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Nonlinear PI/PID Controllers for a High-order Reactor System

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***Abstract*—**The study is carried out on temperature control of a high-order reactor system subject to physical input constraint and output multiplicity. Since many process states are unmeasurable in the real-time evaluation and thermal effects of exothermic reactions usually tend towards operation with stability margins, nonlinear control algorithms derived from the state-space formulation of model-based controller design for nonlinear relative-degree-one and relative-degree-two systems are addressed. With the aid of the equilibrium-based design, the nonlinear PI and PID-types control frameworks are more amenable to industrial implementation. Additionally, the tuning procedure with two controller parameters is relatively simple and straightforward. Through numerical simulations, the low-and-high gain technique and anti-reset windup design are added to enhance the process control performance.

Keywords: Feedback linearization; nonlinear PI/PID control; Anti-reset windup; Polymerization Reactor

I. Introduction

SOME important polymers are industrially produced in continuous stirred tank reactors (CSTRs), for instance polystyrene. In mass and solution free-radical polymerizations, heat transfer is poor due to high viscosities such that thermal effects associated with exothermic reactions and poor heat transfer probably cause the thermal runaway in some PCSTR systems. Therefore, free-radical polymerization reactors not only exhibit highly nonlinear dynamic behavior with many instability features [17, 19], but also their control designs are so attractive as to control other emulsion polymerization reactor systems [7].

While product quality and operation safety are simultaneously maintained, relevant control designs for polymerization reactors are often multivariable [3, 13]. Additionally, the relationship between concentrations and reaction rates has highly nonlinear nature, and the monitoring property related to molecular weight distribution (MWD) is a challenging task [9, 16, 21]. Inspired by feedback linearization methodologies having been widely studied for chemical process applications [10, 15], nonlinear control techniques combined with functional state estimations have been explored for improving productivity of PCSTR systems [9, 23], in which high-gain observers usually provide rapidly estimating unknown polymer properties to recover the performance of partial feedback controls. Besides, some linearization control designs connected with the anti-windup compensation are expected to deal with physical controller constraints [8, 11, 26].

In the last decade, feedback linearization methodologies have been widely explored for the stabilization of chemical reactors [4, 24], and PI-type compensation techniques were applied for the stabilization of a class of chemical reactors in which jacket dynamic is usually neglected [1, 2]. In recent year, Wright et al. [25] proposed nonlinear PI and PID controllers resulted from the application of model-based controller design methods to specific first- and second-order systems, Chang et al. [5] proposed a self-tuning PID controller with a stable adaptation mechanism was carried out on a class of feedback linearizable systems, and Tan et al. [22] used a preload relay into a PID controller such that the robust self-tuning mechanism is suitable for nonlinear systems. Obviously, the conventional PI/PID algorithms are gradually translated into the adaptable, nonlinear PI/PID algorithms.

II. Example

In this paper we consider a jacketed CSTR system in which the free-radical polymerization of styrene takes place [19]. Fig. 1 shows that the reactor is continuously fed with monomer, initiator and solvent. Under the equal-reactivity hypothesis, the quasi-steady-state assumption for all radical species, and ignoring the reaction of chain transfer to the polymer, the process model is described by the following set of equations:

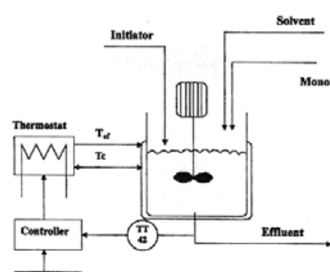

Fig. 1 Polymerization reactor system and its control scheme

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$$\frac{dW_M}{dt} = \frac{Q_F}{\rho V_r}(W_{Mf} - W_M) - (k_p + k_{ttM})W_M C_R - 2fk_d W_I \frac{M_M}{M_I}$$
$$\frac{dW_S}{dt} = \frac{Q_F}{\rho V_r}(W_{Sf} - W_S) - k_{tts} W_M C_R$$
$$\frac{dW_I}{dt} = \frac{Q_F}{\rho V_r}(W_{If} - W_I) - k_d W_I \qquad (1)$$
$$\frac{dT_r}{dt} = \frac{Q_F}{\rho V_r}\left(\frac{c_{pF}}{c_p}T_f - T_r\right) + \frac{UA}{\rho V_r c_p}(T_c - T) - \frac{k_p C_R W_M \Delta H}{M_M c_p}$$
$$\frac{dT_c}{dt} = \frac{Q_c}{V_c}(T_{cf} - T_c) + \frac{UA(T_r - T_c)}{\rho_c V_c c_{pc}}$$

where

$$\rho = \left[\frac{W_M}{\rho_M} + \frac{W_S}{\rho_S} + \frac{1 - W_M - W_S}{\rho_P}\right]^{-1} \text{ and } C_R = \sqrt{\frac{fk_d W_I \rho}{M_I(k_{tc} + k_{td})}}$$

