Optimal Transition and Robust Control Design for Exothermic Continuous Reactors

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The problem of jointly designing the optimal steady-state transition and the related tracking controller for a representative class of exothermic continuous chemical reactors is addressed. The combination of optimal, constructive, and conventional control ideas yields a design methodology with: the identification of the underlying solvability conditions with physical meaning, the construction of the optimal transition, a controller to robustly perform the associated tracking task, and a closed-loop stability criterion coupled with conventional-like tuning guidelines. The controller is driven by a temperature measurement, simultaneously manipulates the heat exchange and reactant feed rates, and its implementation does not require the chemical kinetics model. The control scheme consists of a decentralized feedforward–feedback temperature loop and a ratio-type reactant dosage controller. The proposed transition and control design approach is illustrated with an application example treated with numerical simulations. © 2005 American Institute of Chemical Engineers *AIChE J,* 51: 895–908, 2005
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Introduction

The design and control of transitions between steady-state operations are important and challenging problems in the chemical process industry, when different grades must be produced depending on market needs and plantwide production scheduling. The transition problem has two aspects that must be simultaneously accounted for in the light of safety, operability, and cost considerations: (1) the design of a minimum transition time with minimum off-specification product and (2) the design of a suitable controller to reliably perform the transition task. The transition issue is important in the commodity-oriented large scale as well an in the specialized higher added-value product continuous processes; the situation is well

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exemplified by the polymerization industry (Debling et al., 1994; McAuley and MacGregor, 1992; Sinclair, 1987). In the present globalized economy, especially for commodity-oriented large-scale production processes, the problem of grade transition appears more often than in the past as polymerization companies face increasing pressures to switch part of their production toward more specialized higher added-value materials. Many times, the decision to produce a new more specialized grade in a continuous process depends on the trade-off between the increased valued added by the specialty material and the increased cost generated by the transition. In addition, because these new materials tend to have shorter production campaigns than products already well established in the market, the problem of frequent grade transitions is exacerbated. This is an important motivation for studies that address the problem of optimal grade transitions.

Because of the inherent nonlinear and transient features of continuous reactors, the related joint transition and control design problem resembles the same problem for batch and semibatch processes. In industrial practice, it is well known that process design (that is, equipment and operation policy) affects and is affected by control design, and the interplay between them is handled with some dosage of experience in conjunction with process, control, laboratory-to-plant testing, and scale tools (Seferlis and Georgiadis, 2004). Motivated by the need of systematic design and redesign techniques, the field of batch process system engineering is currently an active research area. The batch and semibatch operations have been designed by standard optimization approaches, whereas tracking controllers have been designed with a diversity of control approaches that include time-scheduled conventional proportional–integral (PI) controllers as well as nonlinear geometric and model predictive techniques, and it is not clear how these two design aspects are connected. Even though there have been important advances in the process and control design parts, their integration is lagging behind, and the integration problem is regarded as an important subject of research. Recently, a methodological avenue has been proposed to jointly address the joint operation and control design for batch processes, by combining ideas from optimal, constructive, and inventory control ideas (Alvarez et al., 2004).

Compared with the batch and semibatch process cases, the transition motion and control design problems for continuous reactors have received far less attention. Basically, in industrial practice the transition problems are addressed in a way that is analogous to those of semibatch reactors. In most industrial cases the transition policy has been based on heuristics; however, this approach is proving increasingly inefficient because of market demands that aim to reduce manufacturing costs. With respect to research studies, they have consisted of open-loop stable transition designs by standard optimization methods (Hicks and Ray, 1971; McAuley and MacGregor, 1992; Takeda and Ray, 1999), and the optimal transition design problem has not been formally connected with the related tracking control problem. Moreover, it is known that an open-loop stable system can be addressed either with sequential (Barton et al., 1998; Sargent and Sullivan, 1979) or simultaneous (Biegler, 1990) optimization techniques, and that the case of an open-loop unstable system must be necessarily treated with the simultaneous technique (Bloss et al., 1999). The similarity between batch transition motion and control design suggests the consideration of the aforementioned joint semibatch motion and control design approach for the continuous transition case, and this in turn constitutes the motivation of the present work.

Because the nominal transition motion is the solution of a nonautonomous problem (that is, forced by time-varying exogeneous inputs d and u), the notion of steady-state stability used in the study of (autonomous) continuous process cannot be directly applied, and the same conclusion holds for the notions of controllability and observability. As mentioned before, the solvability of the optimal reactor transition and its related output feedback control problems are underlined by suitable controllability and observability properties and, consequently, the consideration of the transition-operation design problem within an appropriate stability framework is a necessary conceptual ingredient to connect the previous separate approaches to the optimal transition and feedback control design problems.

With respect to passivity, a geometric controller (Isidori, 1985) is passive if it has a relative degree ≤ 1. Optimal nonlinear controllers are inherently robust and passive with respect to a certain output, and an optimality-based model predictive control scheme is underlined by a passivity property. Presumably, because the recent convergence of optimal [model predictive control (MPC)] and geometric control in the so-called constructive control approach is a rather recent event, in the preceding MPC studies this key connection has not been exploited. Because the control and state constraints are accounted for in the design of the nominal transition, we are looking for a controller that resembles the capabilities of a MPC controller, without the burden of on-line computing Riccati equations for the observer design and Hamiltonian equations to compute the constrained control trajectory over a future horizon.

As mentioned before, the preceding studies on the reactor transition problem have formally addressed only the optimal transition part for open-loop stable transition case, assuming that the control part can be separately performed by the existing tracking control designs, which range from gain-scheduled PI control schemes used in batch processes to the nonlinear observer-based (geometric or MPC) control schemes. Moreover, the conventional type gain-scheduled PI controllers are considerably simpler and less demanding with respect to their nonlinear counterparts, and this constitutes serious complexity and reliability drawbacks for the applicability of the advanced nonlinear controllers. Thus, the consideration of the integrated transition and control design problem constitutes a central point of the present study, in the understanding that, in conjunction with the control oriented study presented in Alvarez et al. (2004), the approach can be extended for the case of nonautonomous process systems in general, including start-up and shutdown operations of continuous processes as well as batch and semibatch processes.

In this paper, the problem of jointly designing the optimal steady-state transition and the related tracking controller for a representative class of exothermic continuous chemical reactors is addressed. The points of departure for the present work are:

(1) The optimal approach to the open-loop reactor transition problem (Hicks and Ray, 1971).

(2) The consideration of a simultaneous optimization ap-

proach to address the open-loop transition case (Bloss et al., 1999).

(3) The joint motion and control design for semibatch exothermic reactors (Alvarez et al., 2004).

(4) The connection between the remarkably robust calorimetric reactor control technique and the conventional-like cascade temperature controller with PI loops.

The combination of the associated optimal, constructive, and conventional control ideas yields a design methodology with the identification of the underlying solvability conditions with physical meaning, the construction of the optimal transition, a controller to robustly perform the associated tracking task, including a stability criterion coupled with conventional-like tuning guidelines. The controller is driven by a temperature measurement, simultaneously manipulates the heat exchange and reactant feed rates, and its implementation does not require the chemical kinetics model. The control scheme consists of a decentralized feedforward–feedback temperature loop and a ratio-type reactant dosage controller. The proposed transition and control design approach is illustrated with an application example treated with numerical simulations.

Transition Tracking Problem

Let us consider a continuous stirred tank reactor with a reversible exothermic reaction

$$\dot{c} = \frac{q}{V}[c_f(t) - c] - r(c, T, p_k) \tag{2.1a}$$

$$\dot{T} = \frac{q}{V}[T_f(t) - T] + \beta r(c, T, p_k) - \gamma(T - T_c) \tag{2.1b}$$

subject to initial conditions

$$c(0) = c_o \tag{2.2a}$$

$$T(0) = T_o \tag{2.2b}$$

The reactor states are the concentration c and the temperature T. The control inputs are the volumetric feedrate q and the coolant temperature T_c; c_f is the feed concentration; T_f is the feed temperature; V is the reactor volume; r is the nonlinear reaction rate; p_k is the vector of kinetics parameters; and the parameters β and γ are given by

$$\beta = \frac{-\Delta H}{\rho C_p V}$$

$$\gamma = \frac{UA}{\rho C_p V}$$

where $-\Delta H$ is the heat of reaction, ρ is the mixture density, C_p is the specific heat capacity, U is the reactor-jacket heat transfer coefficient, and A is the corresponding area. In vector notation, the reactor is given by

$$\dot{x} = f[x, d(t), u, p], \quad y = x, \quad x(t_o) = x_o \tag{2.3}$$

where

$$x = [c, T]'$$

$$d = [c_f, T_f]'$$

$$u = [q, T_c]'$$

$$p = [p_k', p_c']'$$

$$p_c = [V, \beta, \gamma]'$$

and p_c is the vector of "calorimetric" parameters.

