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Successful bounded control for a chemical reactor with non-linear oscillatory consecutive reactions

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Abstract

The closed-loop dynamic behavior of a chemical reactor with two consecutive and oscillatory exothermic reactions is analyzed. When bounds are imposed on the control input, equilibrium points induced by saturation (EPIS) are generated. In this case, the reactor dynamic trajectories are deviated towards the EPIS and their convergence to the set-point is no longer guaranteed. By means of bifurcation analysis, necessary and sufficient conditions are derived to obtain quasi-optimal regulatory control and to avoid the presence of EPIS. Simulation studies proved the advantages of implementing these conditions, giving smooth responses with no oscillation.

Keywords: Process control; Chemical reactors; Mathematical model; Dynamic simulation

1. Introduction

The dynamic behavior of chemical reactors with two consecutive exothermic reactions is highly non-linear, particularly in the case of chemical reactors that present steady-state multiplicity, periodic or chaotic response to perturbations, as shown by Bilous and Amundson [1], Hlavâcek et al. [2], Pikios and Luss [3], Balakotaiah and Luss [4], Jorgensen and Aris [5], and Gray and Scott [6]. For the chemical industries, it is important to control reactors with this type of behavior, over a wide range of operating conditions and in the presence of strong perturbations, in order to achieve successfully high levels of safety and efficiency. Commonly, the industrial control systems are linear in nature; unfortunately, these control schemes are only valid in a small region of the state space around a nominal point. When high productivity and tight quality are demanded for the processes, it is necessary to apply non-linear control algorithms that perform well for a wide range of operating conditions. In addition, most of the actuators have physical bounds to their operation.

In this work, we addressed the non-linear control problem for a chemical reactor, subject to constraints on its control input, in which two consecutive exothermic reactions with oscillatory behavior take place. First, the derivation of the open-loop reactor model is presented, after which the basis for the proposed bounded control strategy is discussed. By means of an exact linear transformation, a non-linear single input–single output control algorithm is developed, which is globally and asymptotically stable and with no saturation. When bounds are imposed to control input, we detected the generation of equilibrium points induced by saturation (EPIS). In this case, the reactor dynamic trajectories are deviated towards the EPIS and their convergence to the set-point is no longer guaranteed. With the help of a bifurcation map of the reactor model, the system's response is forced to behave according to the desired equilibrium state; to avoid the EPIS, necessary and sufficient conditions are derived and proved via numerical simulations.

2. The open-loop reactor

The chemical reactor has been studied previously [5,6]. The reactor temperature is regulated by means of water flowing through a cooling jacket. A stream with a reactant (A) enters into a well-stirred continuous flow reactor, and is converted to an intermediate (B) and to a final product (C). We have

$$A \rightarrow B,\ \text{rate}_1 = k_1(T)a \tag{1}$$

$$B \rightarrow C,\ \text{rate}_2 = k_2(T)b \tag{2}$$

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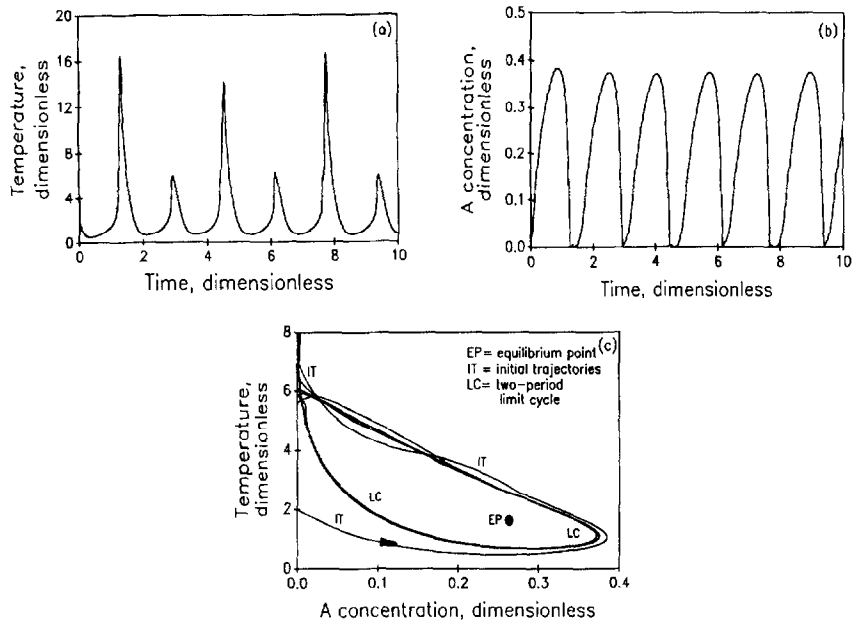

