The Robust Global Stabilization of a Stirred Tank Reactor

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In this paper, a program of analysis is carried out for control of a nonlinear stirred tank reactor. By examining the uniqueness and stability properties of the reactor, the zero dynamics are analyzed. Subsequently, a model reference adaptive controller (MRAC) which explicitly takes into account the nonlinearities of the system is designed; the MRAC successfully compensates for parametric uncertainty. It is shown that even when almost all reactor parameters are unknown, global convergence over the entire phase space is achieved.

Introduction

The control of nonlinear processes has attracted much interest in recent years in the process control literature. This level of interest is borne out by the volume of papers which have appeared more recently in the literature. These include Limqueco et al. (1991), Daoutidis and Kravaris (1991), Gokhale et al. (1991) and Calvet and Arkun (1988).

The usual method of handling nonlinearities is by the traditional Taylor series linearization about a given operating point. This strategy is still perhaps the generic tool for extremely complex nonlinear processes. However, if the process model is relatively simple, then more sophisticated nonlinear control methods can be considered. This viewpoint has led to the development of general methods for classes of nonlinear systems. Those that have found increasing use in chemical process control include the different geometric approach (Kravaris and Kantor, 1990; Alvarez et al., 1989), the reference synthesis (RSS) approach of Bartusiak et al. (1989), and the generic model (GMC) control of Lee et al. (1987). Mclellan et al. (1990) have pointed out the connection between some of these approaches.

Even so, some of the above methods, in their standard forms, are somewhat restrictive. In particular, when full state linearization is not possible, then an input-output linearization (Kravaris and Palanki, 1988; Kravaris and Kantor, 1990; Daoutidis and Kravaris, 1991) is attempted. In performing the input-output linearization, the zero dynamics (Daoutidis and Kravaris, 1991) of the control system is generated. Now, the zero dynamics is generally nonlinear; thus in order to conclude global stability, it is necessary to analyze the stability properties of the zero dynamics. In so doing, it is sufficient to demonstrate, if possible, that the subset of the state corresponding to the zero dynamics has a global attractor. In carrying out such analysis, methods from nonlinear analysis and bifurcation theory become very important (Chang and Chen; 1984; Aluko, 1988; Suárez and Alvarez, 1990). This ability to demonstrate the global stability of the zero dynamics, though not always possible, is the first stage of the design procedure. To be precise, in many control studies, although the local results obtained are useful, practically acceptable and can subsequently be locally extended, the power behind the control scheme is more evident if such local results could be turned into global arrangements. Unfortunately, important as this is, this sort of analysis is rarely performed in the chemical process control literature.

Having completed the first stage, robustness issues are addressed in the second stage. In most of the recent literature (Calvet, 1989; Kravaris and Palanki, 1988; Doyle et al., 1989) robustness has been addressed by employing a fixed gain controller. However, in this paper, we proceed via an adaptive design; in this way, we avoid having to specify a priori bounds on the process parameters. We should emphasize that while adaptive control of chemical processes is not new (Seborg et al., 1986), the present work is quite different from several previous applications in that nonlinearities are taken care of explicitly; this avoids the usual methods of approximating the nonlinear process by a linear model and identifying the parameters of the linear model for purposes of control.

In this study, we carry out the above two-stage program to analyze a nonlinear CSTR; the model selected for analysis is sufficiently complex to incorporate many of the nonlinear features typically exhibited by chemical reactors. Hence, the applicability of the method is not restricted to the system analyzed here; we believe that it is applicable to a much wider class of chemical engineering systems.

Consequently, in the first stage of the work, we derive the control law for the reactor assuming exact knowledge of all reactor parameters and show that it is globally stabilizing. In so doing, we employ topological arguments to characterize the limit sets of the system being analyzed. These arguments allow us to reduce rigorously the behavior of the forced zero dynamics to its unforced counterpart and to extend easily some of the results of Suárez and Alvarez (1990) to certain specialized cases; by reducing the problem to that of analyzing the limiting behavior of a certain class of one or two-dimensional nonautonomous systems, we bypass the need for checking global isothermal stability of certain reaction sequences in high dimensional spaces. The above reduction proves to be extremely useful in stage two where it is central to our ability to construct an adaptive mechanism; this mechanism takes into account system nonlinearities while simultaneously achieving robust global stabilization. By combining the above results establishing the existence of a global attractor for the zero dynamics with a Lyapunov based adaptive design, it is proven that under relatively mild restrictions, we achieve global convergence of the reactor to any desired operating state when essentially all reactor parameters are unknown.

Model

The model employed in this study is that of a nonlinear CSTR undergoing a series reaction. The system is qualitatively similar to one in Suárez and Alvarez (1990) and Kravaris and Kantor (1990) but a somewhat more general scheme is considered. Thus, for the purposes of this study, the reaction is:

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \tag{1}$$

It is assumed that the reaction order for the A to B reactor is of order n, while that of the subsequent stage is m with both n, $m>0$. The situation for $n=0$ or $m=0$ can be handled in the same manner without any modification to the control scheme but slight changes in the arguments which follow. We also assume an Arrhenius type dependence of the rate constants on temperature and that the reaction is operated nonadiabatically. There is a cooling jacket which withdraws heat from the system. For $n=m=1$, some of the nonlinear behavior the uncontrolled system is capable of exhibiting can be found in Jorgensen and Aris (1983). Some more recent work involving singularity theory techniques is presented in Berdouzi (1987) and Byeon and Chung (1989).

A nondimensionalization is possible and perhaps more convenient but this is not too important here. Thus, the model equations for the system become:

$$\dot{C}_A = \frac{F}{V}(C_{Af} - C_A) - k_1(T)C_A^n \tag{2}$$

$$\dot{C}_B = -\frac{F}{V}C_B + k_1(T)C_A^n - k_2(T)C_B^m \tag{3}$$

$$\dot{T} = \frac{F}{V}(T_f - T) + \frac{(-\Delta H)_1 k_1(T)C_A^n}{\rho C_p} + \frac{(-\Delta H)_2 k_2(T)C_B^m}{\rho C_p} - \frac{hA_c}{\rho C_p V}(T - T_j) \tag{4}$$

where V is the reactor volume, F is the flow rate of input and exit streams, and C_A, C_B are the concentrations of A and B respectively within the reactor; h and A_C represent the heat-transfer coefficient and heat-transfer area respectively. The terms involving (ΔH) are the heat of reaction terms, and the reaction rate constants k_1 and k_2 follow an Arrhenius rate dependence on temperature ($k_i = k_{i0}\exp(-E_i/RT) i = 1, 2$). The manipulated variable is the jacket temperature T_j.

