Robust PI Stabilization of a Class of Continuously Stirred-Tank Reactors

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This article deals with the stabilization of continuously stirred-tank reactors in the face of control input saturations and uncertain chemical kinetics. Using ideas from modeling-error compensation techniques, a first-order compensator is designed, and its ability to stabilize the reactor temperature at an arbitrary setpoint is shown. The dynamic part of the proposed controller is interpreted as a type of robust integral action to accommodate the modeling error.

Introduction

Stabilization of chemical reactors is of major interest in the process industry. Industrial chemical reactors are frequently operated at unstable operating conditions, which often corresponds to optimal process performance. Polymerization reactors (Alvarez et al., 1990; Viel et al., 1995) and fluidized catalyst cracking units (Grosdidier et al., 1993) are important examples of large-scale chemical reactors operated at unstable conditions. Important factors such as (1) uncertain nonlinearities induced by chemical kinetics, (2) exothermicity due to the chemical-reaction activity, and (3) control input saturations due to cooling/heating system limitations, must be considered in the control design for actual industrial applications.

During the last decade, several works dealing with the stabilization of continuous stirred-tank reactors (CSTR) have been reported. Input/output (I/O) feedback linearization methodologies have been widely explored (see Hoo and Kantor, 1985; Alvarez et al., 1990; Daoutidis et al., 1990; Viel et al., 1995, for example). However, there is a lack of rigorous results for the problem of robust stabilization against uncertain parameters and chemical kinetics. Kravaris and Palanki (1988) used a Lyapunov redesign approach to provide robust state-feedback controllers that guarantee uniform ultimate boundedness. Doyle et al. (1989) investigated the temperature regulation via the linear state feedback of an exothermic irreversible reaction in a CSTR. In (Alvarez-Ramirez et al., 1997), we used calorimetric balances to propose a robust control scheme in the face of uncertain chemical kinetics. Kosanovich et al. (1995) proposed a Lyapunov-based, linearizing feedback adaptive control structure for a CSTR with unknown parameters. However, their approach requires that unknown parameters appear linearly in the model. Fradkov et al. (1997) studied the viability of defining a stabilizing parameter update law for the case where the reaction kinetics are convex on the unknown parameters. This control scheme suffers from the drawback that perfect knowledge of the parameter structure and concentration measurement are required. Viel et al. (1997) proposed a systematic approach to study the global stabilization of a class of CSTRs with unknown chemical kinetics and an arbitrary number of kinetics. Assuming that the chemical kinetic functionalities are separable with respect to temperature and concentrations, they proposed an adaptive feedback control to estimate the temperature functionality of the chemical kinetics and proved global asymptotic stability at an arbitrary setpoint. The proposed controller requires complete knowledge of the chemical reaction network and its concentration functionality, and measurements of a subset of concentrations.

In this work we continue with the ideas posed in our previous work (Alvarez-Ramirez et al., 1997) to propose an output feedback control structure for a class of CSTR that guarantees stabilization in the face of unknown chemical kinetics functionalities and hard control input saturations. Using ideas from modeling error compensation techniques, a first-order compensator is designed, and its ability to stabilize the reactor temperature at an arbitrary setpoint is proven. The dynamic part of the proposed controller is interpreted as a type of robust integral action to accommodate the modeling error, hence the title of the article.

With respect to existing robust stabilization results available in the literature (Viel et al., 1997; Fradkov et al., 1997; Kosanovich et al., 1995), we make the following extensions:

- Measurements of any chemical species concentration are not required.

• Separability of the chemical kinetics functionality with respect to temperature and concentrations is not assumed. In this way, catalytic reactions whose chemical kinetics functionalities are of the Langmuir type (Froment and Bischoff, 1990) can be considered.

• The proposed controller is of order one, and it is independent of the number of chemical reactions. Moreover, the controller is linear and displays an antireset windup (ARW) structure to deal with control input saturations. When the control input is unsaturated, the control is equivalent to a standard PI compensator, so this work can be seen as an approach to formalize the extensive usage of PI control strategies in actual industrial applications.

The work is organized as follows. In the next section, we present the class of chemical reactors under consideration. We state the control objectives and main assumptions in the third section. The fourth section is devoted to the control design when the chemical kinetics are known. The robust control design is presented in the final section.

System Description

In this section, the class of chemical reactors considered in this work and certain basic properties leading to a natural physical domain are presented.

We consider CSTR's described by the following differential equations:

$$\dot{c} = \theta(c^{\text{in}} - c) + Er(c, T)$$
$$\dot{T} = \theta(T^{\text{in}} - T) + H^T r(c, T) + \gamma(u - T), \qquad (1)$$

where $c \in \mathbb{R}^n$ is the vector of the reactor concentrations of the chemical species, $c^{\text{in}} \in \mathbb{R}^n$ is the vector of nonnegative and constant inlet concentrations, $T \in \mathbb{R}$ is the reactor temperature, $T^{\text{in}} \in \mathbb{R}$ is the inlet temperature, $r(c, T) \in \mathbb{R}^m$ is the vector of the nonnegative reaction kinetics, $E \in \mathbb{R}^{n \times m}$ is the stoichiometric matrix, $H \in \mathbb{R}^m$ is the vector of reaction heats, θ is the dilution rate, γ is a heat-transfer coefficient, and u is the jacket temperature, which is taken as the control input.

In order that Eq. 1 be a well-posed CSTR model with respect to mass conservation, the following assumption is made (Gavalas, 1968; Feinberg, 1987; Viel et al., 1997).

Assumption 1 (Principle of Mass Conservation). There exists a positive vector $\omega \in \mathbb{R}^n$, such that $\omega^T E = 0$. It implies that the polyhedral compact set $\mathbf{C} = \{c \in \mathbb{R}^n: \omega^T(c^{\text{in}} - c) \le 0, c_i \ge 0, 1 \le i \le n\}$ is positively invariant under the dynamics of the CSTR (Proposition 1 in Viel et al., 1997).

Assumption 2. (i) $r(c, 0) = 0$, which implies that there is no reaction activity at the absolute zero (kelvin) temperature; and (ii) $\| r(c, T) \| < \rho$, for all $c \in \mathbf{C}$ and $T \in \mathbb{R}_+ = \{T \in \mathbb{R}: T > 0\}$.

Proposition 1. Assume that the jacket temperature $u(t)$ is positive and bounded for all $t \ge 0$. Under Assumption 1, there exists a temperature $T_1 > 0$ such that the interval of temperatures $(0, T_1)$ is a positively invariant domain.

Proof. From Assumption 2(i), we have that $\dot{T} = \theta T^{\text{in}} + \gamma u > 0$, for $T = 0$ and all $c \in \mathbf{C}$. On the other hand, Assumption 2(ii) implies that

$$\dot{T} < \theta(T^{\text{in}} - T) + \rho + \gamma(u_{\max} - T)$$

for all $c \in \mathbb{C}$, where $u_{\max} = \max_{t \ge 0} u(t) < \infty$. Take $T_1 \stackrel{\text{def}}{=} (\theta T^{\text{in}} + \rho + \gamma u_{\max})/(\theta + \gamma)$. Then $\dot{T} < 0$, for all $c \in \mathbf{C}$ and $T > T_1$. These arguments show that the domain is positively invariant.