Fig. 1. (a) Temperature, (b) reactant A concentration evolution and (c) phase plane of the open-loop reactor with initial conditions $\alpha=0.0$, $\beta=0.0$, $\theta=2.0$.

Both steps are first-order processes: exothermic and with rate constants of Arrhenius temperature dependence. Thus, we have

$$k_i = A_i \exp\left(-\frac{E_i}{RT}\right) \tag{3}$$

Energy and mass balances give the following governing equations:

$$\frac{da}{dt} = \left(\frac{1}{t_{res}}\right)(a_0 - a) - k_1 a \tag{4}$$

$$\frac{db}{dt} = \left(\frac{1}{t_{res}}\right)(b_0 - b) + k_1 a - k_2 b \tag{5}$$

$$C_p\rho\frac{dT}{dt} = \left(\frac{1}{t_{res}}\right)C_p\rho(T - T_0) + (-\Delta H_1)k_1 a + (-\Delta H_2)k_2 b - \left(\frac{1}{V}\right)UA_c(T - T_c) \tag{6}$$

The conditions imposed on the reactor model are as follows: (a) there is no inflow of B or C, i.e. $b_0 = c_0 = 0$; (b) both reactions have the same activation energy, i.e. $E_1 = E_2$; (c) both reactions have the same heats of reaction, i.e. $\Delta H_1 = \Delta H_2$; and (d) the inflow temperature is the same as that of the cooling jacket water, i.e. $T_0 = T_c$.

Using the mean residence time and the reactant A inflow concentration as the time and concentrations scales, we obtain

$$\frac{d\alpha}{d\tau} = 1 - \alpha - \left(\frac{1}{\tau_{ch}}\right)\alpha \exp(\theta) \tag{7}$$

$$\frac{d\beta}{d\tau} = \left(\frac{1}{\tau_{ch}}\right)\alpha \exp(\theta) - \left(\frac{1}{\tau_{ch}}\right)\phi\beta \exp(\theta) - \beta \tag{8}$$

$$\frac{d\theta}{d\tau} = \left(\frac{1}{\tau_{ch}}\right)\theta_j\alpha \exp(\theta) + \left(\frac{1}{\tau_{ch}}\right)\theta_j\phi\beta \exp(\theta) - (1 + \tau_N^{-1})\theta \tag{9}$$

in which the dimensionless concentrations and temperature are given by

$$\alpha = a/a_0,\ \beta = b/a_0,$$

$$\theta = E_1(T - T_c)/RT_c^2,\ \tau = t/t_{res} \tag{10}$$

Parameters such as the chemical time, the reaction rate ratio, the dimensionless temperature of the cooling jacket water and the Newtonian cooling time are respectively given by