Results and Discussion

In this section, we develop the control law that ensures global convergence to the desired set point; an important extension is then briefly discussed. We then implement an adaptive mechanism, which under a mild restriction, is argued to achieve global convergence to the set point when essentially *all* the model parameters are unknown.

Control Law Derivation: Input/Output Linearization

The control law is based on linearizing a subset of the state variables which is designated as the output. For reasons which become clear below, it is natural to select the temperature (T) as the output variable; intuitively, the manipulated input T_j only directly influences T. The control objective is to drive the reactor to an open-loop equilibrium point (E_d^3) which is in physical parameter space. Note that $E_d^3 \in \Re^3 = [C_{Ad}, C_{Bd}, T_d]^T$. The notation ($E_d^3$) employed above is chosen with the benefit of hindsight; it allows for easy extension to a slightly more general situation.

To simplify subsequent analysis, we demand that in closed-loop, the dynamics of the temperature (T) be linear. In order to do this, it is convenient to accomplish this via a reference model and an error system.

Hence we choose a stable reference model (with state T_r) of the form

$$\dot{T}_r = -k(T_r - T_d) \tag{5}$$

where $k>0$. After defining an error $e(=T-T_r)$ the input

$$u = T_j = -g^{-1}\left[\sum_{i=1}^{4} f_i(C_A, C_B, T) + k(T - T_d)\right] \tag{6}$$

with

$$g = \frac{hA_c}{\rho C_p V} \tag{7}$$

$$f_1 = \frac{(-\Delta H)_1 k_{10}\exp\left[\frac{-E_1}{RT}\right]C_A^n}{\rho C_p} \tag{8}$$

$$f_2 = \frac{(-\Delta H)_2 k_{20}\exp\left[\frac{-E_2}{RT}\right]C_B^m}{\rho C_p} \tag{9}$$

$$f_3 = -\left(\frac{F}{V} + g\right)T \tag{10}$$

$$f_4 = \frac{F}{V} T_f \tag{11}$$

will achieve the desired objective. During the above derivation, it is seen that the dynamics of the error system are given by

$$\dot{e} = -ke + \left[\sum_{i=1}^{4} f_i(C_A, C_B, T) + gu + k(T - T_d) \right] \tag{12}$$

where the arguments of the functions f_i $(i = 1, \ldots, 4)$ will usually be omitted in the interest of brevity. The control law in Eq. 6 is easily derived; it belies its underlying power.

Stability/Convergence of the CSTR

From the previous section, the closed-loop system is given by:

$$\dot{C}_A = \frac{F}{V}(C_{Af} - C_A) - k_1(T) C_A^n \tag{13}$$

$$\dot{C}_B = -\frac{F}{V} C_B + k_1(T) C_A^n - k_2(T) C_B^m \tag{14}$$

$$\dot{T} = -k(T - T_d) \tag{15}$$

The purpose of this section is now to argue that the desired equilibrium point E_d^3 is in fact eventually approached in the closed loop; if the system is initiated from any point in physical parameter space (that is, $C_A(0) \in [0, C_{Af}]$, $C_B(0) \geq 0$, $T(0) \in [T_{\min}, T_{\max}]$). In order to do this, we employ a combination of local and global qualitative arguments.

Stability analysis

Local Analysis. The eigenvalues of the closed-loop plant about E_d^3 are determined by the Jacobian of the closed-loop system about E_d^3. It can easily be verified that the eigenvalues of the system are negative about E_d^3. This follows from the fact that the eigenvalues of the Jacobian are its diagonal elements and that E_d^3 belongs to physical parameter space (Thus, C_A and C_B are nonnegative). Therefore, E_d^3 is locally asymptotically stable; which agrees with the results of previous workers in this area.

Global Analysis. The proof of global stability of E_d^3, consists of three parts. First, boundedness of the system solutions is argued. In so doing, the work of Aris and Amundson (1958) on the classic CSTR motivates the construction of a positively invariant set for the system. Next, we show the uniqueness of E_d^3 as the closed-loop critical point. In the final stage of the proof, we show that Eqs. 13 and 14 are 'asymptotically autonomous'; this property allows us to reduce the limiting behavior of the nonautonomous *forced* zero dynamics to that of its *unforced* autonomous counterpart.

