Robust Feedback Stabilization of Chemical Reactors

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***Abstract*—This paper deals with the temperature stabilization of a large class of continuously stirred tank chemical reactors. We design state feedback controllers, and we show their ability to globally stabilize the temperature at an arbitrary set point in spite of uncertainties on the kinetics. Furthermore, it is also shown that these controllers can handle input constraints along the closed-loop trajectories in some instances. For the implementation purpose, we design a robust state observer for the case of partial state measurement, and we prove that its incorporation in the feedback loops does not impair the nominal stabilization properties of the controllers.**

***Index Terms*—Chemical reactors, robust feedback stabilization, robust observer, temperature control.**

I. Introduction

THE DESIGN of stabilizing feedback control laws for unstable chemical reactors has been studied extensively in the past since the pioneering paper of Aris and Admunsen [1]. The engineering motivation relies on the fact that the reactor operation near or at unstable steady states often corresponds to an optimal process performance (like, for instance, an optimum tradeoff between yield and productivity, or between conversion and selectivity, or between catalyst activity and longetivity; see, e.g., [2]).

The feedback control of chemical reactors is a problem which is made difficult by the inherent nonlinear nature of the involved mechanisms. Open chemical reactors, indeed, are well known to exhibit multiple (stable or unstable) steady states, limit cycles, and even chaotic behavior.

In the last ten years, there has been a great deal of activity in the nonlinear feedback control (especially feedback linearization) of chemical reactors. Typical references among others are [3]–[6]. Numerous successful applications have also been reported in the literature.

There are, nevertheless, important theoretical questions that are still open. One of them, which is the main concern of this paper, is the design of feedback control laws that are:

- *globally* stabilizing;
- *robust* against *kinetic uncertainties*;
- *robust* against *control input saturations*.

One of the particular control problems which was most commonly investigated is the temperature regulation of an exothermic irreversible reaction $A \rightarrow B$ in a cooled continuously stirred tank reactor (CSTR). The related robust control problem is to find a feedback law (for the heating rate provided to the reactor) in order to regulate and to globally stabilize the temperature at an arbitrary set point with some robustness against uncertainties in the knowledge of the kinetics. It has been shown in [7] that in the case of first-order kinetics, a simple PI controller can globally stabilize this kind of reactor. Such a controller is robust in the sense that its design does not require an exact knowledge of the kinetics. Considered in [8] and [9] for nth order kinetics is input/output (I/O) linearization (i.e., feedback of concentrations and temperature). In these papers, the uncertainty of the kinetics is restricted to lie in a few constant parameters entering linearly in the model, and a classical adaptive technique model reference adaptive control (MRAC)-type is used, which can globally stabilize the closed loop. In [10], the I/O linearization technique is combined with the robust stabilization methods of [11] and [12]. The proposed controller is time varying (it involves an explicitly time-dependent decaying term) and makes the temperature practically stable at its set point. It is also worth noting that none of these mentioned control methods is able to account for a saturation of the control input along the closed-loop trajectories. It is, however, well known, as illustrated in [13], that saturating the temperature controller of an exothermic reactor can impair its nominal stabilization properties.

In this paper, for a general class of CSTR's, we propose a set of controllers that guarantee the *global* temperature stabilization in spite of strong uncertainties on the dependence of the kinetic functions with respect to the temperature. A main feature of these controllers lies in their capability of handling input constraints in some instances. Moreover, if the reactor is globally asymptotically stable in the isothermal condition, then our results turn into global stabilization of both temperature and concentrations. (Here, we point out that in spite of the global asymptotic stability in the isothermal condition, the overall dynamics of the open-loop reactor can be unstable). The design is based on I/O state feedback linearization with an appropriate dynamic extension.

The stability results that are available in the literature are extended in five main directions.

1) A general class of systems with multiple coupled reactions is considered. The number of involved reactions is arbitrary. In other words, the analysis is not restricted to the special case of systems including only one or two reactions.
2) We do not make any restrictive assumptions regarding the dependence of the kinetic function with respect to the concentrations of the involved chemical species.

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In particular, we do not restrict ourselves to mass-action type kinetics, and we allow for nonmonotonic dependence on both concentrations and temperature.

3) For each proposed controller we give a rigorous proof of the *global* temperature stabilization. By global, we mean that the temperature stabilization is achieved, whatever the initial conditions of the system are. (We only require that the initial conditions are located inside the physical domain of existence of the system.)
4) In some instances, we prove the ability of the controllers to handle input constraints: the control input remains *nonnegative* along the closed-loop trajectories (in accordance with the physical requirements of the problem).
5) Since our controllers are state feedback controllers, they require for implementation purpose the on-line knowledge of the full state, i.e., concentrations and temperature. A robust state observer is designed in the case of partial state measurements. We prove that the incorporation of this observer in the feedback loops does not impair our nominal stabilization properties.

The organization of our paper is as follows: in Section II, we present the general class of CSTR we consider, and we define the control problem. In the third and fourth sections, we address the control design when the kinetics are, respectively, known or uncertain. Section V is devoted to the observer design and to its use together with the nominal stabilizing state-feedback controllers. For the sake of illustration, a simple application is presented in Section VI.

II. System Description and Problem Statement

A. System Description

We will consider throughout the paper CSTR's that are described by the following set of dynamic equations:

$$(S)\begin{cases}\dot{x} = Cr(x,T) + d(x^{in} - x)\\ \dot{T} = B(x,T) - qT + u.\end{cases}$$

In these equations, we have the following.