This CSTR exhibits multiple steady states, and the poor heat removal device usually causes the ignition/extinction behavior or open-loop instability. In general, many polymerization reactor control strategies are multivariable in nature, so the single-loop temperature control connected with PI/PID control framework is rarely employed [17].

Discussion 1: In order to maintain the good product quality of exothermic reactor systems, the cooling jacket is often treated as the feasible heat removal. To examine heat removal effects, Fig. 1 shows the open-loop dynamic of this styrene polymerization reactor in the presence of coolant flowrate changes. However, the low coolant flowrate (Q_c) induces undesired reactor temperature or even thermal runaway. In Fig. 2, the inlet perturbation of initiator in the feed causes the unsymmetrical open-loop responses. Those simulations demonstrate that this reactor has highly nonlinear, unstable dynamical behavior due to thermal effects of polymerization reactions. Referring the issue of process operation in Viel et al. [23], the physical constraints for the safe reactor temperature ($\le T_{r,\max} = 450\text{ K}$) and the proper range of inlet coolant temperature ($300\text{ K} \le T_{cf} \le 450\text{ K}$) are considered. Furthermore, we assume that the PCSTR system is affected by perturbations in the feeds, and the state-space form of reactor model in eq. (1) is written as

$$\begin{aligned} \dot{x} &= f_1(x,\omega) + g_1(x,\omega)\xi \\ \tau_c \dot{\xi} &= f_2(x,\xi) + g_2(x,\xi)\text{sat}(u) \\ y &= h(x) \end{aligned} \qquad (2)$$

where $x = [W_M, W_S, W_I, T_r]'$, $\xi = T_c$, $\tau_c = V_c/Q_c$, $y = T_r$ and $u = T_{cf}$. $\omega \in \Gamma \subset \Re^2$ represents the class of bounded disturbances for both W_{If} and T_f. The saturation function is shown as

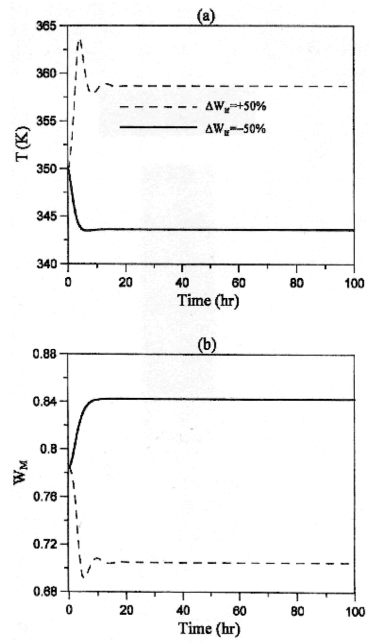

Fig. 2 Open-loop state profiles for step change of initiator in the feed

$$\text{sat}(u) = \begin{cases} u_{\max}, & u \ge u_{\max} \\ u, & u_{\min} < u < u_{\max} \\ u_{\min}, & u \le u_{\min} \end{cases} \qquad (3)$$

Note that the nonlinear vector functions (f_1, g_1, f_2, g_2) can be directly constructed by eq. (1), and $u_{\max}$ =450 K and $u_{\min}$ =300 K.