In order to show boundedness, we *construct the invariant set* as in the old arguments, a trapping region $\mathfrak{M}_3$ which eventually traps all physically possible trajectories. A cube-like region in $\mathfrak{R}^3$ suffices here. This cube is defined by $[0, C_{Af}] \times [0, P] \times [T_{\min}, T_{\max}]$ where P is specified shortly. To see this, note that if C_A equals C_{Af} then $\dot{C}_A$ is negative. Also, when C_A is zero, then $\dot{C}_A$ is positive. Now, if $T_{\min}(>0)$ and $T_{\max}(<\infty)$ are arbitrarily chosen, then T always remains in $[T_{\min}, T_{\max}]$. It is clear that by definition, $T_d \in [T_{\min}, T_{\max}]$. Observe that if C_B is zero, then $\dot{C}_B$ is nonnegative. It now remains to define P. We choose P as $\alpha\ V/F\ C_{Af}^n \sup k_1(T)$ where $\alpha \geq 1$. Note that the supremum required above can be trivially computed from the bounds on T. Let us argue as to why this estimate works. Clearly, if $C_B = P$, then $\dot{C}_B < 0$. Therefore, any trajectory initiated with C_B in $[0, P]$ has C_B trapped in this interval for all time. Certainly, we can make α arbitrarily large so that P is as large as we desire. We can however be slightly less conservative by demanding a relatively small value of P and requiring that even if for some reason, we initiate the system with $C_B > P$, we are still guaranteed to eventually end up within the (now) less conservative trapping region. This motivates the following alternative. We fix $\alpha = 1$ (thus obtaining a smaller value of P) and then, claim that with this choice of $\alpha = 1$, even if a trajectory is initiated with $C_B > P$, C_B enters $[0, P]$ in finite time. To show this, we argue that for $C_B \geq P$, C_B decreases faster than some linear function of time. In so doing, it is clear that for $C_B \geq P$, $\dot{C}_B \leq -k_2(T) P^m \leq \sup(-k_2(T)) P^m$. Note, that $k_2(T)$ for $T \in [T_{\min}, T_{\max}]$ is bounded away from some neighborhood of zero; thus, $\sup(-k_2(T)) < 0$. In effect, for $C_B \geq P$, $\dot{C}_B$ is no greater than a constant negative number $q\ (= \sup(-k_2(T)) P^m)$. Consequently, if $C_B > P$, then C_B decreases faster than a linear function with slope m_1, where $q < m_1 < 0$; this proves the claim. Hence, to summarize thus far, the region $\mathfrak{M}_3 = [0, C_{Af}] \times [0, P] \times [T_{\min}, T_{\max}]$ specified earlier with $P = \alpha\ V/F\ C_{Af}^n \sup k_1(T)$ $(\alpha \geq 1)$ is an invariant set for the system. In addition, if $\alpha = 1$, then this region (now defined as $\mathfrak{M}_{3\infty}$, is an invariant set and furthermore, if a trajectory is initiated with C_B outside of $\mathfrak{M}_{3\infty}$, such a trajectory eventually enters $\mathfrak{M}_{3\infty}$ in finite time. Henceforth, we make no distinction between $\mathfrak{M}_3$ and $\mathfrak{M}_{3\infty}$. We simply refer to either of these regions as the invariant set.

We now have to argue that the trapping region contains E_d^3 (the desired closed-loop equilibrium point) as the *unique equilibrium point* of the system in physical parameter space. To see this, note that at equilibrium, $T = T_d$. In addition, given $T = T_d$, Eq. 13 has exactly one solution $C_{Ae} \in (0, C_{Af})$. This solution is in fact unique in $\mathfrak{R}^+$. This is true because of $k_1(T_d) > 0$ together with the fact that both the first and second terms in Eq. 13 are monotone in C_A. Thus, examining these two functions at the boundaries $C_A = 0$ and $C_A = C_{Af}$ proves the claim. This, together with the fact that E_d^3 is an open-loop equilibrium solution implies that $C_{Ae} = C_{Ad}$. Now, following the same line of reasoning it is clear that Eq. 14 also has exactly one steady-state solution (C_{Be}) in $\mathfrak{R}^+$ which lies in $(0, P)$. To see this, note that the middle term in that equation is strictly positive when $T = T_d$ and $C_A = C_{Ad}$. Transferring the term $k_2(T_d) C_B^m$ to the left and observing the monotonicity of the left and righthand sides proves the uniqueness. To show that C_{Be} lies in $(0, P)$ one observes from Eq. 14 that $C_{Be} < V/F\ k_1(T_d) C_{Ae}^n < \alpha\ V/F\ C_{Af}^n \sup k_1(T) = P$. This uniqueness of C_{Be}, again together with the fact that E_d^3 is an open-loop equilibrium solution implies that $C_{Be} = C_{Bd}$. Consequently, it is clear that E_d^3 is the unique locally stable equilibrium point of the *closed-loop system.*

Asymptotically Autonomous Property. So far, we have an invariant set with the desired equilibrium solution E_d^3 as its

unique locally stable attractor. Therefore, it is clear that within the invariant set, some trajectories approach E_d^3 as $t\to\infty$. The final component of the argument now establishes that, in fact, all the trajectories within the invariant set eventually approach E_d^3. This statement although naively obvious (it is ultimately equivalent to 'slotting' $T=T_d$ into Eqs. 13 and 14 and analyzing the *unforced zero dynamics*), requires an argument. Although Suárez and Alvarez (1990) state a useful theorem here, we prefer to employ a different argument, qualitative in nature and due to Markus (1956). This argument is crucial not only for some of our subsequent extensions, but also for the subsequent design of the adaptive mechanism; it ultimately justifies this 'slotting in' of $T=T_d$ under rather mild conditions. In so doing, to simplify matters, we assume the uniqueness of trajectories. (This assumption is only needed if n or m is less than unity because of trajectories which may hit the nondifferentiable boundaries $C_A=C_B=0$ where the Lipshitz conditions are not easily checked). In order to employ Markus's theorem, it is clear that Eqs. 13 and 14 can be rewritten as:

$$\dot{C}_A=\frac{F}{V}(C_{Af}-C_A)-k_1(T_d)C_A^n-\underbrace{C_A^n(k_1(T)-k_1(T_d))} \tag{16}$$

$$\dot{C}_B=-\frac{F}{V}C_B+k_1(T_d)C_A^n-k_2(T_d)C_B^m \underbrace{+C_A^n(k_1(T)-k_1(T_d))}-\underbrace{C_B^m(k_2(T)-k_2(T_d))} \tag{17}$$