- x is the vector of the concentrations of the involved chemical species (reactants and products), dim $x = n$.
- x^{in} is the vector of nonnegative and constant feed concentrations, dim $x^{in} = n$.
- T is the reactor temperature.
- $r(x,T)$ is the vector of reaction kinetics, dim $r = m$, and $r^T(x,T) = (r_1(x,T), r_2(x,T), \cdots, r_m(x,T))$. Note that m is equal to the number of chemical reactions taking place in the reactor.
- C is the stoichiometric matrix, dim $C = n \times m$.
- $B(x,T)$ is the reaction heat.
- d, q are positive constants (d is the dilution rate, q is a heat transfer coefficient).
- u is the input, i.e., the manipulated heat.
- $r_i(x,T) = k_i(T)\varphi_i(x)$, where $k_i(T)$ is a positive and bounded function of the temperature (for instance, the Arrhenius law), and $\varphi_i(x)$ is a nonnegative function of the concentrations that vanishes if and only if $x_j = 0$ for some reactant j involved in the ith reaction.
- $B(x,T) = K^T(T)\varphi(x)$ with $K^T(T) = (b_1k_1(T), b_2k_2(T), \cdots, b_mk_m(T))$, where the coefficients b_i are constant and $\varphi(x) = (\varphi_1(x), \varphi_2(x), \cdots, \varphi_m(x))^T$.

Note that y^T stands for the transpose vector of y.

Let us introduce the first assumption that will be used throughout the paper.

H1 (Principle of Mass Conservation): There exists a positive vector of dimension $n, w = (w_1, w_2, \cdots, w_n)^T$, $w_i > 0, i = 1, \cdots, n$ such that $w^TC = 0$.

This assumption implies that the reaction system is mass-conservative, or in other words, that what is produced by the reaction system cannot be larger than what is consumed. It also enables one to state a useful result on the boundedness of the concentrations in a chemical reactor described by the model (S).

Lemma A.1 (Uniform Boundedness): Under Assumption H1, the concentrations $x_i(t)$ remain nonnegative for all t if $x_i(0) \geq 0$, and we admit, furthermore, as a positively invariant domain, the compact set $\Omega = \{x \in \Re^n : \forall i, x_i \geq 0, w^Tx \leq w^Tx^{in}\}$.

Proof: The dynamic equation for the ith concentration is given by

$$\dot{x}_i = \sum_j c_{ij}r_j(x,T) + d(x_i^{in} - x_i)$$

and we have $\dot{x}_i(x_i = 0) \geq 0$ since $\Sigma c_{ij}r_j(x,T) \geq 0$ when $x_i = 0$. Hence, the concentrations remain nonnegative provided that $x_i(0) \geq 0, \forall i$. Defining Z as $Z = w^Tx$, we have by Assumption H1: $\dot{Z} = -d(Z - w^Tx^{in})$. Hence, $Z(t) \leq w^Tx^{in}$ for $Z(0) \leq w^Tx^{in}$, and the compact set $\Omega = \{x \in \Re^n : \forall i, x_i \geq 0, w^Tx \leq w^Tx^{in}\}$ is positively invariant by the dynamics of (S). ∎

As a consequence of Lemma A.1, the vector of concentrations x will be restricted to the bounded set Ω throughout the paper. This *uniform* boundedness of the concentrations with respect to the temperature trajectory will be a key point for our future developments.

B. Control Problem Statement

The control problem we consider is to globally stabilize the temperature at a given set point $\boldsymbol{T^* > 0}$ with a nonnegative feedback control $\boldsymbol{u(x,T) \geq 0}$.

The requirement of a *nonnegative* feedback control comes from the fact that the control input u represents a heating rate, provided to the reactor from outside. So, it has to be nonnegative for having a physical meaning.

This control problem will be considered under the following assumptions.

H2) The full state (x,T) is measured.
H3) The functions $k_i(T)$ are positive, bounded, and globally Lipschitz on $]0; \pm\infty[$.
H4) The isothermal dynamics

$$\dot{x} = Cr(x,T^*) + d(x^{in} - x)$$

are globally asymptotically stable at the single equilibrium point $\overline{x} \in \Omega$. By Lyapunov converse theorems [14], we know that there exists a positive definite Lyapunov function $W(x, \overline{x}, T^*)$ such that its time-derivative

$$\left[\frac{\partial W}{\partial x}\right]^T (Cr(x, T^*) + d(x^{in} - x))$$

is negative definite. We further assume that there exists a positive definite function ϕ such that

$$\left\|\frac{\partial W}{\partial x}\right\| \leq a_1 \phi(x - \overline{x})$$

$$\left[\frac{\partial W}{\partial x}\right]^T (Cr(x, T^*) + d(x^{in} - x)) \leq -a_2 \phi^2(x - \overline{x})$$

for some positive constants a_1 and a_2.

We will see in Sections V and VI how Assumption H2 can be relaxed by using an observer. The reader can refer to [15] and [16], where fairly general sufficient conditions on the kinetic scheme are given so that the isothermal stability Assumption H4 holds even in the case of autocatalytic reactions. We point out that in spite of the global asymptotic stability of the isothermal dynamics, the overall dynamics can be open-loop unstable. Note also that the technical Assumption H3 is satisfied when the $k_i(T)$ functions are given by the Arrhenius law.

Two situations for our control problem will be considered.

1) The kinetic rate functions $r(x, T)$ and the reaction heat $B(x, T)$ are assumed to be known.
2) The temperature functions $k_i(T)$ and the b_i constants involved in the kinetic rate functions $r(x, T)$ and in the reaction heat $B(x, T)$ are unknown.

The second situation is motivated by the fact that in many applications, although the stoichiometry and the kinetic scheme are well known, the empirical Arrhenius law may exhibit some uncertainty.

In this paper, we do not take into account any time-varying parametric uncertainty. This type of uncertainty has been considered in [17] for the control of a chemical reactor.

