

Power-Shaping Control of an Exothermic Continuous Stirred Tank Reactor (CSTR)^{*}

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Abstract: The exothermic continuous stirred tank reactor (CSTR) is a classical yet complex case study of nonlinear dynamical systems. Power-shaping control is a recent approach for the control of nonlinear systems based on the physics of the dynamical system. In this paper we present a general methodology to apply the power-shaping control approach to the exothermic CSTR study case. It results in a global Lyapunov function for the exothermic CSTR. This Lyapunov function is then reshaped by the means of a controller in order to stabilize the process at a desired temperature. Some considerations on the local and global convergence to the desired state are presented.

Keywords: Nonlinear control; Power-Shaping Control; exothermic CSTR

1. INTRODUCTION

Thermodynamic systems, and among them chemical reaction systems, are usually nonlinear dynamical systems. They can therefore have a complex behaviour and be difficult to analyze and to control. Stability analysis of nonlinear systems requires the use of abstract mathematical tools such as the two Lyapunov methods or the passivity theory. Over the past years, several works have combined those abstract concepts with the underlying physical phenomena giving rise to the dynamical behaviour of the system. These works include for instance the study of port-Hamiltonian systems (Dalsmo and van der Schaft (1998), Maschke and van der Schaft (2005), Eberard et al. (2006)), energy-balancing passivity based control (PBC) (Ortega et al. (2001), Jeltsema et al. (2004)) or the introduction of the contact formalism for expressing the dynamics of systems in which irreversible phenomena arise (Eberard et al. (2005), Eberard (2006), Favache et al. (2007)). The exothermic continuous stirred tank reactor (CSTR) is a classical study case of nonlinear systems. Indeed, the dynamical behaviour shows complex features, such as multiple equilibrium points. Up to now no exact physical interpretation of the complex behaviour of the exothermic reactor has been found (Favache and Dochain (2009)).

Power-shaping control (Ortega et al. (2003)) has been developed in the past years as an extension of energy-balancing passivity-based control (Ortega et al. (2001), Jeltsema et al. (2004)). In energy-balancing passivity based control, the controller reshapes the energy function of the system so that it has a minimum at the desired equilibrium point. The controller provides to the system

a finite amount of energy so as to drive the system to the desired state. This concept has been widely applied to electro-mechanical systems (Ortega et al. (1999), Maschke et al. (2000), Ortega et al. (2002)) but also to thermodynamic systems where the storage function is the entropy instead of the energy (Alonso et al. (2002), Otero-Muras et al. (2006)). Nevertheless energy-balancing passivity-based control can only be applied to systems without pervasive dissipation, i.e. systems where the power provided by the controller is equal to zero at the desired equilibrium point. To overcome this difficulty the concept of power shaping control was introduced firstly for the stabilization of nonlinear RLC circuits (Ortega et al. (2003)). Contrary to energy-balancing passivity-based control, the storage function used for the control is related to the power and not to the energy. Power-shaping control has subsequently been applied to the control of mechanical and electro-mechanical systems (Garcia-Canseco et al. (2008)). Power-shaping control is based on a particular formulation of the system dynamics, namely the Brayton-Moser equations (Brayton and Moser (1964a), Brayton and Moser (1964b)). Although the first systems which have been described using this formalism are electrical circuits, it is shown in Jeltsema and Scherpen (2003), Jeltsema and Scherpen (2007) and Garcia-Canseco et al. (2008) that mechanical systems can also be expressed in this form.

As the work of Alonso, Ydstie and coworkers (see e.g. Alonso et al. (2002), Antelo et al. (2007), Farschman et al. (1998)), the present research is basically motivated by the objective to connect thermodynamics with process control design (see also Favache and Dochain (2009)). In this paper we apply power-shaping control to the exothermic CSTR case study with the aim of bringing more physical insight in its dynamical behaviour. After a brief presentation of

^{*} The work of A. Favache is funded by a grant of aspirant of Fonds National de la Recherche Scientifique (Belgium).

the main principles of power-shaping control in Section 2 and of the CSTR case study in Section 3, we shall apply the power-shaping control theory to our example. First we shall use the power-shaping approach to analyze the open-loop behaviour (Section 4) and then to design a control action (Section 5). Finally Section 6 presents some general comments on the possibility of extending the power-shaping approach to more complex systems, namely systems with more than one reactant, and/or more than one reaction.

2. POWER-SHAPING CONTROL

In this section, we briefly explain the principles of power-shaping control. The statements are given without any proof. For more details, the reader can refer to Jeltsema and Scherpen (2003), Ortega et al. (2003), Jeltsema and Scherpen (2007), Garcia-Canseco et al. (2008).

2.1 The Brayton-Moser formulation

Let us consider a dynamical system of dimension n with m inputs. The state of the system is given by the vector $x \in \mathbb{R}^n$ and the input is given by vector $u \in \mathbb{R}^m$. The power-shaping control theory is based on the Brayton-Moser formulation of the system dynamics (Brayton and Moser (1964a), Brayton and Moser (1964b)). In this formulation the system dynamics are of the following form:

$$Q(x) \frac{dx}{dt} = \nabla P(x) + G(x) u \quad (1)$$

where $Q(x) : \mathbb{R}^n \rightarrow \mathbb{R}^n \times \mathbb{R}^n$ is a non-singular square matrix, $P(x) : \mathbb{R}^n \rightarrow \mathbb{R}$ is a scalar function of the state and $G(x) : \mathbb{R}^n \rightarrow \mathbb{R}^n \times \mathbb{R}^m$. Additionally the symmetric part of the matrix $Q(x)$ is negative semi-definite, i.e.:

$$Q(x) + Q^t(x) \leq 0 \quad (2)$$

The function $P(x)$ is called the potential function. In electrical and mechanical systems, the potential function has the units of power. In electrical systems it is related to the so-called content and co-content of the resistances (Ortega et al. (2003), Jeltsema and Scherpen (2007)) while it is related to the Rayleigh dissipation function (Jeltsema and Scherpen (2003)) in mechanical systems. In both cases, the potential function $P(x)$ is related to the dissipated power in the system.

