Continuous stirred tank reactors: easy to stabilise?\footnote{This paper was not presented at any IFAC meeting. This paper was recommended for publication in revised form by Associate Editor B. Wayne Bequette under the direction of Editor Sigurd Skogestad.}

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Received 4 April 2001; received in revised form 7 March 2003; accepted 12 May 2003

Abstract

The objective of this work is to make use of methodologies and tools from Lyapunov theory in the design of bounded control laws for the temperature stabilisation of a class of continuous stirred tank reactors with exothermic or endothermic reactions. Simple output feedback control laws, i.e. control laws that feed back only the available measurements, are designed. It is shown that these controllers yield global asymptotic stability and do not require precise knowledge of the system parameters. The capabilities of the proposed method to handle control input constraints and model uncertainties are also discussed. The work is completed with the analysis of a case study: the van der Vusse reaction mechanism.

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Keywords: Chemical reactors; Temperature stabilisation; Input constraints; Bounded output feedback control

1. Introduction

Many processes of industrial interest are difficult to control for the inherent nonlinear behaviour, the presence of input constraints and the lack of measurements. Among these systems, chemical processes have been widely studied and traditionally controlled using linear system analysis and design tools together with linearised models (Aris & Amundson, 1958; Morari & Zafiriou, 1989; Uppal, Ray, & Poore, 1976), or nonlinear methods based on linearisation techniques (Alvarez, Alvarez, & Gonzales, 1989; Alvarez-Ramirez, 1994; Dochain, 1994; Doyle, Packard, & Morari, 1989; Hoo & Kantor, 1985; Kravaris & Chung, 1987; Limqueco & Kantor, 1990). However, the use of linear techniques is very limiting if the analysed chemical process is highly nonlinear, whereas nonlinear control design needs, in general, too much information on the process. During the past decade there has been a significant increase in interest by many industries in the study of appropriate control strategies for batch, semi-batch or continuous reactors, and several researchers have studied the reactor control problem. Conventional Proportional-Integral–Derivative controllers have been traditionally applied for the temperature regulation of chemical reactors. They are usually robust to model uncertainty since their design is partly independent from the model of the system, but dependent on tuning, see Aris and Amundson (1958) for a case study. Feedback linearisation techniques have also been used. In particular, a full state feedback linearisation solution is presented for an exothermic reactor with one reaction (Alvarez et al., 1989; Limqueco & Kantor, 1990). Global stabilisation by state feedback has been numerically demonstrated using the coolant temperature as a manipulated variable and the addition of a state observer (Limqueco & Kantor, 1990). Stabilisation by state feedback has been proved with respect to a well defined domain (Alvarez et al., 1989). Input–output linearising control, an analytical design approach which aims to reduce the original nonlinear control problem to a simpler linear control problem, has been extensively investigated in Daoutidis and Kravaris (1992), and Kurtz and Henson (1997). Various solutions have been proposed to overcome the robustness problem, in particular the addition of an integral action to the controller obtained from input–output linearisation has been proposed (Kravaris & Chung, 1987). Lyapunov-based adaptive linearising techniques have been successively developed in
with modelling error compensation is designed and its
interest in this direction have been obtained
without requiring any knowledge of the concentrations.
region. It must be noted that to be implemented, all the
stabilise the temperature at an arbitrary set-point in spite
inputs and uncertainties on the reaction kinetics and proposed a
robust state observer to overcome the problem of partial
state measurement. Then they extended these results to an
exothermic chemical reactor considering the feed con-
centration as additional input (Viel, Jadot, & Bastin, 1997b).
Another approach has been proposed by Fradkov, Ortega,
and Bastin (1997). Therein a semi-adaptive state feedback
controller was applied in the region of the state space where
convexity can be used to reduce parameter uncertainty and
it is then frozen and switched to a robust scheme outside
this region. It must be noted that to be implemented, all the
above control laws need the on-line measurement of the full
state of the system, represented by the set of concentrations
and the temperatures. In industrial practice it is very easy
to measure temperatures, but usually not concentrations.
The problem of state variable measurement or estimation
can be overcome if we select an output feedback controller
(Antonelli & Astolfi, 1998a,b, 1999) able to regulate and
globally stabilise the reactor temperature at its set-point
without requiring any knowledge of the concentrations.
Interesting results in this direction have been obtained in
Alvarez-Ramirez and Femat (1999), Jadot (1996) and
with modelling error compensation is designed and its
ability to stabilise the temperature of a chemical reactor
is proved (Alvarez-Ramirez & Femat, 1999). Then, the
robust stabilisation of a class of CSTRs with unknown ki-
etics and control input saturations is achieved by means
of modelling error compensation techniques which consist
of interpreting the modelling error signal as a new state,
whose dynamics are observable from output measurements
(Jadot et al., 1999). Finally the stabilisation of chemical
reactors by output feedback with PI-type controllers has
been reviewed and treated in detail in Jadot (1996).

The objective of this work is to use Lyapunov-based meth-
ods to design nonlinear output feedback control laws for
the temperature stabilisation of a class of chemical reactors.
The proposed controllers yield robust stability and guaran-
teed performance also in the presence of input constraints
and uncertainty on the kinetic parameters. The paper is
organised as follows. Section 2 briefly discusses the main fea-
tures of chemical reactors and, in particular, focuses on the
dynamic model of non-isothermal CSTRs. Section 3 and
Section 4 are, respectively, concerned with the problem
statement, some preliminary assumptions and an introd-
utory lemma, which can be regarded as a novel simple tool
in the area of adaptive control. Section 5 contains the main
results of the paper, namely a set of structural stabilisability
properties for a class of CSTRs and a family of dynamic out-
put feedback control laws, delivering bounded control action
and yielding global asymptotic stability or local asymptotic
stability with an explicit estimate of the region of attraction.
In Section 6 the theoretical results are illustrated via the re-
action mechanism known as van der Vusse reaction. Finally
Section 7 provides some concluding remarks.