III. Control Design: Known Kinetics

By known kinetics, we mean that the functions $r(x, T)$ and $B(x, T)$ are known, which implies in particular that all the coefficients involved in these functions are perfectly known.

Our first result to be presented hereafter states that a saturated (lower bounded) state feedback controller resulting from I/O-linearization produces the global stabilization of an endothermic reactor ($\forall i, b_i < 0$) described by the model (S).

Theorem 3.1—Endothermic Case ($\forall i, b_i < 0$)*:* Consider the state feedback controller

$$u(x, T) = \max[0, \beta(T^* - T) + qT] - B(x, T).$$

We have the following.

1) Under Assumptions H1 and H2, for all $\beta > q$, for any initial condition $(x(0), T(0)) \in \Omega \times]0, +\infty[$, the reactor temperature T converges asymptotically to the set point T^*, the feedback control $u(x, T)$ is nonnegative along the closed-loop trajectories, and $(x(t), T(t)) \in \Omega \times]0, +\infty[$ for all t.
2) If, in addition, Assumption H4 is satisfied, then for all $\beta > q$, the closed-loop system is globally asymptotically stable at the equilibrium point $(\overline{x}, T^*)$.

Proof i): By definition, the state feedback controller $u(x, T)$ is always nonnegative $\forall t \geq 0, u(x(t), T(t)) \geq 0$. Moreover, we have

$$\forall T \geq T_l = \frac{\beta T^*}{\beta - q}, \quad \dot{T} < 0.$$

Hence, after a finite time t_l we have $T \geq T_l$ and the state feedback controller reduces to

$$u(x, T) = \beta(T^* - T) + qT - B(x, T)$$

for $t \geq t_l$. Then, the temperature dynamics are

$$\dot{T} = \beta(T^* - T).$$

ii): Now, using H4 and Lemma A.1 together with Theorem A.1 of Appendix A, we obtain that the closed-loop dynamics are globally asymptotically stable (g.a.s.) at the equilibrium point $(\overline{x}, T^*)$. ■

Before considering the exothermic case ($\forall i, b_i > 0$), we introduce the following additional realistic assumption:

H5) The temperature set point T^* is such that $\forall x \in \Omega, qT^* - B(x, T^*) > 0$.

This assumption can be regarded as a kind of feasibility condition on the open-loop system. Indeed, it implies that the static input corresponding to the equilibrium point $(\overline{x}, T^*)$ is positive. Then, we can state the result.

Theorem 3.2—Exothermic Case ($\forall i, b_i > 0$)*:* We have the following.

1) Under Assumptions H1, H2, and H4, for all $\beta > 0$, for any initial condition $(x(0), T(0)) \in \Omega \times]0, +\infty[$, the state feedback controller

$$u(x, T) = \beta(T^* - T) + qT - B(x, T)$$

is such that $(x(t), T(t)) \in \Omega \times]0, +\infty[$ for all t, and the closed-loop system is globally asymptotically stable at the equilibrium point $(\overline{x}, T^*)$.
2) If, in addition, Assumption H5 is satisfied, there exists $\beta^* > 0$ large enough and $\varepsilon > 0$ small enough such that with the state feedback controller

$$u(x, T) = \beta(T) \cdot (T^* - T) + qT - B(x, T)$$
$$\beta(T) = \beta^*, \forall T \in]0; T^*]$$
$$\beta(T) = \min\left[\frac{\varepsilon}{T - T^*}, \beta^*\right], \quad \forall T \in [T^*, +\infty[$$

the closed-loop dynamics are globally asymptotically stable at $(\overline{x}, T^*)$. Moreover, $u(x, T) \geq 0$ on $\Omega \times]0; T_2]$, for some $T_2 > T^*$.

Proof i): Under the feedback controller

$$u(x,T) = \beta(T^* - T) + qT - B(x,T)$$

the temperature dynamics are given by

$$\dot{T} = \beta(T^* - T).$$

Using Assumption H4 and Lemma A.1 together with Theorem A.1 of Appendix A, we conclude that this feedback controller will stabilize (S) at $(\overline{x}, T^*)$.

ii): At first, let us consider the case $T(0) < T^*$. Hence, $\forall t \geq 0, T(0) \leq T(t) \leq T^*$.

Assumption H5 implies that

$$\exists T_1 < T^* \text{ s.t. } \forall \beta^* > 0, \quad \forall x \in \Omega, \quad \forall T \in [T_1, T^*], \quad u(x,T) \geq 0.$$

For $T \in [T(0), T_1]$, we have $u(x,T) \geq \beta^*(T^* - T_1) + qT(0) - B(x,T)$. By choosing β^* such that $\forall (x,T) \in \Omega \times]0, T_1], \beta^* \geq B(x,T)$, the input $u(x,T)$ will be positive. Assume now that $T(0) > T^*$. Hence, $\forall t \geq 0, T^* \leq T(t) \leq T(0)$. Assumption H5 also implies that for $\varepsilon > 0$ such that $\varepsilon < qT^* - B(x,T), \forall x \in \Omega$, then

$$\exists T_2 > T^* \text{ s.t. } \forall x \in \Omega, \quad \forall T \in [T^*, T_2], \quad q^T - B(x,T) \geq \varepsilon.$$

On the set $\Omega \times [T^*, T_2]$, we have $u(x,T) \geq \beta(T) \cdot (T^* - T) + \varepsilon$, and by using $\beta(T) = \min[\varepsilon/(T - T^*), \beta^*]$, we obtain $u(x,T) \geq 0$. ∎

IV. Control Design: Uncertain Kinetics

What we mean precisely by uncertain kinetics is that the functions $k_i(T)$ and the constants b_i of the model (S) are unknown, but the sign of the constants b_i is assumed to be known. To know the sign of b_i is equivalent to knowing whether the ith reaction is exothermic or endothermic. According to Assumption H3, we will denote by α_i the upperbound on the functions $|b_i|k_i(T)$. More precisely, α_i is such that $\alpha_i > |b_i|k_i(T)$. [What we really need is that $\alpha_i > |b_i|k_i(T^*)$.]