Assuming that the reaction rate is Lipschitz continuously differentiable in (x, d, u, r) and that the inputs $d(t)$ and $u(t)$ are piecewise continuous functions of time, each "data" set $\{x_o, d(t), u(t), p\}$ uniquely determines a reactor motion:

$$x(t) = \tau[t, t_o, d(\cdot), u(\cdot), p] \tag{2.4}$$

where τ is the nonlinear transition map that takes the reactor state x_o at time t_o to the state $x(t)$ at time t.

Definition 1 *The unperturbed motion $x(t)$ (Eq. 2.4) of the nonlinear system (Eq. 2.3) is said to be E (exponentially)-stable if, in some neighborhood of x_o, there are two constants A, $L > 0$ so that the (initial state) perturbed motions*

$$\chi(t) = \tau[t, t_o, \chi_o, d(\cdot), u(\cdot), p]$$

are bounded as follows:

$$|\chi(t) - x(t)| \le Ae^{-L(t-t_o)}|\chi_o - x_o|$$

The motion $x(t)$ is said to be RE(exponentially)-stable if, in some neighborhood of $\{x_o, d(t), u(t), p\}$, there are five constants A, L, B_d, B_u, $B_p > 0$ so that the (initial state, exogenous input, model parameter) perturbed motions

$$\chi(t) = \tau[t, t_o, \chi_o, \delta(\cdot), \upsilon(\cdot), \pi]$$

are bounded as follows:

$$|\chi(t) - x(t)| <= Ae^{-L(t-t_o)}|\chi_o - x_o| + (A/L)[B_d\|\delta(t) - d(t)\| + B_u\|\upsilon(t) - u(t)\| + B_p\|\pi - p\|]$$

■

In differential form, the preceding RE-convergence inequality can be restated as follows:

$$|\chi(t) - x(t)| \le s(t) : \dot{s} = -Ls + (A/L) \times [B_d\delta_d + B_u\delta_u + B_p\delta_p] \qquad s(t_o) = s_o = A|\chi_o - x_o| \tag{2.5}$$

where

$$\delta_d = \|\delta(t) - d(t)\|$$

$$\delta_u = \|v(t) - u(t)\|$$

$$\delta_p = \|\pi - p\|$$

In the period $[0, t_o)$, the reactor must be operated at its (possibly open-loop unstable) steady-state $\bar{x}_o$, which is determined (possibly with multiplicity) by the set $(\bar{d}, \bar{u}_o, p)$. At time t_o, the control input $\bar{u}(t)$ must be changed in such a way that the reactor motion $\bar{x}(t)$ reaches, at time t_f, the prescribed final (possibly open-loop unstable) steady-state $\bar{x}_f$, which is determined (possibly with multiplicity) by the set $(\bar{d}, \bar{u}_f, p)$. Once the reactor has reached its final steady state, it must stay there for the period $t > t_f$. Let O_o (or O_f) denote the initial (or final) nominal steady-state operation, and let $\bar{\theta}(t)$ denote the corresponding nominal transition operation:

$$O_o = (\bar{x}_o, \bar{u}_o, \bar{d}, p) \qquad O_f = (\bar{x}_f, \bar{u}_f, \bar{d}, p) \qquad (2.6)$$

$$\bar{\theta}(t) = [\bar{x}(t), \bar{u}(t)] \qquad t \in [t_o, t_f] \qquad \theta(t_o) = O_o \qquad \theta(t_f) = O_f \quad (2.7)$$

Our first problem consists in: (1) designing a nominal reactor transition $\bar{\theta}(t)$ with robustness to model parameter errors $(\pi - p)$, and (2) in designing a temperature-driven and reaction rate model-independent feedback controller to robustly regulate the initial and final nominal operations, and to robustly track the prescribed nominal transition $\bar{\theta}(t)$, by means of a temperature-driven feedback controller whose construction and functioning is independent of the nonlinear reaction kinetics model $r(c, T, p_k)$ and heat transfer information.

Transition Design

In this section the design of an admissible (possibly open-loop unstable) nominal reactor transition that can be robustly tracked by means of a temperature-driven feedback controller is discussed. First, the dynamic inversion algorithm (Hirschorn, 1981) is recalled to establish necessary conditions for the existence of a temperature-feedback robustly stabilizable nominal transition. Then, we discuss how the nominal transition can be constructed by solving a dynamic optimization problem (Hicks and Ray, 1971).

To obtain the underlying necessary condition for the solvability of our controlled transition problem, let us assume the existence of a nominal transition $\bar{\theta}(t) = [\bar{x}(t), \bar{u}(t)]$, obtain its corresponding output $\bar{y}(t) = \bar{x}(t)$, and build the dynamic inverse by taking the time derivative of the output $\bar{y}(t) = [\bar{y}_c(t), \bar{y}_T(t)]'$ to generate a time-varying algebraic equation

$$\dot{\bar{y}}_c(t) = -r[\bar{y}_c(t), \bar{y}_T(t), p_k] + \bar{q}(t)[\bar{c}_f - \bar{y}_c(t)]/V \quad (3.8a)$$

$$\dot{\bar{y}}_T(t) = \beta r[\bar{y}_c(t), \bar{y}_T(t), p_k] + \bar{q}(t)[\bar{T}_f(t) - \bar{y}_T(t)]/V - \gamma[\bar{y}_T(t) - \bar{T}_c(t)] \quad (3.8b)$$

that, with respect to time, can be uniquely and robustly solved for the control input $\bar{u}(t)$:

$$\bar{q}(t) = \{\dot{\bar{y}}_c(t) + r[\bar{y}_c(t), \bar{y}_T(t), p_k]\}V[\bar{c}_f - \bar{y}_c(t)]^{-1} := m_q[\bar{y}_c(t), \bar{y}_T(t), \dot{\bar{y}}_c(t), p_k, V, \bar{c}_f] \quad (3.9a)$$

$$\bar{T}_c(t) = \bar{y}_T(t) + \gamma^{-1}\{\dot{\bar{y}}_T(t) - \beta r[\bar{y}_c(t), \bar{y}_T(t), p_k] - \bar{q}(t)[\bar{T}_f(t) - \bar{y}_T(t)]/V\} := m_q[\bar{y}_c(t), \bar{y}_T(t), \dot{\bar{y}}_T(t), p_k, T_f] \quad (3.9b)$$

For the time-varying algebraic equation pair (Eqs. 3.8a and 3.8b) to be uniquely and robustly solvable for the control input pair $(\bar{q}, \bar{T})(t)$ the following conditions must be met: (i) The heat exchange capability must be larger than a minimum value $\gamma^* > 0$, (ii) the nominal concentration function $\bar{y}_c(t)$ must be smaller than a maximum value c^*, and (iii) the changes of the reaction rate with respect to (x, p_k) must be admissibly bounded:

$$(i) \qquad \gamma > \gamma^* \quad (3.10a)$$

$$(ii) \qquad \bar{y}_c(t) < c^* = \bar{c}_f - \delta^*_{C_f} \quad (3.10b)$$

$$(iii) \qquad \sup[\partial_\alpha r[\bar{c}(t), \bar{T}(t), p_k] \le l^r_\alpha \quad (3.10c)$$

where $\alpha = c, T, p_k$. In addition, the nominal transition $\bar{\theta}(t) = [\bar{x}(t), \bar{u}(t)]$ must meet output and control bounds:

$$(iv) \qquad q^- \le \bar{q}(t) \le q^+ \qquad \bar{T}^-_c \le \bar{T}_c(t) \le \bar{T}^+_c \quad (3.11a)$$

$$(v) \qquad c^- \le \bar{y}_c(t) \le c^+ < c^* \qquad \bar{T}^- \le \bar{y}_T(t) \le \bar{T}^+ \quad (3.11b)$$

Thus, the nominal (open-loop) transition is given by

$$\bar{\theta}(t) = [\bar{x}(t), \bar{u}(t)] \quad (3.12a)$$

$$\bar{x}(t) = [\bar{y}_c(t), \bar{y}_T(t)]' \quad (3.12b)$$

$$\bar{u}(t) = m_q[\bar{y}(t), \dot{\bar{y}}(t), d(t), p] \quad (3.12c)$$

Following Zaldo and Alvarez (1998) for equipment-operation-control design for an emulsion polymerization reactor, by guessing an initial trajectory $\bar{y}(t)$, the iterative application of the dynamic inversion formula leads, in a few steps, to the design of an admissible nominal transition $\bar{\theta}(t) = [\bar{x}(t), \bar{u}(t)]$ that meets adequately the conditions 3.10a–3.10c, and takes, as soon as possible, the reactor from its initial steady state to its final one. This procedure may include the design or redesign of the equipment (that is, the volume, the steady states or the heat exchange system). Alternatively, the transition can be designed by solving a suitable constrained dynamic optimization problem

$$\min_{u(t)} \int_{t_o}^{t_f} \phi[x(\tau), u(\tau), w]d\tau \quad (3.13a)$$

s.t.