2. Dynamics of chemical reactors

Consider a reactor where a set of \( m > 0 \) independent
chemical reactions take place between \( n > 0 \) chemical species. An external jacket is used to remove or supply heat
to the system. In general, a reaction mechanism taking place
in a stirred tank can be expressed in the form (Hill, 1997)

\[
\sum_{j=1}^{n} v_{ji} A_j = 0 \quad i = 1, \ldots, m,
\]

where \( A_j \) denotes the \( j \)th chemical species and \( v_{ji} \) is its sto-
ichiometric coefficient in the \( i \)th reaction. The component
\( A_j \) is defined reactant of the reaction \( i \) if \( v_{ji} < 0 \) and prod-
uct of the reaction \( i \) if \( v_{ji} > 0 \). The information contained
in the reaction scheme (1) can be summarised into a matrix
\( C \), called the characteristic matrix, in which the elements
are the stoichiometric coefficients of reactants and products.
From a dynamic viewpoint, in chemical reactions, the ac-
tual reacted concentration of the generic component \( A_j \)
can be determined by evaluating the reaction rate, which may
have a different numerical value according to the way it is
defined and measured. In general, the reaction rate is a non-
linear function of the temperature \( T \), usually expressed in
Kelvin, and of the vector $x'$ of the concentrations of the reacting species. It expresses the rate of reactant consumption and product formation in the reactor. Usually the reaction rate is a non-negative, possibly time-varying, function. Just for simplicity, this work will consider the case where the reaction rate vector $r(x', T)$ depends only upon $x'$ and $T$ and is separable with respect to its arguments, i.e.

$$r(x', T) = \phi(x') k(T),$$

where the vector $k(T) \in \mathbb{R}^m$ is called rate constant of reaction and it is composed of positive bounded functions of the temperature, while $\phi(x') \in \mathbb{R}^{m \times m}$ is a diagonal matrix whose elements are functions of the vector $x'$ of the concentrations of the reactants. This is related to the vector $x$ of the $n$ concentrations of chemical species involved in the reaction network (reactants and products) by a projection operator, i.e.

$$x'_r = P_r x,$$

where $P_r$ is the operator that projects the concentrations of the reactants of the $i$th reaction into the vector $x'_r$, such that $x' = [x'_1, \ldots, x'_m] \in \mathbb{R}^m$. Moreover, note that the vector $k(T)$ is a continuous and a component wise strictly positive function for all $T > 0$ and that $\lim_{T \to 0} k(T) = 0$, in accordance with the thermodynamic principle that a chemical reaction cannot occur at absolute zero. In the common case when the process kinetics follow the Arrhenius law, the reaction rate vector can be expressed as (Dochain, 1994)

$$r(x', T) = \begin{bmatrix} k_{01} e^{-E_1/RT} \\ \vdots \\ k_{0m} e^{-E_m/RT} \end{bmatrix} \phi_1(x'_1), \ldots, \phi_m(x'_m)), \quad (4)$$

where $k_{0i}$, for $i = 1 \ldots m$, are the constant pre-exponential factors, $E_i$, for $i = 1 \ldots m$, are the activation energies and $R$ is the Joule constant. The functions $\phi_i(x'_i)$, for $i = 1 \ldots m$, are generally nonlinear functions of the concentrations of the reactants involved in the $i$th reaction, i.e. $\phi_i(x'_i) = \prod_{j \in r} \phi_j(x_j)$, $i = 1, \ldots, m$ where, in the presence of elementary reactions (Hill, 1997), $\phi_j(x_j) = x_j^v_j$, with $v_j \in \mathbb{N}$, represents the mass action law.

### 2.1. Continuous stirred tank reactors

A type of reactor widely used in industry is a well-stirred tank into which there is a continuous flow of reacting material and from which the reacted or partially reacted material passes continuously. This reactor is referred to as CSTR. Similarly to other research works in this area (see e.g. Jadot (1996), Kittisupakorn (1996)), in this paper some assumptions have been introduced in the attempt to reduce the model complexity. In particular, we will assume the following.

(Hp1) There is a complete uniformity of concentration and temperature within the reactor and a complete uniformity of temperature inside the jacket.

(Hp2) The reactor and jacket volumes are constant.

(Hp3) The reaction kinetics are $C^1$ functions.

(Hp4) The thermal exchange between the reactor and the jacket is expressed by a constant global heat exchange coefficient $U$ and the amount of heat retained in the reactor walls is negligible.

(Hp5) The reaction enthalpies $\Delta H_{Ri}$ are independent of temperature, positive for endothermic reactions and negative for exothermic reactions.

(Hp6) The heat capacities, $c_p_1$ and $c_p_2$, of the process fluids, i.e reactor content and heat transfer medium, are constant.

Under the above assumptions, the material and energy balances applied to the jacket reactor give the mathematical model (see Gibon-Fargeot, Hammouri, and Celle (1994) for further detail):

$$\dot{x} = Cr(x', T) + d(x^m - x),$$

$$\dot{T} = B(x', T) + q_1(T_j - T) + d(T^m - T),$$

$$\dot{T}_j = -q_2(T_j - T) + u,$$

where $x \in \mathbb{R}^n$ is the vector of the $n$ concentrations of reactants $r$ and products $p$; $x' \in \mathbb{R}^r$ is the vector of the $r$ concentrations of reactants; $C \in \mathbb{R}^{n \times n}$ is the characteristic matrix; $r(x', T) \in \mathbb{R}^m$ is the vector of reaction kinetics, expressed as in Eq. (2); $B(x', T) = H_r^T r(x', T) \in \mathbb{R}$, with $H_r^T = \begin{bmatrix} (\Delta H_{R1})_{p \rightarrow p_1} & \ldots & (\Delta H_{Rm})_{p \rightarrow p_1} \\ \vdots & \ddots & \vdots \\ (\Delta H_{R1})_{p \rightarrow p_m} & \ldots & (\Delta H_{Rm})_{p \rightarrow p_m} \end{bmatrix} \in \mathbb{R}^{m \times m}$ the vector of reaction enthalpies, is the global reaction heat; $T \in \mathbb{R}_+$ is the reactor temperature; $d \in \mathbb{R}_+$ is the dilution rate, that is the ratio between the feed stream flow rate and the volume of the reactor; $x^m \in \mathbb{R}^n$ is the vector of non-negative reactor feed concentrations; $q_1 \in \mathbb{R}_+$ is the side reactor heat transfer parameter; $q_2 \in \mathbb{R}_+$ is the side jacket heat transfer parameter; $T_j \in \mathbb{R}_+$ is the jacket temperature; $T^m \in \mathbb{R}_+$ is the reactor feed temperature; $T^m \in \mathbb{R}_+$ is the jacket fluid stream feed temperature; $u \in \mathbb{R}$ is the manipulated heat.

