutes the most accepted advanced control approach in industrial applications (Bemporad and Morari, 1999). Basically, the MPC on-line solves a model-based constrained optimization problem over a receding time-horizon, and its adequate functioning, depends on suitable choices of control (linear or nonlinear) model, objective function, and tuning parameters (namely, input and output penalizing weights, sampling time, prediction and control horizon) (Bemporad and Morari, 1999). Provided these design choices are appropriately made, the MPC yields robust behavior with constraint handling.

While the linear MPC has been widely studied and tested on nonlinear continuous processes (Qin and Badgwell, 1997), the applicability-oriented development of the nonlinear MPC version lags behind. For instance, the nonlinear MPC controllers for exothermic chemical reactors are perceived as too complex (*i.e.*, nonlinear, strongly coupled, and heavily model dependent) when compared with the conventional control schemes employed in industrial practice (Luyben, 1990; Shinskey, 1988). In fact, there is an on-going controversy on whether the reported benefits of MPC industrial applications (Luyben, 2004) are due to the MPC strategy *per se*, or to the associated upgrade of equipment, and instrumentation, as well as of monitoring and of conventional control components (Ricker, 1990; Luyben, 1990).

According to the nonlinear constructive control design approach (Krstić *et al.*, 1995): (i) optimal controllers are inherently robust (meaning that MPC belongs to this class) and passive with respect to some input-output pair, (ii) in the unconstrained case, the optimization problem can be circumvented via inverse optimality, by designing a passive controller and *a posteriori* verifying its optimality, and (iii) the particular system and its model structure (*i.e.*, controllability and observability) must be exploited to perform an interlaced estimator-control design. Recently, these constructive ideas have been applied to design polymerization reactor (González and Álvarez, 2005; Álvarez and González, 2006) and distillation column (Castellanos-Sahagún *et al.*, 2005;

2006a,b) control schemes with emphasis on the attainment of linearity, decentralization and model independency features. The resulting schemes contain linear and nonlinear components, including PI and material balance elements, and is referred to as PI-inventory control (PIIC). On the basis of theoretical arguments in constructive control, it was claimed that the aforementioned polymer reactor and distillation control schemes: (i) recovered the behavior as an exact model-based nonlinear passive controller, and (ii) were equivalent to an infinite-horizon unconstrained nonlinear MPC. However, the latter equivalence claim has not been comparatively demonstrated against the nonlinear MPC strategy.

In this paper the problem of controlling an exothermic reactor with temperature and flow measurements is addressed within a framework that combines constructive control and MPC ideas. First, the unconstrained case is considered in order to assess the equivalence between the constructive PIIC and nonlinear MPC. Then, the constrained case is addressed by combining the constructive PIIC and MPC approaches, yielding a scheme that: (i) inherits the simplicity and reduced model dependency of the PI-I controller and the constraint handling capability of the MPC, and (ii) is considerably simpler than its conventional nonlinear MPC counterpart. The proposed approach is tested with a representative example through simulations.

2. CONTROL PROBLEM

Consider a continuous chemical reactor (depicted in Figure 1), where a first-order exothermic reaction takes place, heat being removed by means of a jacket with recirculation system. The reactant is fed at rate q, concentration c_e, and temperature T_e, the volume is kept fixed by controlling the exit flow rate $q = q_e$, and the heat removal is performed by feeding a coolant flow rate q_c at temperature T_{je}. The reactor may exhibit steady-state multiplicity. Its dynamics are described by the following mass and energy balances (Aris, 1958; Russo and Bequette, 1995):

$$\begin{aligned} &\dot{c} = -\rho(c,T) + q(c_e - c), && z = c \\ &\dot{T} = \beta\rho(c,T) + q(T_e - T) - \delta(T - T_j), && y_T = T \\ &\dot{T}_j = \delta_1 q_c\,(T_{je} - T_j) + \delta\delta_1\delta_2(T - T_j), && y_j = T_j \end{aligned} \quad (1)$$

where $\rho(c,T) = \phi\, c\, \kappa(T)$ and $\kappa(T) = \exp[T/(1+T/\gamma)]$.