The compact set $\mathbf{D}_p = \mathbf{C} \times [0, T_1]$ can be taken as the *natural* domain of the CSTR. In actual industrial applications, initial conditions that will be eventually attracted to the stabilized setpoint are contained in the neighborhood $W \subset \mathbf{D}_p$ of the operating point. In this way, and from a practical viewpoint, the temperature stabilization of chemical reactors is actually a problem of robust stabilization on compacta.

Control Problem Statement

The control problem under consideration is the stabilization of the reactor temperature at an arbitrary setpoint $T_r > 0$, with respect to a given compact set of initial conditions $W \subseteq \mathbf{D}_p$. The control problem will be studied under the following additional assumptions.

Assumption 3 (Minimum-Phase Assumption). The isothermal dynamics $\dot{c} = \theta(c^{\text{in}} - c) + Er(c, T_r)$ are globally asymptotically stable at the single equilibrium point $\bar{c} \in \mathbf{C}$.

Assumption 4. Only fluid flow rates (θ) and temperatures (T, T^{in}, and u) are available for measurements.

Assumption 5. The vector of reaction kinetics $r(c, T)$ is an unknown function and C^2 with respect to its arguments.

Assumption 6. The jacket temperature is restricted to take values into the domain $[u_{\min}, u_{\max}]$, where $0 < u_{\min} < \bar{u} < u_{\max}$ and the nominal input $\bar{u}$ is given by $\bar{u} = [-\theta(T^{\text{in}} - T_r) - H^T r(\bar{c}, T_r) + \gamma T_r]/\gamma$.

Some comments regarding the preceding assumptions are in order: (1) Several industrial chemical-reaction systems are minimum phase in the sense of Assumption 3 (Feinberg, 1987), including catalytic reactions of the petrochemical industry, (2) temperatures are routinely measured in industry, (3) Assumption 5 considers the worst case where a reaction kinetics model is unavailable, and finally (4) due to limitations in cooling/heating equipment, the jacket temperature is subjected to saturation variations. In actual industrial applications, the operation margin $u_{\max} - u_{\min}$ is on the order of 80 K.

Control Design: State Feedback and Known Kinetics

We start by designing a globally bounded controller by assuming that measurements of the vector concentration $c \in \mathbb{R}^n$ are available and that the vector of reaction kinetics $r(c, T) \in \mathbb{R}^m$ is perfectly known. Such a control design is made the intermediate step toward the final controller of the next section, which will be an output-actuated controller.

Let us introduce the change of coordinates $x = c - \bar{c}$ and $y = T - T_r$. In this coordinates frame, the system (Eq. 1) can be written as follows:

$$\dot{x} = \theta(x^{\text{in}} - x) + ER(x, y)$$
$$\dot{y} = -\tau_n^{-1} y + H^T R(x, y) + \beta(T_r) + \gamma u, \qquad (2)$$

where $x^{\text{in}} = c^{\text{in}} - \bar{c}$, $R(x, y) = r(x + \bar{c}, y + T_r)$, $\tau_n^{-1} = \theta + \gamma > 0$, and $\beta(T_r) = \theta(T^{\text{in}} - T_r) + \gamma T_r$. The physical domain $\mathbf{D}_p =$

$\mathbf{C} \times [0, T_1]$ is then mapped to the translated physical domain $\mathbf{D} = \mathbf{C}' \times [-T_r,\ T_1 - T_r]$, where $\mathbf{C}' = \{x \in \mathbb{R}^n : x = c - \bar{c},\ c \in \mathbf{C}\}$.

Note that the system (Eq. 2) has relative degree one with respect to the control input u and the regulated output y. Consider that the desired closed-loop performance is specified through the reference model $\dot{y} = -\tau_c^{-1} y$, where τ_c is a prescribed closed-loop time constant. This closed-loop behavior can be attained by linearizing the input/output map of Eq. 2 via the following state-feedback function:

$$u = \phi(x, y), \tag{3}$$

where

$$\phi(x, y) = \left[-H^T R(x, y) - \beta(T_r) + \left(\tau_n^{-1} - \tau_c^{-1}\right) y \right] / \gamma. \tag{4}$$

Remark 1. Note that the setting $\tau_c = \tau_n$ yields $u = [-H^T R(x, y) - \beta(T_r)]/\gamma$, which by virtue of Assumption 2 is a globally bounded feedback on the physical domain $\mathbf{D}$. In this way, the setting $\tau_c = \tau_n$ provides a type of minimum-energy-control design, where τ_n is the natural time constant induced by dilution and heat transfer effects.

The proof of the following proposition can be easily established by using Assumption 3 and Viel et al. (1997, Lemma A.1).

Proposition 2. The closed-loop system formed by the system (Eq. 2) and the feedback (Eqs. 3, 4) is globally asymptotically stable about the origin with respect to the physical domain $\mathbf{D}$.

To accomplish a bounded input constraint (Assumption 6), we consider a saturating version of the control law (Eq. 3) (Alvarez et al., 1991):

$$u = \mathrm{Sat}(\phi(x, y)), \tag{5}$$

where the saturation function is given by

$$\mathrm{Sat}(v) = \begin{cases} u_{\min} & \text{if} \quad v \le u_{\min} \\ v & \text{if} \quad u_{\min} < v < u_{\max} \\ u_{\max} & \text{if} \quad u_{\max} \le v. \end{cases} \tag{6}$$

The resulting closed-loop system is

$$\dot{z} = f_0(z), \tag{7}$$

where $z = (x, y^T)^T \in \mathbb{R}^{n+1}$, and

$$f_0(z) = \begin{bmatrix} \theta(x^{\mathrm{in}} - x) + ER(x, y) \\ -\tau_n^{-1} y - H^T R(x, y) + \beta(T_r) + \gamma\, \mathrm{Sat}(\phi(x, y)) \end{bmatrix}.$$

It is likely that in some cases control input saturations might defeat the global stabilization property (Alvarez et al., 1991). However, preservation of the asymptotic stability of the equilibrium under the saturated feedback (Eq. 5) is ensured by the assumption that $u_{\min} < \bar{u} < u_{\max}$ (Alvarez et al., 1991). In fact, in the neighborhood of the origin, $\mathrm{Sat}(\phi(x, y)) = \phi(x, y)$. This implies the existence of a region of attraction of the origin for the closed-loop system (Eq. 7) whose "size" depends strongly on the control input limits $u_{\min}$ and $u_{\max}$.

From the fact that the origin of the closed-loop system (Eq. 7) is asymptotically stable and based on Lyapunov converse theorems (Massera, 1956), there exist a maximal domain containing the origin $\Delta \subset \mathbb{R}^{n+1}$ and a maximal Lyapunov function $V(z)$: $\Delta \to \mathbb{R}$, such that $V(0) = 0$ and $[\partial V/\partial z]^T f_0(z)$ is negative definite, for all $z \in \Delta$. For technical reasons related to the tools used to prove our main result (Esfandiari and Khalil, 1992), we further assume the following.

Assumption 7. (i) $\beta_1 \| z \|^2 \le V(z) \le \beta_2 \| z \|^2$; (ii) $[\partial V/\partial z]^T f_0(z) \le \beta_3 \| z \|^2$; (3) $\| \partial V/\partial z \| \le \beta_4 \| z \|$, for all $z \in \Delta$, where β_1 to β_4 are positive constants.