Theorem 4.1—General Case (Endothermic or Exothermic): Consider the dynamic state feedback controller

$$u(x,T,\theta) = \beta(T^* - T) + qT - g^T(\theta)\varphi(x)$$
$$\dot{\theta}_i = (T - T^*)\,\text{sign}\,(b_i)\theta_i\varphi_i(x) \qquad i = 1, \cdots, m$$

with $\beta > 0, \theta = (\cdots, \theta_i, \cdots)^T \in \Re_+^m$ and $g(\theta) = (\cdots, \text{sign}\,(b_i)(\alpha_i\theta_i/(\alpha_i + \theta_i)), \cdots)^T$. Then, we have the following.

1) Under Assumptions H1–H3, for $\beta > 0$ large enough, for any initial condition $(x(0), T(0), \theta(0)) \in \Omega \times]0, +\infty[\times \Re_+^m$, the state $(x(t), T(t), \theta(t)) \in \Omega \times]0, +\infty[\times \Re_+^m$ for all time t, the reactor temperature T converges to the set point T^*, and the variables θ_i are bounded.
2) If, in addition, Assumption H4 is satisfied, then for $\beta > 0$ large enough, the concentrations x and the reactor temperature T globally converge to $\overline{x}$ and T^* (for any initial condition $(x(0), T(0), \theta(0)) \in \Omega \times]0, +\infty[\times \Re_+^m$).

Proof i): The closed-loop dynamics can be written as

$$\dot{T} = \beta(T^* - T) + [\Delta K(T)]^T\varphi(x) + [K(T^*) - g(\theta)]^T\varphi(x)$$
$$\dot{\theta}_i = (T - T^*)\,\text{sign}\,(b_i)\theta_i\varphi_i(x)$$

with $\Delta K(T) = K(T) - K(T^*)$.

It is easy to check that for $\beta > 0$ large enough, the set $\Omega \times]0, +\infty[\times \Re_+^m$ is positively invariant by the closed-loop dynamics.

Let us consider the candidate Lyapunov function

$$V = \tfrac{1}{2}(T^* - T)^2 + \sum_i (\alpha_i \ln(\alpha_i + \theta_i) - |b_i|k_i(T^*)\ln(\theta_i)).$$

Note that this function is differentiable, has a global minimum, and is radially unbounded on $\Re \times \Re_+^m$. We obtain

$$\dot{V} \leq -\beta(T^* - T)^2 + ||\Delta K(T)|| \cdot ||\varphi(x)|| \cdot |T^* - T|.$$

Using Lemma A.1 together with Assumption H3, there exists a positive constant M such that

$$\dot{V} \leq -\beta(T^* - T)^2 + M(T^* - T)^2.$$

Hence, by choosing $\beta > 0$ large enough, we have

$$\dot{V} \leq (-\beta + M)(T^* - T)^2 \leq 0.$$

Using the properties of our Lyapunov function V, it then follows that the reactor temperature T and the variables θ_i are bounded. (Remember that by Lemma A.1, the concentrations x are already bounded.) So, we can invoke the Invariance Principle [18] to claim that whatever the concentration trajectory is, the reactor temperature T will converge to T^*.

ii): It remains to prove now that under Assumption H4, the concentrations will converge to their equilibrium point $\overline{x}$. To do so, we introduce a new Lyapunov function. From Assumption H4, there exists a positive definite function $W(x, \overline{x}, T^*)$ such that in isothermal operation, its time derivative is negative definite. Then, consider the candidate Lyapunov function $V + W$. We have

$$\dot{V} + \dot{W} \leq (-\beta + M)(T^* - T)^2 + \left[\frac{\partial W}{\partial x}\right]^T \cdot (Cr(x,T^*) + d(x^{in} - x)) + \left|\left|\frac{\partial W}{\partial x}\right|\right| \cdot ||Cr(x,T) - Cr(x,T^*)||.$$

From Assumption H4, we know that

$$\left[\frac{\partial W}{\partial x}\right]^T (Cr(x,T^*) + d(x^{in} - x)) \leq -a_2\phi_2(x - \overline{x})$$

and

$$\left|\left|\frac{\partial W}{\partial x}\right|\right| \leq a_1\phi(x - \overline{x}).$$

Now, using Lemma A.1 and Assumption H3, we obtain

$$||Cr(x,T) - Cr(x,T^*)|| \leq a_3|T - T^*|$$

for some constant $a_3 > 0$. So, there exist two positive constants a_2 and a_4 such that

$$\dot{V} + \dot{W} \leq (-\beta + M)(T^* - T)^2 - a_2\phi^2(x - \overline{x}) + a_4\phi(x - \overline{x})|T - T^*|.$$

Eventually, it is easy to check that for $\beta > 0$ large enough, the right-hand side of the preceding inequality is negative definite. More precisely, for $\beta > 0$ large enough, there exists a positive definite matrix P such that

$$\dot{V} + \dot{W} \leq -(\phi(x - \overline{x}), |T - T^*|)P(\phi(x - \overline{x}), |T - T^*|)^T.$$

Hence, it follows from the Invariance Principle [18] that the concentrations x converge to their equilibrium point $\overline{x}$. ■

The design of the dynamic state feedback controller of Theorem 4.1 is based on the I/O-linearization technique together with an appropriate dynamic extension. The dynamic extension has been obtained via the Lyapunov redesign method using a Lyapunov function inspired from the one considered in [15] for the open-loop analysis of a class of isothermal reactors. The additional state θ is an internal and bounded state of the controller which is able to asymptotically compensate for the model uncertainties. Let us point out that our model uncertainties do not satisfy the structural property known as the *matching condition* since they also appear in the control-free dynamics of the concentrations. The technical keypoint to overcome this situation lies in the use of the uniform boundedness of the concentrations (Lemma A.1). For the use of the matching condition in the robust control of chemical processes, the reader can refer to [19], where the practical stabilization of two isothermal reactors has been obtained.