$$\tau_{ch} = 1/k_1 t_{res},\ \phi = A_2/A_1,$$

$$\theta_j = (-\Delta H_1)a_0 E_1/C_p\rho RT_c^2 \tag{11}$$

$$\tau_N = t_N/t_{res} = C_p\rho V/UA_c t_{res} \tag{12}$$

The dynamic behavior of the autonomous reactor is highly complex for the following parameter values: $\tau_{ch} = 1.81$, $\theta_j = 17.5$, $\phi = 0.01$ and $\tau_N = 0.14$. In this case, the reactor has one unstable equilibrium point, $e_p = (\alpha_e = 0.2634, \beta_e = 0.7166, \theta_e = 1.6261)$. The instability of this equilibrium point stems from the values of the Jacobian eigenvalues: $\lambda = (-1.0299,\ 0.3227 + 4.3534i,\ 0.3227 - 4.3534i)$, producing chaotic behavior or limit cycles with one, two, four or eight periods [6]. Fig. 1(a) and 1(b) show the open-loop dynamic behavior of the reactor for the parameter values mentioned above. In Fig. 1(a), we can see a two-period oscillatory behavior of the dimensionless temperature. Fig. 1(c) shows the phase plane of the autonomous reactor. Here, we see the two-period limit cycle and the equilibrium point position. Reactors with this type of behavior make the application of a linear control scheme a difficult task.

3. The closed-loop reactor without saturation

To develop the control law, the reactor temperature is selected as the controlled variable and the temperature of the

cooling water is taken as the manipulated variable. This choice of the manipulated variable is made to simplify the control problem, because a simple relation between the volumetric flow and temperature of the cooling water exists, by means of a heat balance, in the cooling jacket [7].

Using the standard notation for dynamical systems, the reactor mathematical model can be expressed as

$$\begin{bmatrix}\dot{x}_1\\ \dot{x}_2\\ \dot{x}_3\end{bmatrix}=\begin{bmatrix}f_1(x)\\ f_2(x)\\ f_3(x)\end{bmatrix}+\begin{bmatrix}g_1(x)\\ g_2(x)\\ g_3(x)\end{bmatrix}\begin{bmatrix}u_1\\ u_2\\ u_3\end{bmatrix}^T \tag{13}$$

where

$$[x_1\ x_2\ x_3]=[\alpha\ \beta\ \theta] \tag{14}$$

$$\begin{bmatrix}f_1(x)\\ f_2(x)\\ f_3(x)\end{bmatrix}=\begin{bmatrix}1-\alpha-[\alpha\exp(\theta)]/\tau_{ch}\\ [\alpha\exp(\theta)](1-\beta)/\tau_{ch}-\beta\\ -(1+\tau_N^{-1})\theta\end{bmatrix} \tag{15}$$

$$\begin{bmatrix}g_1(x)\\ g_2(x)\\ g_3(x)\end{bmatrix}=\begin{bmatrix}0\\ 0\\ \exp(\theta)(\alpha+\phi\beta)/\tau_{ch}\end{bmatrix} \tag{16}$$

and

$$[u_1\ u_2\ u_3]=[0\ 0\ \theta_j] \tag{17}$$

The output error can be defined as

$$\epsilon(t)=\theta(t)-\theta_{sp} \tag{18}$$

where the temperature set-point is chosen as the open-loop equilibrium temperature, i.e. $\theta_{sp}=\theta_e=1.6261$. If an integral control action is desired, then one can impose on the error the behavior that

$$\dot{\epsilon}+K\epsilon=0 \tag{19}$$

and it is guaranteed that

$$\lim_{t\to\infty}\epsilon(t)=0,\quad \lim_{t\to\infty}\theta(t)=\theta_{sp} \tag{20}$$

whenever the control gain **K** is greater than zero.

From Eqs. (13)–(19), the following control law is obtained:

$$u_3(x)=\left[\frac{1}{g_3(x)}\right][-K\epsilon-f_3(x)] \tag{21}$$

The reactor will be controllable under the control law given by Eq. (21) if $g_3(x)\neq 0$; as we can see in Eq. (16), this is satisfied, because all the parameters of the system are greater than zero.