Let $x_{ss} \in \mathbb{R}^n$, $T_{ss} \in \mathbb{R}$, $T_{ss}^m \in \mathbb{R}$, $u_{ss} \in \mathbb{R}$ be steady state values of the state and input variables, respectively, and define, as in Alvarez-Ramirez and Femat (1999), the deviation variables

$$\psi = x - x_{ss}, \quad \zeta = T - T_{ss}, \quad \eta = T_j - T_{ss}^m,$$

$$\delta u = u - u_{ss}.$$ (6)

Let

$$\psi_r = P_r \psi, \quad \psi_r' = P_r \psi_r,$$ (7)

1 By assumption (Hp5), the components $b_i$ of the vector of reaction enthalpies $H_r^T$ are negative for endothermic reactions and positive for exothermic reactions. The constant $\rho$ is the reactor content density.
where $P_f$ is as in (3), and $(\psi')^T = [\psi_1', \ldots, \psi_m'] \in \mathbb{R}^m$, then system (5) can be rewritten as

$$
\dot{\psi} = C\hat{r}(\psi', \zeta) + d(\psi - \psi),
$$

$$
\dot{\zeta} = -(q_1 + d)\zeta + q_1 \eta + B(\psi', \zeta),
$$

$$
\hat{\eta} = q_2 \zeta - q_2 \eta + B_0 \eta + \delta u,
$$

where $\beta(T_{ss}, T_{in}) = q_1(T_{in} - T_{ss}) + d(T_{in} - T_{ss})$, $\hat{r}(\psi', \zeta) = r(\psi + x_{ss} \zeta + T_{ss})$, $\psi = x_{in} - x_{ss} \in \mathbb{R}^n$ and the reaction heat $B(\psi', \zeta) = B(\psi' + x_{ss} \zeta + T_{ss})$ can be expressed as

$$
\hat{\eta} = B_0 + B_1 \psi' + B_2 \zeta.
$$

In particular, if the kinetics follow the **Arrhenius law**, one has

$$
B_0 = B_0(x_{ss}, T_{ss}) = H(T)^T = \begin{bmatrix}
\varphi_1(x_{ss}^T k_0) \exp(-E_1/R T_{ss}) \\
\vdots \\
\varphi_m(x_{ss}^T k_0) \exp(-E_m/R T_{ss})
\end{bmatrix},
$$

$$
B_1 = B_1(x', T) = H(T)^T = \begin{bmatrix}
B_{11} & 0 & \ldots & 0 \\
0 & B_{12} & \ldots & \vdots \\
\vdots & \vdots & \ldots & 0 \\
0 & 0 & \ldots & B_{1m}
\end{bmatrix}
$$

with

$$
B_{1i} = B_{1i}(x_i', T) = \left(\frac{\varphi_i(x_i') - \varphi_i(x_{ss})}{x_i - x_{ss}^T}\right) k_0 e^{-E_i/R T_{ss}}
$$

and

$$
B_2 = B_2(x_{ss}, T) = H(T)^T = \begin{bmatrix}
\varphi_1(x_{ss}^T k_0) \exp(-E_1/R T_{ss}) \\
\vdots \\
\varphi_m(x_{ss}^T k_0) \exp(-E_m/R T_{ss})
\end{bmatrix}.
$$

The functions $\varphi_i(x_i')$ are the components of the diagonal matrix $\varphi(x')$ as in the reaction rate (2). It must be noted that, by definition of deviation coordinates, the system (8) takes the simplified form

$$
\dot{\psi} = C\hat{r}(\psi', \zeta) + d(\psi - \psi),
$$

$$
\dot{\zeta} = -(q_1 + d)\zeta + q_1 \eta + B_1 \psi' + B_2 \zeta,
$$

$$
\hat{\eta} = q_2 \zeta - q_2 \eta + \delta u.
$$

3. **Main assumptions and problem statement**

Together with Assumptions (Hp1)–(Hp6), which are used to derive the mathematical description (5), further assumptions are now introduced to describe the dynamic behaviour of the system in particular operating conditions, to characterise the heat exchange of the reaction and to define the control bounds and the location of the measurement devices. A detailed analysis of the dynamic properties of system (5) may be found e.g. in Jadot (1996), Jadot et al. (1999), Viel et al. (1997a, b).

**Assumption 1.** For any initial value $x(0) \in \mathbb{R}^n$, $x(t) \in \mathbb{R}^n$ for all $t \geq 0$.

This assumption expresses the **non-negativity property** of the concentration variables.

**Assumption 2.** For the isothermal condition, $T = T_{ss}$, the system

$$
\dot{x} = Cr(x', T) + d(x_{in} - x)
$$

has a single equilibrium point $x = x_{ss}$, which is **globally exponentially stable**.

This assumption states that the concentrations of the $n$ components of the reaction mixture reach their steady state values when the temperature is at its steady state value. Several industrial chemical reaction processes verify this assumption. The dynamics (15) can also be interpreted as the **isothermal dynamics** of the reactor (5). Moreover, by Lyapunov converse theorems (Khalil, 1996), Assumption 2 may be reformulated as follows.