Although the result presented in Theorem 4.1 is general (it covers for instance the situation where a mixture of endothermic and exothermic reactions take place), the nonnegativeness of the input along the closed-loop trajectory is not ensured. However, in the endothermic case (the constants b_i are all negative), we have the deeper result.

Theorem 4.2—Endothermic Case ($\forall i, b_i < 0$)*:* Consider the dynamic state feedback controller

$$u(x, T, \theta) = \max(0, \beta(T^* - T) + qT] - h(T)g^T(\theta)\varphi(x)$$
$$\dot{\theta}_i = (T^* - T)\theta_i\varphi_i(x) \qquad i = 1, \cdots, m$$

with $\beta > q, \theta = (\cdots, \theta_i, \cdots)^T \in \Re_+^m, g(\theta) = (\cdots, -(\alpha_i\theta_i/(\alpha_i + \theta_i)), \cdots)^T$ and $h(T)$ a decreasing positive C_0^1;$+\infty$[-function such that $h(T) = 1$ for $T \leq T^*$ and $h(T) = 0$ for $T \geq T_l$, where $T_l = \beta T^*/(\beta - q)$. Then, we have the following.

1) Under Assumptions H1–H3, for $\beta > q$ large enough, for any initial condition $(x(0), T(0), \theta(0)) \in \Omega\times]0, +\infty[\times\Re_+^m$, the state $(x(t), T(t), \theta(t)) \in \Omega\times]0; +\infty[\times\Re_+^m$ for all t, the reactor temperature T converges to the set point T^*, the variables θ_i are bounded, and the input is nonnegative along the closed-loop trajectories.
2) If in addition Assumption H4 is satisfied, then for $\beta > q$ large enough, the concentrations x and the reactor temperature T globally converge to $\overline{x}$ and T^* (for any initial condition $(x(0), T(0), \theta(0)) \in \Omega\times]0, +\infty[\times\Re_+^m$).

Proof i): By definition, the input is nonnegative $\forall t \geq 0, u(x(t), T(t), \theta(t)) \geq 0$. Moreover, we have

$$\forall T \geq T_l, \forall \theta \in \Re_+^m, \qquad \dot{T} < 0.$$

(Note that this property holds because of the role played by the $h(T)$ function in the feedback control law.) Hence, after a finite time t_l we have $T \leq T_l$, and the feedback control reduces to

$$u(x, T, \theta) = \beta(T^* - T) + qT - h(T)g^T(\theta)\varphi(x)$$

for $t \geq t_l$. Then, we can consider the closed-loop dynamics

$$\dot{T} = \beta(T^* - T) + [\Delta K(T)]^T\varphi(x) + [K(T^*) - h(T)g(\theta)]^T \cdot \varphi(x)$$
$$\dot{\theta}_i = (T^* - T)\theta_i\varphi_i(x)$$

with $\Delta(K)T = K(T) - K(T^*)$. As a candidate Lyapunov function, we choose

$$V = \tfrac{1}{2}(T^* - T)^2 + \sum_i (\alpha_i \ln(\alpha_i \ln(\alpha_i + \theta_i) + b_i k_i(T^*) \ln(\theta_i)).$$

We obtain

$$\dot{V} \leq -\beta(T^* - T)^2 + ||\Delta K(T)|| \cdot ||\varphi(x)|| \cdot |T^* - T| + (T - T^*)\sum_i \varphi_i(x)\frac{\alpha_i\theta_i}{\alpha_i + \theta_i}(h(T) - 1).$$

Since $h(T) - 1$ vanishes for $T \leq T^*$ and is negative for $T > T^*$, we have

$$\dot{V} \leq -\beta(T^* - T)^2 + ||\Delta K(T)|| \cdot ||\varphi(x)|| \cdot |T^* - T|.$$

Using Assumption H3 and Lemma A.1, there exists a positive constant M such that

$$\dot{V} \leq -\beta(T^* - T)^2 + M(T^* - T)^2.$$

Hence, by choosing $\beta > 0$ large enough, we have

$$\dot{V} \leq (-\beta + M)(T^* - T)^2 \leq 0.$$

So, T converges to T^*.

ii): The rest of the proof is similar to that of Theorem 4.1. ■

Corollary 4.1—Single Reaction Case: In the single reaction case ($m = 1$), if all the reactants are fed to the reactor (the zero entries of the vector x_{in} correspond to reaction products), then in addition to the statements of Theorems 4.1 and 4.2, the variable θ globally converges to the constant $\overline{\theta} \in \Re_+$ such that $g(\overline{\theta}) = K(T^*)$.

The proof of this Corollary directly follows from the application of the Invariance Principle [18] to our Lyapunov function V and from the fact that the variable θ is scalar.

V. Control Design with State Observer

So far in the paper we have assumed that the temperature T and the state vector x of concentrations are fully measurable and available for feedback. From now on, we shall assume that in addition to the temperature T, a *subset* of the concentrations only is available for on-line measurement. The vector of these measurements is denoted x_1, while the vector of the remaining nonmeasured concentrations is denoted x_2.