Let $\mathbf{L}(V, \alpha) = \{z \in \mathbb{R}^{n+1} : V(z) < \alpha,\ \alpha \ge 0\}$ be the α-level set of the Lyapunov function $V(z)$. For each $\alpha > 0$, and by virtue of Assumption 7, $\mathbf{L}(V, \alpha)$ is a compact domain containing the origin. Let $\Omega_0 \overset{\mathrm{def}}{=} \mathbf{L}(V, \alpha_{\max})$ be the maximal level set contained in domain Δ. Then all trajectories of the closed-loop system (Eq. 7) starting into the domain Ω_0 converge asymptotically to the origin. Hence, we will take the domain Ω_0 as a maximal estimate of the region of attraction of the origin for the CSTR under the saturated state-feedback control (Eq. 5). The estimate Ω_0 can be conservative because of the quadratic-type conditions imposed on the Lyapunov function $V(z)$. If $\mathbf{D} \subseteq \Omega_0$, we will say that the closed-loop system (Eq. 7) is GAS with respect to the physical domain $\mathbf{D}_P$. Our analysis of the robust stabilization of the CSTR system (Eq. 2) will be restricted to the domain Ω_0.

Control Design: Output Feedback and Unknown Kinetics

The feedback control (Eq. 5) cannot be implemented because the modeling error signal $\eta(t) \overset{\mathrm{def}}{=} H^T R(x(t), y(t))$ is unknown. Let $\bar{\eta}(t)$ be an estimate of the modeling error. Then the certainty equivalence control law becomes

$$u = \mathrm{Sat}(\varphi(y, \bar{\eta})), \tag{8}$$

where

$$\varphi(x, \bar{\eta}) = \left[-\bar{\eta} - \beta(T_r) + \left(\tau_n^{-1} - \tau_c^{-1}\right) y \right] / \gamma. \tag{9}$$

To construct an estimator for the modeling error signal $\eta(t)$, let us represent the system (Eq. 5) as an extended-state system in the following form:

$$\begin{aligned} \dot{x} &= \theta(x^{\mathrm{in}} - x) + ER(x, y) \\ \dot{y} &= -\tau_n^{-1} y + \eta + \beta(T_r) + \gamma u \\ \dot{\eta} &= \Gamma(x, y, u), \end{aligned} \tag{10}$$

where $\Gamma(x, y, u)$ is the time derivative of the modeling error signal $\eta(t) = H^T R(x(t), y(t))$ and is given by

$$\Gamma(x, y, u) = H^T \left[\partial_x R f_1(x, y) + \partial_y R f_2(x, y, u) \right], \tag{11}$$

where $f_1(x, y) = \theta(x^{\mathrm{in}} - x) + ER(x, y)$ and $f_2(x, y, u) = -\tau_n^{-1} y + H^T R(x, y) + \beta(T_r) + \gamma u$. Note that since the modeling error signal $\eta(t)$ is unknown, its time derivative $\Gamma(x(t), y(t), u(t))$ is also unknown. In the state-space representation

(Eq. 10), the modeling error η is seen as a new state whose dynamics can be reconstructed from measurements of the system temperatures T, T^{in}, and u. In fact, we have that $\eta(t) = \dot{y}(t) + \tau_n^{-1} y(t) - \beta(T_r) - \gamma u(t)$, which evidences a kind of strong observability (Diop and Fliess, 1991) of the modeling error signal $\eta(t)$. We can take advantage of this observability property to propose an observer-based estimator for the modeling error signal $\eta(t)$.

Let $\sigma_m = \dot{y} + \tau_n^{-1} y - \beta(T_r) - \gamma u$ be an equivalent measured output. Note that σ_m depends only on measured signals and the output time derivative $\dot{y}$. Moreover, $\sigma_m(t) \equiv \eta(t)$, for all $t \geq 0$. To estimate the modeling error signal $\eta(t)$, the following reduced-order observer is proposed:

$$\dot{\overline{\eta}} = \tau_e^{-1}(\sigma_m - \overline{\eta}), \tag{12}$$

where $\tau_e > 0$ is the estimation time constant. Since $\sigma_m = \dot{y} + \tau_n^{-1} y - \beta(T_r) - \gamma u$, we have that

$$\dot{\overline{\eta}} = \tau_e^{-1}\left(\dot{y} + \tau_n^{-1} y - \beta(T_r) - \gamma u - \overline{\eta}\right). \tag{13}$$

To avoid the use of derivators in the righthand side of Eq. 13, let us introduce the estimator variable $w = \tau_e \overline{\eta} - y$. Thus the estimator (Eq. 13) is equivalent to the following:

$$\begin{aligned} \dot{w} &= \tau_n^{-1} y - \beta(T_r) - \gamma u - \tau_e^{-1}(w + y) \\ \overline{\eta} &= \tau_e^{-1}(w + y). \end{aligned} \tag{14}$$

This estimator can be initialized as follows. Since the signal $\eta(t)$ is unknown, the initial estimate $\overline{\eta}(0) = 0$ can be taken, so that $w(0) = -y(0)$.

The proposed controller is therefore composed by the first-order filter (Eq. 14), which provides an estimate of the modeling error signal $\eta(t) = H^T R(x(t), y(t))$, and the certainty equivalence feedback function, Eq. 8.

The structure of the proposed control law

The following result clarifies the structure of the control law (Eqs. 8 and 14).

Proposition 3. The control law given by the feedback function (Eq. 8) and the modeling error estimator (Eq. 14) is equivalent to a PI controller with antireset windup (ARW) structure.

Proof. Take

$$u_c \overset{\text{def}}{=} \varphi(x, \overline{\eta}) = \left[-\overline{\eta} - \beta(T_r) + \left(\tau_n^{-1} - \tau_c^{-1}\right) y\right] / \gamma \tag{15}$$

as the computed control input and $u = \text{Sat}(u_c)$ as the actual control input. From Eqs. 9 and 13, we obtain that the computed control input is given by

$$\begin{aligned} u_c = \frac{1}{(\tau_e s + 1)} u - \frac{\tau_e s}{\gamma(\tau_e s + 1)} \beta(T_r) \\ + \frac{\tau_e\left(\tau_n^{-1} - \tau_c^{-1} - \tau_e^{-1}\right) s - \tau_c^{-1}}{\gamma(\tau_e s + 1)} y, \end{aligned} \tag{16}$$

where s denotes the Laplace variable. If the control input is not subjected to saturations, then $u = u_c$. In this case, the computed control input becomes

$$u_c = -\frac{\beta(T_r)}{\gamma} - K_c\left(1 + \frac{1}{\tau_I s}\right) y, \tag{17}$$

which can be seen as a control law composed of the precompensator $-\beta(T_r)/\gamma$ and of a standard PI compensator with control gain K_c and integral time $\tau_I > 0$ given by

$$\begin{aligned} K_c &= \frac{\tau_e^{-1} + \tau_c^{-1} - \tau_n^{-1}}{\gamma} \\ \tau_I &= \tau_e \tau_c\left(\tau_e^{-1} + \tau_c^{-1} - \tau_n^{-1}\right). \end{aligned} \tag{18}$$

In the general case, where the computed control input is subjected to saturation, the corresponding controller equations can be written as follows:

$$u_c = -\frac{\beta(T_r)}{\gamma} + K_c\left[-y + \tau_I^{-1}\int_0^t\left(-y + \frac{\tau_I}{K_c \tau_e}[u_c - u]\right) dt\right], \tag{19}$$

which shows that the proposed control law contains an ARW feedback-like structure (Khotare et al., 1994) given by

$$\frac{\tau_I}{K_c \tau_e}[u_c - u]. \tag{20}$$

In this way, when the control input is saturated, the feedback signal just given drives the error $u_c - u$ to zero by recomputing the integral such that the controller output u_c is exactly at the saturation limit. This prevents the controller from winding up (Khotare et al., 1994).