The *states* are, in dimensionless form, the reactant concentration c, and the reactor (or jacket) temperature T (or T_j). The coolant flow q_c is the *control input*. The concentration c is the *regulated-unmeasured output z*, the temperature T is the *measured-regulated output* y_T, and y_j is the jacket temperature measurement. The feed composition c_e and the reactor (or jacket) feed temperature T_e (or T_{je}), are *exogenous disturbances*, with T_e and T_{je} (or c_e) being a measured (or unmeasured) variable. The controllability test for the affine nonlinear control system in (1) can be accomplished by means of a rank condition assessment (Isidori, 1995).

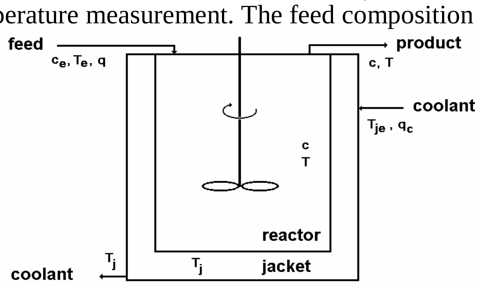

Fig. 1. Jacketed CSTR.

3. PI-INVENTORY CONTROL

In this section, the constructive approach-based PII control scheme, originally developed in the context of polymer (González and Álvarez, 2005; Álvarez and González 2006), and non-monotonic (Díaz-Salgado *et al*., 2006) reactors is recalled, with one difference: here, the two-state EKF estimator for the concentration control component (Díaz-Salgado *et al*., 2006) is replaced by a single-state geometric estimator.

3.1 Control model

The idea behind the constructive PII reactor control design is an interlaced estimator-control design on the basis of a control model with maximum linearity, decentralization and model independency features, according to a suitable controllability-detectability structure. For this aim, let us rewrite the reactor nonlinear system (1) in the form:

$$\dot{c} = -r + q(c_e - c); \quad \dot{T} = a_T T_j + b_T; \quad \dot{T}_j = a_j\, q_j + b_j\,, \quad (2)$$

where $a_j \approx \bar{\delta}_1\bar{\delta}(\bar{T}_{je} - \bar{T})$, $a_T \approx \bar{\upsilon}$, r=ρ(c,T), $b_j = a\upsilon(T - T_j)$, $b_T = \beta\rho(c,T) + q(T_e - T) - \upsilon T$ and a_j and a_T are approximated steady-state values. Since the terms b_T and b_j are observable, in the sense that they can be quickly reconstructed via a suitable observer, they are assumed to be in slow varying regime with respect to the observer dynamics, which is a standard assumption in signal derivative estimation (Papoulis, 1965). Accordingly, the *control model* is given by:

$$\begin{aligned} &\dot{c} = -r + q\,(c_e - c), \quad z = c, \quad y_r = r = \rho(c,T) \\ &\dot{T} = a_T T_j + b_T, \quad y_T = T, \quad \dot{b}_T \approx 0 \\ &\dot{T}_j = a_j\, q_j + b_j\,, \quad y_j = T_j, \quad \dot{b}_j \approx 0 \\ &r = \{b_T + b_j / [a(1 - y_j / y_T)] - q(T_e - y_T)\}/\beta \end{aligned} \quad (3)$$

where the reaction rate value r is determined, via the dynamic heat balances, by the observable pair (b_T, b_j), and consequently, y_r is regarded as a "virtual measurement" (González and Álvarez, 2005: Díaz-Salgado *et al*., 2006). This model has the following controllability-detectability structure:

$rd(q_j, y_T) = 2$, $rd(q, z) = 1$, stable ZD (4a)

$eo(b_T, y_T) = eo(b_j, y_j) = eo(c, y_r) = 1$ (4b)

where *rd* denotes "relative degree", ZD "zero-dynamics" (*i.e*, the concentration dynamics in isothermal regime), and *eo* denotes "estimation order".

3.2 Interlaced estimator-control design

From the enforcement of the temperature-composition closed-loop dynamics

$$\dot{T} = -k_T\,(T - T_{sp})\,, \qquad \dot{c} = -k_c\,(c - c_{sp})$$

upon the control model (3), the PI-inventory control scheme follows (González and Álvarez, 2005; Díaz-Salgado *et al*., 2006):