Let us now assume that the system dynamics are given by the following relation:

$$\frac{dx}{dt} = f(x) + g(x) u \quad (3)$$

where $f(x) : \mathbb{R}^n \rightarrow \mathbb{R}^n$ and $g(x) : \mathbb{R}^n \rightarrow \mathbb{R}^n \times \mathbb{R}^m$. The system (3) can be written in the form (1) if there exists a non-singular matrix $Q(x)$ fulfilling (2) and that solves following partial differential equation:

$$\nabla(Q(x) f(x)) = \nabla^t(Q(x) f(x)) \quad (4)$$

This condition is equivalent to the existence of the potential function $P(x)$ (i.e. if the potential function $P(x)$ exists, its Jacobian matrix must be symmetric). This one is the solution of the following partial differential equation system:

$$\nabla P(x) = Q(x) f(x) \quad (5)$$

Finally the function $G(x)$ is given by the following relation:

$$G(x) = Q(x) g(x)$$

2.2 Power-shaping control

Let us assume that the system dynamics can be expressed using the Brayton-Moser equations presented above. The desired equilibrium state is denoted by x^* . The rationale of power-shaping control is to choose the input $u(x)$ such that in closed loop the system dynamics are given by the following relation:

$$Q(x) \frac{dx}{dt} = \nabla P_d(x)$$

where $P_d(x) : \mathbb{R}^n \rightarrow \mathbb{R}$ is the reshaped potential function. The desired equilibrium point x^* must be a local minimum of the potential function $P_d(x)$ in order to be locally asymptotically stable. The function $P_d(x)$ cannot be arbitrarily chosen since the following relation has to be fulfilled:

$$g^\perp(x) Q^{-1}(x) \nabla P_d(x) = 0 \quad (6)$$

where $g^\perp(x) : \mathbb{R}^n \rightarrow \mathbb{R}^{n-m} \times \mathbb{R}^n$ is a full-rank left annihilator of $g(x)$ (i.e. $g^\perp(x) g(x) = 0$ with $\text{rank}(g^\perp(x)) = n - m$) and $P_d(x) = P_d(x) - P(x)$. The condition (6) ensures the existence of a function $u(x)$ such that:

$$Q(x) (f(x) + g(x) u(x)) = \nabla P(x) + \nabla P_d(x)$$

Under these conditions, the control input $u(x)$ that achieves to reshape $P(x)$ into $P_d(x)$ is the following one:

$$u(x) = (G^t(x) G(x))^{-1} G^t(x) \nabla P_d(x) \quad (7)$$

where $G(x) = Q(x) g(x)$

3. THE EXOTHERMIC CONTINUOUS STIRRED TANK REACTOR (CSTR)

In our research, we have applied the power-shaping methodology to a classical process control case study: the exothermic continuous stirred tank reactor (CSTR), illustrated in Figure 1. The reaction that is taking place is $A \rightarrow B$. In order to simplify the model, the following assumptions have been considered:

- the reactor is liquid phase and the volume V is constant.
- the density ρ and the specific heat c_p of the mixture are constant (i.e. independent of the temperature or of the composition).
- the reaction heat is independent of the temperature.
- the reaction is irreversible.
- the reaction kinetics obey to the mass action law, i.e. $r = k(T) n_A$ where $k(T)$ is the kinetic constant, depending only on the temperature T and n_A is the number of moles of component A . The function $k(T)$ is assumed to be monotonically increasing. Moreover let us assume that $\lim_{T \rightarrow 0} k(T) = 0$, $\lim_{T \rightarrow \infty} k(T) = k_0$ and

$$\lim_{T \rightarrow 0} \frac{dk}{dT} = \lim_{T \rightarrow \infty} \frac{dk}{dT} = 0$$

- the dynamics of the jacket can be neglected.

¹ These assumptions on $k(T)$ are for instance fulfilled by the commonly used Arrhenius law.

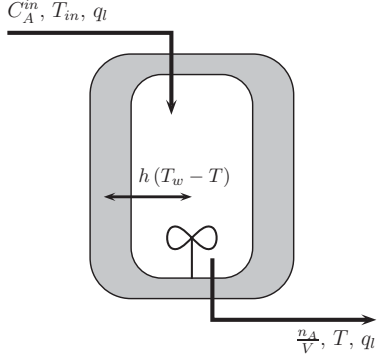


Fig. 1. Schematic view of the CSTR

- the heat exchange between the reactor and the jacket is proportional to the temperature difference between them, with h the heat exchange coefficient.
- the system is controlled by the cooling fluid flow rate. It acts directly on the heat transfer coefficient h . Therefore we shall consider in the sequel that the control input is the quantity $\frac{h}{\rho c_p V}$.

Under these assumptions the dynamic model of the system is given by following equations:

$$\begin{cases} \frac{dn_A}{dt} = \frac{q_l}{V} (C_A^{in} V - n_A) - k(T) n_A \\ \frac{dT}{dt} = \frac{q_l}{V} (T_{in} - T) + \frac{(-\Delta_r H)}{\rho c_p V} k(T) n_A \\ \quad + \frac{h}{\rho c_p V} (T_w - T) \end{cases} \quad (8)$$

where q_l is the volumetric inlet and outlet flow rate, C_A^{in} is the inlet concentration of A , T_{in} is the inlet temperature, $(-\Delta_r H)$ is the reaction heat and T_w is the temperature of the cooling fluid. Using the notations of (3), we have:

$$f(x) = \begin{pmatrix} \delta (C_A^{in} V - n_A) - k(T) n_A \\ \delta (T_{in} - T) + \gamma k(T) n_A \end{pmatrix}$$

$$g(x) = \begin{pmatrix} 0 \\ T_w - T \end{pmatrix}$$

with $x = [n_A, T]^t$, $u = \frac{h}{\rho c_p V}$, $\delta = \frac{q_l}{V}$ and $\gamma = \frac{(-\Delta_r H)}{\rho c_p V}$.

It can be shown that this system can have up to three equilibrium points in open loop (i.e. for $u = 0$), depending on the numerical values of the parameters (see e.g. Aris and Amundson (1958), Uppal et al. (1974)). Here we shall consider the case with three equilibrium states, two being stable and one being unstable.