The control law derived will affect only θ (or x_3); the dynamics of α (or x_1) and β (or x_2) then constitute the internal dynamics of the system [8]. To ensure the stability of the closed-loop system, the internal dynamics must also be stable. Given that the control law regulates only the behavior of θ, analysis of the internal dynamics is limited to the behaviors of α and β while θ is kept constant; therefore, Eq. (13) is reduced to the pair of equations

$$\dot{x}_1^*=1-(1+C_1)x_1^* \tag{22}$$

$$\dot{x}_2^*=C_1x_1^*-(1+C_2)x_2^* \tag{23}$$

where

$$C_1=[\exp(\theta_{sp})]/\tau_{ch},\quad C_2=[\phi\exp(\theta_{sp})]/\tau_{ch} \tag{24}$$

Solving Eqs. (22) and (23) gives

$$x_1^*=\left[x_{10}^*-\left(\frac{1}{1+C_1}\right)\right]\exp[-(1+C_1)\tau]+\left(\frac{1}{1+C_1}\right) \tag{25}$$

$$x_2^*=[x_{20}^*-(C_3+C_4)]\exp[-(1+C_2)\tau]+C_3\exp[-(1+C_1)\tau]+C_4 \tag{26}$$

where

$$C_3=\left(\frac{1}{\phi-1}\right)\left\{x_{10}^*-\left[\frac{1}{1+\exp(\theta_{sp})/\tau_{ch}}\right]\right\} \tag{27}$$

and

$$C_4=\frac{[\exp(\theta_{sp})]/\tau_{ch}}{\{1+[\exp(\theta_{sp})]/\tau_{ch}\}\{1+[\phi\exp(\theta_{sp})]/\tau_{ch}\}} \tag{28}$$

From Eqs. (25) and (26), the reactor internal dynamics are asymptotically stable, provided that C_1 and C_2 are always greater than zero, with

$$\lim_{\tau\to\infty}x_1^*=\frac{1}{[1+\exp(\theta_{sp})]/\tau_{ch}}=\alpha_e \tag{29}$$

and

$$\lim_{\tau\to\infty}x_2^*=\frac{\exp(\theta_{sp})/\tau_{ch}}{\{1+[\exp(\theta_{sp})]/\tau_{ch}\}\{1+[\phi\exp(\theta_{sp})]/\tau_{ch}\}}=\beta_e \tag{30}$$

From Eqs. (18)–(20), (29) and (30), it is easy to see that, for the closed-loop reactor without bounds on the control input, its equilibrium point (x_c) corresponds to the equilibrium point of the open-loop reactor (e_p):

$$\lim_{t\to\infty}x(t)=x_c=e_p=[\alpha_c,\ \beta_c,\ \theta_e] \tag{31}$$

Numerical simulations of the closed-loop reactor without saturation allow us to obtain the time evolution of the dimensionless A concentration and temperature, respectively, as depicted in Fig. 2(a) and 2(b) for a control gain of $K=1.0$, and for the initial conditions $A=(0.0,\ 0.5,\ 0.5)$, $B=(0.0,\ 0.5,\ 3.0)$, $C=(1.0,\ 0.5,\ 0.5)$ and $D=(1.0,\ 0.5,\ 3.0)$. We can observe the disappearance of oscillatory behavior, and the stabilization of these variables at the reference values. Fig. 2(c) shows the time evolution of the control input in the absence of bounds; the control input reaches unrealistic values, as a result of the absence of bounds. The phase plane of Fig. 2(d) shows the convergence of all the trajectories towards the set-point; this proves the asymptotic stability of the reactor operating under the control algorithm without bounds on the control input.