Cascade temperature controller

$$\dot{\chi}_T = -\omega_T\,\chi_T - \omega_T^2\,T - \omega_T\,a_T\,T_j\,, \qquad \hat{b}_T = \chi_T + \omega_T\,T$$

$$\dot{\chi}_j = -\omega_j\,\chi_j - \omega_j^2\,T_j - \omega_j\,a_j\,q_j, \qquad \hat{b}_j = \chi_j + \omega_j\,q_j$$

$$\dot{T}_j^* = -(\dot{b}_T + k_T\,\dot{T})/a_T \tag{5a}$$

$$q_j = \left\{-\left[\dot{b}_T + k_T(a_T T_j^* + b_T)\right]/a_T - b_j - k_j(T_j - T_j^*)\right\}/a_j \tag{5b}$$

Composition controller

$$\partial_c\rho(\hat{c}, y_T) = \frac{\partial\rho(c, y_T)}{\partial c} = \phi k(y_T)$$

$$q = \left[-k_c(\hat{c} - c_{sp}) + y_r\right]/(c_e - \hat{c}) \tag{6a}$$

$$\dot{\hat{c}} = -y_r + q\,(c_e - \hat{c}) + \left[\frac{\omega_c}{\partial_c\rho(\hat{c}, y_T)}\right][y_r - \rho(\hat{c}, y_T)] \tag{6b}$$

$$y_r = \left[\hat{b}_T - q(T_e - T) + \hat{b}_j/a + a_T T_j\right]/\beta$$

As mentioned before, here the two-state EKF concentration component (Díaz-Salgado *et al.*, 2006) has been replaced by a single-state geometric estimator, because the present reaction rate is monotonic with concentration. Component (5) is a linear-decentralized cascade controller with primary and secondary PI loops, and component (6) is an observer-based material balance controller driven by the information contained in the integral states of the temperature controller. Excepting its nonlinear innovation gain, the concentration dynamic controller is linear, meaning that it suffices to have a reasonable tendency reaction rate model. According to theoretical arguments (González and Álvarez 2005, Álvarez and González, 2006), the preceding controller: (i) recovers the behavior of an exact model-based nonlinear passive controller, and (ii) is equivalent to an unconstrained nonlinear MPC with respect to a meaningful objective function over an infinite receding horizon.

3.3 Convergence and tuning

The closed-loop robust convergence assessment coupled to easy-to-apply conventional-like tuning guidelines can be seen elsewhere (González and Álvarez, 2005; Álvarez and González, 2006), and here it suffices to mention that closed-loop robust nonlocal stability is attained by tuning: (i) the secondary temperature control gain sufficiently faster than its primary counterpart ($k_j > k_T$), (ii) the temperature observer gains sufficiently faster than the control gains ($\omega_T, \omega_j > k_T, k_j$), but not faster than the high-frequency unmodeled dynamics, and (iii) the concentration observer gain (ω_c) sufficiently faster than the related control gain (k_c), but not faster than the temperature observer gains.

Summarizing, the PI-I controller (5) is equivalent to an unconstrained nonlinear MPC over an infinite receding horizon, has rather modest modeling requirements, namely two static parameters (a_T and a_j), and a tendency reaction rate model to perform the innovation in the concentration estimator (6b). The cascade T controller (5) is linear and decentralized, and the composition controller (6) is nearly a linear filter. The tuning can be efficiently performed with conventional tuning rules employed in industrial practice. If the reaction rate is non-monotonic (i.e., ρ has a maximum with c), the term $\partial_c\rho$ vanishes at maximum reaction rate, and the geometric concentration estimator component (5) must be replaced by an EKF (Diaz-Salgado *et al.*, 2005)

4. CONSTRUCTIVE MPC

As it stands, the PII controller (5) can only contribute to prevent input saturation because of its inherent optimality-based non-wasteful feature, but cannot anticipate and cope with saturation in the way the MPC controller does. This consideration motivates the pursuit, in this section, of a combined constructive-MPC design.