The system (S) can therefore be rewritten as

$$\begin{aligned}\dot{x}_1 &= C_1 r(x_1, x_2, T) + d(x_1^{in} - x_1)\\ \dot{x}_2 &= C_2 r(x_1, x_2, T) + d(x_2^{in} - x_2)\\ \dot{T} &= B(x_1, x_2, T) - qT + u\end{aligned}$$

with appropriate definitions of the vectors x_1^{in} and x_2^{in}, and of the matrices C_1 and C_2.

The objective of this section is to develop a state observer for the on-line reconstruction of the nonmeasured partial state x_2. The observer design must, however, account for the fact that the kinetic function $r(x_1, x_2, T)$ is assumed to be partially unknown. We therefore use a methodology proposed in [20] and [21], based on the concept of "chemical invariants" [22] and on the technique of observers for linear systems with unknown disturbance input as discussed, e.g., in [23] and [24].

The application of the methodology requires one to introduce the following additional assumptions.

H6) $\dim x_1 \geq \operatorname{rank} C$: the number of measured species is larger or equal to the rank of the stoichiometric matrix.

H7) $\operatorname{rank} C_1 = \operatorname{rank} C$.

Assumptions H6 and H7 will be used to relax the demanding condition of H2 in our preceding results. They explicit the conditions that allow partial state measurement. In the single reaction case, these assumptions mean that only one single species must be measurable (whatever the number of chemical species involved in the reaction) as it is illustrated in Section VI: this is certainly a realistic and weak requirement.

Under these assumptions, it is obvious that a matrix N exists such that

$$NC_1 + C_2 = 0.$$

We define the auxiliary partial state

$$z = Nx_1 + x_2$$

whose dynamics are easily shown to be

$$\dot{z} = -dz + d(Nx_1^{in} + x_2^{in}).$$

Note that this equation is clearly independent of the unknown kinetic function $r(x_1, x_2, T)$. A simple and natural observer is then derived from the last two equations as follows:

$$\begin{aligned}\dot{\hat{z}} &= -d\hat{z} + d(Nx_1^{in} + x_2^{in})\\ \hat{x}_2 &= \hat{z} - Nx_1\end{aligned}$$

where $\hat{z}$ and $\hat{x}_2$ denote on-line estimates of z and x_2, respectively. The exponential convergence of this observer is evident since the dilution rate d is a positive constant. However, the speed of convergence is not assignable and is completely determined by the value of the dilution rate d. This is why this algorithm is called an *asymptotic* observer in [20].

We will now examine the effect of the closed-loop dynamics when this observer is combined with the nominal stabilizing controllers of Section VI (uncertain kinetics).

Let us denote by $\hat{x} = (x_1, \hat{x}_2)^T$ the vector of measured and estimated concentrations. It can be noted that $\hat{x}$ might take values outside the domain Ω. When incorporating the observer into the loop, we therefore introduce a nonnegative function $\tilde{\varphi}(\hat{x})$ such that $\tilde{\varphi}(\hat{x}) = \varphi(\hat{x})$ when $\hat{x} \in \Omega$ and $\tilde{\varphi}(\hat{x})$ is globally Lipschitz on $\Re^n$.

Let us address the following question.

Q: Will the temperature stabilization properties of the nominal controllers (Theorems 4.1 and 4.2) remain valid when the observer is incorporated in the loop?

First, we consider the controller of Theorem 4.1 using the observer. The resulting control structure is

$$(C1)\begin{cases} u(\hat{x}, T, \theta) = \beta(T^* - T) + qT - g^T(\theta)\tilde{\varphi}(\hat{x})\\ \dot{\theta}_i = (T - T^*)\operatorname{sign}(b_i)\theta_i\tilde{\varphi}_i(\hat{x})\\ \dot{\hat{z}} = -d\hat{z} + d(Nx_1^{in} + x_2^{in})\\ \hat{x}_2 = \hat{z} - Nx_1. \end{cases}$$

The answer to the above question is positive as shown in the following theorem.

Theorem 5.1—General Case (Endothermic or Exothermic): Assume that the above controller $(C1)$ is applied to the system (S). Then, we have the following.

1) Under Assumptions H1, H3, H6, and H7, for $\beta > 0$ large enough, for any initial condition $(x(0), \hat{x}(0), T(0), \theta(0)) \in \Omega \times \Omega \times]0; +\infty[\times \Re_+^m$, the reactor temperature T still converges to the set point T^*.
2) If, in addition, Assumption H4 is satisfied, then for $\beta > 0$ large enough, the concentrations x and the reactor temperature T still globally converge to $\overline{x}$ and T^* (for any initial condition $(x(0), \hat{x}(0), T(0), \theta(0)) \in \Omega \times \Omega \times]0; +\infty[\times \Re_+^m$).

Proof i): Let us consider the candidate Lyapunov function $V + \hat{V}$ with

$$V = \frac{1}{2}(T^* - T)^2 + \sum_i (\alpha_i \ln(\alpha_i + \theta_i) - |b_i| k_i(T^*) \ln(\theta_i))$$

$$\hat{V} = \frac{d}{2}||x - \hat{x}||^2 = \frac{d}{2}||e||^2.$$

On the one hand, we have

$$\dot{V} \leq (-\beta + M)(T^* - T)^2 + |T - T^*| \cdot ||K(T^*)|| \cdot ||\tilde{\varphi}(x) - \tilde{\varphi}(\hat{x}||$$

where M is a positive constant.