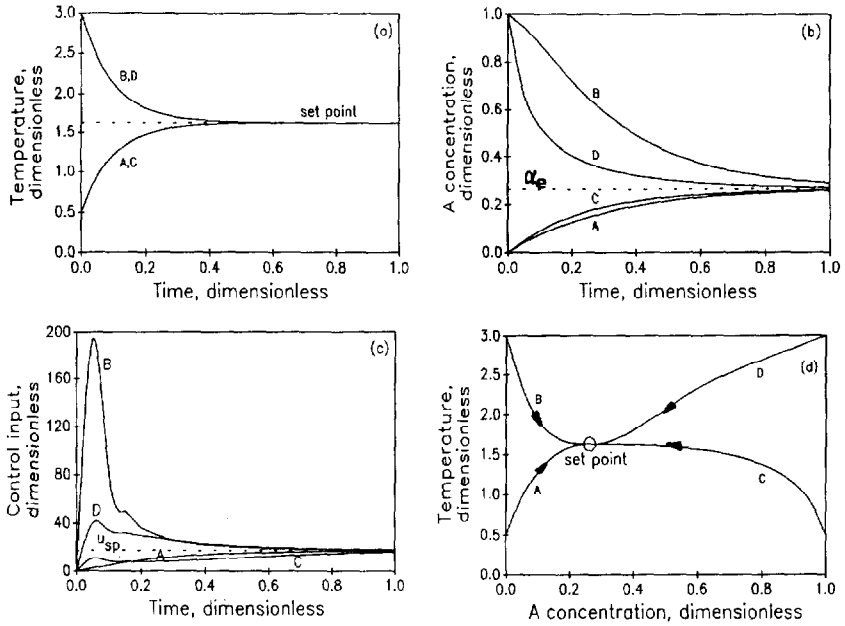

Fig. 2. (a) Temperature evolution for the closed-loop reactor without bounds on the control input, where the control gain $K = 1.0$. (b) Reactant A concentration evolution. (c) Control input evolution. (d) Phase plane of the closed-loop reactor. Initial conditions in all cases: $A = (0.0, 0.5, 0.5)$, $B = (0.0, 0.5, 3.0)$, $C = (1.0, 0.5, 0.5)$ and $D = (1.0, 0.5, 3.0)$.

4. The saturation control problem

It is well known that all process variables have lower and upper bounds that arise from factors such as the equipment size, design conditions and safe operating conditions. A reactor operating under bounds on the control input can be expressed mathematically as

$$\dot{x} = f(x) + g(x)u_{sat}(x) \tag{32}$$

where

$$u_{sat}(x) = \begin{cases} u^+ & \text{if } u(x) \geq u^+ \\ u(x) & \text{if } u^- < u(x) < u^+ \\ u^- & \text{if } u(x) \leq u^- \end{cases} \tag{33}$$

and u^- and u^+ are the lower and upper bounds of the control input u respectively. The equilibrium point of the reactor under input saturation (x_s) can be obtained by solving

$$f(x_s) + g(x_s)u_{sat}(x_s) = 0 \tag{34}$$

Commonly, $x_s \neq x_c$, which means that the control input saturation creates new equilibrium points, deviating the trajectories far away from the set-point and destroys the asymptotic stability of the reactor. To illustrate this, numerical simulations were carried out; the results can be seen in Fig. 3 for $u_3^- = 0$ and $u_3^+ = 10.0$, and the initial conditions A, B, C and D mentioned above. Fig. 3(a) and 3(b) show the curves for the dimensionless temperature and reactant A concentration, and its stabilization far away from its reference values. Fig. 3(c) shows the time evolution of the control input for this case; the control input reaches its maximum value fixed by its upper bound, and remains saturated for the entire time period considered. Fig. 3(d) shows the phase plane for this bounded case, indicating the presence of an EPIS. Fortunately, x_s can be determined from a bifurcation analysis of the open-loop reactor, in which the bifurcation parameter is the input control variable, as shown in Fig. 4. For this analysis, the equilibrium points of the open-loop reactor are obtained by solving Eqs. (7)–(9) at the steady state and taking as the bifurcation parameter the control input θ_j.

If the bound values are known, then one can locate the EPIS. In Fig. 4, the lower and upper bounds of the control input are located at the horizontal axis, and the corresponding equilibrium value of dimensionless temperature is located through the bifurcation curve at the vertical axis. $u_{sp} = 17.5$ is the control input associated with θ_{sp}, i.e. the dimensionless temperature set-point, and can be found by equating the output error to zero for the control law given by Eq. (21). Thus, we have

$$u_{sp} = -\frac{f_3(x_c)}{g_3(x_c)} \tag{35}$$

For example, for $u_3^+ = 10.0$, Fig. 4 predicts that the dimensionless temperature will be stabilized at 0.6304, which is verified in the phase plane shown in Fig. 3(d).