$$\dot{x} = f[x, \bar{d}, u(t), \pi] \quad (3.13b)$$

$$x(t_o) = \bar{x}_o \quad (3.13c)$$

$$x \in X \quad (3.13d)$$

$$u \in U \quad (3.13e)$$

$$x(t_f) = \bar{x}_f \quad (3.13f)$$

in the understanding that the analysis and adequate fulfillment of the above discussed solvability conditions should lead to a robust or well-posed optimization problem. ϕ is the Lagrangian functional and w represents adjustable parameters or weights. In principle, the dynamic inversion inspection-based approach should be used to gain valuable insight on the nature of the transition and to provide an adequate initial trajectory guess of the optimization routine. It must be pointed out that the solution of this dynamic optimization approach presents some drawbacks: (i) the choice of the Lagrangian function is by no means a trivial task, and its determination requires a certain dosage of trial and error; (ii) the majority of the dynamic optimization routines are intended for state transitions that are open-loop stable (Biegler, 2001); there are no systematic schemes to address the case of an unstable or poorly stable open-loop transition. A further discussion on this important subject is beyond the scope of the present work, and here it suffices to say that one of our application examples is an open-loop unstable transition (from unstable to unstable steady state).

Finally, it must be pointed out that the robust dynamic invertibility of the reactor about its nominal transition motion $\bar{x}(t)$ implies the robust solvability of the state-feedback tracking control problem with *LNPA* (linear, noninteractive, pole assignable) output error dynamics (Alvarez, 1996; Isidori, 1985). In fact, the difficult problem of control with input saturation can be eliminated or minimized if the nominal transition is judiciously designed so that the control constraints are not met for a set of prescribed exogenous input, initial state, and parameter errors.

Controller Construction

In this section a candidate temperature-driven controller to robustly track a (possibly open-loop unstable) prescribed admissible reactor transition is constructed. The points of departure are: the nonlinear geometric state-feedback controller with *LNPA* (Alvarez, 1996; Isidori, 1985) concentration-temperature tracking error dynamics, the proportional–integral (*PI*) estimator-based nonlinear geometric temperature tracking controller (Alvarez and Lopez, 1999), and its connection with the so-called calorimetric control approach (Tyner et al., 1999). The methodology is along the spirit of the constructive nonlinear geometric idea (Isidori, 1985); it regards the control structure as design degree of freedom, and resorts to a stability analysis to assess the corresponding performance and robustness properties. In this section we circumscribe ourselves to the constructive part, in the understanding that the corresponding robust stability analysis will be executed a posteriori in the next section.

Two-input state-feedback control

For construction and comparison purposes, in this section the following auxiliary state-feedback control problem is considered: given the actual parameter model parameter p, and assuming that the state $x = [c, T]'$ and the exogenous input $d = [c_f, T_f]$ about $\bar{d}$ are measured on-line; build a state-feedback controller with a d-feedforward path so that the closed-loop reactor robustly tracks the prescribed nominal transition motion $\bar{x}(t)$ with *LNPA* error dynamics:

$$\dot{e}_c = -\omega_c e_c \qquad e_c(t_o) = e_{co} = c_o - \bar{c}_o \qquad e_c = c - \bar{c}(t) \qquad e = [e_c, e_T]' \quad (4.14a)$$

$$\dot{e}_T = -\omega_T e_T \qquad e_T(t_o) = e_{To} = T_o - \bar{T}_o \qquad e_T = T - \bar{T}(t) \quad (4.14b)$$

where ω_c (or ω_T) is the concentration (or temperature) control gain. The combination of this equation with the open-loop reactor model (Eqs. 2.1a and 2.1b) yields the following state-feedback controller:

$$\begin{aligned} q^o &= \{\dot{\bar{y}}_c(t) - \omega_c[c - \bar{y}_c(t)] + r[c, T, p_k]\}V[c_f(t) - \bar{y}_c(t)]^{-1} \\ &:= \mu_c^o[x, d(t), p, \omega, t] \end{aligned} \quad (4.15a)$$

$$\begin{aligned} T_c^o &= \bar{y}_T(t) + \gamma^{-1}\{\dot{\bar{y}}_T(t) - \omega_T[T - \bar{y}_T(t)] - \beta r[c, T, p_k] \\ &\quad - q[T_f(t) - \bar{y}_T(t)]/V\} \\ &:= \mu_T^o[x, d(t), p, \omega, t] \end{aligned} \quad (4.15b)$$

where the superindex "o" denotes "evaluated with the exact arguments." The application of the preceding controller to the reactor (Eq. 2.3) yields the closed-loop system

$$\dot{x} = \{x, d(t), \mu^o[x, d(t), p, \omega, t], p\} \qquad y = x \qquad x(t_o) = x_o \quad (4.16)$$

and its corresponding closed-loop motion and transition, respectively

$$x(t) = \tau_c[t, t_o, x_o, d(\cdot), \omega, p] \quad (4.17a)$$

$$\theta(t) = [x(t), u(t)] \qquad u(t) = \mu[\bar{y}(t), d(t), p, t] \quad (4.17b)$$

When there are neither initial ($x_o = \bar{x}_o$ or $e_o = 0$ in Eqs. 4.15a and 4.15b) nor exogenous input [$d(t) = \bar{d}$] errors, the preceding state-feedback controller (4.16) coincides with the dynamic inverse (3.9a–3.9b), implying that the closed-loop reactor transition (4.17b) coincides with the nominal one (3.9a–3.9b) [that is, $\theta(t) = \bar{\theta}(t)$]. If there are exogenous input disturbances $d(t) \neq \bar{d}$, the closed-loop motion $x(t)$ still coincides with the nominal one $\bar{x}(t)$, and the corresponding input $u(t)$ becomes a perturbation of the nominal one $\bar{u}(t)$, depending on the kind and sizes of the initial condition (e_o) exogenous input [$e_d(t) = d(t) - \bar{d}$] errors and according to the following expression:

$$e_u(t) = u(t) - u^o(t) = \mu^o[\bar{x}(t), d(t), p, \omega, t] - \mu^o[\bar{x}(t), \bar{d}, p, \omega, t] \qquad |e_u(t)| \le L_d^{\mu^o}|e_d(t)|$$

where $L_d^{\mu^o}$ is the Lipschitz constant of the nonlinear map μ^o with respect to its argument d. In the case that the nominal transition had been incorrectly designed overlooking the adequate fulfillment of the robust dynamic invertibility conditions, say by having a very small transfer coefficient to reactor heat capacitance ratio (that is, γ very small) and/or setting a concentration trajectory $\bar{c}(t)$ that at some point is very close to $\bar{c}_f + d_c(t) = c_f(t)$, the ill-conditioning of the built-in dynamic inverse equation pair should imply an excessive sensitivity of the control $u(t)$ with respect to the exogenous input disturbance $e_d(t)$. In the next proposition these features of the state-feedback controller are summarized, and generalized for the case of having also model parameter errors.