4. THE OPEN LOOP BEHAVIOUR

The methodology described in Section 2.1 has been applied to the system described in Section 3. The first step was to find the square matrix $Q(x)$ that meets the required properties (2) and (4). The partial differential equation (4) for the open-loop CSTR is written as follows:

$$\begin{aligned} & -q_{11} n_A \frac{dk}{dT} - q_{12} \delta + q_{12} \gamma n_A \frac{dk}{dT} \\ & + \frac{\partial q_{11}}{\partial T} (\delta (C_A^{in} V - n_A) - k n_A) \\ & + \frac{\partial q_{12}}{\partial T} (\delta (T_{in} - T) + \gamma k n_A) \\ & = -q_{21} \delta - q_{21} k + q_{22} \gamma k + \frac{\partial q_{21}}{\partial n_A} (\delta (C_A^{in} V - n_A) - k n_A) \\ & + \frac{\partial q_{22}}{\partial n_A} (\delta (T_{in} - T) + \gamma k n_A) \end{aligned} \quad (9)$$

where q_{ij} is the entry in position (i, j) of the matrix $Q(n_A, T)$. We first transformed (9) into an algebraic equation by restricting ourselves to a subset of possible matrices $Q(n_A, T)$. This algebraic equation then has been solved and a possible matrix has been found². In our case, the symmetric part of matrix $Q(x)$ was found to be definite negative.

Remark 1. Indeed a family of possible matrices $Q(n_A, T)$ has been found that both satisfy (2) and (4). But since they all have a similar form apart from a constant parameter, we shall treat them in the sequel as one unique matrix.

Next the potential function is found by integrating (5). The general form of the potential form is given by the following expression:

$$P(n_A, T) = \int p(T) dT + \omega [\gamma (C_A^{in} V - n_A) + (T_{in} - T)]^2 \quad (10)$$

where ω is a positive constant and $p(T) : \mathbb{R} \rightarrow \mathbb{R}$ is a non-linear function of $k(T)$ and T . The quadratic term of (10) is clearly linked to the convection phenomena, whereas the integral term is related to the reaction kinetics.

Remark 2. Actually the function $p(T)$ is not unique. It depends directly on the matrix $Q(x)$. Since we have found a family of matrices $Q(x)$, there is a corresponding family of functions $p(T)$ that are similar apart from a constant parameter.

Let us now consider the equilibrium points $\bar{x} = (\bar{n}_A, \bar{T})$ of the open-loop CSTR:

$$Q(\bar{x}) \left. \frac{dx}{dt} \right|_{\bar{x}} = \nabla P(\bar{x}) = 0$$

Since the matrix $Q(x)$ is non-singular, the equilibrium points \bar{x} are also critical points of the potential function $P(x)$ (i.e. $\nabla P(\bar{x}) = 0$) and conversely. The analysis of the Hessian matrix of the obtained potential function (10) at each of the equilibrium points shows that the stable ones are local minima of the function $P(x)$ whereas the unstable one is a saddle point. The level curves of the function $P(x)$ are given in Figure 2.

The variation of function $P(x)$ along the trajectories of the system are given by the following relation:

² Calculation details can be found in Favache and Dochain (2008).

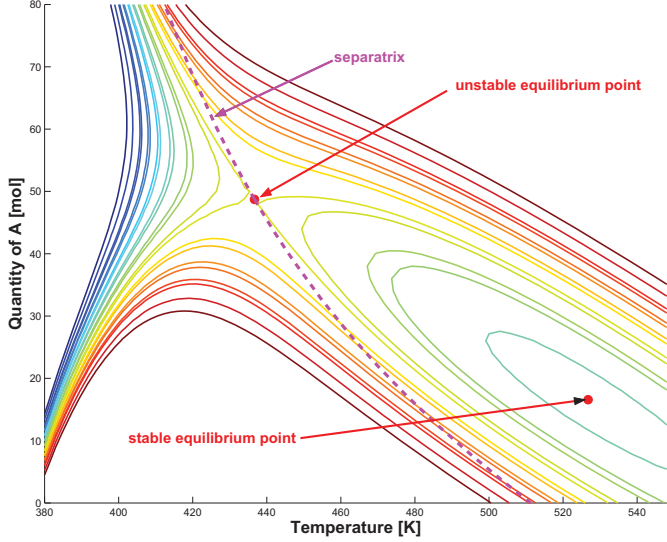


Fig. 2. Level curves of the potential function

$$\begin{aligned} \frac{dP}{dt} &= \nabla^t P(x) f(x) \\ &= \nabla^t P(x) Q^{-1}(x) \nabla P(x) \\ &= \frac{1}{2} \nabla^t P(x) \left(Q^{-1}(x) + (Q^t(x))^{-1} \right) \nabla P(x) \end{aligned}$$

Since the symmetric part of $Q(n_A, T)$ is negative definite, we have $\frac{dP}{dt} \leq 0$ where the equality holds only for $\nabla P(x) = 0$, i.e. for the equilibrium points. As a consequence $P(n_A, T)$ is decreasing along the trajectories. Moreover $P(x)$ is radially unbounded. Therefore the potential function $P(n_A, T)$ is a global Lyapunov function for the system (Khalil (2002)).

5. POWER-SHAPING CONTROL OF THE CSTR

5.1 Controller design

Let us denote by $x^* = [n_A^*, T^*]^t$ the desired equilibrium state. Since the input has an effect only on the temperature dynamics, the values of n_A^* and T^* cannot be chosen independently. This is stated in the following lemma:

Lemma 1. Let us consider some control input $u(x)$ such that the closed loop system has at least one equilibrium point. The equilibrium points of the closed loop system are contained in the following set:

$$(n_A^*, T^*) \in \left\{ (n_A, T) \left| \begin{array}{l} n_A = \frac{\delta C_A^{in} V}{k(T) + \delta} \\ T \in]0, +\infty[\setminus \{T_w\} \end{array} \right. \right\} \quad (11)$$

Proof. Let $x^* = (n_A^*, T^*)$ be an equilibrium point of the closed loop system for the control input $u(x)$. By definition of an equilibrium point, we have:

$$\begin{cases} 0 = \frac{q_l}{V} (C_A^{in} V - n_A^*) - k(T^*) n_A^* \\ 0 = \frac{q_l}{V} (T_{in} - T^*) + \frac{(-\Delta_r H)}{\rho c_p V} k(T^*) n_A^* \\ \quad + u(x^*) (T_w - T^*) \end{cases} \quad (12)$$

The first equation can be directly rewritten as follows:

$$n_A^* = \frac{\delta C_A^{in} V}{k(T^*) + \delta}$$

Let us now assume that $T^* = T_w$ is a possible equilibrium of the open loop system. If we replace in the second equation of (12), we find the following relation:

$$0 = \frac{q_l}{V} (T_{in} - T_w) + \frac{(-\Delta_r H)}{\rho c_p V} k(T_w) \frac{\delta C_A^{in} V}{k(T_w) + \delta}$$

This relation implies that T_w is an equilibrium point of the open-loop system. But, except an unlikely particular case, there is no reason that the temperature of the cooling fluid is exactly equal to an equilibrium temperature of the open-loop CSTR. Hence T_w cannot be an equilibrium temperature of the closed-loop system. \square

Lemma 2. (11) is a necessary condition for $x^* = (n_A^*, T^*)$ to be a local minimum of $P_d(x)$.