III. Nonlinear PI Control Scheme

Obviously, the state-space form of eq. (2) can be denoted as a two-time-scale nonlinear system [14, 27]. A quasi-steady-state equation while τ_c=0 is shown as

$$0 = f_2(x, \xi_s) + g_2(x, \xi_s)u \qquad (4)$$

where ξ_s represents a quasi-steady-state value. The solution of ξ_s by eq. (4) is described by

$$\xi_s = \varphi(x, u) \qquad (5)$$

The reduced-order linearizable system is expressed as

$$\dot{e}_1 = L_{f_1}h + \varphi(x,u)L_{g_1}h$$
$$\dot{\eta}_1 = L_{f_1}\eta_1 \tag{6}$$

where the function $\eta_1(x) \in \Re^{n-1}$ satisfies $L_{g_1}\eta_1(x) = 0$. In general, the static state feedback control cannot reduce steady state errors in the presence of step disturbances or structured modeling errors. Thus, a first-order reference model as an error compensator is introduced

$$\dot{y}_m = \varepsilon_1(y_{sp} - y) \tag{7}$$

and the control law is given by

$$u = \varphi^{-1} \circ \left[\left(\varepsilon_1(y_{sp} - y) - (y - y_m)/\varepsilon_2 - L_{f_1}h \right) \Big/ L_{g_1}h \right] \tag{8}$$

where $\varepsilon_1, \varepsilon_2 > 0$ are denoted as tuning parameters, and $y_m \in \Re$ is the reference output. Moreover, the closed-loop linearizable system is augmented

$$\varepsilon_2\dot{z}_1 = -z_1, \quad \dot{y}_m = -\varepsilon_1 y_m + \varepsilon_1\delta, \quad \dot{\eta}_1 = L_{f_1}\eta_1 \tag{9}$$

where $z_1 = y - y_m$ and $\delta = y_{sp} - y + y_m$. Both parameters ($\varepsilon_1$, ε_2) dominates the closed-loop transient response.

Remark 1: If the integration of first-order reference model is shown as

$$y_m = y_{m,b} + \varepsilon_1 \int_0^t (y_{sp} - y)d\tau \tag{10}$$

where $y_{m,b}$ represents the initial of reference model. Moreover, the PI–type state feedback control by eqs (8) and (10) is represented as

$$u = u_{PI}(x,y) + K_c^{PI}(x,y) \times \left[(y_{sp} - y) + \frac{1}{\tau_I^{PI}} \int_0^t (y_{sp} - y)d\tau \right] \tag{11}$$

where

$$u_{PI} = \varphi^{-1} \circ \left[\left((y_{m,b} - y)/\varepsilon_2 - L_{f_1}h \right) \Big/ L_{g_1}h \right]$$
$$K_c^{PI} = \varphi^{-1} \circ \left(\varepsilon_1 / L_{g_1}h \right) \tag{12}$$
$$\tau_I^{PI} = \varepsilon_2$$

Note that the modes of PI configuration are parameterized by both tuning parameters ε_1 and ε_2. Active input constraints often degrade the PI control performance due to the pure integral effect. The anti-reset windup design for the nonlinear gain K_c^{PI} is introduced

$$\text{sat}(K_c^{PI}) = \varphi^{-1} \circ \left(\text{sat}(\varepsilon_1) / L_{g_1}h \right) \tag{13}$$

with

$$\text{sat}(\varepsilon_1) = \begin{cases} \varepsilon_1 & \text{if } \left| u - u_{b,ss} \right| \le b_d \\ \sigma & \text{if } \left| u - u_{b,ss} \right| > b_d \end{cases} \tag{14}$$

where $u_{b,ss}$ is control bias, and $\sigma \ge 0$ is a adjustable parameter.

Discussion 2: For a demonstration, Fig 3(a) and 3(b) depict that the nonlinear PI control with two kinds of tuning constants can ensure the convergent temperature trajectory around the same boundaries while an unknown disturbance, ΔT_F, appears in the inlet flow. It is noted that both parameters ε_1 and ε_2 can individually perform the same high-gain effect for the output regulation. Under the actuator constraints ($300\ \text{K} \le u \le 450\ \text{K}$), Fig. 4(a) shows that the added anti-reset windup design can keep the stable output regulation, and Fig. 4(b) depicts that controller is unsaturated by adjusting $\sigma = 0$.