Proposition 1 (*Proof in Appendix A*). *Let the robust dynamic invertibility solvability conditions* (*i*) *and* (*ii*) *be met along the nominal transition motion* $\bar{\theta}(t) = \{\bar{x}(t), \bar{u}(t)\}$, *with the initial condition* (x_o), *and assume that the exogenous input* $d(t)$ *and the control parameter* π *have deviations about their nominal* ($\bar{d}$) *and actual* (p) *values, respectively,*

$$e_o = [c_o, T_o]' - [\bar{c}_o, \bar{T}_o]', \; e_d(t) = d(t) - \bar{d}, \qquad d(t) = [c_f, T_f]; \; e_p = \pi - p$$

Then, the application of the state-feedback controller with $[d(t), \pi]$ *yields a closed-loop reactor transition* $\theta_c(t)$ *that RE-converges to the nominal one* $\bar{\theta}(t)$, *according to the following inequalities* (L_d^f *is the Lipschitz constant of* f *with respect to* d).

$$|c(t) - \bar{c}(t)| \le e^{-\omega_c(t-t_o)}|c_o - \bar{c}_o| + L_p^{f_c}|\pi - p|/\omega_c$$

$$|T - \bar{T}| \le e^{-\omega_T(t-t_o)}|T_o - \bar{T}_o| + L_p^{f_T}|\pi - p|/\omega_T$$

$$|q^o(t) - \bar{q}(t)| \le L_x^{\mu_c^o}|x(t) - \bar{x}(t)| + L_d^{\mu_c^o}|d(t) - \bar{d}| + L_p^{\mu_T^o}|\pi - p|$$

$$|T_c^o(t) - \bar{T}_c(t)| \le L_x^{\mu_T^o}|x(t) - \bar{x}(t)| + L_d^{\mu_T^o}|d(t) - \bar{d}| + L_p^{\mu_T^o}|\pi - p|$$

■

As can be seen in the Appendix, the Lipschitz conditions grow with the sizes of the disturbances and become excessively large when the robust solvability conditions (i), (ii), and (iii) are poorly met. When there are neither input disturbances $[d(t) = \bar{d}]$ nor initial condition ($x_o = \bar{x}_o$) and control parameter ($\pi = p$) errors, the closed-loop transition $\theta_c(t) = \{x(t), u(t)\}$ coincides with the prescribed nominal one $\bar{\theta}(t) = \{\bar{x}(t), \bar{u}(t)\}$. If there is only initial condition error ($x_o \neq \bar{x}$), the closed-loop transition $\theta_c(t)$ exponentially (that is, asymptotically without offset) approaches the nominal one $\bar{\theta}(t)$, with adjustable convergence rate. If there is initial condition error ($x_o \neq \bar{x}_o$) and exogenous input deviations $[d(t) \neq \bar{d}]$ the closed-loop reactor motion $x(t)$ exponentially converges, with adjustable rate, to the nominal motion $\bar{x}(t)$; and the control input $u^o(t)$ RE-converges, with adjustable rate, to the nominal input $\bar{u}(t)$, with an offset depending on the size of the initial error and of the exogenous input deviation. In the most general case of (initial condition and parameter) errors and (exogenous input) deviations, the closed-loop reactor transition $\theta_c(t)$ RE-converges to the nominal one $\bar{\theta}(t)$, with adjustable convergence rate and with a deviation that depends on the size of the errors and deviations.

Single-input/single-output dynamic temperature-driven controller

Because only temperatures can be measured on-line, the direct application of the standard geometric approach suggests the consideration of a relative degree one estimator-based controller (Alvarez, 1996), with a preprogrammed feed flow rate model–based input $\bar{q}(t)$, and with the control target of tracking the prescribed temperature time-varying setpoint $\bar{y}_T(t)$. For this purpose, one must require the temperature–flow rate forced (zero) dynamics

$$\dot{\bar{c}} = -r[\bar{c}, \bar{y}_T(t), p_k] + \bar{q}(t)[\bar{c}_f - c]/V \qquad \bar{c}(t_o) = \bar{c}_o \tag{4.18}$$

to have a nominal (zero-dynamics) restricted concentration motion

$$\bar{c}(t) = \tau_c[t, t_o, \bar{c}_o, \bar{y}_T(\cdot), \bar{q}(\cdot), \bar{c}_f, V, p_k] \tag{4.19}$$

that is RE-stable with respect to disturbances $\{c_o, y_T(t), q(t), c_f(t), \hat{V}, \pi_k\}$ about $\{\bar{c}_o, \bar{y}_T(t), \bar{q}(t), \bar{c}_f, V, p_k\}$. In this case, the corresponding PI estimator-based (Alvarez and Lopez, 1999) RE-convergent tracking controller (Alvarez et al., 2000) is given by

$$\dot{\hat{c}} = -r(\hat{c}, \hat{T}, \pi_k) + \bar{q}(t)[c_f(t) - \hat{c}]/\hat{V} \tag{4.20a}$$

$$\dot{\hat{T}} = \hat{\beta}r(\hat{c}, \hat{T}, \pi_k) + \bar{q}(t)[T_f(t) - \hat{T}]/\hat{V} - \hat{\gamma}[\hat{T} - T_c] + \chi_T + 2\xi_o\omega_o[y_T(t) - \hat{T}] \tag{4.20b}$$

$$\dot{\chi} = \omega_o^2[y_T(t) - \hat{T}] \tag{4.20c}$$

$$T_c = \bar{y}_T(t) + \hat{\gamma}^{-1}\{\dot{\bar{y}}_T(t) - \omega_T[\hat{T} - \bar{y}_T(t)] - \hat{\beta}r(\hat{c}, T, \pi_k) - q[T_f(t) - \bar{y}_T(t)]/\hat{V}\} := \mu^p[\hat{x}, d(t), \pi, \omega, t] \tag{4.20d}$$

$$\hat{c}(0) = \hat{c}_o \tag{4.20e}$$

$$\hat{T}(0) = \hat{T}_o \tag{4.20f}$$

where $y_c = c$, $y_T = T$, $\pi = [\pi_k', \pi_c']'$, and $\pi_c = [\hat{V}, \hat{\beta}, \hat{\gamma}]'$. π is an approximation of the parameter vector p, and χ_m is a fast convergent estimate of the persistent modeling errors in the estimator input ($\bar{q}$, T_f)–output (y_T) path so that the controller asymptotically (that is, without offset) tracks the prescribed output temperature. Referring to the formulation of our control problem, this controller has four drawbacks: (1) the controller requires a model of the reaction function r; (2) the corresponding modeling error manifests itself in the deviation $[c(t) - \bar{c}(t)]$ of the closed-loop transition motion, (3) the feed flow rate cannot be adjusted to compensate for the concentration deviations; and (4) the functioning of the controller depends on meeting the RE-stability requirement on the zero-dynamics concentration motion (Eq. 4.19).

Calorimetric estimation-based controller

Let us recall the construction of the (static) two-input state-feedback static and (dynamic) temperature-driven estimator-based controller, and build our candidate dynamic controller according to the following rationale:

(1) In Eq. 4.20b, eliminate the heat-generation term [that is, $\hat{\beta}r(\hat{c}, \hat{T}, \pi_k) = 0$].

(2) In Eqs. 4.20a and 4.20b replace the integral action χ term by the estimate $\hat{Q}$ of $Q = \beta r(c, T, p_k)$.

(3) In Eq. 4.20a replace $r(\hat{c}, \hat{T}, \pi_k)$ by $r(\hat{c}, \hat{T}, \pi_k)/\hat{\beta}$.

(4) In Eq. 4.20d replace $\hat{\beta}r(\hat{c}, T, \pi_k)$ by $\hat{Q}/\hat{\beta}$.

(5) Incorporate the q-state-feedback controller (Eq. 4.15a) with $[r(c, T, p_k), c, V, c_f]$ replaced by $[\hat{Q}/\hat{\beta}, \hat{c}, \hat{V}, \bar{c}_f]$. The result is the following two-input temperature-driven dynamic tracking controller

$$\dot{\hat{c}} = -\hat{Q}/\hat{\beta} + q(t)(\bar{c}_f - \hat{c})/\hat{V} \tag{4.21}$$

$$\dot{\hat{T}} = \hat{Q} + q[T_f(t) - \hat{T}]/\hat{V} - \hat{\gamma}[\hat{T} - T_c] + 2\xi_o\omega_o[y_T(t) - \hat{T}] \tag{4.22}$$

$$\dot{\hat{Q}} = \omega_o^2[y_T(t) - \hat{T}] \tag{4.23}$$

$$q = \{\dot{\bar{y}}_c(t) - \omega_c[\hat{c} - \bar{y}_c(t)] + \hat{Q}/\hat{\beta}\hat{V}\}[\bar{c} - \bar{y}_c(t)]^{-1} \tag{4.24}$$

$$T_c = \bar{y}_T(t) + \hat{\gamma}^{-1}\{\dot{\bar{y}}_T(t) - \omega_T[\hat{T} - \bar{y}_T(t)] - \hat{Q} - q[T_f(t) - \hat{T}]\hat{V}^{-1}\} \tag{4.25}$$

$$\hat{c}(t_o) = \hat{c}_o = \bar{c}_f - \hat{Q}_o/[\hat{\beta}q(t_o)]^{-1} \tag{4.26}$$

$$\hat{T}(t_o) = \hat{T}_o \tag{4.27}$$

$$\hat{Q}(t_o) = \hat{Q}_o = \hat{\beta}r(\hat{c}_o, \hat{T}_o, \pi_k) \tag{4.28}$$

with model-based initial condition $(\hat{c}_o, \hat{Q}_o)$.

This controller has a cascade q-to-T_c interconnection. The state pair (T, Q) is RE-observable (Alvarez and Lopez, 1999) along any possible practical reactor transition or, equivalently, instantaneously or locally weakly observable (Hermann and Krener, 1977) along any reactor motion. Once the heat generation rate estimate $\hat{Q}$ is available, the preceding controller amounts to the use of dynamical heat and mass balances in conjunction with feedback from the calorimetric-based on-line estimate pair $(\hat{T}, \hat{Q})$.