so that what we have is an autonomous vector field in $\Re^2$ perturbed by time varying terms (in underbraces). (Note that all the trajectories are already trapped within the invariant set). Now, it is clear that because $T\to T_d$ and $k_1(T)$ and $k_2(T)$ are continuous in T, then all the terms in underbraces also vanish as $t\to\infty$ uniformly on every compact set in C_A-C_B space. Under these conditions, Markus tells us that we can compare the limiting behavior of this 2-dimensional nonautonomous system to the solutions of the unperturbed autonomous vector field ($\mathcal{S}^{3\infty}$). Clearly, $\mathcal{S}^{3\infty}$ eventually has all its orbits in $[0, C_{Af}]\times[0, P]$. Therefore, we reduce to analyzing the qualitative behavior of an autonomous system in $\Re^2$ which has all its orbits trapped in an invariant set. If n and m are at least unity, the negative criterion of Bendixson quickly establishes that $\mathcal{S}^{3\infty}$ has neither periodic orbits nor homoclinic orbits; clearly, heteroclinic phenomena are also impossible. This leads us to conclude that the only possible candidates for the limit set of all the trajectories are critical points. But E_d^3 is the unique critical point of the closed-loop system. It follows then that every trajectory within the invariant set approaches E_d^3 as $t\to\infty$. If n or m is less than unity ($\in(0, 1)$), it is clear that $\mathcal{S}^{3\infty}$ has no homoclinic/heteroclinic orbits because the only critical point in the invariant set is locally asymptotically stable and thus, not a saddle. In addition, there are no periodic orbits since the C_A subsystem for $\mathcal{S}^{3\infty}$ is a one-dimensional autonomous system (independent of C_B) which qualitatively, will always approach the unique critical point. It therefore follows in this case as well, that every trajectory of the closed-loop system approaches E_d^3 as $t\to\infty$.

Remarks

In Suárez and Alvarez (1990) the authors argue global stability for a generalized sequence of first-order reactions. In Kravaris and Kantor (1990), the authors work with the case $n=2$ and $m=1$ for a two stage reaction; however global stability was not concluded in that study. Thus, the analysis here in a sense, generalizes the work in the above papers. Actually, it bypasses the need for checking the global isothermal stability of a generalized nonlinear reaction sequence in $\Re^q$, this may be difficult if q is large. We digress briefly in order to establish this claim; in so doing, we work with an N-stage reaction and as before, assume the uniqueness of trajectories. Essentially, we find a trapping region (including the temperature) in $\Re^{N+1}$ where $N+1$ is the number of components in the system, and then, decompose the system into a sequence of asymptotically autonomous first-order systems whose limit sets must be critical points; hence, the procedure is constructive. We thus consider the system

$$A_1 \overset{k_1,\ n_1}{\rightarrow} A_2 \overset{k_2,\ n_2}{\rightarrow} A_3 \overset{k_3,\ n_3}{\rightarrow} \cdots A_{N+1} \tag{18}$$

taking place nonisothermally in the CSTR for some finite N with Arrhenius rate constants $k_i(T)$, $(i=1,2,\ldots N)$ and orders n_i, $(i=1,2,\ldots N)$ with $n_i>0\forall i$; in effect, $k_i=k_{io}e^{-E_i/RT}$, $(i=1,2,\ldots N)$. It is assumed that the system is initiated with $C_{A1}(0)\in[0, C_{A1f}]$, $C_{Ai}(0)\geq 0$, $(i=2,3,\ldots N)$, $T(0)\in[T_{\min}, T_{\max}]$. The control problem is to drive the reactor to an open-loop equilibrium $E_d^{N+1}=[C_{A_1d}, C_{A_2d}, C_{A_3d}, \ldots C_{A_Nd}, T_d]$.

We begin with the component A_1 and 'move down the chain' incrementing i at each stage. Thus, the trapping region for A_1 is $[0, C_{A_1f}]$. A trapping region for the ith component $(i\geq 2)$ is clearly given by $[0, \alpha_i\ V/F\ \sup\{k_{i-1}(T)C_{A_{i-1}}^{n_i-1}\}]$ with $\alpha_i\geq 1\forall i(\geq 2)$. As was argued for the case $N=2$, one can set α_i to be unity for all such i; also, the suprema required above are readily computable from the bounds on T. At the end of this procedure $(i=N)$, a positively invariant set, $\mathfrak{M}_{N+1}$ has been constructed.

Clearly, given $T=T_d$, C_{A_1} is uniquely determined at steady state. Thus, using the same arguments as for the case $N=2$, one moves down the chain one at a time to argue that at any critical point, T_d and $C_{A_{i-1}}$, uniquely determine $C_{A_i}(\forall i\geq 2)$. Thus, E_d^{N+1} is the *unique* critical point in $\mathfrak{M}_{N+1}$.

Now instead of 'decomposing' into $\Re^2$ as was done for the case $N=2$, we can decompose into $\Re$ by moving down the chain; this procedure makes it unnecessary to examine the global stability of the nonlinear zero-dynamics subsystem in $\Re^N$ and it simplifies the analysis considerably. To be precise, we write the equation for A_1 as

$$\dot{C}_{A_1}=\frac{F}{V}(C_{A_1f}-C_{A_1})-k_1(T_d)C_{A_1}^{n_1}-\underbrace{C_{A_1}^{n_1}(k_1(T)-k_1(T_d))} \tag{19}$$

Since $T\to T_d$ and $k_1(T)$ is continuous, the term in underbraces vanishes uniformly on compact subsets of C_{A_1}. Thus, we reduce to examining the autonomous part of a one-dimensional system with all its orbits trapped in the invariant set; thus, $C_{A_1}\to C_{A_{1d}}$ as $t\to\infty$. Now for the ith component with $2\leq i\leq N$, we write

$$\dot{C}_{A_i} = -\frac{F}{V} C_{A_i} + k_{i-1}(T_d) C_{A_{i-1}d}^{n_{i-1}} - k_i(T_d) C_{A_i}^{n_i} + \underbrace{(k_{i-1}(T) C_{A_{i-1}}^{n_{i-1}} - k_{i-1}(T_d) C_{A_{i-1}d}^{n_{i-1}})} - \underbrace{C_{A_i}^{n_i}(k_i(T) - k_i(T_d))} \quad (20)$$

Since $C_{A_{i-1}}$, $k_{i-1}(T)$ and $k_i(T)$ approach $C_{A_{i-1}d}$, $k_{i-1}(T_d)$ and $k_i(T_d)$ respectively as $t \to \infty$, the terms in underbraces vanish uniformly on compact subsets of C_{A_i} and we again reduce to examining the trajectories of the one-dimensional autonomous portion of the C_{A_i} vector field; therefore, $C_{A_i} \to C_{A_i d}$ as $t \to \infty$.