Proof. A necessary condition for x^* to be a local minimum of $P_d(x)$ is the following one:

$$\nabla P_d(x^*) = \nabla P(x^*) + \nabla P_a(x^*) = 0$$

By replacing $\nabla P(x)$ and $\nabla P_a(x)$ by their expressions, the following relation is obtained:

$$\begin{aligned} -\nabla P(x^*) &= -Q(x^*) f(x^*) \\ &= \nabla P_a(x^*) = Q(x^*) g(x^*) u(x^*) \end{aligned}$$

Since $Q(x^*)$ is invertible, this can be rewritten as :

$$f(x^*) + g(x^*) u(x^*) = 0 \quad (13)$$

When replacing $f(x)$ and $g(x)$ by their respective expression, (12) is obtained. Thus the rest of the proof of Lemma 1 also applies here. \square

The control action is then found by applying the methodology described in Section 2.2. First we solve (6) using the previously found expression for the matrix $Q(x)$. The left annihilators of $g(x)$ are given as follows:

$$g^\perp(x) = [\varphi \ 0]$$

with $\varphi \in \mathbb{R}^*$. (6) is thus written as follows:

$$\frac{\varphi}{\det Q(x)} \left(q_{22}(n_A, T) \frac{\partial P_a}{\partial n_A} - q_{12}(n_A, T) \frac{\partial P_a}{\partial T} \right) = 0$$

where $q_{12}(n_A, T)$ and $q_{22}(n_A, T)$ are the elements of $Q(x)$ in position (1, 2) and (2, 2), respectively. With our matrix $Q(x)$ the solution of this partial differential equation is given as follows:

$$P_a(n_A, T) = f_a \left(n_A + \int w(T) dT \right)$$

where $w(k(T))$ is a rational function of the kinetic coefficient $k(T)$. $f_a(z) : \mathbb{R} \rightarrow \mathbb{R}$ can be any smooth real-valued function. In our case we have chosen $f_a(z)$ to be a second order polynomial. Using now (7), the control action of the following form is obtained for stabilizing the desired equilibrium point:

$$u(n_A, T) = \frac{-\mu(n_A - n_A^* + W_{T^*}(T)) + u^*(T_w - T^*)}{T_w - T} \quad (14)$$

where $W_{T^*}(T) : \mathbb{R}^{*+} \rightarrow \mathbb{R}$ is given by the following expression:

$$W_{T^*}(T) = \int_{T^*}^T w(k(\tau)) d\tau$$

Obviously $W_{T^*}(T^*) = 0$. $\mu \in \mathbb{R}$ is a parameter of the controller and u^* is the value of the input at the equilibrium state:

$$u^*(T_w - T^*) = -\delta(T_{in} - T) - \gamma\delta(C_A^{in}V - n_A^*)$$

In order to ensure that x^* is a local minimum of $P_d(x^*)$, μ has to be lower bounded. The bounds are obtained by imposing that the Jacobian matrix of $P_d(x^*)$ is positive definite at the desired closed-loop equilibrium point. The control action $u(x)$ acts in (8) via the term

$$g(x)u(x) = \begin{pmatrix} 0 \\ -\mu(n_A - n_A^* + W_{T^*}(T)) + u^*(T_w - T^*) \end{pmatrix}$$

which does not depend on $(T_w - T)$ anymore. This means that the actual control input is the transferred heat which is equal to:

$$-\mu(n_A - n_A^* + W_{T^*}(T)) + u^*(T_w - T^*)$$

5.2 Considerations on local and global convergence

The controller designed in the previous section only guarantees a local convergence to the desired set point, i.e. the system will converge to desired point if and only if the initial conditions are close enough to it. Global convergence is ensured if and only if the shaped potential function $P_d(x)$ does not have other local minima, i.e. if and only if x^* is a global minimum of the function $P_d(x)$.

Let us assume that the point $x^\# = [n_A^\#, T^\#]^t$ is another local minimum of the function $P_d(x)$. For the same reasons as stated before, the following relation has to be fulfilled:

$$n_A^\# = \frac{\delta C_A^{in} V}{k(T^\#) + \delta} \quad (15)$$

Moreover, for $x^\#$ to be a closed loop equilibrium of (8), the following relation has to be fulfilled:

$$\begin{aligned} &\delta(T_{in} - T^\#) + \delta\gamma(C_A^{in}V - n_A^\#) \\ &+ u^*(T_w - T^*) - \mu(n_A^\# - n_A^* + W_{T^*}(T^\#)) = 0 \end{aligned} \quad (16)$$

By analogy with (15), let us define the function $\tilde{T}^\#(n_A)$ by the following implicit relation:

$$k(\tilde{T}^\#(n_A)) = \frac{\delta C_A^{in} V}{n_A} - \delta$$

Consider the following function:

$$\begin{aligned} \Delta(n_A) &= \delta(T_{in} - \tilde{T}^\#) + \delta\gamma(C_A^{in}V - n_A) \\ &+ u^*(T_w - T^*) - \mu(n_A - n_A^* + W_{T^*}(\tilde{T}^\#)) \end{aligned}$$

where the dependence of $\tilde{T}^\#(n_A)$ on n_A has been omitted for sake of clarity. The equilibrium points x^* and $x^\#$ are zeros of the function $\Delta(n_A)$. Therefore x^* is the unique convergence point if it is the unique zero of $\Delta(n_A)$.