In terms of a closed-loop estimation scheme, the preceding controller is given by

$$\dot{\hat{c}} = \dot{\bar{y}}_c(t) - \omega_c[\hat{c} - \bar{y}_c(t)] \qquad \hat{c}(t_o) = \hat{c}_o \tag{4.29a}$$

$$\dot{\hat{T}} = \dot{\bar{y}}_T(t) - \omega_T[\hat{T} - \bar{y}_T(t)] + 2\xi_o\omega_o[y_T(t) - \hat{T}] \qquad \hat{T}(t_o) = \hat{T}_o \tag{4.29b}$$

$$\dot{\hat{Q}} = \omega_o^2[y_T(t) - \hat{T}] \qquad \hat{Q}(t_o) = \hat{Q}_o \tag{4.29c}$$

$$\begin{aligned} q &= \{\dot{\bar{y}}_c(t) - \omega_c[\hat{c} - \bar{y}_c(t)] + \hat{Q}/\hat{\beta}\}\hat{V}[\bar{c} - \bar{y}_c(t)]^{-1} \\ &:= \mu_c(\hat{Q}, \hat{c}, \bar{c}, \pi_C, t) \end{aligned} \tag{4.29d}$$

$$\begin{aligned} T_c &= \bar{y}_T(t) + \hat{\gamma}^{-1}\{\dot{\bar{y}}_T(t) - \omega_T[\hat{T} - \bar{y}_T(t)] - \hat{Q} - q[T_f(t) - \hat{T}]\hat{V}^{-1}\} \\ &:= \mu_T[\hat{T}, \hat{Q}, \hat{c}, \bar{c}, T_f(t), \pi_C, t] \end{aligned} \tag{4.29e}$$

It must be pointed out that the closed-loop estimator is a linear one, in agreement with the *LNPA* property of the underlying kinetics model-based nonlinear state-feedback controller; the elimination of the unknown reaction rate model rendered a linear static state-feedback map (d and e) and, consequently, the closed-loop dynamic linear controller is a linear one with respect to the dynamical state set $(\hat{T}, \hat{Q}, \hat{c})$. This remarkable linearity property is a consequence of basing the controller on the linear mass and energy balances in conjunction with the "instantaneous" (that is, local weak observability; Hermann and Krener, 1977) observability property of the temperature–heat motion $[T(t), Q(t)]'$ of any practically possible reaction transition.

Controller and estimator tuning

To design the nonlinear closed loop control system we will assume that the controlled variables are the product composition (c) and reactor temperature (T), whereas the manipulated variables are the volumetric feedstream flow rate (q) and cooling temperature (T_c). The input/output pairings are selected as follows,

$$q \rightarrow c$$

$$T_c \rightarrow T$$

If we agree that the states (c, T) are also the measured variables:

$$y_c = c \tag{4.30}$$

$$y_t = T \tag{4.31}$$

then

$$\frac{dy_c}{dt} = \frac{dc}{dt} = \frac{1}{\theta}(c_f - c) - r \tag{4.32}$$

$$\frac{dy_t}{dt} = \frac{dT}{dt} = \frac{1}{\theta}(T_f - T) + Jr - \alpha u(T - T_c) \tag{4.33}$$

The right-hand sides of Eqs. 4.32 and 4.33, which represent nonlinear terms, can be cast in linear form as

$$\frac{dy_c}{dt} = \nu_c \quad (4.34)$$

$$\frac{dy_t}{dt} = \nu_t \quad (4.35)$$

By combining the right-hand sides of Eqs. 4.32 and 4.34 (and replacing $\theta = V/q$) and the right-hand sides of Eqs. 4.33 and 4.35, we obtain the equations for computing the closed-loop value of the manipulated variables:

$$q = \frac{(\nu_c + r)V}{(c_f - c)} \quad (4.36)$$

$$T_c = T - \frac{\left[\frac{q}{V}(T_f - T) + Jr - \nu_t\right]}{\alpha u} \quad (4.37)$$

The ν_c and ν_t terms can be obtained from the following proportional + integral control laws:

$$\nu_c = \dot{c} + k_c(c^d - c) + \hat{x}_m^c$$

$$\nu_t = \dot{T} + k_T(T^d - T) + \hat{x}_m^T$$

The estimator dynamics is represented by the following set of equations:

$$\dot{\hat{c}} = f_1(\hat{c}, \hat{T}, \hat{p}) + S_o K_1^{oc}(y_1 - \hat{c}) + \hat{x}_m^c \quad (4.38)$$

$$\dot{\hat{T}} = f_2(\hat{c}, \hat{T}, \hat{p}) + S_o K_1^{oT}(y_2 - \hat{T}) + \hat{x}_m^T \quad (4.39)$$

$$\dot{\hat{x}}_m^c = S_o^2 K_2^{oc}(y_1 - \hat{c}) \quad (4.40)$$

$$\dot{\hat{x}}_m^T = S_o^2 K_2^{oT}(y_2 - \hat{T}) \quad (4.41)$$

where f_1 and f_2 stand for the right-hand sides of the mass and energy balances, respectively.

To implement the estimator initial conditions must be supplied. In this work the following initial conditions were used:

$$\hat{c} = c^s$$

$$\hat{T} = T^s$$

$$\hat{x}_m^c = 0$$

$$\hat{x}_m^T = 0$$

where c^s and T^s stand for the steady-state concentration and temperature, as defined by Eqs. 2.1a and 2.1b and by the set of system parameters.

Controller

$$k_c = S_c \omega_c^c \quad (4.42)$$

$$k_T = S_c \omega_T^c \quad (4.43)$$

where ω_c^c and ω_T^c stand for the process characteristic times. In this case:

$$\omega_c^c = \omega_T^c \approx \frac{1}{\theta} \quad (4.44)$$

$$S_c = 3 \quad (4.45)$$

Estimator

$$K_1^{oc} = n_r S_c \omega_c \quad (4.46)$$

$$K_1^{oT} = n_r S_c \omega_T \quad (4.47)$$

$$K_2^{oc} = (n_r S_c \omega_c)^2 \quad (4.48)$$

$$K_2^{oT} = (n_r S_c \omega_T)^2 \quad (4.49)$$

where

$$\omega_c = \omega_T \approx \frac{1}{\theta} \quad (4.50)$$

$$n_r S_c = S_o \quad (4.51)$$

Therefore if the estimator dynamics is required to be 10-times faster than the closed-loop process dynamics:

$$S_o = n_r S_c = (10)(3) = 30 \quad (4.52)$$

Closed-Loop Transition Motion Stability

The application of the candidate calorimetric controller yields the closed-loop reactor:

$$\dot{\hat{T}} = \dot{\bar{y}}_T(t) - \omega_T[\hat{T} - \bar{y}_T(t)] + 2\xi_o\omega_o(T - \hat{T}) \qquad \hat{T}(t_o) = \hat{T}_o \quad (5.53a)$$

$$\dot{\hat{Q}} = [\hat{\gamma} + \mu_c(\hat{Q}, \hat{c}, \bar{c}, \pi_C, t)/\hat{V}]2\xi_o\omega_o + \omega_o^2(T - \hat{T}) \qquad \hat{Q}(t_o) = \hat{Q}_o \quad (5.53b)$$

$$\dot{\hat{c}} = \dot{\bar{y}}_c(t) - \omega_c[\hat{c} - \bar{y}_c(t)] \qquad \hat{c}(t_o) = \hat{c}_o \quad (5.53c)$$

$$\dot{c} = -r(c, T, p_k) + \mu_c(\hat{Q}, \hat{c}, \bar{c}, \pi_C, t)[c_f(t) - c]/V \qquad y_c = c \qquad c_0 = c_o \quad (5.53d)$$

$$\dot{T} = \beta r(c, T, p_k) + \mu_c(\hat{Q}, \hat{c}, \bar{c}, \pi_C, t)[T_f(t) - T]/V \\ - \gamma\{T - \mu_T[\hat{T}, \hat{Q}, \hat{c}, \bar{c}, T_f(t), \pi_C, t]\} \quad T(0) = T_o \tag{5.53e}$$

$$\dot{Q} = f_Q(x, d, u, p) \tag{5.53f}$$

The zero-dynamics concentration RE-stability requirement of the kinetics model-based dynamic single-input/single-output (SISO) nonlinear geometric estimator-based controller has been removed by the proposed calorimetric controller because the feedrate control is now active with two correcting terms: one ratio-type attributed to the estimate $\hat{R} = \hat{Q}/\hat{\beta}$ of the unknown reaction rate, and another one $\omega_c[\hat{c} - \bar{y}_c(t)]$ generated by the combination of the mass balance (Eq. 5.53c) with the estimate of $\hat{R}$.