In the above sequential manner, one establishes the convergence (in closed-loop) of the general system of $N+1$ components to the desired open-loop equilibrium point; this proves our claim of generalization; therefore, carrying out the analysis for $N=2$ is sufficient for our purposes. Henceforth, we continue with the specific case ($N=2$) with the understanding that all subsequent results extend to the general case with $N+1$ components having various positive reaction orders n_i, ($i=1, 2, \ldots N$).

From the above detailed analysis, global convergence has been established. However, all this work pays off because in the next section, we use the stability of the zero dynamics to advantage in constructing an adaptive mechanism for the reactor. At this point, it is clear that the algebraic problem of establishing that there exists a controller which structurally solves the global stabilization problem is complete. In effect, Stage 1 of our two part program is achieved. The next section which addresses Stage 2 completes the program.

Adaptive Global Convergence: Lyapunov Design

In this section, we motivate and develop an adaptive mechanism for the CSTR. We emphasize that the *sole* justification for adaption is to address problems associated with model uncertainty. Although adaptive control of chemical processes is not new (Seborg et al., 1986; Sela, 1990), in most instances in the past, adaptation has been accomplished in a somewhat approximate sense (and with good results). More precisely, because most of the processes were nonlinear, they were usually approximated with linear models whose parameters were updated with time. Examples of very successful instances of this approach to some chemical reactors include Farber and Ydstie (1986), Kwalik and Schork (1988), and Temeng and Schork (1989). Some other work is also available in Sela (1990). Instances of adaptive control of chemical processes which directly account for process nonlinearities are uncommon in the literature. One of the few examples available is presented in Slotine and Ydstie (1989). In that work, the authors incorporated a physical process model based on fundamental modeling into their adaptive design for the classic CSTR (Aris and Amundson, 1958; Uppal et al., 1974).

Here, we also incorporate a nonlinear model into the adaptive mechanism; but from an alternative viewpoint. Actually, the approach adopted here is indicative of a general philosophy in line with classical MRAC. We elaborate briefly on this issue not only to rigorously justify the entire design program, but also to systematize its development. To be precise, the first part of the design program has in a certain sense identified the 'significant' output and in a sense, allows us to forget about the zero dynamics. The question now is what part does the zero dynamics play in the stability analysis of our subsequent adaptive strategy? The answer is little, except that the stability of the zero dynamics ensures the boundedness of the error derivative which is required for the global convergence of the adaptive system. In effect, from a stability viewpoint, the only information really needed from the zero dynamics is its boundedness; usually, the parameters in the zero dynamic subsystem need not be known during the construction of the adaptive mechanism. Thus, from the viewpoint of classic MRAC (Narendra and Annaswamy, 1989; Sastry and Isidori, 1989; Praly et al., 1990) the first part of the design procedure solves the algebraic part of the adaptive design, while the second part comprises the analytic portion of the adaptive design. With the above comments in mind, we return to the specific problem under consideration.

For the system at hand, uncertainties in process parameters may arise from several sources; for instances, the heat-transfer coefficient (h) may be unknown, in which case, g is unknown. In addition, knowledge of the preexponential factors (k_{1o}, k_{2o}), the heats of reaction ($(\Delta H)_1$), $(\Delta H)_2$)) and the activation energies (E_1, E_2) may be imprecise. For reasons which become clear shortly, we assume that E_1 and E_2 are known. This, together with the assumption that $T=0$ is not encountered by the adaptive mechanism are the *only restrictions* in our analysis. Thus, the task at hand now is that of constructing an adaptive mechanism which will ensure that even if all reactor parameters (excluding E_1 and E_2) are unknown, global convergence to the set point E_d^3 is achieved; the construction of this mechanism essentially mimics the procedure for that of a standard linear MRAC and is not overly complicated (Narendra and Annaswamy, 1989; Sastry and Bodson, 1989). The important point to note is that the *stability of the forced* zero dynamics provides the theoretical basis for this approach; the strategy is to *focus relentlessly on the temperature loop*. In so doing, the error system previously defined now becomes useful.

We proceed by noting the control

$$u = T_j = -g^{-1}\left[\sum_{i=1}^{4} f_i(C_A, C_B, T) + k(T - T_d)\right] \quad (21)$$

was applied with the error system (Eq. 12) given by

$$\dot{e} = -ke + \left[\sum_{i=1}^{4} f_i(C_A, C_B, T) + gu + k(T - T_d)\right] \quad (22)$$

and the f_i, ($i=1, \ldots, 4$) previously defined. The unknown parameters are now isolated by writing:

$$f_1 = \delta_1 f_1', \; f_2 = \delta_2 f_2', \; f_3 = \delta_3 f_3', \; f_4 = \delta_4 f_4' \quad (23)$$

where

$$\delta_1 = \frac{(-\Delta H)_1 k_{10}}{\rho C_p}, \; f_1' = \exp\left[\frac{-E_1}{RT}\right] C_A^n \quad (24)$$

$$\delta_2 = \frac{(-\Delta H)_2 k_{20}}{\rho C_p}, f_2' = \exp\left[\frac{-E_2}{RT}\right] C_B^m \tag{25}$$

$$\delta_3 = -\left(\frac{F}{V} + g\right), f_3' = T \tag{26}$$

$$\delta_4 = 1, f_4' = f_4 \tag{27}$$

Since f_4' is a function of solely the residence time (V/F) and the feed temperature (T_f) (both of which are usually known to a high degree of accuracy in practice), we assume f_4' is known. (Actually, this assumption is entirely unnecessary since we can in fact pick $f_4' = 1$, $\delta_4 = (F/V)T_f$ and then assume δ_4 is unknown). Thus, all the unknown parameters have been isolated in g, δ_1, δ_2, δ_3 and (possibly) δ_4. Note that $\mathrm{Sgn}(g)(=1)$ is known on physical grounds.