The function $\Delta(n_A)$ is linear in the parameter μ . Therefore it can be written as follows:

$$\Delta(n_A) = \Delta_0(n_A) + \mu\Delta_\mu(n_A)$$

Remark 3. In Favache and Dochain (2009), we have presented several old and new results that aim at linking the thermodynamics and the system theory concepts via

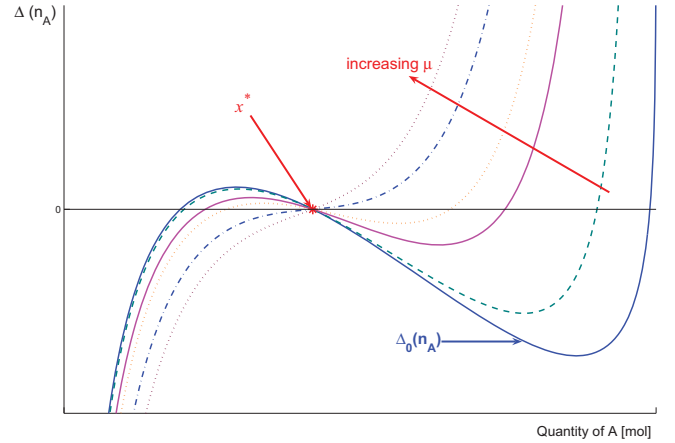


Fig. 3. Influence of μ on $\Delta(n_A)$

the CSTR study case³ In this paper we have introduced a function of the state, denoted $\Delta_{eq}(T)$. By integrating the notations and assumptions of the present paper, this function is given by the following expression:

$$\begin{aligned} \Delta_{eq}(T) &= k(T)n_A V(-\Delta_r H) \\ &- \rho c_p V [u(n_A, T)(T - T_w) + \delta(T - T^{in})] \end{aligned}$$

It can be seen directly that $\Delta_{eq}(T)$ and $\Delta(n_A)$ are linked by the following relation:

$$\Delta(n_A) = \frac{\Delta_{eq}(\tilde{T}^\#(n_A))}{\rho c_p V}$$

It can be shown that the assumptions on the form of $k(T)$ described in Section 3 and the existence of three open loop equilibria implies that $\Delta_0(n_A)$ is increasing for low and high temperatures, but decreasing on one determined interval⁴ As a consequence, $\Delta(n_A)$ can have several zeros, depending on the term $\mu\Delta_\mu(n_A)$.

If the function $w(T)$ has been adequately chosen, then $\Delta_\mu(n_A) > 0$ for $n_A > n_A^*$ and $\Delta_\mu(n_A) < 0$ for $n_A < n_A^*$. This means that if μ is chosen sufficiently large and positive, then the term $\mu\Delta_\mu(n_A)$ reshapes the initial function $\Delta_0(n_A)$ so as to make the two undesired zeros to vanish (see Figure 3). As a conclusion, there is a lower bound on the parameter μ in order to ensure global convergence.

5.3 Simulation results

In this section we present some simulation results of the controlled system. First the performance of the controller for reference tracking is shown in Figure 4. Then Figures 5 and 7 show the cases where only local convergence and global convergence, respectively, to the desired equilibrium point is ensured. These figures show the temperature evolution for different initial conditions. The corresponding level curves of the potential function $P_d(x)$ are shown for

³ In Favache and Dochain (2009) we have considered a CSTR with a reversible reaction, but the results can be applied directly for an irreversible reaction by setting the kinetic reaction coefficient of the reverse reaction equal to zero.

⁴ This can be deduced from the form of $\Delta_{eq}(T)$ in Favache and Dochain (2009) using the fact that $\tilde{T}^\#(n_A)$ is a strictly decreasing function.

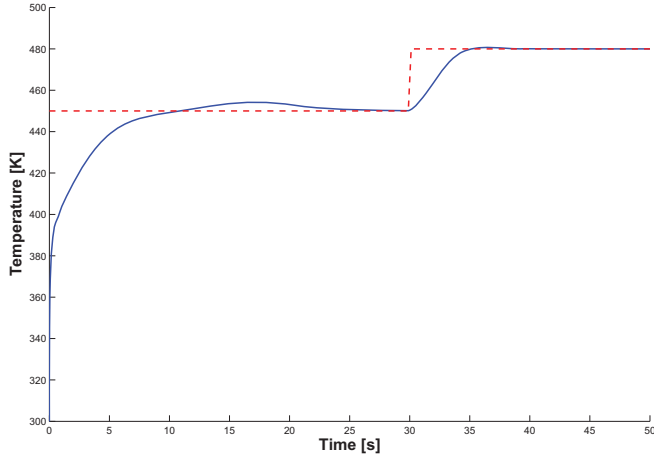


Fig. 4. Reference tracking

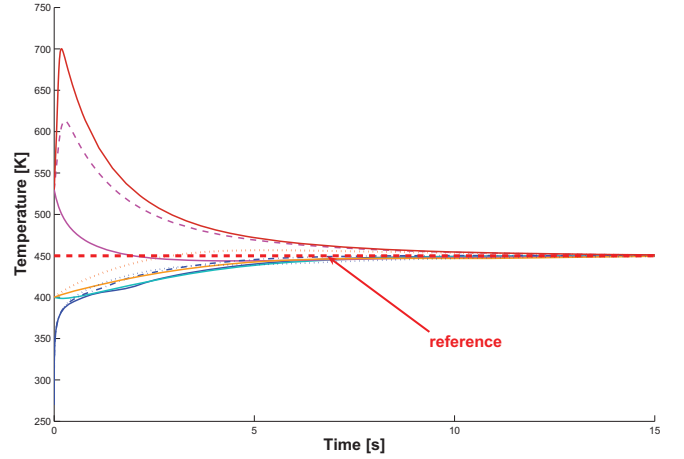


Fig. 7. Temperature evolution for different initial conditions (global convergence)

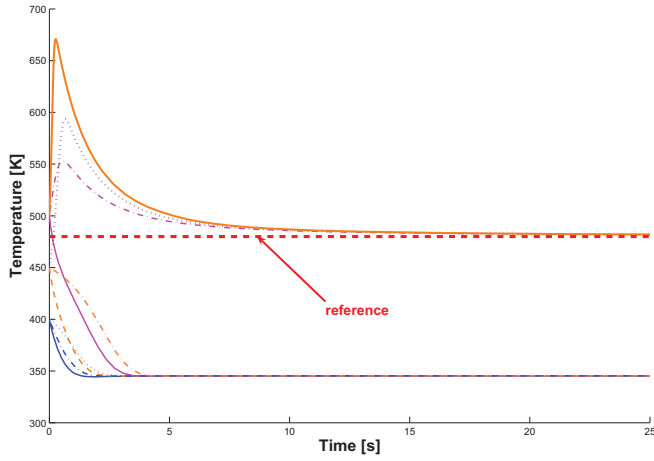


Fig. 5. Temperature evolution for different initial conditions (local convergence)