There exist a positive definite and radially unbounded function $W(\psi)$ and positive constants $a_0$, $a_1$, $a_2$ and $a_3$ such that $a_0 \|\psi\|^2 \leq W(\psi) \leq a_1 \|\psi\|^2$.

$$
\dot{W} \leq -a_2 \|\psi\|^2 \leq 0,
$$

$$
\|\frac{\partial W}{\partial x}\| \leq a_3 \|\psi\|.
$$

**Assumption 3.** The functions $k_i(T) \in \mathbb{R}^m$ satisfy the Lipschitz condition at $T = T_{ss}$, i.e. there exists a positive number $M$ such that, for all $T$,

$$
\|Cr(x', T) - Cr(x', T_{ss})\| \leq M|T - T_{ss}|.
$$

**Assumption 4.** The variables available for feedback are the dilution rate $d$, and the temperatures $T$, $T_j$ and $T_{in}$.

In what follows, system (5) and Assumptions 1–4 are considered. The objective consists in finding, if possible, a static control law, described by equations of the form

$$
w = w(y),
$$
where \( w^T = [u, d, T^{in}] \) and \( v^T = [T, T_s, T^{in}, d] \), or a dynamics control law with state \( \theta \), described by equations of the form
\[
\dot{\theta} = \Theta(\theta, v) \quad w = w(\theta, v)
\]
(20)
such that the closed loop system (5)–(19) or (5)–(20) is globally asymptotically stable or locally asymptotically stable with a computable bound on the region of attraction. Moreover, the manipulated variables \( w^T = [u, d, T^{in}] \) take value inside a compact set \( \mathcal{D} \subset \mathbb{R}^3 \) which depends on the specific application.

4. A preliminary result

This section provides a simple result, which is instrumental in proving the main results of this work.

Lemma 1. Consider the system
\[
\dot{z} = f(z) + g(z)u
\]
(21)
with state \( z \in \mathbb{R}^n \) and control \( u \in \mathbb{R} \). Suppose that there exist an unknown constant control \( u = u_{sa} \) and a positive definite and radially unbounded function \( V(z) \) such that
\[
\dot{V}(z) = \frac{\partial V}{\partial z} f(z) + \frac{\partial V}{\partial z} g(z)u_{sa} < 0
\]
(22)
for all nonzero \( z \). Then for any \( u \) and \( \tilde{u} \) such that \( u < u_{sa} < \tilde{u} \), there exists a dynamic control law, which does not require knowledge of \( u_{sa} \), namely
\[
\dot{\theta} = \Theta(z, \theta) \quad u = \theta
\]
(23)
with \( \theta(0) \in (\tilde{u}, u) \), such that the closed loop system (21)–(23) is stable in the sense of Lyapunov, the variable \( z \) converges to zero and, along the trajectories of the closed loop system, \( \theta(t) = u(t) \in (\tilde{u}, u) \).

Proof. Consider the function
\[
V(z) + \omega(\theta),
\]
(24)
where
\[
\omega(\theta) = \ln((\tilde{u} - \theta)^{\tau k}) - \ln((\theta - u)^{(\tau + 1)k})
\]
(25)
with \( k > 0, \tau = (u_{sa} - \tilde{u})/(\tilde{u} - u) < 0 \) and \( \tau + 1 > 0 \). Note that \( V(z) + \omega(\theta) \) is positive definite and radially unbounded in \( \Omega_{\theta} = \{(z, \theta) \in \mathbb{R}^{n+1} | u < \theta < \tilde{u}\} \), i.e. \( \lim_{(z, \theta) \to \partial \Omega_{\theta}} V(z) + \omega(\theta) = +\infty \). Setting \( \dot{\theta} = (\partial V/\partial z) g(z) \sigma(\theta) \), with
\[
\sigma(\theta) = k(\theta - \tilde{u})(\theta - u)
\]
(26)
and noting that \( \theta - u_{sa} + (\tilde{u} \omega/\partial \theta) \sigma(\theta) = 0 \), yields
\[
\dot{V}(z) + \dot{\omega}(\theta) = (\partial V/\partial z)[f(z) + g(z)u_{sa}] < 0
\]
(27)
for all nonzero \( z \). As a result the closed loop system
\[
\dot{z} = f(z) + g(z)\theta \quad \dot{\theta} = \frac{\partial V}{\partial z} g(z) \sigma(\theta)
\]
(28)
is locally stable and any trajectory starting in the set \( \Omega_{\theta} \) remains in \( \Omega_{\theta} \) for any \( t \geq 0 \) and it is such that \( z \) converges to zero and \( \theta(t) = u(t) \in (\tilde{u}, \tilde{u}) \) for all \( t \).

From Eq. (26) it is easy to show that, if \( v = (\partial V/\partial z) g(z) \) is the measurable variable, then the considered dynamic control law may be interpreted as the nonlinear PI controller
\[
u = \tilde{u} [u(0) - u] - [u(0) - \tilde{u}] \phi_{ui}(v),
\]
where \( \phi_{ui}(v) = \exp[k(\tilde{u} - u ) f(z)\sigma(\theta)] \) and \( u(0) \) is the value of the control input at the initial time.

Remark 1. The Lyapunov function (24) is positive definite and radially unbounded in the set \( \Omega_{\theta} \). Hence, no trajectory of the closed loop system (28) can be such that \( \sup_{t \in [0, \infty)} \theta(t) = \tilde{u} \), or \( \inf_{t \in [0, \infty)} \theta(t) = u \). Despite this theoretical result, in practical implementations, where numerical errors are relevant, it may be necessary to implement the proposed control law in the following form:
\[
\dot{\theta} = \begin{cases} 
\max \left(0, \frac{\partial V}{\partial z} g(z) \sigma(\theta) \right) & \text{if } \theta \in [u + \epsilon, \tilde{u} - \epsilon], \\
\min \left(0, \frac{\partial V}{\partial z} g(z) \sigma(\theta) \right) & \text{if } \theta \in [\tilde{u} - \epsilon, \tilde{u}], 
\end{cases}
\]
for some \( \epsilon > 0 \) and sufficiently small. This modification has been used in the experiments carried out in Escobar, Chevreau, Ortega, and Mendes (2002), where the adaptive control problem for a power system has been addressed, and in Antonelli, Harmand, Steyer, and Astolfi (2002), where the problem of robust control of a biochemical reactor has been studied. Moreover, the modification has been used also in the simulation results reported in Section 6.