In view of Eq. 21 and the above definitions, we can rewrite Eq. 21 as

$$u = T_j = -g^{-1}\left[\sum_{i=1}^{4} \delta_i f_i'(C_A, C_B, T) + k(T - T_d)\right] \tag{28}$$

Now since g and δ_i, $(i = 1, \ldots, 4)$ are unknown, Eq. 28 motivates proposing the 'mimicking' control law

$$u = T_j = \sum_{i=1}^{4} -k_i' f_i'(C_A, C_B, T) - k_5'(T - T_d) \tag{29}$$

where adaptive update laws for k_i', $(i = 1, \ldots, 5)$ are to be derived. From Eqs. 22 and 29, the error system then becomes

$$\dot{e} = -ke + \left[\sum_{i=1}^{4} (\delta_i - gk_i') f_i'(C_A, C_B, T) - (gk_5' - k)(T - T_d)\right] \tag{30}$$

so that selecting the candidate Lyapunov function

$$V_l = \frac{1}{2}\left[e^2 + \frac{1}{|g|}\sum_{i=1}^{4} (\delta_i - gk_i')^2 + \frac{1}{|g|}(gk_5' - k)^2\right] \tag{31}$$

gives

$$\dot{V}_l = e\dot{e} - \mathrm{Sgn}(g)\left[\sum_{i=1}^{4} (\delta_i - gk_i')\dot{k}_i' + [(gk_5' - k)\mathrm{Sgn}(g)\dot{k}_5')\right] \tag{32}$$

in which case slotting in Eq. 30 into Eq. 32 implies that by choosing:

$$\dot{k}_i' = \mathrm{Sgn}(g) f_i'(C_A, C_B, T)e, \quad (i = 1,2\ 3,4) \text{ and } \dot{k}_5' = \mathrm{Sgn}(g)(T - T_d)e \tag{33}$$

ensures that

$$\dot{V}_l = -ke^2 \leq 0 \tag{34}$$

Under our assumption that trajectories are bounded away from some small neighborhood of $T = 0$, then the control law u is well defined for all time. Therefore, the equilibrium point $(e, k_1', k_2', k_3', k_4', k_5') = (0, g^{-1}\delta_1, g^{-1}\delta_2, g^{-1}\delta_3, g^{-1}\delta_4, g^{-1}k)$ is stable in the large and e and all the k_i', $(i = 1, \ldots, 5)$ are bounded ($\in \mathcal{L}_\infty$); in addition, $e \in \mathcal{L}_2$. The boundedness of e together with the stability of the reference plant implies that T is bounded. It remains to argue that the crucial error derivative $\dot{e}$ is bounded. Now invoking the arguments previously used, clearly C_A is bounded. Furthermore, C_B is bounded because it is nonnegative together with the fact that the middle term ($W^{\mathrm{def}} = k_1(T)C_A^n$) in Eq. 14 is bounded. Therefore if $C_B > V/F \sup(W)$, then $\dot{C}_B < 0$. The continuity of the $f_i'(C_A, C_B, T)$ $(i = 1, 2, 3, 4)$ cleary implies that all these functions are bounded since they are now defined on arbitrary but compact domains of C_A, C_B, and T. In effect, u and $\dot{e}$ are bounded. Thus, $e \in \mathcal{L}_2 \cap \mathcal{L}_\infty$, $\dot{e} \in \mathcal{L}_\infty$ and thus $e \to 0$ as $t \to \infty$; in effect, $\lim_{t\to\infty} T = T_d$; more precisely, $\lim_{t\to\infty} T = T_d$ uniformly on arbitrary compact sets of $C_A - C_B$ space. Consequently, we have now reduced to the similar situation where the forced zero dynamics have already been analyzed. The same topological result of Markus involved in that argument can now be used to draw the desired conclusion that $\lim_{t\to\infty}[C_A, C_B, T] = [C_{Ad}, C_{Bd}, T_d]$.

Remarks

It is clear that we obtain global convergence *without* explicitly trying to identify the plant. The stability of the forced zero dynamics was crucial in establishing the boundedness of the error derivative and the convergence of the temperature T to its desired value T_d. The convergence of the zero dynamics to its global attractor then follows from the result of Markus.

The restrictions in the above section show the limitations of the proposed scheme. In practice, precise estimates of the activation energies E_1 and E_2 are not easy to obtain. The difficulty is that they appear in a complicated fashion within the functions $(f_i', i = 1, 2)$. This is as yet an unsolved problem with this approach.

The assumption that trajectories are bounded away from some neighborhood of $T = 0$ is however not so serious. It appears possible that with appropriate modifications to the adaptive scheme, one can ensure that an a priori specified σ-band around $T = 0$ is actually not encountered in the closed-loop. Note also that with appropriate modifications, an adaptive mechanism with less than five gains can be constructed by combining some of the composite functions; this may be important for practical implementations.

Other issues of practical interest relate to input constraints; these could perhaps be addressed by introducing adaptive gains into the definition of the Lyapunov function and evaluating the system performance by simulation. In so doing, the positive adaptive gains then essentially serve as detuning parameters which multiply the adaptive update laws.

It should also be noted that even though, we have assumed that the parameters compensated for are *constant*, it is clear that they can be piecewise constant provided that they change at very infrequent time intervals; the argument being that at the time of change, the adaptive mechanism is perturbed from its rest position momentarily, but subsequently, begins its globally stabilizing updates towards the set point immediately afterwards. This could be important when effects such as fouling

could lead to changes in some of these parameters after prolonged operation.

Taking into account the above comments, and since the entire two-stage program is now complete, a precise statement of what has been accomplished in this study is in order. This is contained in:

Theorem 1. Let $E_d^3 = [C_{Ad}, C_{Bd}, T_d]^T$ *be an open-loop equilibrium point in physical parameter space for the reaction scheme in Eqs. 2 through 4. Assume that only Sgn(g) together with the activation energies* E_1 *and* E_2 *are known. Suppose further that the control law (Eq. 29) and adaptation laws (Eq. 33) are employed, and that for some* $\sigma > 0$, *the* σ*-neighborhood of* $T = 0$ *is not encountered in the closed-loop. Then, all the signals in the closed-loop plant are uniformly bounded; and furthermore, independent of initial conditions in physical parameter space, the closed-loop reactor converges to* E_d^3 *as* $t \to \infty$.

Simulation Results

In this section, we present simulation results for a case study. The results were generated by employing routines both from the NAG library and the public domain bifurcation software AUTO. No serious attempt was made to enhance numerical stability; the reactor equations in their most basic forms were simulated as is; nondimensionalization and/or scaling were not carried out and numerical Jacobians were employed in all simulations. This may possibly result in some slight loss in accuracy of the computed solutions; however, the qualitative picture is not compromised.