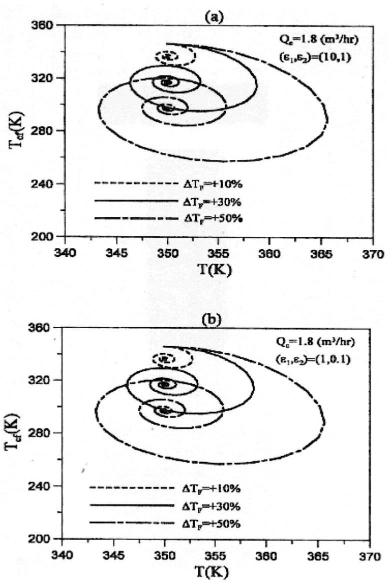

Fig. 3 Closed-loop state trajectories with respect to step change in the feed temperature using the PI-type state feedback controller

Control based on an equilibrium manifold

In fact, the state information of control laws in eq. (11) is unavailable for practical applications. Inspired by the equilibrium-based control strategy [20] for output regulation of nonlinear systems, the PI-type state feedback control will be extended to involve this useful feedforward design.

It is assumed that smooth maps $x^e : \Gamma \to \Re^4$ and $u^e : \Gamma \to \Re$ are determined by solving the following algebraic equations

$$\begin{cases} F\left(x^e(\omega), u^e(\omega), \omega\right) = 0 \\ \quad h\left(x^e(\omega)\right) - y_{sp} = 0 \end{cases} \tag{15}$$

where $F \triangleq f_1\left(x^e(\omega), \omega\right) + g_1\left(x^e(\omega), (\omega)\right)\varphi\left(x^e(\omega), u^e(\omega)\right)$, and both functions x^e and u^e are specified the equilibrium manifold with the nominal equilibrium point, $x_{ss} = x^e(0)$. If

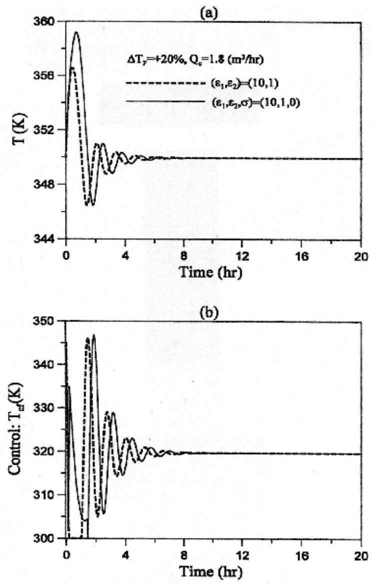

Fig. 4 Disturbance rejection of step change in the feed temperature using the PI-type state feedback controller without or with anti-reset windup design

the equilibrium function of x^e is determined from the off-line approach, then a PI-type feedforward/output feedback control is written as

$$u = u_{PI}(x^e(\omega), y) + K_c^{PI}(x^e(\omega), y) \times \left[(y_{sp} - y) + \frac{1}{\tau_I^{PI}} \int_0^t (y_{sp} - y) d\tau \right] \tag{16}$$

and also suppose that the following term

$$\frac{\partial F\left(x^e(\omega), u^e(\omega), \omega\right)}{\partial x} + \frac{\partial F\left(x^e(\omega), u^e(\omega), \omega\right)}{\partial u} u_{PI}\left(x^e(\omega), y_{sp}\right) \tag{17}$$

has only negative-real-part eigenvalue for $\omega \in \Gamma$. Basically, the approximation of equilibrium function x^e for this PCSTR system can be easily obtained through numerical approaches, e.g. an interpolation combination [6].

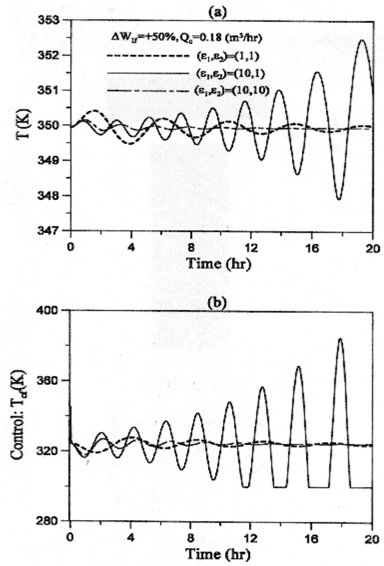

Fig. 5 Disturbance rejection of step change of initiator in the feed using the PI-type feedforward/output feedback controller:

Discussion 3: Two modes of above PI configuration are nonlinear and parameterized, so the tuning interaction between ε_1 and ε_2 are worthily investigated. Inspired by the low-and-high gain design technique in Saberi et al. [18], both tuning parameters are expected to perform low-and-high gain effects for stable output regulation. In Fig. 5(a), the tuning constants $(\varepsilon_1, \varepsilon_2) = (10,10)$ provide the satisfactory output regulation for an unknown disturbance, ΔW_{If}, but the pure high-gain approach $(\varepsilon_1, \varepsilon_2) = (10,1)$ may destabilize the closed-loop system.