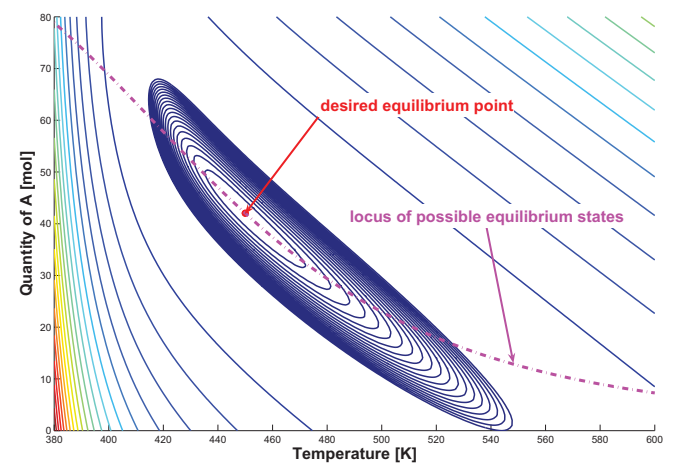


Fig. 8. Level curves of $P_d(x)$ (global convergence)

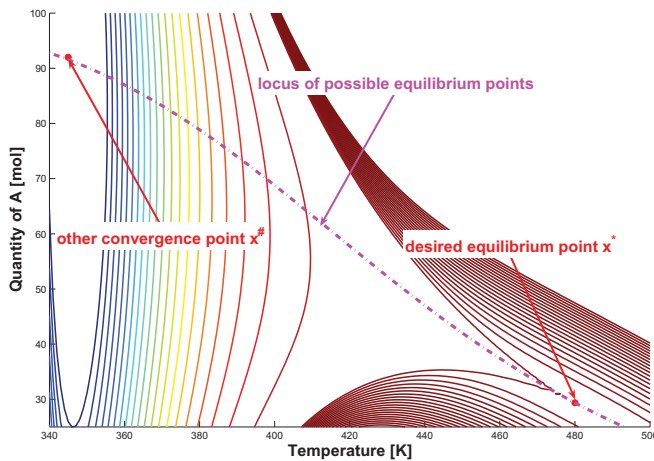


Fig. 6. Level curves of $P_d(x)$ (local convergence)

both cases in Figures 6 and 8, respectively. It can be clearly seen on Figure 5 that there exist two convergence points, depending on the initial condition. This is confirmed by the level curves of the function $P_d(x)$ in Figure 6 where two local minima can be distinguished.

5.4 Robustness analysis

The control law given in (14) requires the complete state feedback. Moreover it also requires the knowledge of the temperature dependence of the kinetic coefficient $k(T)$ that appears in the expression of $W_{T^*}(T)$. In most practical applications, the kinetic coefficient is determined experimentally and the on-line measurement of the concentration is not always achievable. In this section we shall analyze the effect on the closed-loop convergence and stability of modeling errors in the kinetic coefficient $k(T)$.

Let us assume that there is a modeling error on the kinetic coefficient. The aim is to stabilize the state (n_A^*, T^*) . The controller is designed using the function $\hat{k}(T)$ instead of the real kinetic coefficient $k(T)$:

$$\hat{k}(T) = (1 + \xi(T)) k(T) \quad (17)$$

with $\xi(T) > -1$.

Assumption 1. Despite the error on $k(T)$, the equilibrium value of n_A is known:

$$n_A^* = n_A^{eq}(T^*) = \delta \frac{C_A^{in} V}{\delta + k(T)} \neq \delta \frac{C_A^{in} V}{\delta + \hat{k}(T)}$$

Assumption 2. Despite the error on $k(T)$, the equilibrium value of the control input u^* is known:

$$\begin{aligned} u_c^* &= -\delta (T_{in} - T^*) - \gamma k(T^*) n_A^* \\ &\neq -\delta (T_{in} - T^*) - \gamma \hat{k}(T^*) n_A^* \end{aligned}$$

Assumption 3. The control input has been designed such that, based on the estimated value of the kinetic coefficient, the desired equilibrium is asymptotically stable.

From (14), the control input applied to the system is given by the following expression:

$$\begin{aligned} u_c(T_w - T) &= \mu \left(n_A^* - n_A - \int_{T^*}^T \hat{w}(\tau) d\tau \right) + u_c^*(T_w - T^*) \end{aligned}$$

where we have introduced the following notation, for the sake of clarity: $\hat{w}(T) = w(\hat{k}(T))$. Assumptions 1 and 2 imply that (n_A^*, T^*) is still an equilibrium of the closed-loop system. Assumption 3 implies that the function $w(y)$ and the parameter μ have been chosen such that the following matrix is negative definite:

$$\hat{\Lambda} = \begin{pmatrix} -(\delta + \hat{k}^*) & -n_A^* \frac{d\hat{k}}{dT} \Big|_{T^*} \\ \gamma \hat{k}^* - \mu & -\delta + \gamma n_A^* \frac{d\hat{k}}{dT} \Big|_{T^*} - \mu \hat{w}(T) \end{pmatrix}$$

$\hat{\Lambda}$ is the matrix of the linearized system around the desired equilibrium state if the kinetics was indeed equal to $\hat{k}(T)$. As a consequence we have:

$$\text{tr } \hat{\Lambda} < 0 \quad \text{and} \quad \det \hat{\Lambda} > 0$$

The actual matrix of the linearized system around (n_A^*, T^*) is written as follows:

$$\Lambda = \begin{pmatrix} -(\delta + k^*) & -n_A^* \frac{dk}{dT} \Big|_{T^*} \\ \gamma k^* - \mu & -\delta + \gamma n_A^* \frac{dk}{dT} \Big|_{T^*} - \mu \hat{w}(T) \end{pmatrix}$$