4.1 Conventional nonlinear MPC

In this subsection, the nonlinear MPC (NMPC) reactor control scheme (Biagiola and Figueroa, 2004) is recalled, with: (i) a Luenberger-type nonlinear observer

$$\dot{\hat{x}} = f(\hat{x}) + g(\hat{x})\,u + \vartheta^{-1}(\hat{x})G\;(y - C\,\hat{x}) \tag{7}$$

where x represents the CSTR states (i.e. c, T and T_j), y is the vector of measurements (i.e. T and T_j), and $\vartheta^{-1}(\hat{x})G$ is the innovation gain, and G is an adjustable gain, and (ii) the discrete nonlinear state-feedback controller as the on-line solution of the optimization problem (Meadows and Rawlings, 1997; Allgöwer and Zheng, 1991)

$$\min_{u(k|k),u(k+1|k),\ldots,u(k+M-1|k),} J = \Phi\left[x(k+P\mid k)\right] + \sum_{j=0}^{P-1} L\left[x(k+j\mid k), u(k+j\mid k), \Delta u(k+j\mid k)\right] \tag{8}$$

subject to (input, state, output) constraints

$$\Delta u(k+j|k) = u(k+j|k) - u(k+j-1|k)$$

where $u(k+1|k)$ is the input calculated from information at time k, $x(k+1|k)$ is the one-step ahead prediction of the state, M is the control horizon, P is the prediction horizon and Φ and L are (possibly) nonlinear weight functions that must be chosen to effectively penalize state deviations and control effort. The use of a detailed nonlinear process model is intended to fully exploit the information on the process dynamics.

The combination of the state-feedback MPC with the nonlinear observer (7) yields the output-feedback MPC. At each time-step, the solution of the optimization problem (8) yields the future input sequence, its first entry is applied to the process, and then, in the next step, a new measurement is incorporated, the future sequence input is recomputed, its first entry is applied to the process, and so on.

The advantages of this controller are its robustness and constraint handling capability, and its disadvantages are: (i) the complexity (nonlinearity and strong interaction) of the control system, when compared with its industrial counterparts, (ii) the tuning of the observer-controller is a complex procedure that depends heavily on designer experience and skills, and (iii) the design overlooks the controllability-observability properties that determine the control capabilities and limitations.

4.2 Constructive MPC

Motivated by the aforementioned advantages and limitations of the PIIC and NMPC approaches, in this section is considered a combined constructive PIIC-MPC (CMPC) approach to the reactor control problem, according to the following rationale: (i) the linear model and the associated estimator of the PIIC, underlie by a robust controllability-detectability structure, are employed, and (ii) the constrained controller is built according to the MPC technique.

The constructive MPC is built as follows: (i) the estimator (5a) (linear-decentralized model plus data assimilation mechanism) of the PII control, is rewritten in discrete-time form (9),

$$
\begin{aligned}
c(k+1) &= T_s\left(-r+q(k)(c_e-c(k))\right)+c(k) \\
T(k+1) &= T_s\left(a_T T_j(k)+\hat{b}_T\right)+T(k) \\
T_j(k+1) &= T_s\left(a_j\, q_j(k)+\hat{b}_j\right)+T_j(k)
\end{aligned}
\tag{9}
$$

where T_s is the time interval, and (ii) the PII state-feedback controller is replaced by the on-line solution of the constrained optimization (8).

By doing so, the resulting *constructive MPC* (8-9): (i) is more linear, decentralized and model independent than its conventional nonlinear MPC counterpart (7-8), (ii) includes the design of a suitable model on the basis of the reactor controllability-detectability structure, (iii) attains optimality-based robustness with constrained handling capability.

The tuning of the estimator is performed according to the tuning guidelines of the PIIC controller, and the tuning of the controller is performed according to the guidelines of the MPC. Moreover, the tools of the stability-oriented PIIC can be applied to assess the closed-loop stability of the proposed CMPC.

5. CLOSED-LOOP BEHAVIOR

5.1. Open-loop behavior

To set a severe test for the control schemes, the reactor is set so that it has three steady-sates, two stable ones (ignition and extinction), and one unstable (saddle-type)

$$(c, T, T_j, V)^T = (0.5818, 2.6000, 0.1149, 1)^T$$

which constitutes the prescribed operation. The model parameters are in Nagrath *et al.* (2002) and Russo and Bequette (1995); and the control variables are q_c=0.6687, q=1.

Figure 2 presents the reactor response, from the neighbourhood of the unstable steady-state, with a +1% deviation in concentration. As it can be seen in the figure, the reactor reaches the extinction regime, and this in turn displays the control objective: to maintain the closed-loop reactor about the open-loop unstable steady-state (Biagiola and Figueroa, 2004).