IV. Nonlinear PID Control Scheme

Above PI control design procedures are superior to a two-time-scale PCSTR system with $\tau_c << 1$, but the extended design procedure for a relative-degree-two system is developed. First, the augmented transformation is defined as

$$z_1 = y - y_m, \quad z_2 = \varepsilon_2(\alpha_1 - \dot{y}_m) + z_1 \tag{18}$$

where $\alpha_1 = L_{f_1}h + \xi L_{g_1}h$. Moreover, the time derivative of z_1 and z_2 are expressed as

$$\begin{aligned} \varepsilon_2 \dot{z}_1 &= -z_1 + z_2 \\ \dot{z}_2 &= \varepsilon_2 \alpha_2 + \alpha_1 + \left(\varepsilon_2 \frac{\partial \alpha_1}{\partial \xi} g_2 \right) u + \varepsilon_1 \varepsilon_2 \dot{y} - \dot{y}_m \end{aligned} \tag{19}$$

where $\alpha_2 = \frac{\partial \alpha_1}{\partial x}(f_1 + \xi g_1) + \frac{\partial \alpha_1}{\partial \xi} f_2$. If the state feedback control law is set as

$$u=\left(\varepsilon_2\frac{\partial\alpha_1}{\partial\xi}g_2\right)^{-1}\left[-z_2/\varepsilon_2-\alpha_2-\varepsilon_1\varepsilon_2\dot{y}+\dot{y}_m\right] \tag{20}$$

Then the closed-loop system can be written as

$$\begin{aligned}&\varepsilon_2\dot{z}_1=-z_1+z_2, \qquad \varepsilon_2\dot{z}_2=-z_2\\&\dot{y}_m=\varepsilon_1(y_{sp}-y), \qquad \dot{\eta}_2=L_{f_1}\eta_2\end{aligned} \tag{21}$$

where $\eta_2(x)\in\Re^{n-2}$. Similarly, the stable nonlinear inversion and the stable internal dynamic $\dot{\eta}_2$ are required. Using the reference model in eq. (7), the novel PID-type state feedback control is written as

$$\begin{aligned}u=&u_{PID}\left(\varsigma,y\right)+K_c^{PID}\left(\varsigma,y\right)\\&\cdot\left[\left(y_{sp}-y\right)+\frac{1}{\tau_I^{PID}}\int_0^t\left(y_{sp}-y\right)d\tau+\tau_D^{PID}\frac{de}{dt}\right]\end{aligned} \tag{22}$$

where $\varsigma\triangleq\begin{bmatrix}x\\\xi\end{bmatrix}$ and

$$\begin{aligned}u_{PID}&=\left(\varepsilon_2\frac{\partial\alpha_1}{\partial\xi}g_2\right)^{-1}\left[-\alpha_1-\alpha_2-y/\varepsilon_2+y_{m,b}/\varepsilon_2\right]\\K_c^{PID}&=\left(\varepsilon_2\frac{\partial\alpha_1}{\partial\xi}g_2\right)^{-1}(\varepsilon_1+\varepsilon_2)\\\tau_I^{PID}&=\frac{\varepsilon_2(\varepsilon_1+\varepsilon_2)}{\varepsilon_1}\\\tau_D&=\frac{\varepsilon_1\varepsilon_2}{\varepsilon_1+\varepsilon_2}\end{aligned} \tag{23}$$