The trace and the determinant of Λ are given by the following relations:

$$\text{tr } \Lambda = \Psi^* - \delta - \mu \hat{w}(T^*)$$

$$\det \Lambda = -\delta \Psi^* + \mu \left[(\delta + k^*) \hat{w}(T^*) - n_A^* \frac{dk}{dT} \Big|_{T^*} \right]$$

with

$$\Psi^* = -(k^* + \delta) + \frac{dk}{dT} \Big|_{T^*} \gamma n_A^* \quad (18)$$

Using (17), we can define the following quantity $\hat{\Psi}^*$ by analogy with (18):

$$\begin{aligned} \hat{\Psi}^* &= \gamma n_A^* \frac{d\hat{k}}{dT} \Big|_{T^*} - (\hat{k}^* + \delta) \\ &= \Psi^* (1 + \xi^*) + \gamma n_A^* k^* \frac{d\xi}{dT} \Big|_{T^*} + \delta \xi^* \end{aligned}$$

where $\xi^* = \xi(T^*)$. As a consequence the trace and the determinant of $\Lambda^{(cl)}$ can be rewritten as follows:

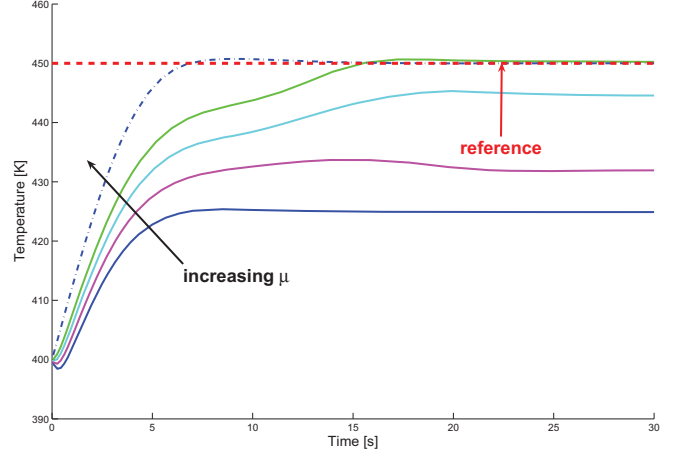


Fig. 9. Influence of the modelling error on $k(T)$ for different values of μ

$$\begin{aligned} (1 + \xi^*) \text{tr } \Lambda &= \underbrace{\hat{\Psi}^* - \delta - \mu \hat{w}(T^*)}_{\text{tr } \hat{\Lambda}^{(cl)} < 0} \\ &\quad - \left[\frac{d\xi}{dT} \Big|_{T^*} \gamma k^* n_A^* + 2\xi^* \delta + \mu \xi^* \hat{w}(T^*) \right] \end{aligned}$$

By applying the same development on the determinant, the following expression is obtained:

$$\begin{aligned} (1 + \xi^*) \det \Lambda &= \det \hat{\Lambda} + \xi^* \delta (\delta + \mu \hat{w}(T^*)) \\ &\quad + n_A^* k^* \frac{d\xi}{dT} \Big|_{T^*} (\gamma \delta + \mu) \end{aligned}$$

The closed-loop equilibrium is asymptotically stable if and only if the trace is strictly negative and the determinant is strictly positive. Using the inequalities of Assumption 3, this means that if $\xi^* > 0$ and $\frac{d\xi}{dT} \Big|_{T^*} \geq 0$, the closed-loop equilibrium is asymptotically stable. But if these two conditions are not fulfilled, then the closed-loop equilibrium can become unstable. Nevertheless, if the function $w(y)$ has been taken sufficiently large such that:

$$(\delta + k^*) \hat{w}(T^*) - n_A^* \frac{dk}{dT} \Big|_{T^*} > 0$$

then $\det \Lambda^{(cl)}$ is increasing with μ such that there is a lower bound on μ that ensures the local asymptotic convergence (see Figure 9).

6. EXTENSION TO MORE COMPLEX SYSTEMS

The power-shaping approach has given interesting results on the simplified CSTR case study. It is therefore of major interest to see if this approach can be extended to more complex systems, and more particularly to systems with more than one reacting chemical species and/or with multiple reactions.

We keep the same assumptions as before, but we consider more complex kinetics. Under these assumptions, the general form of the dynamics of a non-isothermal CSTR can be deduced from (8).

Let us now consider a CSTR with N_r independent reactions. From all the chemical species in the mixture, it is only necessary to consider those that intervene in the

kinetics of the reactions. Let N_c be the number of chemical species which intervene in the expression of the reaction kinetics. For each species i the time evolution is given by the following differential equation (with $i = 1, \dots, N_c$):

$$\frac{dn_i}{dt} = \delta(C_i^{in}V - n_i) + \sum_{l=1}^{N_r} \Gamma_{il}r_l(T, n) \quad (19)$$

where Γ_{il} is the stoichiometric coefficient of species i in the reaction l . The temperature dynamical equation becomes as follows:

$$\frac{dT}{dt} = \delta(T^{in} - T) + \sum_{l=1}^{N_r} \gamma_l r_l(T, n)$$

where $\gamma_l = \frac{(-\Delta_r H)_l}{\rho c_p V}$ and $(-\Delta_r H)_l$ is the reaction heat of the reaction l . The time evolution equations of n_A and T have a similar form and the dynamics of the system can be written as follows (see Dochain et al. (1992)):

$$\frac{dx}{dt} = \delta(x^{in} - x) + \Gamma r(x) \quad (20)$$

where $x = [n_A, \dots, n_{N_c}, T]^t$, $\Gamma \in \mathbb{R}^{N_c+1} \times \mathbb{R}^{N_r}$ is a matrix that contains the stoichiometric coefficient of species i in the reaction l in position (i, l) if $1 \leq i \leq N_c$ and that contains γ_l in the l^{th} column if $i = N_c + 1$.