We conclude that the modeling error estimation scheme (Eq. 14) provides the proposed controller with a *natural* ARW structure. Because of this structure, the first-order filter (Eq. 14) is able to provide an asymptotic estimate of the modeling error signal $\eta(t)$ in spite of control input saturations.

Remark 2. It is interesting to note the following. The setting $\tau_c = \tau_n$ yields $\gamma K_c = \tau_e^{-1}$ and $\tau_I = \tau_n$. This control gain and integral time setting is analogous to the IMC tuning rules for first-order plants, which are commonly used in the process industry (Morari and Zafiriou, 1989). These IMC tuning rules are derived by solving an H_2-optimal control problem and provides the better nominal performance with minimum control effort. In this way, by setting $\tau_c = \tau_n$, we take advantage of the natural damping capabilities of the CSTR, which are induced by heat transfer and input flow effects.

Remark 3. If γ and τ_n are interpreted to be the identified high-frequency gain and open-loop time constant, respectively, of a given plant, Eq. 18 yield an interesting (τ_c, τ_e)-parameterization of the control gain and integral time for standard PI control. This parameterization is quite interesting because it provides a configuration for the design of better, faster, and more efficient tuning procedures (Gawthrop, 1986). In fact, the tuning of τ_c and τ_e is particularly easy to carry out in view of the fact that, up to the point where the influence of nonmodeled plant behavior is no longer negligible, the velocity of response of the closed-loop system in-

creases monotonically with τ_c and the sensitivity of the closed-loop system in the face of load-disturbances and uncertainties increases monotonically with τ_e.

Stability analysis

To study the stability properties of the controlled CSTR, let us compute the closed-loop equations. To this end, introduce the estimation error $\zeta \overset{\text{def}}{=} \eta - \bar{\eta} \in \mathbb{R}$. The $u = \text{Sat}[\varphi(y, \eta - \zeta)] = \text{Sat}\{\varphi[y, H^T R(x, y) - \zeta]\}$, which together with Eq. 11 give

$$\begin{aligned}\Xi(x, y, \zeta) &\overset{\text{def}}{=} \Gamma\left\{x, y, \text{Sat}\left[\varphi\left(y, H^T R(x, y) - \zeta\right)\right]\right\} \\ &= H^T\Big[\partial_x R f_1(x, y) \\ &\quad + \partial_y R f_2\Big(x, y, \text{Sat}\left[\varphi\left(y, H^T R(x, y) - \zeta\right)\right]\Big)\Big] \end{aligned} \tag{21}$$

Note that $\varphi[y, H^T R(x, y)] \equiv \phi(x, y)$. Thus, the certainty equivalence control law (Eq. 8) becomes the ideal control law (Eq. 5), as the estimation error $\zeta \to 0$. Thus, from Eqs. 5, 7, and 10, and using the fact that $\eta(t) \equiv \sigma_m(t)$, the resulting closed-loop equations can be written as follows:

$$\begin{aligned}\dot{z} &= f_0(z) + \gamma b_1\Big[\text{Sat}\Big\{\varphi\Big[y, H^T R(x, y) - \zeta\Big]\Big\} - \text{Sat}(\phi(x, y))\Big] \\ \tau_e \dot{\zeta} &= -\zeta + \tau_e \Xi(x, y, \zeta),\end{aligned} \tag{22}$$

where $b_1 = [0, 0, \ldots, 0, 1]^T \in \mathbb{R}^{n+1}$. For small values of the estimation time constant $\tau_e > 0$, the closed-loop system, Eq. 22, is a singularly perturbed system with $z \in \mathbb{R}^{n+1}$ and $\zeta \in \mathbb{R}$ as the fast and the slow variables, respectively. Furthermore, as a consequence of the global boundedness of the control input function, $\text{Sat}(\varphi(y, \bar{\eta}))$, the righthand side of the slow variable equation is a bounded function of the fast variable $\zeta \in \mathbb{R}$. The stability of this special structure of singularly perturbed nonlinear system was studied by Esfandiari and Khalil (1992) in a work related to the output stabilization problem of nonlinear systems via high-gain observers.

Our main result can be described in the following theorem.

Theorem 1. Consider the CSTR described in Eq. 1 and suppose that Assumptions 1 to 7 are satisfied. Given any compact set W contained in the interior of $\Omega_0 \subseteq \mathbb{R}^{n+1}$ and a prescribed closed-loop time constant $\tau_c > 0$, there exists a maximum estimation time constant τ_e^* for the PI controller with antireset windup structure (Eqs. 8, 14) such that, for all $0 < \tau_e < \tau_e^*$, the equilibrium point $(\bar{c}, T_r) \in \mathbb{R}^{n+1}$ of the closed-loop system is asymptotically stable and the set W is included in the region of attraction.

Proof. With reference to Esfandiari and Khalil (1992, theorem 2), take $\epsilon = \tau_e$ as the perturbation parameter, $r = n + 1$ as the dimension of the slow variable, and $p = 1$ as the dimension of the fast variable. With

$$\begin{aligned}\bar{f}(z, \zeta) &= \gamma b_1\Big[\text{Sat}\Big\{\varphi\Big[y, H^T R(x, y) - \zeta\Big]\Big\} - \text{Sat}[\phi(x, y)]\Big] \\ \bar{g}(z, \zeta) &= \Xi(x, y, \zeta) \\ A_f &= [-1],\end{aligned}$$

it can be verified that the closed-loop system, Eq. 22, satisfies all the assumptions of theorem 2 in Esfandiari and Khalil (1992) with $D_1 = \Omega_0$. Since the set W is in the interior of Ω_0, there exists a positive constant $\alpha_1 < \alpha_{\max}$ such that $W \subseteq \mathbf{L}(V, \alpha_1) \subset \Omega_0$. Thus, we can take $\bar{\Omega}_1 = \mathbf{L}(V, \alpha_1)$, and the given compact set W is a subset of $\bar{\Omega}_1$. On the other hand, since $\bar{\eta}(0) = 0$, we have that the initial condition $\zeta(0)$ satisfies $\|\zeta(0)\| \le \vartheta$, where $\vartheta = \max_{z \in W} |H^T R(x, y)| < \infty$. It follows from Esfandiari and Khalil's results that there exists a maximum estimation time constant $\tau_e^* > 0$ such that, for all $0 < \tau_e < \tau_e^*$, the origin of the closed-loop system, Eq. 22, is asymptotically stable and all trajectories starting in W converge to the origin as $t \to \infty$. Moreover, for all initial states in W, the trajectory $z(t)$ under the output feedback tends to the trajectory $z(t)$ under state feedback, as the modeling error estimation is carried out faster and faster (that is, $\tau_e \to 0$).