Remark 2. The hypothesis that the system (21) in closed loop with the constant control \( u = u_{sa} \) is globally asymptotically stable can be experimentally verified and this kind of information is in general available in real applications, although the precise value of the constant stabilising \( u_{sa} \) is not known or might depend on the operating conditions.

5. Main results

In this section it is shown how the problem of asymptotic stabilisation for system (8), under suitable assumptions, can be solved using dynamic control laws which require only partial state information and provide a bounded control action. The result established in Lemma 1 will be instrumental in deriving the control laws. However, as already discussed,
the application of Lemma 1 requires the property that the system can be stabilised with constant control action. This property is closely related to the features of the temperature sub-system and, in particular, to the degree of exothermicity of the reaction taking place in the reactor. These are in turn related to the properties of the mappings $B_1$ and $B_2$ given in Eqs. (11) and (13). It must be noted that a CSTR can be controlled using different variables. To begin with, the heat supplied or removed from the jacket, $u$, is considered to be the manipulated variable and the jacket temperature $T_j$ is assumed to be the measured variable. Then, multivariable extensions, in which the manipulated variables are the pairs $(u, T_m)$ or $(u, d)$ and the measured variables are $(T, T_j, d)$, are considered. In all cases the control laws provide bounded control action and, in particular, the positivity constraints associated with some variables, e.g. the dilution rate $d$, will be satisfied for all time.

5.1. Stabilisation through control of the supplied or removed heat $u$

**Proposition 1.** Consider the CSTR described by equation (8) and suppose that Assumptions 1–4 hold. Consider the reaction heat $B(q, \zeta)$ expressed by Eq. (9) and suppose that the functions $B_1$ and $B_2$ defined in (11) and (13) are such that

$$B_2 + \frac{x_2 M}{\bar{x}_2} \tilde{Q} < d,$$  

where $\bar{B}_2 = \max_{T \in \mathbb{R}_+} B_2$, $M$ is as in (18), $d$ is the dilution rate, $\bar{x}_2$ and $x_2$ are as in (16) and (17), respectively, and $\tilde{Q} = \max_{T \in \mathbb{R}_+} ||P^\top B_1^\top||$ with $P^\top$ as in (7).

Then there exist a constant feedback law $u = u_{ss}$, (30) two real-valued functions, $W(q)$ and $V(\zeta, \eta)$, which are positive definite and proper, and a real positive constant $\lambda^*$ such that $W + \lambda^* V < 0$, for all $(q, \zeta, \eta) \neq (0, 0, 0)$. Therefore, the constant control (30) globally asymptotically stabilises the system (8) at the equilibrium point $(0, 0, 0)$.

**Remark 3.** Before presenting the proof of Proposition 1, it is convenient to briefly discuss condition (29). This condition implies that $B_2 < d$ which is always verified if the reaction network is globally endothermic (in fact, for endothermic reactions $B_2 < 0$ for all $T \in \mathbb{R}_+$). By a simple property of any projection operator, condition (29) can be simplified as $\max_{T \in \mathbb{R}_+} ||B_2^\top|| < (x_2/x_2 M)(d - \bar{B}_2)$. Moreover, $||B_1^\top||$ and $B_2$ are bounded functions of their arguments and this assumption can be satisfied if the dilution rate $d$ is sufficiently large, which is in agreement with common process industry experience. It is also worth noting that the functions $B_1$ and $B_2$ and the variables $M$, $x_2$ and $x_3$ can be, in practical applications, experimentally estimated.

**Proof of Proposition 1.** Let $W(q)$ be as in Assumption 2 and let $V(\zeta, \eta)$ be defined as

$$V(\zeta, \eta) = \frac{q_2}{2} \zeta^2 + \frac{q_1}{2} \eta^2.$$  

Then $\dot{W} \leq -x_2 ||\psi||^2 + x_3 ||\psi|| M ||\zeta||$, and, for $u = u_{ss}$,

$$\dot{V} = -q_2 (q_1 + d - B_2) \zeta^2 - q_1 q_2 \eta^2 + 2 q_1 q_2 \zeta \eta + q_2 B_1 \psi \zeta.$$

Suppose now that condition (29) is satisfied. Then for any $\lambda > 0$, and after simple manipulations, one has

$$\dot{W} + \lambda \dot{V} \leq -\frac{\sqrt{x_2}}{2} ||\psi|| - \frac{x_2 M}{\sqrt{2} x_2} ||\zeta||^2 - \frac{\sqrt{x_2}}{2} ||\psi|| - \frac{\lambda q_2 (B_1)^\top}{\sqrt{2} x_2} ||\zeta||^2 - \left( \sqrt{x_1 q_2 \eta} - \sqrt{\lambda q_1 q_2 \zeta} \right)^2 - \frac{\lambda q_2 (d - B_2)}{2 x_2} + \frac{\lambda^2 q_2 ||(P^\top)^\top B_1^\top||^2}{2 x_2} \zeta^2.$$

The first three terms of the last equation are non-positive for any non-zero value of the variables $q$, $\zeta$ and $\eta$, while the sign of the fourth term is unknown and depends on the choice of $\lambda$. However, this last term can be made negative if there exists a $\lambda > 0$ such that

$$q_2 ||(P^\top)^\top B_1^\top||^2 \lambda^2 - 2 q_2 x_2 (d - B_2) \lambda + x_2^2 M^2 < 0.$$  

Such a $\lambda$ indeed exists and it is given by

$$\lambda^* = \frac{x_2 (d - \bar{B}_2)}{2 q_2 \max_{T \in \mathbb{R}_+} ||(P^\top)^\top B_1^\top||^2} > 0.$$  

It is straightforward to conclude that the function $W(q) + \lambda^* V(\zeta, \eta)$ is a Lyapunov function for system (8) with $u = u_{ss}$, hence the equilibrium point $(0, 0, 0)$ of the closed loop system (8)–(30) is globally asymptotically stable. □

Proposition 1 can be combined with the result established in Lemma 1 as expressed in the following corollary, in which, instead of the constant control $u = u_{ss}$, a dynamic control law, which requires only knowledge of the jacket temperature and of its set-point value, is used.