Some remarks are in order about units. Naturally, all temperatures are in Kelvin. However, all other units are not provided (and are unnecessary) since for any set of data with consistent units, we can *always* find a set of reactor parameters to match the data. With this understanding, we proceed directly to the case study.

For the reactor conditions simulated, the reactor parameters employed were $n = 2$, $m = 1$, $C_{Af} = 3.0$, $(-\Delta H)_1/\rho C_p = 1{,}100.0$, $(-\Delta H)_2/\rho C_p = 1{,}200.0$, $k_1(T) = 50.0 \exp -(3{,}000.0/T)$, $k_2(T) = 40.0 \exp -(4{,}000.0/T)$, $(hA_c/\rho C_p V) = 3.0$, $T_f = 340$ K, $u = T_j = 300$ K. In order to determine an appropriate operating region, a very brief numerical study was conducted with AUTO using the residence time (V/F) as distinguished parameter. Since this paper is not really on bifurcation analysis, several unnecessary details are suppressed; we merely determined regions in the regions in the residence time space where multiple steady states are possible. The result of the numerical study is presented in Figure 1. As seen in that figure, there is a wide range of residence times over which multiple equilibria exist. For our purposes, we decided to operate at a residence time value of 1.0. Under these conditions, there are *at least* two equilibria; actually, elementary reactor theory tells us there will be at least three. The upper one shown in the figure is open-loop *unstable* which is where we choose to operate. The actual co-ordinates of the corresponding critical point are given by $E_d^3 = [C_{Ad}, C_{Bd}, T_d]^T = [2.3000, 0.6897, 505.488]^T$.

The open-loop phase portrait is shown in Figure 2 for the residence time of 1.0. Note that the plot is presented in only $C_A - T$ space; it is unnecessary to plot C_B since analysis has established that C_A and T uniquely determine C_B at equilibrium. We emphasize that only portions of this portrait which are germane to this presentation are depicted. It is clear that

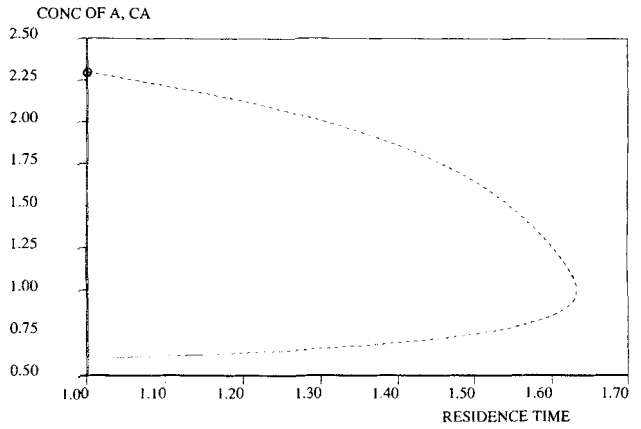

Figure 1. Open-loop bifurcation diagram; Unstable (dashed line) and stable (solid line) equilibria.

Reactor parameters are: order of reaction A to B, $n = 2$; order of reaction B to C, $m = 1$; $C_{Af} = 3.0$; $(-\Delta H)_1/\rho C_p = 1{,}100.0$; $(-\Delta H)_2/\rho C_p = 1{,}200.0$; $k_1(T) = 50.0e(-3{,}000.0/T)$; $k_2(T) = 40.0e(-4{,}000.0/T)$; $(hA_c/\rho C_p V = 3.0$; $T_f = 340$K, $T_j = 300$ K.

this picture supports the information from AUTO presented earlier in Figure 1; the location of the stable steady state at about $C_A = 0.6$ confirms the results from AUTO. The existence of another stable steady state (at about $C_A = 2.96$) is also revealed by the dynamic simulation; this same information would probably have been revealed by AUTO if we had continued the solution branch or initiated tracing of another branch close to zero conversion. In any event, it is seen that the existence of the desired equilibrium E_d^3 is not revealed by the dynamic simulation since it is open-loop unstable. It is important also to observe the thermal runaway behavior exhibited by some reactor trajectories near this degenerate operating point; maintaining safe reactor operating temperatures here is thus crucial.

For the purposes of closed-loop simulations, in all cases, the gain of the reference model was set at $k = 0.50$; this choice

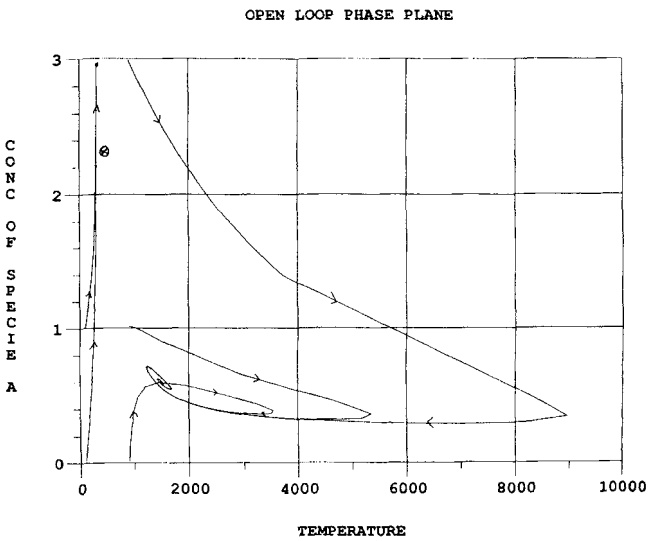

Figure 2. Open-loop dynamic simulation at residence time of 1.0.

(All other parameters are identical to those in Figure 1). •, Stable equilibria; ⊗, unstable equilibria. Note the qualitative agreement with Figure 1.