Remark 4. The preceding result gives a regional (semiglobal) stabilization result with respect to the estimate of the region of attraction under state feedback and known chemical kinetics. A drawback of this regional result is that the estimate of the region of attraction Ω_0 is only a subset of the actual region of attraction, and it could be a conservative one. The result shows that all trajectories starting in any compact domain W contained in Ω_0 can be stabilized via output feedback despite the fact that the reaction kinetics are unknown. In other words, *almost any initial condition stabilized via state-feedback control with perfect knowledge can be stabilized via a PI control with ARW*. In this sense, the PI control with ARW is a universal output feedback stabilizer (in the sense defined by Ilchmann, 1991) for the class of CSTRs considered in this article.

Remark 5. The determination of the actual boundary of the region of attraction $\partial\Omega_0$ is a very hard problem (Alvarez et al., 1991). In the generic case, $\partial\Omega_0$ is composed by unstable invariant sets (such as equilibrium points and limit cycles) and their unstable manifolds. However, the result in Theorem 1 states that the maximal region of attraction under input saturation can be achieved in the limit as $\tau_e \to 0$.

Examples

Some numerical results are presented in this section. The objective is twofold: first, to illustrate the performance of the proposed controller, and second, to show that the ARW may be necessary to achieve semiglobal stability.

Example 1

For clarity of presentation in this subsection we have chosen an academic example with a first-order reaction $A \to B$:

$$\begin{aligned}\dot{c}_A &= \theta\left(c_A^{\text{in}} - c_A\right) - \kappa(T) c_A \\ \dot{c}_B &= -\theta c_B + \kappa(T) c_A \\ \dot{T} &= \theta(T^{\text{in}} - T) + H\kappa(T) c_A + \gamma(u - T),\end{aligned} \tag{23}$$

where $\kappa(T) = \kappa_0 \exp(-E_a/RT)$ is the so-called Arrhenius functionality, E_a is the activation energy, and R is a universal constant. It is easy to check Assumption 1 with $\omega = (1,1)^T$ and the global asymptotic stability of the isothermal dynamics $\dot{c} = -[\theta + \kappa(T_r)]c_A + \theta c_A^{\text{in}}$. Although this model is very simple, it retains the main characteristics of CSTR dynamics, namely, multiplicity of equilibrium points and exothermic reactions. In fact, under the parameters— $\theta = 1$, $c_A^{\text{in}} = 1$, $\kappa_0 =$

exp(25), $E_a/R = 10^4$, $T^{in} = 350$, $H = 200$, $\gamma = 1$, and the nominal control input value $\bar{u} = 350$—the open-loop reactor exhibits three equilibrium points. One of these equilibrium points, which is located at $(\bar{c}, T_r) = (0.5, 400)$, is (saddle-type) unstable. The CSTR model (Eq. 23), along with the preceding set of parameters was reported by Aris and Amundson in their pioneering article (Aris and Amundson, 1958), and is commonly used in the chemical engineering literature as a benchmark problem to test the performance of control algorithms for chemical reactors.

Assume that the control objective is to stabilize the reactor at the open-loop unstable equilibrium point ($T_r = 400$). Alvarez et al. (1991) showed that the control input bounds $u_{min} < 232$ and $u_{max} > 373$ suffice for the global asymptotic stabilization of the chemical reactor under the saturated state feedback control, Eq. 4. Let us assume that $u_{min} = 320$ and $u_{max} = 380$. To take advantage of the natural damping of the CSTR dynamics, choose $\tau_c = \tau_n = (\theta + \gamma)^{-1} = 0.5$. Moreover, choose the initial conditions equal to the inlet conditions (startup operation) and suppose a setpoint change from $T_r = 400$ to $T_r = 410$, which also corresponds to an open-loop unstable equilibrium point, at time $t = 8$.

Figure 1 shows the reactor and the jacket temperatures (control input) for three different values of the estimation time constant τ_e. For the sake of comparison, Figure 1 also shows these temperatures under state feedback and perfect

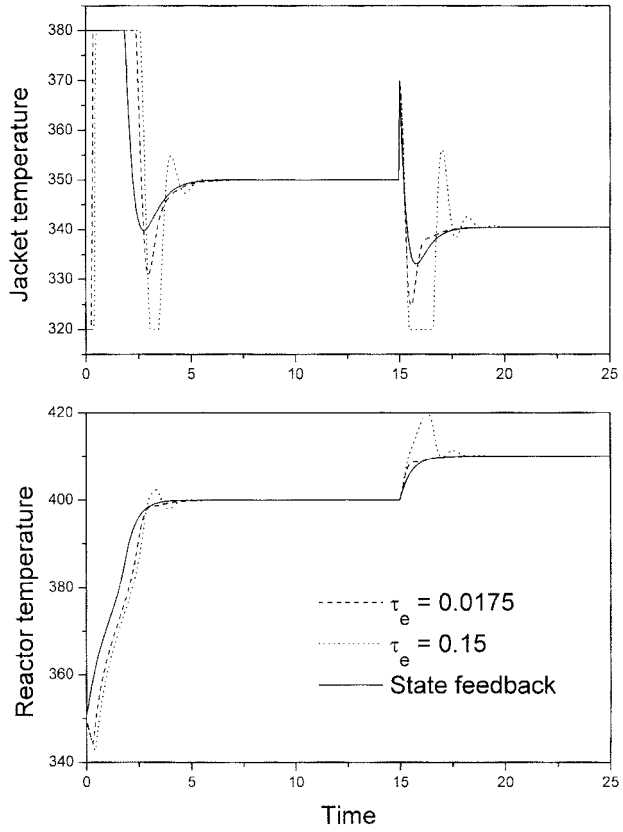

Figure 1. Dynamics of reactor and jacket temperatures for two different values of the estimated time constant (Example 1).

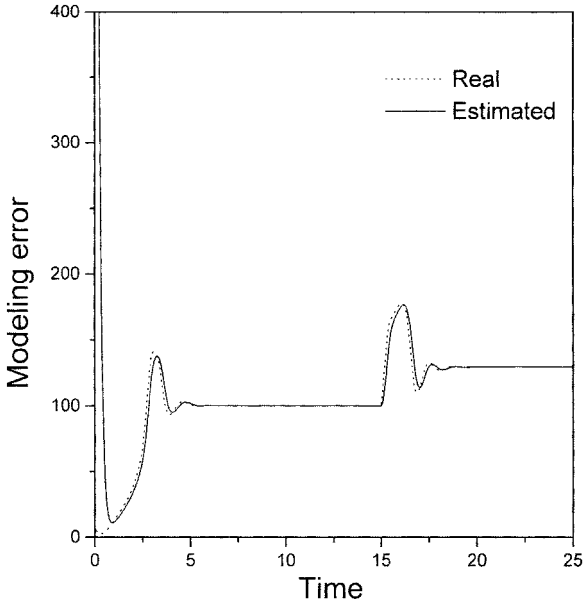

Figure 2. Real and estimated modeling error for Example 1.

knowledge of the chemical kinetics. The value $\tau_e^* \cong 0.21$ was found via numerical simulations. On the other hand, notice that the smaller the estimation time-constant value, the closer the behavior to that obtained under state feedback and perfect knowledge. Figure 2 shows the dynamics of the real $\eta(t) = 200 \exp[25 - (10^4/T)]$ and the estimated $\bar{\eta}(t)$ modeling errors. For $\tau_e < \tau_e^* \cong 0.21$, $\bar{\eta}(t) \to \eta(t)$ after a short transient.