5.2 Tuning

The application of its tuning guidelines yielded a PIIC (5-6) with the following gains:

$$k_T=k_i=20,\ k_c=2,\ \text{and}\ \omega_T=\omega_j=\omega_c=5 \tag{10}$$

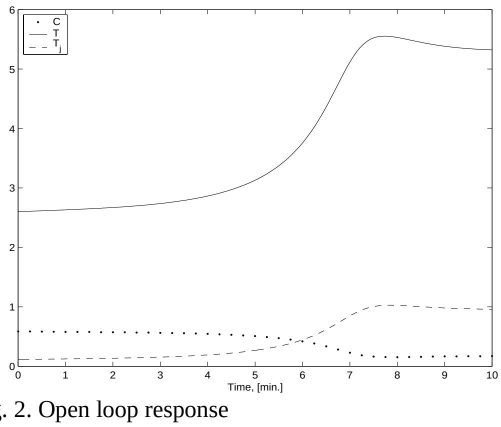

Fig. 2. Open loop response

The *conventional NMPC* was set with: (i) a Luenberger-type nonlinear observer (Papoulis, 1965) and constant innovation gain G =[1.15 0; 1.32 0.25; 0 0.75], and (ii) the quadratic objective function

$$\Phi=\left[x(k+j\mid k)-x_s(k)\right]^T Q\left[x(k+j\mid k)-x_s(k)\right]$$

$$
\begin{aligned}
L=&\left[x(k+j\mid k)-x_s(k)\right]^T Q\left[x(k+j\mid k)-x_s(k)\right]+ \\
&\left[\Delta u(k+j\mid k)-\Delta u_s(k)\right]^T S\left[\Delta u(k+j\mid k)-\Delta u_s(k)\right]
\end{aligned}
\tag{11}
$$

where u_s and x_s are steady-state targets for u and x, respectively. The values selected for the weights were: Q = diag{50, 1000, 0}; S = diag{1, 3}. The time interval was T_s=0.05, and the state and input horizons were P=20 and M=5, respectively.

It must be pointed out that the tuning of the constructive PIIC was considerably simpler than the one of the NMPC.

The *constructive MPC* was with: (i) the estimator model and gains (5) of the PIIC (10), and (ii) the objective function (11) of the NMPC. For comparison purposes, the gains of the constructive MPC were not retuned, in the understanding that better (smoother) can be obtained with further tuning.

5.3 Closed-loop behavior without constraints

The performances of the observer-based controllers are illustrated through simulation results, for tracking of concentration and temperature trajectories. The initial state conditions are: c(0)=0.58, T(0)=2.60, and T_j(0)=0.12. The reactor closed-loop behaviors with PIIC, NMPC and constructive MPC are presented in Figure 3, showing that: (i) the three controllers yield the same overall behavior, (ii) the PIIC and conventional NMPC have similar responses, and (iii) with the gains inherited from the PIIC and NMPC designs, the CMPC yields a more oscillatory response, that can be improved by retuning (not shown here).

These results verify that, as claimed on the basis of theoretical grounds (González and Álvarez, 2005; Álvarez and González, 2006): indeed, the constructive approach-based PI-inventory controller (5-6) behaves like an unconstrained nonlinear MPC (subsection 4.1). With a considerably simpler construction, the constructive MPC yields a behavior than resembles the one of its nonlinear MPC counterpart.

5.4 Closed-loop behavior with constraints

Let us assume that the coolant system flow is limited as follows $0\le q_c\le 2$ (Nagrath *et al.*, 2002), and that a 2.6-to-2.4 temperature decrease must be tracked. The reactor closed-loop behaviors with PIIC (5-6), NMPC (7-8) and constructive MPC (8-9) are presented in Fig. 4. Note that: (i) in all the cases the reactor is stabilized in the presence of constraints, however, for the NMPC the concentration exhibits an overshoot which makes this option inadmissible, (ii) at the cost of more control effort, the PIIC yields a faster response, (iii) the CMPC displays a better constraint handling capability, (iv) the optimality property that underlies the PIIC design manifests itself to deal well with constrains which is due to the nonwasteful feature of optimal controllers.