**Corollary 1.** Consider the CSTR described in Eq. (8) and suppose that Assumptions 1–4 hold and that condition (29) is verified. Assume moreover that $u$ is the only manipulated variable, that $u \in (u, \bar{u})$ and that $u_{ss} \in (u, \bar{u})$. 

Then the initialized dynamic output feedback control law
\[ u = 0, \]
\[ \theta = k_0(\theta - \tilde{u})(\theta - y) \eta \]
with \( k_0 > 0 \), is such that the equilibrium \((0,0,0,u_{ss})\) of the closed loop system (8)–(35) is locally stable and, for any initial conditions \((\psi(0), \zeta(0), \eta(0), \theta(0))\) with \( \theta(0) \in (\tilde{u}, \tilde{u}) \), \((\psi(t), \zeta(t), \eta(t))\) converges asymptotically to \((0,0,0)\) and the control variable \( \theta(t) \in (u, \tilde{u}) \).

5.2 Stabilisation through control of the supplied or removed heat \( u \) and of the inlet stream temperature \( T^m \)

The stabilising control (35) has a very simple structure, however it requires that condition (29), concerning the level of exothermicity of the reaction network, is satisfied. This condition, which might be too restrictive, can be relaxed increasing the complexity of the control structure, i.e. introducing extra manipulated variables to compensate the physical limitations of the heat exchange when a highly exothermic reaction takes place.

For, consider system (5) and, in addition to the variables (6), introduce the new deviation variable \( \delta T^m = T^m - T_{ss} \in \mathbb{R} \), and regard \( T^m \) as a new manipulated variable. As a result, system (5) can be rewritten as
\[ \dot{\psi} = C\tilde{r}(\psi, \zeta) + d(\psi^m - \psi), \]
\[ \dot{\zeta} = -(q_1 + d)\zeta + q_1 \eta + dT^m + B_1 \psi' + B_2 \zeta, \]
\[ \dot{\eta} = -q_2 \eta + q_2 \zeta + bu, \] (36)
which is the starting point in deriving a multivariable version of Proposition 1.

**Proposition 2.** Consider the CSTR described by equations (36) and suppose that Assumptions 1–4 hold. Consider the reaction heat \( \tilde{B}(\psi', \zeta) \), defined in (9), and suppose that for a given \( k_{in} \geq 0 \),
\[ \tilde{B}_2 + \frac{x_3 M}{x_2} \tilde{Q} < d + k_{in}d, \] (37)
where \( B_2 \) is as in (13), \( \tilde{B}_2 = \max_{\psi, t \in \mathbb{R}} \tilde{B}_2 \), \( M \) is as in (18), \( d \) is the dilution rate, \( x_2 \) and \( x_3 \) are as in (16) and (17), respectively, and \( \tilde{Q} = \max_{\psi, t \in \mathbb{R}} \|(P')^T B_1^T\| \), with \( B_1 \) as in (11).

Then there exist two positive constants \( u_{ss} \) and \( T_{ss} \) such that the equilibrium \((0,0,0,0)\) of the system (36) in closed loop with the feedback law
\[ u = u_{ss}, \]
\[ T^m = T_{ss} - k_{in}(T - T_{ss}) \]
(38)
is globally asymptotically stable. Moreover, if
\[ 0 \leq k_{in} \leq T_{ss} \frac{x_3}{x_2} M \frac{q_2}{q_1 + q_2} \] (39)
with \( \tilde{V} = \max ||\psi|| \), then all trajectories of the closed loop system (36)–(38) such that \( T(0) \) and \( T(0) \) are in the set
\[ \mathcal{M} = \left\{ (T, T_j) \mid (T - T_{ss})^2 + \frac{q_1}{q_2} (T_j - T_{ss})^2 \leq \left( \frac{T_{in}}{k_{in}} \right)^2 \right\} \]
remain in the set \( \mathcal{M} \), and are such that \( T^m = T_{ss} - k_{in}(T - T_{ss}) \) is non-negative for all \( t \geq 0 \).

**Proof.** We break up the proof in two steps.

**Step 1:** Global asymptotic stability. Consider the positive definite and radially unbounded function \( W(\psi) + \lambda V(\zeta, \eta) \) where \( W(\psi) \) and \( V(\zeta, \eta) \) are as in the proof of Proposition 1 and \( \lambda \) is a positive constant to be determined. Then, along the trajectories of the closed loop system (36)–(38) one has, after simple manipulations,
\[ \dot{W} + \lambda \dot{V} \leq - \left[ \frac{x_2}{2} ||\psi||^2 - \frac{x_3 M}{x_2} ||\zeta||^2 \right] \]
\[ \leq - \left[ \frac{x_2}{2} \psi - \lambda q_2 (B_1 P')^T \right] \]
\[ \leq - \left[ \lambda q_2 (d + k_{in}d - B_2) - \frac{x_3 M^2}{2x_2} \right] \]
\[ \leq \frac{x_2}{2} q_2^2 ||(P')^T B_1^T||^2 \] (38)
Applying arguments similar to those used in the proof of Proposition 1, it is easy to conclude that there exists a positive constant \( \lambda^* \) such that \( \dot{W} + \lambda^* V < 0 \), for all \( (\psi, \zeta, \eta) \neq (0,0,0) \), hence the claim.