To illustrate the fact that the underlying ARW structure is of major importance for the stabilization of the chemical reactor, Figure 3 presents the dynamics of the reactor and jacket (control input) temperatures for the cases with and without ARW, and $\tau_e = 0.1$. Reactor temperature stabilization is only possible when the ARW structure is used.

Remark 6. For the sake of clarity in presentation, we considered only uncertainties related to the chemical kinetics. In actual industrial applications, uncertainties in the heat-transfer coefficient γ also must be considered. In fact, the heat-transfer coefficient γ depends in a complex way of heat-transfer surface conditions, physical properties of the fluids (density, viscosity, etc.), and temperature. For instance, in polymerization reactors where the viscosity of the polymer mixture changes drastically with composition and temperature, relative variations of the heat-transfer coefficients are of the order of -75% (Alvarez et al., 1990). The ideas presented in this work also can be used to handle uncertainties in the heat-transfer coefficient by taking the modeling-error signal as $\eta(t) \stackrel{def}{=} H^T R(x(t), y(t)) + (\gamma - \bar{\gamma})u(t)$, where $\bar{\gamma} > 0$ is an estimate of the real heat-transfer coefficient γ. In this case, the resulting output feedback controller is given as before (Eqs. 8, 9, and 14), but using the estimate parameter $\bar{\gamma}$ instead of the real parameter γ. To illustrate the performance of the proposed control strategy, Figure 4 shows the dynamics of the controlled CSTR for $\tau_e = 0.1$ and two different values of the estimated heat-transfer coefficient, which corresponds to $+50\%$ and -50% of error in the estimation of γ. Reactor stabilization is attained in spite of strong un-

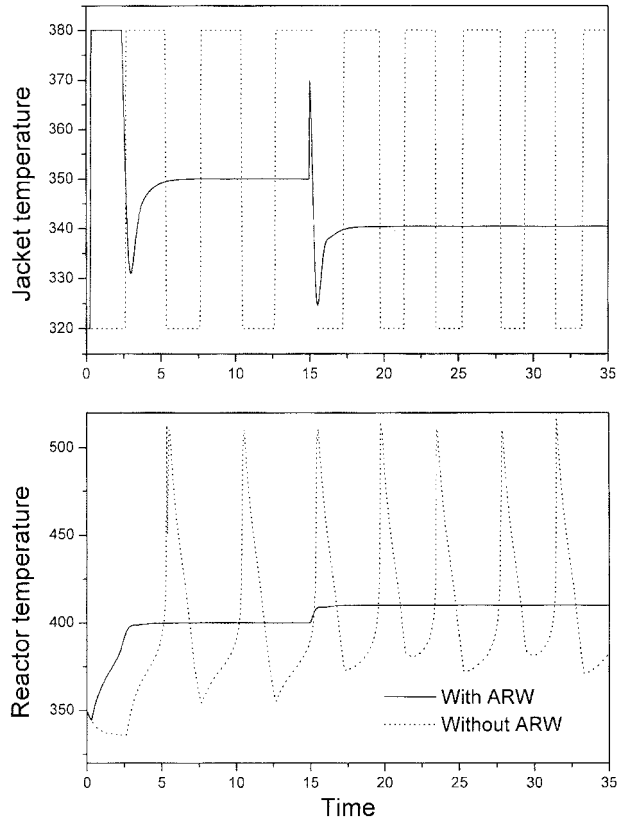

Figure 3. Dynamics of reactor and jacket temperatures with and without antireset windup for Example 1.

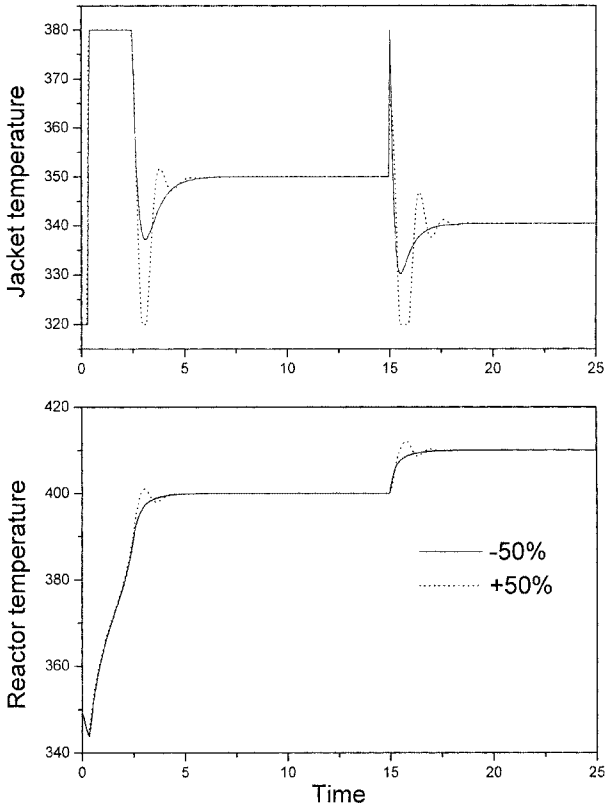

Figure 4. Dynamics of reactor and jacket temperatures for Example 1, with strong uncertainties in the heat-transfer coefficient.

certainties in the heat-transfer coefficient and the chemical kinetics. These simulation results demonstrate that the PI feedback-control structure with ARW presented in this work can efficiently handle uncertainties in the heat-transfer coefficient γ. The proof of this result can be obtained along the lines of the proof of Theorem 1.

Example 2

We consider the oxidation of benzene (B) to maleic anhydride (MA) in a fluidized-bed reactor as described in Kendi and Doyle (1996). The oxidation reaction to produce MA from B is highly exothermic. Therefore, careful temperature control is required. In practical applications, the temperature of the bed is measured and relayed to a controller that regulates the jacket temperature. The oxidation of B to MA is modeled under the following assumptions: (a) a simple two-phase model; (b) a perfectly mixed dense phase: and (c) plug flow in the bubble phase. The resulting *dimensionless* model has the same structure as a CSTR model, and is detailed below:

$$\dot{c}_B = \theta_1\left(c_B^{\text{in}} - c_B\right) - a_1\left[\kappa_{1f}\zeta_1(T) + \kappa_{3f}\zeta_3(T)\right]c_B$$

$$\dot{c}_{MA} = \theta_1\left(c_{MA}^{\text{in}} - c_{MA}\right) + a_1\left[\kappa_{1f}\zeta_1(T)c_B - \kappa_{2f}\zeta_2(T)c_{MA}\right]$$

$$\dot{T} = \theta_2(T^{\text{in}} - T) + a_2\left[\kappa_{1f}H_{r1}\zeta_1(T) + \kappa_{3f}H_{r3}\zeta_3(T)\right]c_B + a_2\kappa_{2f}H_{r2}\xi_2(T)c_{MA} + \gamma(u - T) \quad (24)$$

where

$$\zeta_i(t) = \exp\left(\frac{\beta_i T}{1 + (T/B_m)}\right), \qquad i = 1 \text{ to } 3,$$

and c_B and c_{MA} are, respectively, the mole fraction of benzene and maleic anhydride; and T and u are, respectively, dimensionless reactor and jacket temperatures. The definition and meaning of the dimensionless reactor-modeling parameters are described in table 3 of Kendi and Doyle's article. The numerical values of these parameters are given in Table 1. Initial values for the dimensionless variables $c_B(0) = 0.238$, $c_{MA}(0) = 0.383$, and $T = 2.12$.