5. Solution of the bounded control problem

Traditionally, the bounded control problem has been bypassed by transferring it to the tuning step, in which the control gain is maintained around a small value to avoid control input saturation [9]. However, this approach produces control systems with conservative dynamic responses,

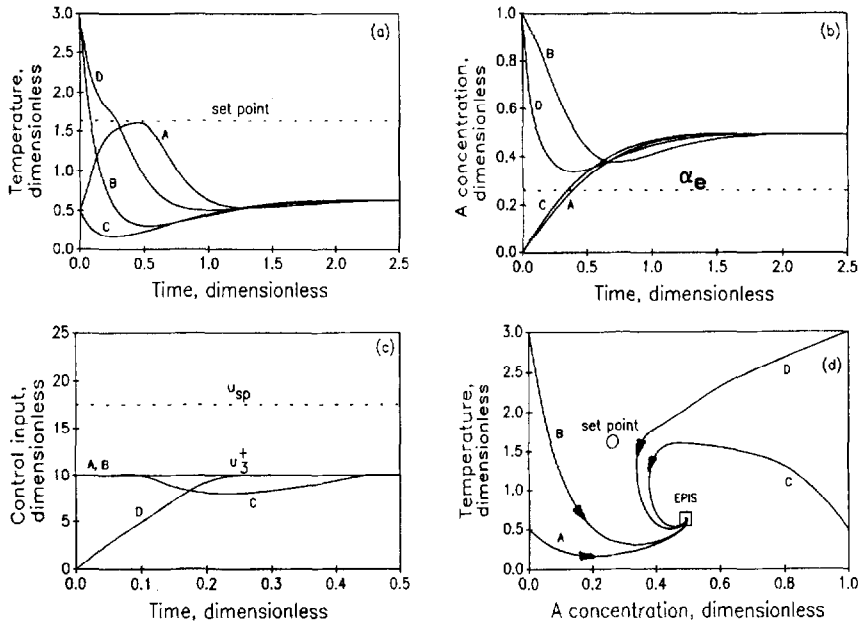

Fig. 3. (a) Temperature evolution for the closed-loop reactor with bounds on the control input, where the control gain $K=1.0$, and the bounds are $u_3^- = 0.0$ and $u_3^+ = 10.0$. (b) Reactant A concentration evolution. (c) Control input evolution. (d) Phase plane of the closed-loop reactor. Initial conditions in all cases: $A=(0.0, 0.5, 0.5)$, $B=(0.0, 0.5, 3.0)$, $C=(0.0, 0.5, 0.5)$ and $D=(1.0, 0.5, 3.0)$.

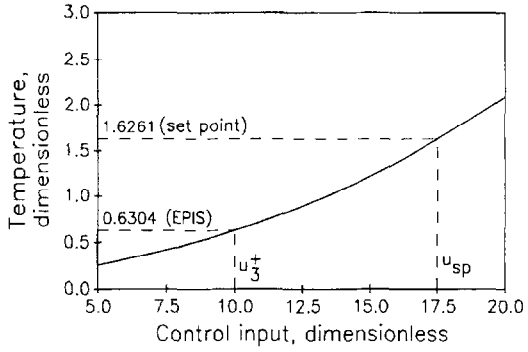

Fig. 4. Bifurcation map of the chemical reactor for EPIS locating.

which are unacceptable for high efficiency and productivity operating conditions. Following Alvarez et al. [9], the bounded control problem given by Eq. (32) can be solved if, for certain values of the upper and lower bounds, it is verified that $x_s = x_e$, i.e. if the equilibrium point of the closed-loop reactor under bounds on the control input is the same as the equilibrium point of the closed-loop reactor without bounds on the control input.