Summarizing, from the constructive and engineering judgment developments of the present section one is led to conjecture that the proposed calorimetric controller: (i) unlike the estimator-based nonlinear geometric controller, does not bear the zero-dynamics concentration motion RE-stability condition; (ii) should have a strongly robust tracking capability, as a result of the on-line estimation of the unknown reaction rate; and (iii) should approach the performance of the exact state-feedback controller by making the (T, Q) estimation dynamics sufficiently fast (with the only limit being the noise propagation), in agreement with its PI-estimator–based nonlinear geometric control counterpart (Alvarez et al., 2000). The rigorous verification of the truthfulness of these conjectures constitutes the central subject of the next section.

Application Example

Stable to stable steady-state transition

Let us consider a continuous stirred tank reactor with a reversible exothermic reaction:

$$\frac{dc}{dt} = \frac{q}{V}(c_f - c) - r \tag{6.54}$$

$$\frac{dT}{dt} = \frac{q}{V}(T_f - T) + Jr - \alpha F_w(T - T_c) \tag{6.55}$$

The states of the reactor are the concentration c and the temperature T; the control inputs are the feed flow rate q and coolant temperature T_c; r is the reaction rate; V is the volume; c_f is the feed concentration; T_f is the feed temperature; J is the adiabatic temperature rise (that is, heat of reaction divided by the mixture density times heat capacity); α is the dimensionless heat transfer area; and F_w is the coolant flow rate. Parameter values are given elsewhere (Hicks and Ray, 1971).

Having analytically established the existence of a closed-loop robustly stable optimal nominal trajectory (using a two-input, two-output controller) the actual nominal transition is obtained from the numerical solution of a standard dynamic optimization problem (Hicks and Ray, 1971) using the following objective function:

$$\phi = \alpha_1(\bar{c} - c_f)^2 + \alpha_2(\bar{T} - T_f)^2 + \alpha_3(\bar{q} - q_f)^2 + \alpha_4(\bar{T}_c - T_{cf})^2$$

Table 1. Initial and Final Steady States for Dynamic Optimization Calculations

	Initial Steady State	Final Steady State
c	0.4081	0.4493
T	329.76	322.94
q	100	99.95
T_c	290	278.4

where $\alpha_1 = 5 \times 10^4$, $\alpha_2 = 1 \times 10^3$, and $\alpha_3 = \alpha_4 = 10^{-1}$. Because the work done by Hicks and Ray (1971) considered only one input (F_w), we adapted their problem formulation to our case of two inputs. Optimal control computations were carried out using the RIOTS optimal control Matlab toolbox (Schwartz et al., 1997). The open-loop dynamic trajectories were sought between the following sets of initial and final input and output values as shown in Table 1.

Figure 1 displays the closed-loop optimal output transition profiles when the exact full-state feedback controller is used. As expected, the closed-loop trajectory $\Theta_c(t)$ closely tracks the nominal one $\bar{\Theta}(t)$. Figure 1 shows also the manipulated variables changes to track the desired signals. Because of the scale of the plot it is difficult to observe any difference between the open-loop output optimal desired trajectories and the corresponding closed-loop trajectories.

Next the closed-loop performance of the measurement-driven controller was assessed. To test the robustness of the proposed tracking methodology, a 20% modeling error in the activation energy was considered. Figure 2 displays the closed-loop tracking of the desired trajectories and in the same figure the behavior of the manipulated variables is also shown. The closed-loop output response clearly shows that, when the initial states were those given earlier, the estimator integral action was able to compensate the kinetics modeling errors. Similarly, a −20% modeling error in the activation energy was considered; as shown in Figure 3 the closed-loop tracking of the trajectories was also possible and only small differences with respect to the desired trajectories were observed. However, stronger control actions were required. Finally, a completely unknown reaction rate expression was assumed; even in this limited case, good closed-loop transition trajectories were obtained, as depicted in Figure 4.

Unstable to unstable steady-state transition

The computation of dynamic optimal transition trajectories between open-loop unstable processes is a problem that, as far as we know, has not been systematically addressed in the open literature. Sometimes an ad hoc procedure is used to "solve" this problem. This approach consists, in the first place, in using a controller to closed-loop stabilize the process and, once the system is stable, to use standard dynamic optimization techniques to compute the optimal transition trajectory.

Recently we proposed a simultaneous finite-element orthogonal collocation procedure to address the problem of computing optimal transition trajectories between unstable steady states; see Silva et al. (2002) for details about parameter values that were modified for multiplicity emergence, the optimization formulation, and computed dynamic trajectories. To test the closed-loop performance of the nonlinear model–based controller to track the trajectories, the worst-case scenario, an

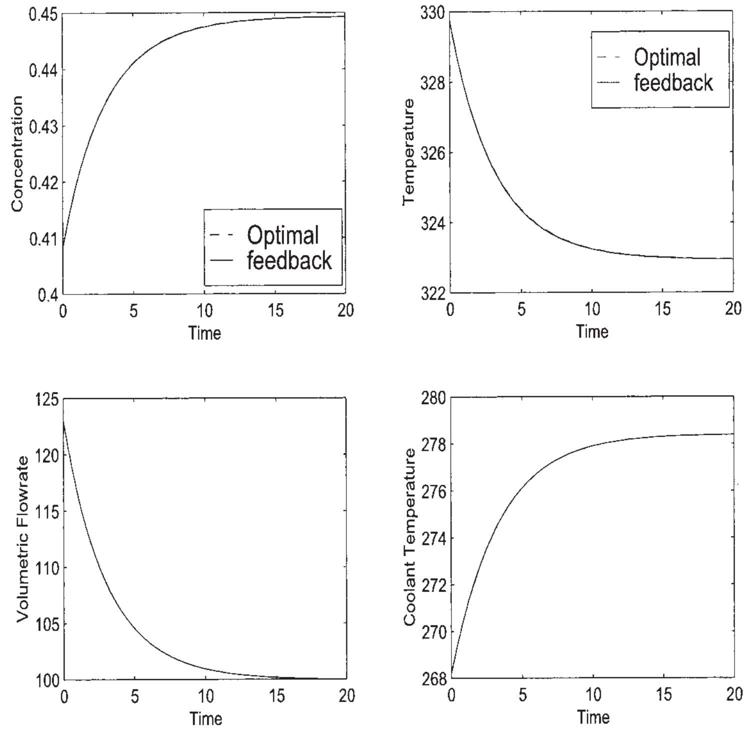

Figure 1. Closed-loop output and input trajectories using the full-state feedback nonlinear geometric controller.

unstable–unstable optimal trajectory, was analyzed in the hope that other types of transitions (stable–unstable or unstable–stable) might be easier to track. Figure 5 displays the controller performance that seems to be good if one recalls that, besides the unstable nature of the steady states, reaction kinetics is completely unknown.

To test the robustness characteristics of our control plus observer scheme, errors in the observer initial conditions were

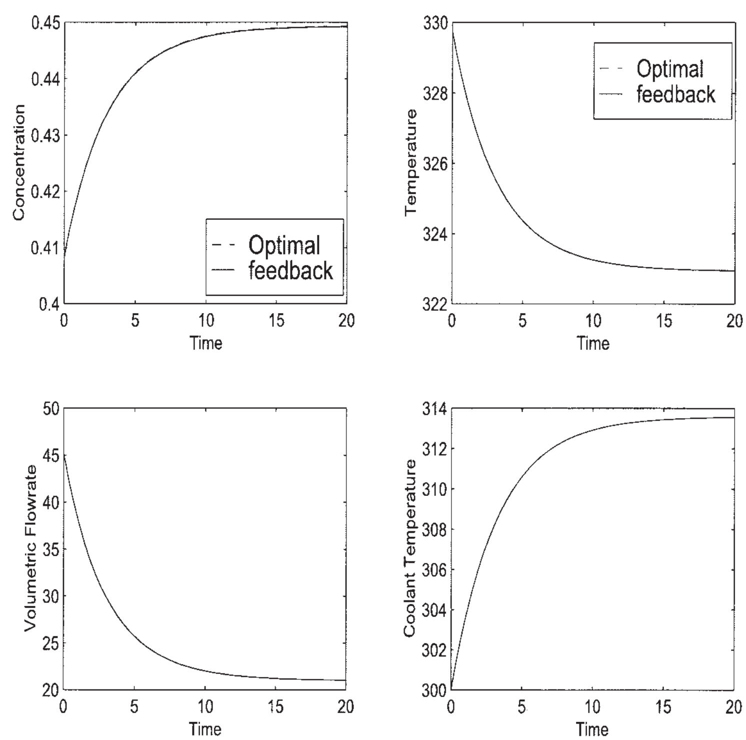

Figure 2. Closed-loop output and input trajectories using the temperature-driven estimator and considering +20% modeling error in the activation energy.