On the other hand, we have

$$\dot{\hat{V}} \leq -d||x - \hat{x}||^2.$$

From the smoothness of the function $\tilde{\varphi}$, we deduce that there exists a positive constant c such that

$$\dot{V} + \dot{\hat{V}} \leq (-\beta - M)(T^* - T)^2 + c|T - T|^* \cdot ||x - \hat{x}|| - d||x - \hat{x}||^2.$$

It is then easy to check that for $\beta > 0$ large enough, there exists a positive definite matrix P_1 such that

$$\dot{V} + \dot{\hat{V}} \leq (||x - \hat{x}||, |T - T^*|) P_1 (||x - \hat{x}||, |T - T^*|)^T$$

$(x(t), e(t), T(t), \theta(t))$ being bounded, we can use the Invariance Principle [18] to conclude that T still converges to T^*.

ii): It remains to prove now that under the Assumption H4, the concentrations will converge to their equilibrium point $\overline{x}$. From Assumption H4, we know that there exists a positive definite function $W(x, \overline{x}, T^*)$ such that in isothermal operation, its time derivative is negative definite. Consider the candidate Lyapunov function $V + \hat{V} + W$. Using the same technique as in the proof of Theorem 4.1, it can be shown that for $\beta > 0$ large enough

$$\dot{V} + \dot{\hat{V}} + \dot{W} \leq -(\phi(x - \overline{x}), ||x - \hat{x}||, |T - T^*|) \cdot P_2 (\phi(x - \overline{x}), ||x - \hat{x}||, |T - T^*|)^T$$

where P_2 is a positive definite matrix and ϕ is the positive definite function defined in Assumption H4. So, it follows again from the Invariance Principle [18] that the concentrations x converge to their equilibrium point $\overline{x}$. ■

Consider now the controller of Theorem 4.2 using the observer. The resulting control structure is

$$(C2) \begin{cases} u(\hat{x}, T, \theta) = \max[0, \beta(T^* - T) + qT] - h(T) g^T(\theta) \cdot \tilde{\varphi}(\hat{x}) \\ \dot{\theta}_i = (T^* - T) \theta_i \tilde{\varphi}_i(\hat{x}) \\ \dot{\hat{z}} = -d\hat{z} + d(N x_1^{in} + x_2^{in}) \\ \hat{x}_2 = \hat{z} - N x_1. \end{cases}$$

Theorem 5.2 Endothermic Case $(\forall i, b_i < 0)$*:* Assume that the controller $(C2)$ is applied to the system (S). Then, we have the following.

1) Under Assumptions H1, H3, H6, and H7, for $\beta > q$ large enough, for any initial condition $(x(0), \hat{x}(0), T(0), \theta(0)) \in \Omega \times \Omega \times]0; +\infty[\times \Re_+^m$, the reactor temperature T still converges to the set point T^*, and the input is nonnegative along the closed-loop trajectories.
2) If, in addition, Assumption H4 is satisfied, then for $\beta > q$ large enough, the concentrations x and the reactor temperature T still globally converge to $\overline{x}$ and T^* (for any initial condition $(x(0), \hat{x}(0), T(0), \theta(0)) \in \Omega \times \Omega \times]0; +\infty[\times \Re_+^m$).

The proof of this result is left to the reader. The mechanism of the proof is similar to that of Theorem 5.1.

Corollary 5.1—Single Reaction Case: In the single reaction case $(m = 1)$, if all the reactants are fed to the reactor (the zero entries of the vector x_{in} correspond to reaction products), then in addition to the statements of Theorems 5.1 and 5.2, the variable θ globally converges to the constant $\overline{\theta} \in \Re_+$ such that $g(\overline{\theta}) = K(T^*)$.

It has been shown in [25] and [26], for instance, that the problem of output feedback stabilization can be solved in a semiglobal manner, according to the terminology of [27]. Here it is worth noting that Theorems 5.1 and 5.2 are really *global* results. Indeed, the tuning of the control parameter β is independent of the initial states.

VI. Application

For the sake of illustration of these results, let us consider the following CSTR in which the first-order reaction $A \rightarrow B$ takes place:

$$(S_{AB}) \begin{cases} \dot{x}_A = -k(T) x_A + d(x_A^{in} - x_A) \\ \dot{x}_B = k(T) x_A - d x_B \\ \dot{T} = bk(T) x_A - qT + u. \end{cases}$$

Assumption H1 is satisfied with $w^T = (1, 1)$. Hence, by Lemma A.1, the concentrations in (S_{AB}) admit as a positively invariant domain the compact set $\Omega = \{x_A \geq 0, x_B \geq 0, x_A + x_B \leq x_A^{in}\}$. Suppose for instance that $k(T)$ is given by an Arrhenius law with unknown coefficients. Then, Assumption H3 holds. It is also straightforward to check that the isothermal stability Assumption H4 holds. However, the reactor described by the system (S_{AB}) may have an open-loop *unstable* behavior. It can be shown that (S_{AB}) may exhibit up to three different equilibrium points for some constant values of the input u**.** These equilibrium points are either asymptotically stable or unstable [7]. For economic and practical reasons, it can be desirable to regulate the reactor at an open-loop unstable equilibrium point. Suppose now that the temperature T and the concentration x_B of the product B are measured. As a consequence, Assumptions H6 and H7 are also satisfied.