Remark 2: Obviously, the system has not restricted in a two-time-scale form, and the control law connected with the derivative output will induce the nonlinear PID configuration. The state-dependent nonlinear function u_{PID} is similar to a bias of PID algorithm, K_c^{PID} is a state-dependent nonlinear gain, and τ_I^{PID} and τ_D are parameterized by both tuning parameters (ε_1 , ε_2). A small ε_2 or a large ε_1 will produce the fast mode so that both tuning parameters are related to high-gain effect. Moreover, if the saturated composite gain K_c^{PID}/τ_I^{PID} is described as

$$\text{sat}\left(K_c^{PID}/\tau_I^{PID}\right)=\text{sat}(\varepsilon_1)\Big/\left(\varepsilon_2^2\frac{\partial\alpha_1}{\partial\xi}g_2\right) \tag{24}$$

then eq. (22) is modified to

$$\begin{aligned}u=&u_{PID}\left(\varsigma,y\right)+K_c^{PID}\left(\varsigma,y\right)\left[\left(y_{sp}-y\right)+\tau_D^{PID}\frac{de}{dt}\right]\\&+sat\left(\frac{K_c^{PID}}{\tau_I^{PID}}\right)\int_0^t\left(y_{sp}-y\right)d\tau\end{aligned} \tag{25}$$

Similarly, the equilibrium-based design is added to establish a PID-type feedforward/output feedback control

$$\begin{aligned}u=&u_{PID}\left(\varsigma^e(\omega),y\right)+K_c^{PID}\left(\varsigma^e(\omega),y\right)\\&\times\left[\left(y_{sp}-y\right)+\frac{1}{\tau_I^{PID}}\int_0^t\left(y_{sp}-y\right)d\tau+\tau_D^{PID}\frac{de}{dt}\right]\end{aligned} \tag{26}$$

where the smooth map $\varsigma^e\triangleq\begin{bmatrix}x^e(\omega)\\\varphi\left(x^e(\omega),u^e(\omega)\right)\end{bmatrix}$, and also suppose that the following term

$$\begin{aligned}&\frac{\partial F\left(x^e(\omega),u^e(\omega),\omega\right)}{\partial x}\\&\quad+\frac{\partial F\left(x^e(\omega),u^e(\omega),\omega\right)}{\partial u}u_{PID}\left(\varsigma^e(\omega),y_{sp}\right)\end{aligned} \tag{27}$$

has only negative-real-part eigenvalue for $\omega\in\Gamma$.

Remark 3: The above PID-type nonlinear control scheme is derived from the I/O linearization approach, but the closed-loop stability should depend on limitations of positive parameters $\left(\varepsilon_1,\varepsilon_2\right)$, the stable internal model $\dot{y}_m$, and stable internal dynamics $\dot{\eta}_2$. The control performance relies on the choice of both parameters $\left(\varepsilon_1,\varepsilon_2\right)$. Essentially, the developed nonlinear PID control schemes are implemented to a relative-degree-two system subject to input constraints. Since the derivative mode can make the smooth output trajectory and increase the closed-loop stability, the PID controller design can improve the drawback of the previous nonlinear PI controller.

Discussion 4: To demonstrate above PID control schemes, Fig. 6(a) depicts that the PID-type state feedback control can effectively reject an unmeasured disturbance on the output, and the corresponding control action in Fig. 6(b) is unsaturated by exploiting the anti-windup compensation with $\sigma=2$.

V. Conclusion

The study is carried out on temperature control of a free-radical PCSTR system subject to physical input constraint and output multiplicity. Through the I/O linearization method as a base of controller syntheses, the state-space formulation of PI- and PID-types state feedback control frameworks are applied for nonlinear relative-degree-one and relative-degree-two systems, respectively. With the aid of the equilibrium-based design, the novel nonlinear PI/PID controllers are developed. Whatever PI or PID control configuration, only two tuning constants are implemented to reduce input constraints as well as reset windup problems. In addition, the proposed issues for closed-loop stability analyses are quite straightforward from the basis feedback linearization approach and equilibrium manifold.

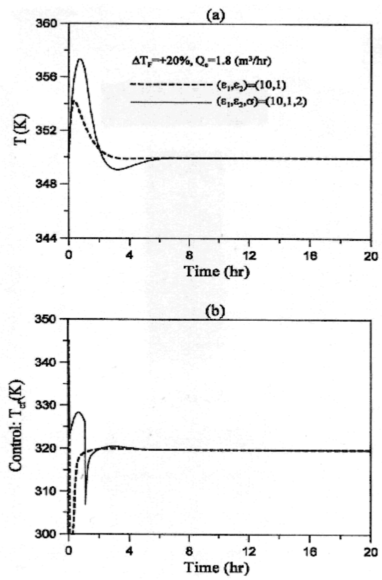

Fig. 6 Disturbance rejection of step change in the feed temperature using the PID-type state feedback controller without or with anti-reset windup design

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