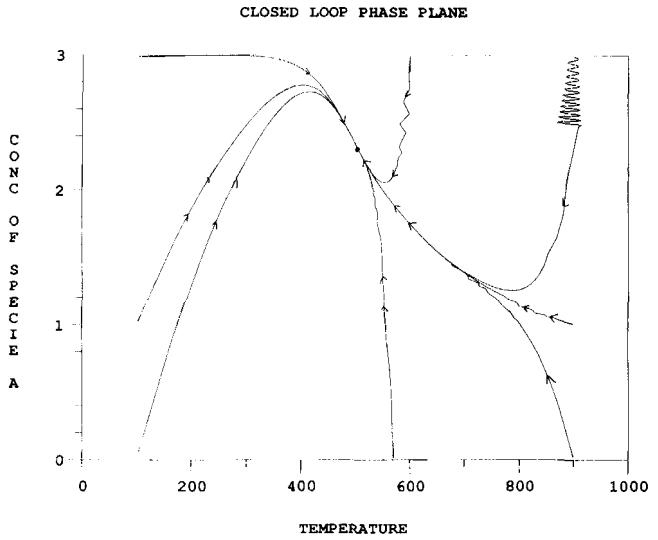

Figure 3. Closed-loop phase portrait when only E_1 and E_2 are assumed known.

All other parameters are assumed unknown. Operation is at the unstable equilibrium which exists at a residence time of 1.0 (depicted in Figures 1 and 2). Some of the initial conditions for C_A, C_B and T are identical to those in Figure 2. Note global convergence to this equilibrium point under closed-loop operation.

of k was arbitrary. In our evaluations, we have tried to be objective by including an instance where the initial transient closed response is slightly poor. This is sometimes to be expected; in a certain sense, it is the price paid for achieving global robustness. In very few instances, some trajectories did 'hit' the $T=0$ boundary but in most cases, this was not a problem; except in these degenerate cases, as is predicted by our analysis, the reactor always converged to the desired operating condition. Thus, for the closed-loop trajectories presented in Figure 3 we have again shown only the $C_A - T$ phase plane for a wide range of initial conditions; some of the initial conditions for C_A, C_B and T in this figure are identical to those in Figure 2; note that in this particular figure, the reactor was usually initiated at temperatures of over 350 K from the desired operating point. In a few cases, the initial response is somewhat oscillatory. As was earlier stated, this should sometimes be expected since the demands on the control system are quite ambitious. In addition, we emphasize that no attempt was made to vary k, thus it may be possible to improve the initial transient response for some of the trajectories shown in the figure. In any event, as is seen in the Figure 3, the runaway behavior evident in some of the trajectories depicted in Figure 2 has been eliminated. Moreover, the desired equilibrium is indeed globally attracting, thereby providing direct numerical confirmation of our global predictions.

Conclusion

In this paper, a global stability analysis of a highly nonlinear reactor under nonlinear feedback control has been carried out. In the initial portion of the analysis, the zero dynamics of the system was analyzed using methods from nonlinear analysis. In the final stages of the analysis, a MRAC was incorporated into the design to address issues of robustness; the stability of the zero dynamics was a crucial factor in establishing the global convergence of the entire scheme, even when model parameters were assumed completely unknown. At the moment, issues not addressed, but which are equally important for actual implementation include the incorporation of a state estimator, the handling of constraints and the robustness of the adaptive mechanism itself to unmodelled dynamics. As was stated earlier though, an ad-hoc approach toward the constraint issue is by introducing adaptive gains into the Lyapunov design and evaluating the resulting inputs by simulation; these gains essentially function as detuning parameters and are used to scale the adaptive update laws.

Finally, the application illustrates the important issues which arise from the study; namely that an understanding of the nonlinear dynamics of processes and their attractors is invaluable in gaining insight into designing control strategies for complex chemical processes. This approach, probes the core of the system deeply, but the effort involved is eventually justified in the sense that global inferences can be made. Thus, it is hoped that these methods continue to find use within the process control community.

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Notation

A = specie A
A_c = heat-transfer area of reactor
A_i = specie A_i, $i=1,2,\ldots N$
B = specie B
C_A = concentration of specie A in reactor
C_{Ad} = desired concentration of specie A in reactor
C_{Ae} = equilibrium concentration of specie A in reactor
C_{Af} = feed concentration of specie A
C_{Ai} = concentration of specie i in reactor, $i=1,2,\ldots N$
C_{Ai_d} = desired concentration of specie i in reactor, $i=1,2,\ldots N$
C_{A1_f} = feed concentration of specie A_1
C_B = concentration of specie B in reactor
C_{Bd} = desired concentration of specie B in reactor
C_{Be} = equilibrium concentrations of specie B in reactor
C_p = specific heat capacity of reactor contents
e = state of the error system
E_d^3 = desired equilibrium point of two-stage reaction
E_d^{N+1} = desired equilibrium point for N-stage reaction
E_i = activation energy for reactor stage i
f_i, f_i' = reactor specific functions used in the design, $i=1,\ldots,4$
F = volumetric flow rate of feed
g = control input multiplier
h = heat-transfer coefficient
$(-\Delta H)_i$ = heat of reaction for reaction stage i
k = gain of reference model
k_i' = adaptation gains
k_{io} = frequency factor for reaction stage i
m = order of second stage reaction in two-stage reaction
n = order of first stage reaction in two-stage reaction
n_i = order of stage i in N-stage reaction, $i=1,\ldots,N$
N = dummy variable used for number of reaction stages
$\mathfrak{M}_3, \mathfrak{M}_{3\infty}$ = invariant sets for two-stage reaction
$\mathfrak{M}_{N+1}$ = invariant set for N-stage reaction
P = used in construction of invariant set

R = universal gas constant
$S^{3\infty}$ = limiting autonomous system for zero dynamics of two-stage reaction
t = time
T, T_d = reactor temperature, desired reactor temperature
T_j = cooling jacket temperature
T_f = feed temperature
T_{min}, T_{max} = min and max reactor temperature respectively
T_r = state of the reference plant
u = manipulated variable
V = volume of reactor
V_l = Lyapunov function
W = dummy variable, used in adaptive design

Greek letters

α = parameter for selecting invariant set for two-stage reaction
α_i = parameter for trapping regions for N-stage reaction, $i=2, \ldots N$
δ_i = uncertain parameters of reactor, $i=1, \ldots, 4$
ρ = density of reacting medium

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