Let $T^* > 0$ be the temperature set point. Let the nonnegative function $\tilde{\varphi}(\hat{x}_A)$ and the positive constant $\overline{\theta}$ be, respectively, defined by

$$\operatorname{sign}(b) \frac{\alpha \overline{\theta}}{\alpha + \overline{\theta}} = bk(T^*)$$
$$\tilde{\varphi}(\hat{x}_A) = \hat{x}_A \cdot 1_{\{\hat{x}_A \geq 0\}}.$$

From Theorem 5.1 and Corollary 5.1, we can deduce that there exists $\beta > 0$ large enough such that for any initial condition $(x(0), \hat{x}(0), T(0), \theta(0)) \in \Omega \times \Omega \times \Re_+ \times \Re_+$, the following control structure:

$$(C1) \begin{cases} u(\hat{x}_A, x_B, T, \theta) = \beta(T^* - T) + qT - \operatorname{sign}(b) \cdot \dfrac{\alpha\theta}{\alpha + \theta} \tilde{\varphi}(\hat{x}_A) \\ \dot{\theta} = (T - T^*) \operatorname{sign}(b) \theta \tilde{\varphi}(\hat{x}_A) \\ \dot{\hat{z}} = -d\hat{z} + d x_A^{in} \\ \hat{x}_A = \hat{z} - x_B \end{cases}$$

produces the global asymptotic stability of the closed-loop dynamics at the equilibrium point $(\overline{x}, \overline{x}, T^*, \overline{\theta})$. By the way, if the set point T^* is chosen such that $(\overline{x}, T^*)$ is an open-loop unstable equilibrium point of (S_{AB}), then the preceding result means that we are able to regulate the system at this open-loop unstable equilibrium point.

In the endothermic case (we then have $b < 0$), according to Theorem 5.2 and Corollary 5.1, there exists $\beta > q$ large enough such that for any initial condition $(x(0), \hat{x}(0), T(0), \theta(0)) \in$

$\Omega \times \Omega \times \Re_+ \times \Re_+$, the following control structure:

$$(C2)\begin{cases} u(\hat{x}_A, x_B, T, \theta) = \max[0, \beta(T^* - T) + qT] + h(T) \\ \quad \cdot \dfrac{\alpha\theta}{\alpha + \theta}\tilde{\varphi}(\hat{x}_A) \\ \dot{\theta} = (T^* - T)\theta\tilde{\varphi}(\hat{x}_A) \\ \dot{\hat{z}} = -d\hat{z} + dx_A^{in} \\ \hat{x}_A = \hat{z} - x_B \end{cases}$$

which also produces the global asymptotic stability of the closed-loop dynamics at the equilibrium point $(\overline{x}, \overline{x}, T^*, \overline{\theta})$. Furthermore, in this case, the input $u(\hat{x}_A, x_B, T, \theta)$ is nonnegative along the closed-loop trajectories.

VII. Conclusion

In this paper, we investigated the global temperature stabilization problem for CSTR. More precisely, the control problem we considered was the design of feedback control laws that allow the global temperature stabilization, that are robust against kinetic uncertainties, and robust against control input saturations.

We have proposed a set of controllers that can guarantee the global temperature stabilization of CSTR in spite of strong uncertainties on the dependence of the kinetic function with respect to the temperature. The uniform boundedness of the concentrations with respect to the temperature was the keypoint in our proofs. The design of the stabilizing controllers was based on I/O state feedback linearization with an appropriate dynamic extension. We ensure the nonnegativeness of the input in the endothermic case.

To be implemented, our state feedback controllers require the on-line knowledge of the full state: the concentrations and the temperature. In the case of partial state measurement, we have used a robust state observer. This observer provides an exponentially converging estimation error, the rate of which is determined by the dilution rate. We proved that the incorporation of this observer in the feedback loops does not impair the nominal stabilization properties of our controllers.

As a general conclusion, we have obtained control structures that are capable of performing the global temperature stabilization of CSTR with uncertain kinetics but also of guaranteeing the nonnegativeness of the input in the endothermic case. A practical consequence of these results lies in the opportunity of operating chemical reactors at unstable open-loop steady states that correspond to optimal operating conditions.

In our control problem framework, several theoretical questions are still left open. In the endothermic case, we have only considered lowerbounds on the input. It can be of some interest to address the problem when we take into account some upperbounds. It is likely that in some cases, this might defeat the global stabilization property.

In the exothermic case, a robust stabilizing feedback controller such that the input is nonnegative along the closed-loop trajectories is lacking here. However, this problem has been recently addressed, and a solution has been proposed by the authors in [29].

Appendix A
Stability of Globally Minimum Phase Systems

Consider the normal form

$$(N)\begin{cases} \dot{Z} = f(Z, \xi) \\ \dot{\xi} = A\xi \end{cases}$$

that one obtains when the I/O-linearization technique for nonlinear systems is applied. Assume that f is smooth, $f(0,0) = 0$, and the matrix A is stable. It has been shown in [28] that the global asymptotic stability of the subsystem $\dot{Z} = f(Z, 0)$ (then (N) is said to be globally minimum phase) does not imply that (N) is globally asymptotically stable at zero. However, the following result holds.

Theorem A.1—Stability of Cascade Nonlinear Systems: Consider the following cascade nonlinear system:

$$(S)\begin{cases} \dot{Z} = f(Z, \xi) \\ \dot{\xi} = g(\xi) \end{cases}$$

where f and g are smooth, Z and ξ evolve in $\Re^{n-k}$ and $\Re^k$ respectively, and $f(0,0) = g(0) = 0$. Assume that:

C1) $\dot{Z} = f(Z, 0)$ is globally asymptotically stable at $0 \in \Re^{n-k}$;

C2) $\dot{\xi} = g(\xi)$ is globally asymptotically stable at $0 \in \Re^k$.

Then, under Conditions C1 and C2, we have the following.

1) (S) is asymptotically stable at $0 \in \Re^n$.
2) Any trajectory of $(S), \Lambda(Z(0), \xi(0)) = \{(Z(t), \xi(t)), t \in \Re\}$, such that its semitrajectory, $\Lambda^+(Z(0), \xi(0)) = \{(Z(t), \xi(t)), t \geq 0\}$ is bounded, belongs to the basin of attraction of $0 \in \Re^n$.

The proof of this result is given in [25].

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