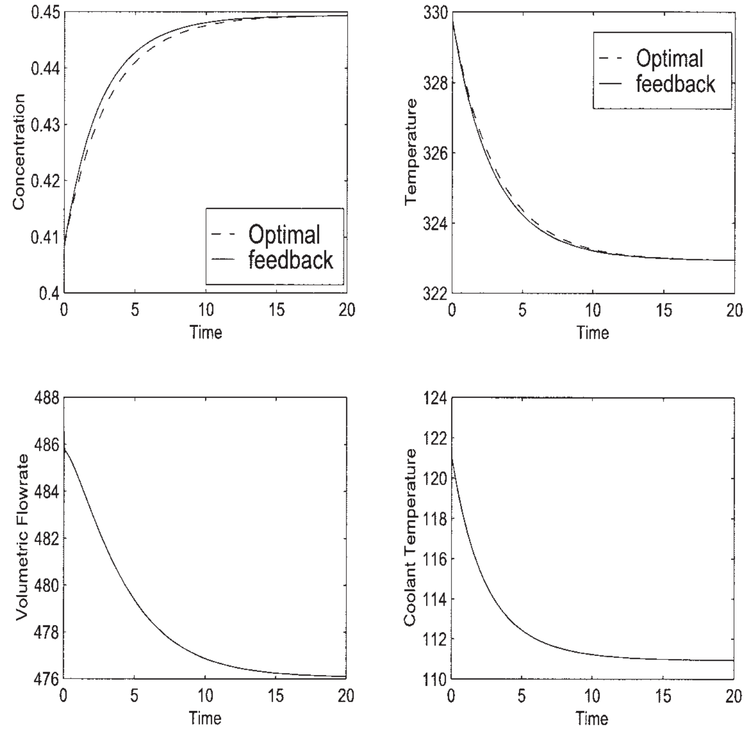

Figure 3. Closed-loop output and input trajectories using the temperature-driven estimator and considering −20% modeling error in the activation energy.

also assessed. Figures 6 and 7 display the closed-loop response when the observer initial conditions are over- and underestimated by +10% and −10%, respectively. As before, reaction kinetics is completely unknown. As might be expected, the closed-loop performance deteriorates compared to the case of solid knowledge of the observer initial conditions. However,

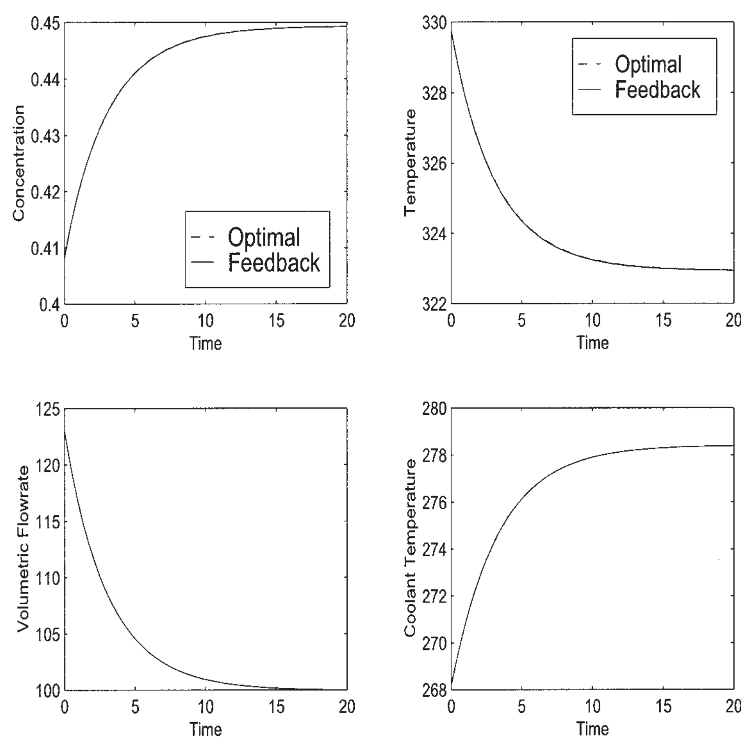

Figure 4. Closed-loop output and input trajectories using the temperature-driven estimator and without complete knowledge of the kinetic reaction rate expression.

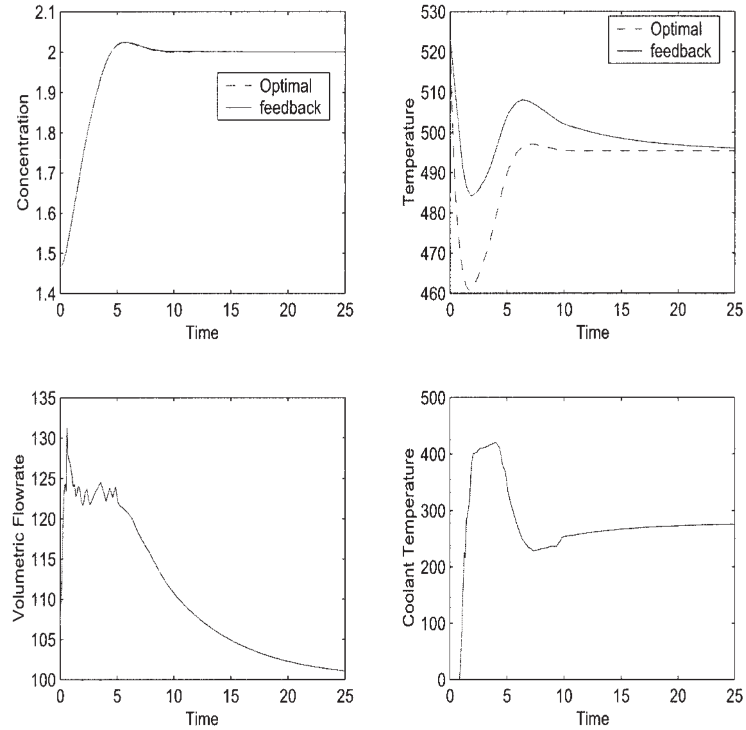

Figure 5. Closed-loop output and input trajectories between two unstable steady states using the temperature-driven estimator and without complete knowledge of the kinetic reaction rate.

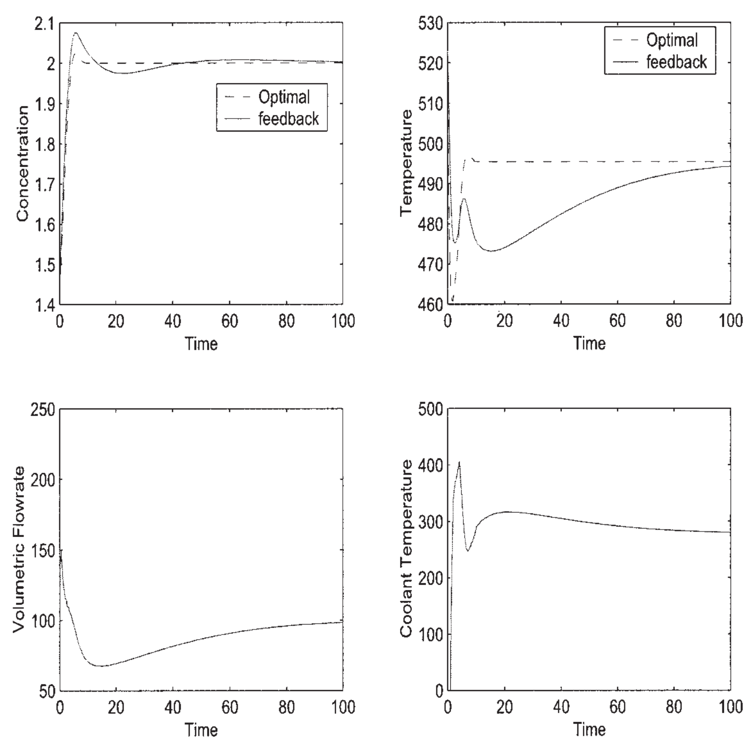

Figure 6. Closed-loop output and input trajectories between two unstable steady states using the temperature-driven estimator, without complete knowledge of the kinetic reaction rate and +10% overestimation of observer initial conditions.