**Step 2:** Invariance of the set \( \mathcal{M} \). Note that the control \( T^m \) defined in (38) is non-negative for all \( T \leq T_{ss} + T_{in}/k_{in} \). Hence, a simple calculation shows that it is non-negative within the set \( \mathcal{M} \). Therefore, to establish the claim, it must be proved that the set \( \mathcal{M} \) is positively invariant. To this end, consider the function \( V \) in Step 1, and note that
\[ V \leq -q_1 q_2 ((T - T_{ss}) - (T_j - T_{ss}))^2 \]
\[ -q_2 (d + k_{in}d - B_2)(T - T_{ss})^2 \]
\[ + q_2 (T - T_{ss})^2 \] (39)
If \( k_{in} \) satisfies condition (39) then, as detailed in Antonelli (2001), the function \( V \) is positive semidefinite in a compact set properly contained in \( \mathcal{M} \), and negative elsewhere. Hence the claim. □

The control law (38) cannot be implemented because it requires knowledge of the steady state variables \( u_{ss} \) and \( T_{ss} \). However, as already discussed, this problem can be easily overcome, as stated in the following corollary.
Corollary 2. Consider the CSTR described in (36) and suppose that Assumptions 1–4 hold. Suppose that condition (37) is satisfied. Assume that \( u \) and \( T^m \) are the manipulated variables, that \( u \in (u_0, \bar{u}) \) and \( T^m \in (T^m_0, \bar{T}^m) \), and that \( u_0 \in (u_0, \bar{u}) \) and \( T^m_0 \in (T^m_0, \bar{T}^m) \).

Then the initialized dynamic output feedback control law \( u = 0 \),
\[
\dot{\theta} = k_0(\theta - u)(\theta - \bar{u})\eta,
\]
\[
\dot{T}^m = \gamma - k_m(T - T_{ss}),
\]
\[
\dot{\gamma} = k_r(\gamma - \bar{T}^m)(\gamma - \bar{T}^m)\zeta
\]
\[\text{with } k_0 > 0, k_m \geq 0 \text{ and } k_r > 0, \text{ is such that the equilibrium point } (0, 0, 0, u_0, T^m_0) \text{ of the closed loop (36)–(41) is locally stable and, for any initial conditions } \theta(0), \zeta(0), \eta(0), \bar{T}(0), \gamma(0) \text{ with } \theta(0) \in (u_0, \bar{u}) \text{ and } \gamma(0) \in (T^m_0, \bar{T}^m), \text{ the system converges asymptotically to } (0, 0, 0) \text{ and the control variables are such that } \theta(t) \in (u_0, \bar{u}) \text{ and } \gamma(t) \in (T^m_0, \bar{T}^m).\]

Moreover, if condition (39) holds then every trajectory of the closed loop system starting in \( \mathcal{H} \) remains in \( \mathcal{H} \) and \( T^m \geq 0 \) for all \( t > 0 \).

5.3. Stabilisation through control of the supplied or removed heat \( u \) and of the dilution rate \( d \)

Consider now the reactor system described by (5), let the dilution rate, \( d \), be a new control input, which is acting together with the manipulated transferred heat \( u \), and introduce the new deviation variable \( \delta d = d - d_{ss} \in \mathbb{R} \). As a result, the system (5) becomes
\[
\dot{\psi} = C\dot{\zeta}(\psi', \zeta) + d(\psi - \psi),
\]
\[
\dot{\zeta} = -(q_1 + d_{ss} + \delta d - B_2)\zeta
\]
\[
+ q_1\eta + \delta d(T^m - T_{ss}) + B_1P^s\psi,
\]
\[
\dot{\eta} = -q_2\eta + q_2\zeta + \delta u.
\]
\[\text{In the following proposition it is shown how this system can be stabilised at the desired equilibrium and how condition (29) is modified by the introduction of a further control input, namely the dilution rate } d.\]

Proposition 3. Consider the CSTR described in (42) and suppose that Assumptions 1–4 hold. Consider the reaction heat \( \tilde{B}(\psi', \zeta) \) as in (9). Suppose that\(^3\)
\[
B_2(T^m) + \frac{\alpha_3 M}{\bar{z}^2} \Omega_{\text{in}}^m \leq d_{ss},
\]
\[\text{where } B_2(T^m) \text{ is as in (13) with } T = T^m, d \text{ is the dilution rate, } x_2 \text{ as in (16), } x_3 \text{ as in (17), } M \text{ as in (18), } \Omega_{\text{in}}^m = \max_{\forall \psi} \left\| (P^s)^T B_1(T^m) \right\| \text{ and } B_1(T^m) \text{ is as in (11) with } T = T^m. \text{ Then there exist a feedback control law}
\]
\[
u = u_{ss},
\]
\[
d = d_{ss} + k_d \left[ \text{sat}(T - T_{ss})\text{sat}(T - T^m) \right]
\]
\[\text{with } k_d = \min(d_{ss} - \bar{d}, \bar{d} - d_{ss}) \text{ and sat a saturation function, two real-valued functions, } W(\psi) \text{ and } V(\zeta, \eta), \text{ which are positive definite and proper, and a real constant } \lambda^* \text{ such that } W + \lambda^* V < 0, \text{ for all } (\psi, \zeta, \eta) \neq (0, 0, 0). \text{ Therefore, the control law (44) globally asymptotically stabilises the system (42) at the equilibrium point } (0, 0, 0).\]

Proof. The proof is similar to the proof of Proposition 1. See also Antonelli (2001) for details.

Obviously, even in this case, the control law (44) can be modified to avoid the use of the steady state variables \( u_{ss} \) and \( d_{ss} \).

Corollary 3. Consider the CSTR described in (36), suppose that Assumptions 1–4 hold and that condition (43) is verified. Assume moreover that \( u \) and \( d \) are the manipulated variables, that \( u \in (u_0, \bar{u}) \) and \( d \in (\bar{d}, \tilde{d}) \), and that \( u_{ss} \in (u_0, \bar{u}) \) and \( d_{ss} \in (\bar{d}, \tilde{d}) \).