When the input control is upper saturated, it can be verified from Eqs. (21), (33) and (34) that

$$f_3(x) + g_3(x)u_3^+ = 0 \tag{36}$$

and

$$\frac{1}{g_3(x)}\left[-K(\theta_s - \theta_e) - f_3(x)\right] \geq u_3^+ \tag{37}$$

where θ_s and θ_e are the closed-loop equilibrium reactor temperatures with and without saturation on the control input respectively. From Eqs. (36) and (37), we obtain the inequality

$$\theta_s \leq \theta_e \tag{38}$$

Similarly, for lower saturation, we have

$$f_3(x) + g_3(x)u_3^- = 0 \tag{39}$$

and

$$\frac{1}{g_3(x)}\left[-K(\theta_s - \theta_e) - f_3(x)\right] \leq u_3^- \tag{40}$$

which implies that

$$\theta_s \geq \theta_e \tag{41}$$

Eqs. (38) and (41) give the necessary conditions to obtain equilibrium points induced by upper or lower saturation. When these conditions are reversed, we obtain the necessary and sufficient conditions to avoid the presence of equilibrium

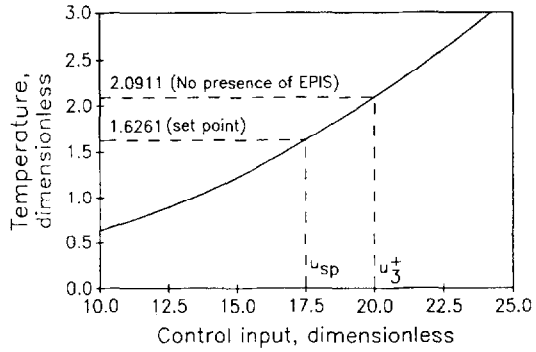

Fig. 5. Bifurcation map of the chemical reactor for the avoidance of EPIS.

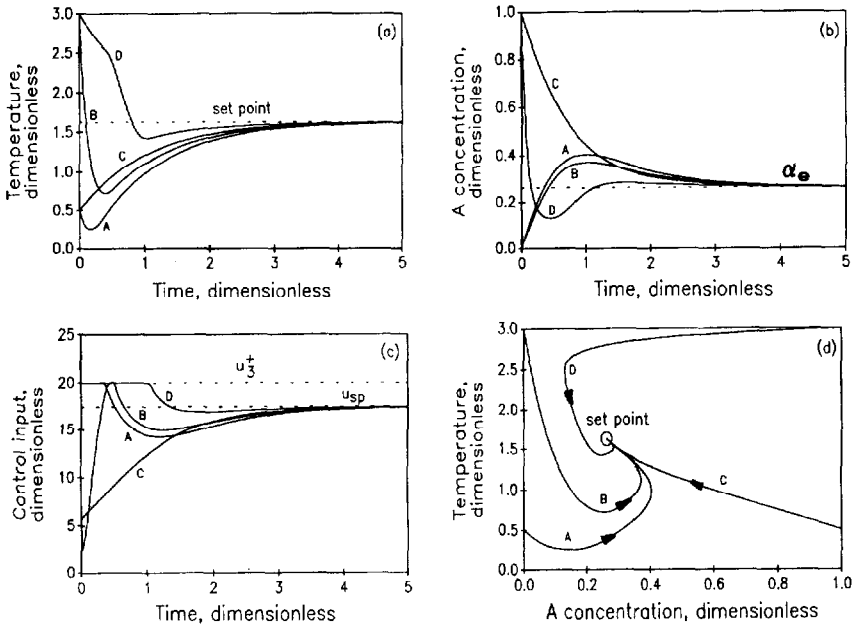

Fig. 6. (a) Temperature evolution for the closed-loop reactor with bounds on the control input and satisfying the conditions found here, where the control gain $K=1.0$, and the bounds are $u_3^- = 0.0$ and $u_3^+ = 20.0$. (b) Reactant A concentration evolution. (c) Control input evolution. (d) Phase plane of the closed-loop reactor. Initial conditions in all cases: $A = (0.0, 0.5, 0.5)$, $B = (0.0, 0.5, 3.0)$, $C = (1.0, 0.5, 0.5)$ and $D = (1.0, 0.5, 3.0)$.