Assume that the estimated value of the heat-transfer coefficient is $\bar{\gamma} = 0.015$. This numerical value corresponds to $+50\%$ error in the estimation of this parameter. As in Example 1, to take advantage of the natural damping of the CSTR

Table 1. Dimensionless Parameters for the Example 2 Model

$\beta_m = 19.1172$	$\gamma = 0.01$
$\beta_1 = 1.1626$	$H_{r1} = 1.5165 \times 10^6$
$\beta_2 = 0.6747$	$H_{r2} = 1.1521 \times 10^6$
$\beta_3 = 1.1626$	$H_{r3} = 2.6885 \times 10^6$
$\theta_1 = 0.6225$	$\kappa_{1f} = 0.1186 \times 10^{-4}$
$\theta_2 = 0.014$	$\kappa_{2f} = 0.0525 \times 10^{-4}$
$a_1 = 12{,}847$	$\kappa_{3f} = 0.0509 \times 10^{-4}$
$a_2 = 0.0005457$	

dynamics, choose the closed-loop time constant τ_c of the order of the natural time constant $\tau_n = (\theta_2 + \bar{\gamma})^{-1} = 46$ s. We pick $\tau_c = 30$ s, the control input bounds as $u_{\min} = 580$ K and $u_{\max} = 660$ K, and the temperature reference as $T_r = 650$ K.

Figure 5 shows the reactor and the jacket temperatures (control input) for two different values of the estimation time constant τ_e, which are of the order of the closed-loop time constant τ_c. The proposed control strategy is able to drive the reactor temperature to the reference value despite strong model uncertainties. Moreover, the convergence increases as the estimation time constant becomes smaller, although more severe input saturations are displayed.

We then evaluated the performance of the controller under setpoint changes and abrupt parameter changes. To this end, we considered the following changes: the reference temperature is changed at $t = 100$ s from 650 K to 670 K, and the inlet reactor temperature is changed at $t = 500$ s from 633 K to 640 K. Figure 6 shows the time evolution of the reactor and jacket temperatures for the two different values of the estimation time constant used previously. Notice that the effects of the disturbances in the reactor temperature are reduced more efficiently, as the estimation time constant takes smaller values. Of course, in actual applications, arbitrarily small values of the time-constant estimation cannot be used because of measurement noise and unmodeled dynamics, which limit the achievable closed-loop performance (Morari and Zafiriou, 1989).

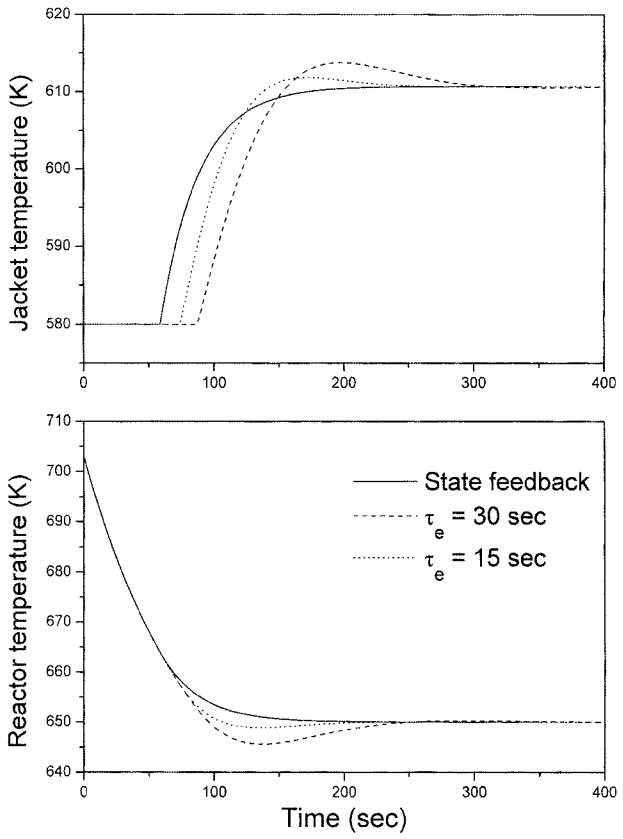

Figure 5. Time evolution of reactor and jacket temperatures for two different values of the estimation time constant (Example 2).

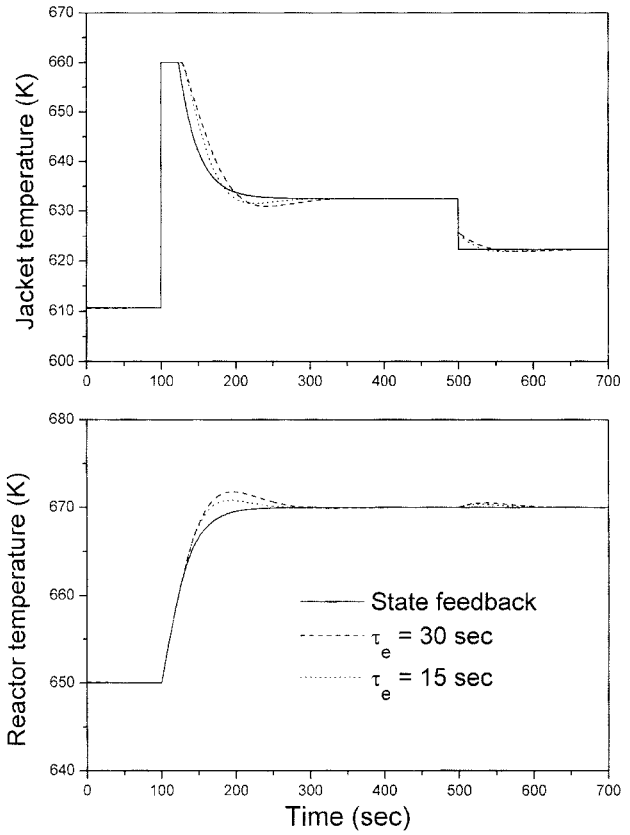

Figure 6. Time evolution of reactor and jacket temperatures under setpoint and parameter disturbance step changes (Example 2).

Finally, to test the control algorithm in the face of several non-first-order reactions, let us assume that the actual kinetics of oxidation of benzene to maleic anhydride are given by $\kappa_{1f}\zeta_1(T)c_B^{1.25} + \kappa_{3f}\zeta_3(T)c_B^{1.5}$ and $\kappa_{1f}\zeta_1(T)c_B^{1.25} - \kappa_{2f}\zeta_2(T)c_{MA}^{1.4}$. Figure 7 shows the time evolution of the reactor and jacket temperature for $\tau_c = 30$ s and $\tau_e = 20$ s, and the same step disturbances as in Figure 6. The proposed control strategy is able to handle efficiently the step disturbances despite the unknown nonlinear chemical kinetics.