Then the initialized dynamic output feedback control law
\[
\dot{\theta} = k_0(\theta - u)(\theta - \bar{u})\eta,
\]
\[
d = v + k_0[\text{sat}(T - T_{ss})\text{sat}(T - T^m)],
\]
\[
\dot{\psi} = v + k_0(T^m - T_{ss})(\psi - \bar{d})\zeta
\]
\[\text{with } k_0 > 0, k_d > 0 \text{ and } k_v > 0, \text{ is such that the equilibrium } (0, 0, 0, u_{ss}, d_{ss}) \text{ of the closed loop system (42)–(45) is locally stable and, for any initial conditions } \psi(0), \zeta(0), \eta(0), \bar{T}(0), \gamma(0) \text{ with } \theta(0) \in (u_0, \bar{u}) \text{ and } \gamma(0) \in (T^m_0, \bar{T}^m), \text{ the system converges asymptotically to } (0, 0, 0) \text{ and the control variables are such that } \theta(t) \in (u_0, \bar{u}) \text{ and } \gamma(t) \in (T^m_0, \bar{T}^m).\]

6. Case study: the van der Vusse reaction

Consider the complex reaction mechanism, known as the van der Vusse reaction, as described in Chen, Kremling, and Allgower (1995), see also Antonelli (2001) for further detail. The main reaction is the transformation of cyclopentadiene (component \( A \)) to the product cyclopentanol (component \( B \)). A parallel reaction takes place producing the by-product dicyclopentadiene (component \( D \)). Furthermore, cyclopentenol reacts again giving the undesired product cyclopentandiol (component \( C \)). All these reactions

\[\text{Condition (43) differs from condition (29), as it imposes a constraint on the exothermicity of the reaction only for } T = T^m \text{ and not for all temperatures } T.\]
Fig. 1. Reactor temperature $T$ (top-left), jacket temperature $T_j$ (top-right), control signals (bottom-left) and concentration $x_B$ of the product B for the van der Vusse reaction described in (46) with the control laws (35) (solid line), (41) (dashed line) and (45) (dotted line), respectively.

The reaction rates $k_i$ are functions of the reactor temperature $T$ and follow the Arrhenius law. It is worth pointing out that, whatever the initial conditions of the system are, the concentration trajectories obtained in isothermal condition, i.e. $T = T_{ss}$, for the system

\[
\begin{align*}
\dot{x}_A &= \frac{\dot{V}}{V_R}(x_{A}^m - x_A) - k_1(T)x_A - k_{in}(T)x_A^2, \\
\dot{x}_B &= -\frac{\dot{V}}{V_R}x_B + k_1(T)x_A - k_2(T)x_B, \\
\dot{T} &= \frac{\dot{V}}{V_R}(T_{in} - T) + \frac{k_w A_R}{\rho C_p V_R} (T_j - T) \\
&\quad - \frac{k_1(T)x_A \Delta H_{AB} + k_2(T)x_B \Delta H_{BC} + k_{in}(T)x_A^2 \Delta H_{AD}}{\rho C_p}, \\
\dot{T}_j &= \frac{1}{m_K C_p}[u + k_w A_R(T - T_j)].
\end{align*}
\]

(46)

As usual, the control input $u$ is the heat removal while the additional control variables are the reactor feed temperature $T_{in}$ and the dilution rate $d = \dot{V}/V_R$ expressed as the flowrate normalised by the reactor volume. These manipulated variables are constrained by $-150 \text{kJ/min} \leq u \leq 0 \text{kJ/min}$, $95^\circ \text{C} \leq T_{in} \leq 130^\circ \text{C}$, and $0.05 \text{min}^{-1} \leq d \leq 0.53 \text{min}^{-1}$.

The reaction rates $k_i$ are functions of the reactor temperature $T$ and follow the Arrhenius law. It is worth pointing out that, whatever the initial conditions of the system are, the concentration trajectories obtained in isothermal condition, i.e. $T = T_{ss}$, for the system

\[
\begin{align*}
\dot{x}_A &= \frac{\dot{V}}{V_R}(x_{A}^m - x_A) - k_1(T_{ss})x_A - k_{in}(T_{ss})x_A^2, \\
\dot{x}_B &= -\frac{\dot{V}}{V_R}x_B + k_1(T_{ss})x_A - k_2(T_{ss})x_B
\end{align*}
\]

(47)

converge all to the same equilibrium point $x_{ss} = (x_{A_{ss}}, x_{B_{ss}})$. Hence, the stability properties of this system can be studied by applying the control design proposed in Section 5. The results shown in Fig. 1 are obtained when the dynamic output feedback control laws (35), (41) and (45) are implemented. Because of the high rate of heat production by the reaction, the performance of the multivariable controllers (41) and (45) are better than the performance of the single input controller (35). In fact, for the single input controller, the
cooling rate goes to its lower bound for a longer period of time during which $T$ and $T_i$ cannot be controlled. These simulation results clearly demonstrate the improvement that can be obtained by using additional control variables.

7. Conclusions

This work has considered the output feedback regulation of endothermic and exothermic chemical reactors. In particular, the problem of global temperature control for a general class of chemical reactors has been addressed and solved using Lyapunov techniques. A nonlinear reactor model has been used to synthesize output feedback control laws, i.e. feedback control laws which generate the control signals on the basis of the available measurements only. Under reasonable and easy to test assumptions, global temperature control has been achieved in presence of control bounds. The proposed approach offers some important advantages including constraint handling capability and computational simplicity: the only conditions to be fulfilled are simple and natural feasibility conditions, namely that the steady state control signals are admissible. The result is that the difficulty in the measurement or in the estimation of some state variables has been overcome given that all proposed controllers are based on partial state measurements. Finally some numerical simulations, illustrating the theoretical results, are presented.

References


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