points induced by saturation (i.e. allowing $x_s = x_e$). Thus, for upper saturation of the control input, we have

$$\theta_s \geq \theta_e \tag{42}$$

and, for lower saturation, we have

$$\theta_s \leq \theta_e \tag{43}$$

To illustrate the application of these necessary and sufficient conditions, numerical simulations were carried out for a lower bound $u_3^- = 0.0$ and an upper bound $u_3^+ = 20.0$. From the bifurcation map plotted in Fig. 5, the dimensionless equilibrium temperature under saturation (θ_s) associated with the upper bound is equal to 2.0911. For this case, it is easy to see that the condition given by Eq. (42) is verified, which means that $\theta_s > \theta_e$. In this case, the only equilibrium point will be the set-point, despite the bounds imposed on the control input; all the trajectories converge towards the set-point, although the control input is temporarily saturated.

Fig. 6(a) and 6(b) present the time evolution of dimensionless temperature and reactant A concentration for the initial conditions A, B, C and D mentioned earlier. The values of the state variables are asymptotically stable and converge to the reference values. Fig. 6(c) shows the control input that corresponds to these initial conditions and a control gain of $K=1.0$. At the beginning of the simulation, the control input is saturated for initial conditions A and D; however, as time proceeds, the control input is desaturated, allowing θ to reach its set-point, as is foreseen by the conditions derived here. Finally, Fig. 6(d) presents the phase plane for this case, showing the convergence of all the trajectories to the set-point, despite the imposed bounds on the control input.

6. Conclusions

The imposition of bounds on the control input for a chemical reactor in which there occurs two consecutive exothermic chemical reactions results in the presence of equilibrium points induced by saturation, which deviate the state variable trajectories of the reactor far away from the set-point, destroying the reactor asymptotic stability. For a single input–single output non-linear control algorithm, the solution of the bounded control problems was proved possible whenever some conditions developed in this work are satisfied. Numerical simulation results indicate the avoidance of the equilibrium points induced by saturation and, consequently, the reactor stabilization at the set-point, despite the imposed bounds on the control input.

Appendix A. Nomenclature

a	reactant A concentration
a_0	concentration of A in feed
b	reactant B concentration
b_0	concentration of B in feed
A_c	effective jacket heat transfer area
A_i	Arrhenius constant for reaction $i = 1, 2$
C_i	internal dynamic constants, $i = 1, 2, 3, 4$
C_p	specific heat of reacting mixture
E_1	activation energy for reaction (1)
E_2	activation energy for reaction (2)
e_p	state vector for the open-loop equilibrium point
k_1	rate constant for reaction (1)
k_2	rate constant for reaction (2)

K control gain
R universal gas constant
t time
t_N Newtonian cooling time
t_{res} mean residence time
T reactor temperature
T_c cooling water temperature
T_0 feed temperature
U overall heat transfer coefficient
u_{sat} bounded control input
u_{sp} control input associated to temperature set-point
u^- lower bound of the control input
u^+ upper bound of the control input
u_3 control input (θ_j)
V reactor volume
x_1 state variable (dimensionless concentration of reactant A)
x_1^* state variable (x_1) for reactor internal dynamics
x_2 state variable (dimensionless concentration of reactant B)
x_2^* state variable (x_2) for reactor internal dynamics
x_3 state variable (dimensionless temperature of reactor)
x_e state vector for the closed-loop equilibrium point without input bounds
x_s state vector for the closed-loop equilibrium point with input bounds

α dimensionless concentration of reactant A
α_e α value at open-loop equilibrium point
β dimensionless concentration of reactant B
β_e β value at open-loop equilibrium point
ΔH_1 heat of reaction for reaction (1)
ΔH_2 heat of reaction for reaction (2)
ϵ output error
ρ density of reacting mixture
ϕ reaction ratio
θ reactor dimensionless temperature
θ_j dimensionless temperature of cooling water
θ_e θ value at open-loop equilibrium point
θ_{sp} set-point for reactor dimensionless temperature
τ dimensionless time
τ_{ch} dimensionless chemical time
τ_N dimensionless Newtonian cooling time

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