5.5 Closed-loop behavior with model errors

As a robustness test, the model heat of reaction (β)

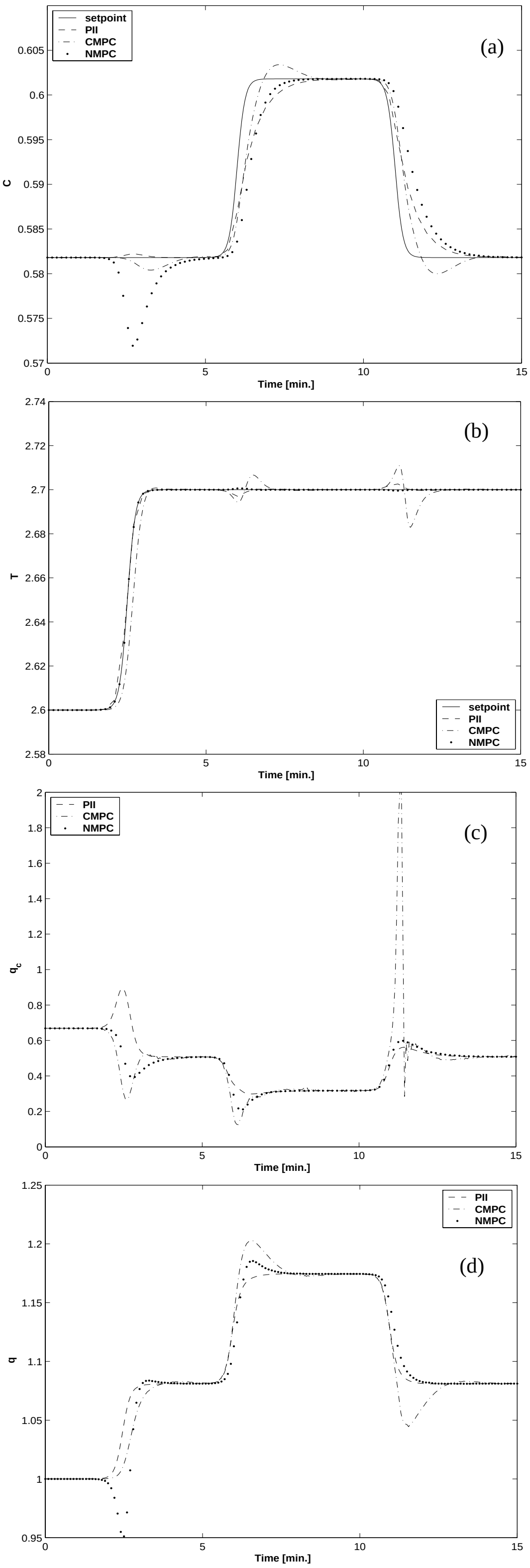

Fig. 3. (a) Concentration, (b) Temperature, (c) Coolant flow rate (q_c) and (d) Feed flow rate response (q) responses with unconstrained PIIC, NMPC and CMPC.

was set 5% greater than its actual value. The corresponding closed-loop responses of the PIIC, NMPC and CMPC without constraints are presented in Fig. 5, showing that: (i) the three controllers stabilize the reactor, (ii) the three controllers yield some (rather small) concentration offset, with the CMPC (or PIIC) yielding the largest (or smallest) offset, and (iii) while the PIIC and CMPC tracks the temperature without offset, the NMPC yields some offset. The excessive excursions of the temperature response with CMPC can be attenuated by estimator-control gain retuning (not shown here).

5.6 Concluding remarks

From the preceding tests the next conclusions follow: (i) as is predicted by the constructive control theory (González and Álvarez, 2005; Álvarez and González, 2006), the PIIC is a particular case of unconstrained NMPC, and behaves accordingly, (ii) CMPC can manage the regulation-stabilization control problem subject to constraints while construction and tuning procedures are considerably simpler than the ones of the conventional NMPC as well as less modelling dependant~~,~~ and (iii) suitable estimator-control running guidelines as well as more systematic objective function selection criteria should be developed for the proposed CMPC technique.