Conclusions

In this work, we studied the stabilization of a class of continuous stirred-tank reactors (CSTR) where unknown chemical kinetics and control input saturations were assumed. The new idea we proposed for robust stabilization is based in modeling error-compensation techniques, and consists of interpreting the modeling error signal as a new state, whose dynamics are observable from temperature measurements. In this way, we used a reduced-order observer to estimate the modeling error signal, which is subsequently used in the saturated version of an I/O feedback linearizing feedback. The resulting controller is shown to be equivalent to a standard PI controller with an antireset windup structure. Our stability analysis showed that, as $\tau_e \to 0$, such a standard PI controller is able to recover the closed-loop performance under state feedback and perfect knowledge of the chemical kinetics.

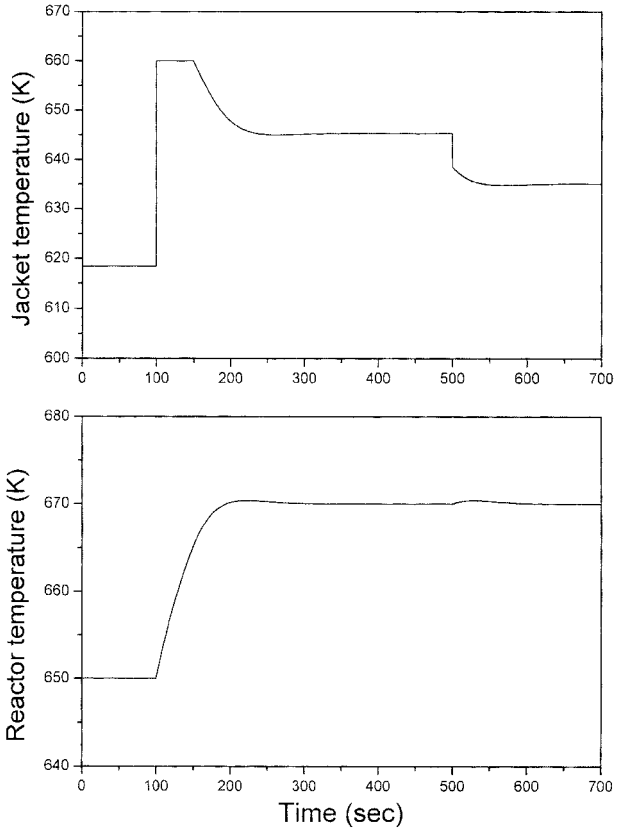

Figure 7. Time evolution of reactor and jacket temperatures for $\tau_c = 30$ s and $\tau_e = 20$ s, in the nonlinear chemical kinetics model.

We extended the stability results available in the literature (see Viel et al., 1997; Fradkov et al., 1997; Kosanovich et al., 1995) in several directions: (1) the order of the proposed controller does not depend on the number of chemical reactions involved; (2) we do not make any restrictive assumption of the functionality of the chemical kinetics, that is, nonseparable chemical kinetics functionalities $r(c, T)$ are allowed; and (3) the implementation of our controller does not require the measurement of any chemical species concentration.

Acknowledgment

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Literature Cited

Alvarez, J., J. Alvarez-Ramirez, and R. Suarez, "Nonlinear Bounded Control of Continuous Agitated Tank Reactor," *Chem. Eng. Sci.*, **46**, 3235 (1991).

Alvarez, J., R. Suarez, and A. Sanchez, "Nonlinear Decoupling Control of Free Radical Polymerization Continuous Stirred Tank Reactors," *Chem. Eng. Sci.*, **45**, 238 (1990).

Alvarez-Ramirez, J., R. Suarez, and R. Femat, "Control of Continuous Stirred Tank Reactors: Stabilization with Unknown Reaction Rates," *Chem. Eng. Sci.*, **51**, 4183 (1996).

Aris, R., and N. R. Amundson, "An Analysis of Chemical Reactor Stability and Control—I, II, II," *Chem. Eng. Sci.*, **7**, 121 (1958).

Daoutidis, P., M. Soroush, and C. Kravaris, "Feedforward/Feedback Control of Multivariable Nonlinear Processes," *AIChE J.*, **36**, 1471 (1990).

Diop, S., and M. Fliess, "On Nonlinear Observability," *Proc. European Control Conf.*, European Control Society, Brussels, Belgium, p. 152 (1991).

Doyle, F. J., III, A. K. Packard, and M. Morari, "Robust Controller Design for a Nonlinear CSTR," *Chem. Eng. Sci.*, **44**, 1929 (1989).

Esfandiari, F., and H. K. Khalil, "Output Feedback Stabilization of Fully Linearizable Systems," *Int. J. Control*, **56**, 1007 (1992).

Feinberg, M., "Chemical Reaction Network Structure and the Stability of Isothermal Reactors—I The Deficiency Zero and Deficiency One Theorems," *Chem. Eng. Sci.*, **29**, 2229 (1987).

Fradkov, A., R. Ortega, and G. Bastin, "Semiadaptive Control of Convexity Parameterized Systems with Application to Temperature Regulation of Chemical Reactors," *Proc. IFAC-ADCHEM*, Banff, Canada (1997).

Froment, G. F., and K. B. Bischoff, *Chemical Reactor Analysis and Design*, Wiley, New York (1990).

Gavalas, G. R., *Nonlinear Differential Equations of Chemical Reacting Systems*, Springer-Verlag, New York (1968).

Gawthrop, P. J., "Self-Tuning PID Controllers: Algorithms and Implementation," *IEEE Trans. Automat. Contr.*, **AC-31**, 201 (1986).

Grosdidier, P., A. Mason, A. Aitolahti, P. Heinonen, and V. Vanhumaki, "FCC Unit Regenerator-Reactor Control," *Comput. Chem. Eng.*, **17**, 165 (1993).

Hoo, K. A., and J. C. Kantor, "An Exothermic Continuous Stirred Tank Reactor Is Equivalent to a Linear System," *Chem. Eng. Commun.*, **37**, 1 (1985).

Ilchmann, A., "Non-Identifier-Based Adaptive Control of Dynamical Systems: A Survey," *IMA J. Math. Control Inf.*, **8**, 321 (1991).

Kendi, T. A., and F. J. Doyle III, "Nonlinear Control of a Fluidized Bed Reactor Using Approximate Feedback Linearization," *Ind. Eng. Chem. Res.*, **35**, 746 (1996).

Kosanovich, K. A., M. J. Piovoso, V. Rokholenko, and A. Guez, "Nonlinear Adaptive Control with Parameter Estimation of a CSTR," *J. Proc. Contr.*, **5**, 137 (1995).

Kothare, M. V., P. J. Campo, M. Morari and C. N. Nett, "A Unified Framework for the Study of Anti-Windup Designs," *Automatica*, **30**, 1869 (1994).

Kravaris, C., and S. Palanki, "Robust Nonlinear State Feedback Under Structured Uncertainty," *AIChE J.*, **34**, 1119 (1988).

Massera, J. L., "Contribution to Stability Theory," *J. Differential Equations*, **64**, 182 (1956).

Morari, M., and E. Zafiriou, *Robust Process Control*, Prentice Hall, Englewood Cliffs, NJ (1989).

Viel, F., E. Buesvelle, and J. P. Gauthier, "Stability of Polymerization Reactors Using I/O Linearization and a High-Gain Observer," *Automatica*, **31**, 971 (1995).

Viel, F., F. Jadot, and G. Bastin, "Robust Feedback Stabilization of Chemical Reactors," *IEEE Trans. Automat. Contr.*, **AC-42**, 473 (1997).

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