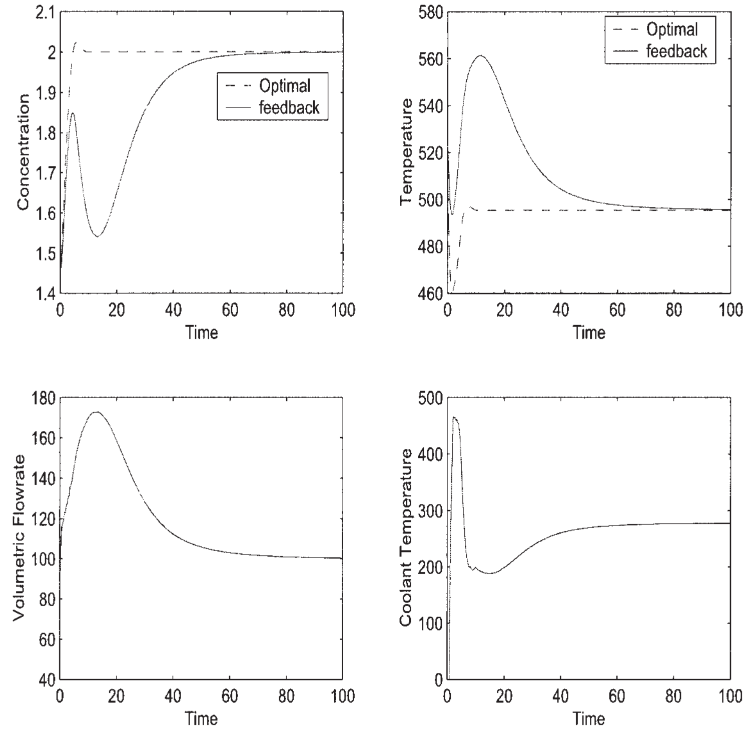

Figure 7. Closed-loop output and input trajectories between two unstable steady states using the temperature-driven estimator, without complete knowledge of the kinetic reaction rate and −10% underestimation of observer initial conditions.

our proposed control scheme is able to reach the final desired steady state, although the dynamic transition trajectory does not resemble the desired optimal one. These results clearly demonstrate that setpoint changes should not be carried out before the observer initial conditions match process operating conditions.

Conclusions

In this work connections among the theoretically oriented constructive nonlinear control, the application-oriented calorimetric control, and dynamic optimization approaches have been shown. We have shown that, even in the worst-case scenario, meaning unknown reaction rate and unstable to unstable optimal control tracking, our nonlinear robust model–based controller plus calorimetric estimator was able to effectively track the desired optimal trajectories. Presently we are addressing the problem of extending this approach to the optimal control of complex polymerization reaction systems.

We think that our robust optimal control tracking trajectory approach might be applied to almost any process involving changes between setpoints. In addition to the specific problem addressed in this work other problems include batch operation, start-up and shutdown operations, and polymer grade transitions.

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Appendix: Proof of Proposition 1

The closed-loop tracking dynamics are given by

$$\dot{e}_c = -\omega_c e_c + q_c(\varepsilon_Q, \varepsilon_c, \tilde{c}_e, \tilde{p}_C, \cdots) \qquad e_c(t_o) = e_{co} \quad \text{(A1)}$$

$$\dot{e}_T = -\omega_T e_T + q_T(\varepsilon_T, \varepsilon_Q, \varepsilon_c, \tilde{c}_e, \tilde{p}_C, \cdots) \qquad e_T(t_o) = e_{To} \quad \text{(A2)}$$

and are bounded as follows:

$$|e_c(t)| \le s_c(t) : \dot{s}_c = -\omega_c s_c + L|\varepsilon_Q| + L|\varepsilon_c| + L|\tilde{c}_e| + L|\tilde{p}_C| \qquad s_c(t_o) = s_{co} = |e_{co}| \quad \text{(A3)}$$

$$|e_T(t)| \le s_T(t) : \dot{s}_T = -\omega_T s_T + L|\varepsilon_T| + L|\varepsilon_Q| + L|\varepsilon_C| + L|\tilde{c}_e| + L|\tilde{p}_C| \qquad s_T(t_o) = s_{To} = |e_{To}| \quad \text{(A4)}$$

On the other hand, the estimation error dynamics are bounded as follows:

$$|\varepsilon_T(t)| \le \sigma_T(t) : \dot{\sigma}_T = -L\sigma_T + (a_T/L)[|f_Q| + L|\tilde{p}_C|] \qquad \sigma_T(t_o) = \sigma_{To} = a_t|\varepsilon_{co}| \quad \text{(A5)}$$

$$|\varepsilon_Q(t)| \le \sigma_Q(t) : \dot{\sigma}_Q = -L\sigma_Q + (\kappa a_T/L) \times [|f_Q| + L|\tilde{p}_C|] +^* \delta_\gamma +^* \delta_V \qquad \sigma_Q(t_o) = \sigma_{Qo} = a_Q|\varepsilon_{Qo}| \quad \text{(A6)}$$

$$|\varepsilon_c(t)| \le \sigma_c(t) : \dot{\sigma}_c = -\theta_* \sigma_c + [\kappa a_T/(L\theta_*)] \times [|f_Q| + L|\tilde{p}_C|] +^* \delta_{ce} +^* \delta_\beta +^* \delta_\gamma +^* \delta_V \qquad \sigma_Q(t_o) = \sigma_{Qo} = a_c|\varepsilon_{Qo}| \quad \text{(A7)}$$

$$\dot{\varepsilon}_1 = -2\xi\omega\varepsilon_1 + \varepsilon_2 \quad \text{(A8)}$$

$$\dot{\varepsilon}_2 = \omega^2\varepsilon_1 + f_g(\varepsilon, \tilde{p}_c, \cdots) - f_Q \quad \text{(A9)}$$

$$\begin{aligned} -f_Q(x, d, u, p) &= -\beta[(\partial_c r) f_c + (\partial_T r) f_T] \\ &= -\beta(\partial_c r)[\dot{\bar{c}} - \omega_c e_c + q_c(\varepsilon_Q, \varepsilon_c, \tilde{c}_f, \tilde{p}_c, \cdots)] \\ &\quad - \beta(\partial_T r)[\dot{\bar{T}} - \omega_T e_T + q_T(\varepsilon_T, \varepsilon_Q, \varepsilon_c, \tilde{c}_f, \tilde{p}_c, \cdots)] \\ &= \beta(\partial_c r)\omega_c e_c + \beta(\partial_T r)\omega_T \varepsilon_1 - \beta(\partial_c r) \times [\dot{\bar{c}} + q_c(\varepsilon_Q, \varepsilon_c, \tilde{c}_f, \tilde{p}_c)] \\ &\quad - \beta(\partial_T r)[\dot{\bar{T}} + q_T(\varepsilon_Q, \varepsilon_c, \tilde{c}_f, \tilde{p}_c)] \end{aligned} \quad \text{(A10)}$$

$$\dot{\varepsilon}_1 = -2\xi\omega\varepsilon_1 + \varepsilon_2 \quad \text{(A11)}$$

$$\dot{\varepsilon}_2 = -[\omega^2 - \beta(\partial_T r)\omega_T]\varepsilon_1 + f_g(\varepsilon, \tilde{p}_c, \cdots) + \beta(\partial_c r)\omega_c e_c + F(\varepsilon_T, \varepsilon_Q, \varepsilon_c, \tilde{c}_f, \tilde{p}_c, \cdots) \quad \text{(A12)}$$

Necessary condition: $\omega^2 > \beta(\partial_T r)\omega_T$

$$\omega^* = [\omega^2 - \beta(\partial_T r)\omega_T]^{1/2} \quad \text{(A13)}$$

$$2\xi\omega = 2\xi(\omega/\omega^*)\omega^* \qquad 2\xi^*\omega^* \qquad \xi^* = \xi(\omega/\omega^*) \qquad \xi^* < \xi \quad \text{(A14)}$$

$$\dot{\varepsilon}_1 = -2\xi^*\omega^*\varepsilon_1 + \varepsilon_2 \quad \text{(A15)}$$

$$\dot{\varepsilon}_2 = -(\omega^*)^2\varepsilon_1 + \beta(\partial_c r)\omega_c e_c + f_g(\varepsilon, \tilde{p}_c, \cdots) + F(\varepsilon_T, \varepsilon_Q, \varepsilon_c, \tilde{c}_f, \tilde{p}_c, \cdots) \quad \text{(A16)}$$

$$|e_c(t)| \le s_c(t) : \dot{s}_c = -\omega_c s_c + L|\varepsilon_Q| + L|\varepsilon_c| + L|\tilde{c}_f| + L|\tilde{p}_c| \qquad s_c(t_o) = s_{co} = |e_{co}| \quad \text{(A17)}$$

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