We shall now apply the same approach as in Section 4, i.e. we shall first look for a matrix $Q(x)$ that fulfills the conditions (2) and (4). By using (20), we have the following relations ($i, j = 1, \dots, N_c + 1$):

$$(Q(x) f(x))_i = \sum_{k=1}^{N_c+1} q_{ik} (\delta(x_k^{in} - x_k) + \Gamma_{kl}r_l(x))$$

and thus:

$$\begin{aligned} (\nabla(Q(x) f(x)))_{ij} &= -\delta q_{ij} + \sum_{k=1}^{N_c+1} \left[q_{ik} \sum_{l=1}^{N_r} \Gamma_{kl} \frac{\partial r_l}{\partial x_j} \right] \\ &+ \sum_{k=1}^{N_c+1} \frac{\partial q_{ik}}{\partial x_j} (\delta(x_k^{in} - x_k) + \Gamma_{kl}r_l(x)) \end{aligned}$$

Consequently, condition (4) can be rewritten as follows:

$$\begin{aligned} &-\delta q_{ij} + \sum_{k=1}^{N_c+1} \left[q_{ik} \sum_{l=1}^{N_r} \Gamma_{kl} \frac{\partial r_l}{\partial x_j} \right] \\ &+ \sum_{k=1}^{N_c+1} \frac{\partial q_{ik}}{\partial x_j} (\delta(x_k^{in} - x_k) + \Gamma_{kl}r_l(x)) \\ &= -\delta q_{ji} + \sum_{k=1}^{N_c+1} \left[q_{jk} \sum_{l=1}^{N_r} \Gamma_{kl} \frac{\partial r_l}{\partial x_i} \right] \\ &+ \sum_{k=1}^{N_c+1} \frac{\partial q_{jk}}{\partial x_i} (\delta(x_k^{in} - x_k) + \Gamma_{kl}r_l(x)) \end{aligned} \quad (21)$$

for all $i, j = 1, \dots, N_c + 1$.

In the simplified CSTR case, we have first restricted the set of possible matrices $Q(x)$ to find a solution for (4) by transforming the partial differential equation into an algebraic one which is simpler to solve. The same can be done in the more complex case by adequately restricting the set of possible solutions.

A general solution of the algebraic form of (21) has not been found yet. Despite of this, some characteristics of the

solution (if it exists) have already been derived in Favache and Dochain (2008). We shall now look at some particular cases of more complex reactions to get a first intuition of the existence of non-singular and negative semi-definite solutions of the algebraic form of (21). The detailed solution for the three particular cases (namely parallel reactions, reactions with two reactants and consecutive reactions) is given in Favache and Dochain (2008). In the three cases it has been assumed that the kinetic functions can be expressed as powers of the concentration of the reactants, i.e.:

$$r_l(n, T) = k_l(T) \prod_{i \in \Theta_l} (n_i)^{\zeta_{il}}$$

where Θ_l is the set of reactants of reaction l and ζ_{il} is some positive constant.

6.1 Parallel reactions and reactions with two reactants

In this case a solution has been found, but the obtained matrix has not a negative semi-definite symmetric part. Thus the corresponding potential function cannot be used as a Lyapunov function for the open-loop system because they are not decreasing along the system trajectories.

As shown in Garcia-Canseco et al. (2008), given a matrix $Q(x)$ that fulfills (4), other solutions to (4) can be built departing from the first one. Applying this methodology on the matrices that have been found could lead to another matrix $Q(x)$ that would be negative-definite and hence give a Lyapunov function for the open-loop system.

Remark 4. In the particular case of parallel reactions with first order kinetics, another solution for the matrix $Q(x)$ has been found. This solution does not exist for higher order kinetics. This particular solution has a very similar form of that of the matrix proposed for the case with one reaction. This seems to indicate that the matrix $Q(n_A, T)$ that has been used in Section 4 is a particular solution of (9) that exists only in the case of first-order kinetics.

6.2 Consecutive reactions

In this case the algebraic form of (21) has no non-singular solution. This does not mean that the dynamics cannot be put into the Brayton-Moser form. But if the Brayton-Moser form exists, then the partial differential equation (21) has to be solved.

7. CONCLUSION

A general description of the power-shaping control approach of the CSTR has been given in this paper. The main results that were obtained by this approach have been presented and illustrated by some simulation results. A detailed mathematical analysis is provided in Favache and Dochain (2008). Contrary to previous works and approaches, a global Lyapunov function for the exothermic CSTR has been found using the power-shaping approach. This Lyapunov function could then be used to design a controller for stabilizing the reactor at a desired temperature. Some results about the local and global convergence of the controller have also been shown.

The Lyapunov function that was found is the potential function of the Brayton-Moser formulation of the CSTR

dynamics. Although the potential function has a physical meaning for the Brayton-Moser formulation of electrical or mechanical systems, a precise physical interpretation of the potential function of the CSTR has still to be found. This interpretation should give more physical insight on the reasons of the existence of multiple open loop equilibria, and also on the action of the controller.

The controller obtained by the power-shaping control approach depends on the on-line measurements of the concentration and of the knowledge on the reaction kinetics. Both quantities are usually not exactly known. We have shown, that if the parameters of the controller are adequately chosen, the control action is robust with respect to modeling errors on the kinetics. But a robustness study on the influence of the concentration measurement errors should also be of great interest before applying it to a real reactor.

Finally we studied the possibility of extending the previous work to more complex systems, and more precisely to CSTRs with multiple reactions and/or multiple reactants. The extension seems to be rather complex, even for simple cases such as two parallel reactions or two consecutive reactions with mass action law kinetics. Indeed, in the simple CSTR case with a single first-order kinetics reaction, the solution of the partial differential equation needed to write the system dynamics in the Brayton-Moser form has been found by transforming it into an algebraic one. For the three considered particular cases the corresponding algebraic equation system has either no non-singular solution (consecutive reactions) or an indefinite solution (parallel reactions, reaction with two reactants). The study presented here is only embryonic since it does not imply that the power-shaping control approach cannot be applied. But the Brayton-Moser form of the dynamics (if it exists) actually needs the solution of the partial differential equation, and not of its simplified version which is the algebraic equation. Nevertheless in the cases where an indefinite matrix has been found, the work presented in Garcia-Canseco et al. (2008) offers the possibility of finding an alternative negative semi-definite matrix without having to solve the partial differential equation. Also in this study we have only considered a particular form of the kinetics, namely we have assumed that the kinetics can be written as a product of powers of the concentration (i.e. a more general form of the mass action law) and a kinetic term. This is only a restricted class of the possible kinetic laws. Indeed it could also be interesting to apply the power-shaping control to other forms of kinetics such as the Monod kinetics (biological systems) or the Michaelis-Menten kinetics (enzymatic reactions), for instance.

ACKNOWLEDGEMENTS

This paper presents research results of the Belgian Network DYSCO (Dynamical Systems, Control, and Optimization), funded by the Interuniversity Attraction Poles Programme, initiated by the Belgian State, Science Policy Office. The scientific responsibility rests with its authors.

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