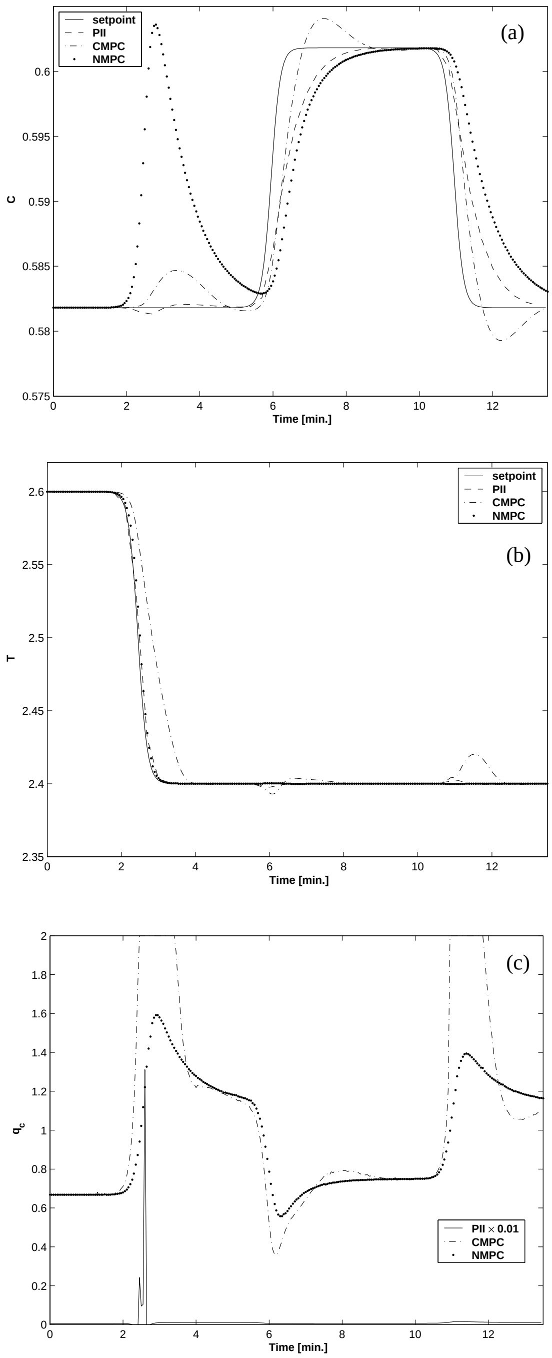

Fig. 4. (a) Concentration, (b) Temperature and (c) Coolant flow rate response with constrained PIIC and CMPC.

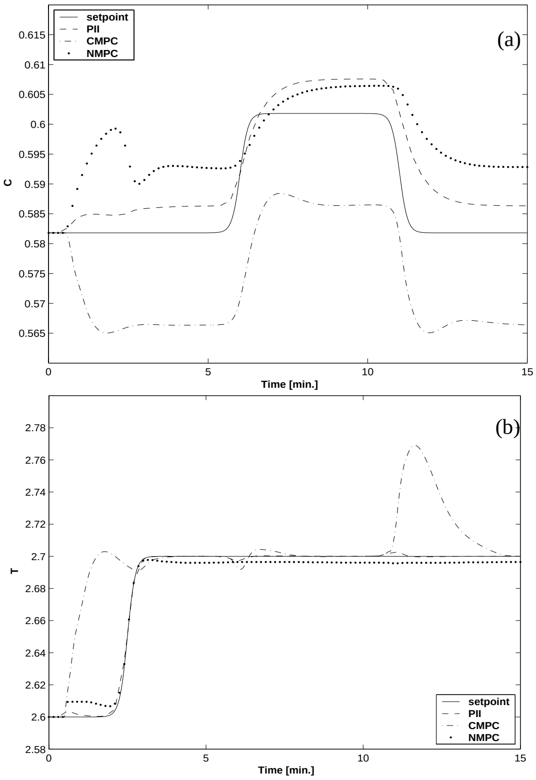

Fig. 5. Closed-loop PIIC, NMPC and CMPC composition (a) and temperature (b) response with model error.

6. CONCLUSIONS

The problem of controlling a (possible open-loop unstable) CSTR with flow and temperature measurements, with emphasis on the attainment of control robustness, linearity, decentralization, and model independency features, has been addressed via constructive MPC. The proposed approach was illustrated and tested with a representative example through simulations, finding that: (i) as predicted on theoretical grounds, the previous constructive approach-based PIIC scheme is equivalent to an unconstrained infinite-horizon NMPC, and (ii) even when it is less modeling dependant than conventional NMPC, the proposed CMPC can stabilize the reactor in the presence of control constraints. These results suggest further studies on: (i) the exploitation of the PIIC-NMPC connection to draw more systematic procedures to set the objective function of the CMPC, (ii) the derivation of tuning guidelines for the CMPC, coupled with a suitable closed-loop robust stability assessment, along the methodological avenue employed in Álvarez and González (2006).

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