Automatica 46 (2010) 1877–1883

Contents lists available at ScienceDirect

Automatica

journal homepage: www.elsevier.com/locate/automatica

Brief paper

Power-shaping control of reaction systems: The CSTR case☆

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ARTICLE INFO

Article history:
Received 12 October 2009
Received in revised form
16 April 2010
Accepted 1 July 2010
Available online 25 August 2010

Keywords:
Nonlinear dynamical systems
Non-isothermal CSTR
Power-shaping control
Brayton–Moser form

ABSTRACT

Power-shaping control is a recent approach for the control of nonlinear systems based on the physics of the dynamical system. It rests on the formulation of the dynamics in the Brayton–Moser form. One of the main obstacles for using the power-shaping approach is to write the dynamics in the required form, since a partial differential equation system submitted to sign constraints has to be solved. This work comes within the framework of control design approaches that could possibly generate a closer link between the notions of energy that are specific to reaction systems as derived from thermodynamics concepts, and the dynamic system stability theory. The objective of this paper is to address the design of power-shaping control to reaction systems, and more particularly the step of solving the partial differential equation system. In order to illustrate the approach, we have selected the classical yet complex continuous stirred tank reactor (CSTR) as a case study. We show how using the power-shaping approach leads to a global Lyapunov function for the unforced exothermic CSTR. This Lyapunov function is then reshaped by means of a controller in order to stabilize the process at a desired temperature.

1. Introduction

Nonlinear dynamical systems can 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 recent 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 & van der Schaft, 1998), energy-balancing passivity based control (PBC) (Jeltsema, Ortega, & Scherpen, 2004; Ortega, van der Schaft, Mareels, & Maschke, 2001) or the introduction of the contact formalism for expressing the dynamics of systems in which irreversible phenomena arise (Eberard, Maschke, & van der Schaft, 2007; Favache, Maschke, & Dochain, 2007).

Power-shaping control (Ortega, Jeltsema, & Scherpen, 2003) has been developed in recent years as an extension of energy-balancing PBC (Jeltsema et al., 2004; Ortega et al., 2001) and has been applied to electro-mechanical systems (Maschke, Ortega, & van der Schaft, 2000; Ortega, van der Schaft, Maschke, & Escobar, 2002) and to thermodynamic systems (Alonso, Ydstie, & Banga, 2002; Otero-Muras, Szederkényi, Alonso, & Hangos, 2006). However this control approach cannot be applied to systems with pervasive dissipation. To overcome this difficulty power-shaping control has been introduced, firstly for the stabilization of nonlinear RLC circuits (Ortega et al., 2003). Contrary to energy-balancing PBC, 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 electromechanical systems (García-Canseco, Jeltsema, Ortega, & Scherpen, 2010).

The central objective of this work is to come with control design approaches that could possibly generate a closer link between the notions of energy that are specific to reaction systems as derived from thermodynamics concepts, and the dynamic system stability theory. Thermodynamic systems, and among them chemical reaction systems, are usually nonlinear dynamical systems. The non-isothermal continuous stirred tank reactor (CSTR) is clearly the most representative example of such a system in dynamical system theory. In particular its dynamical behaviour exhibits complex features, such as multiple equilibrium points. Up to now no precise physical interpretation of the complex behaviour of the non-isothermal reactor has been found (Favache & Dochain, 2009c). Hence the power-shaping approach seems to offer a promising way to achieving this objective.

☆ 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. The work of A. Favache has been funded by a grant of aspirant of Fonds National de la Recherche Scientifique (Belgium). The material in this paper was partially presented at ADCHEM, July 12–15, 2009, Istanbul, Turkey. This paper was recommended for publication in revised form by Associate Editor Michael A. Henson under the direction of Editor Frank Allgöwer.

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doi:10.1016/j.automatica.2010.07.011

Model-predictive control (MPC) has been widely applied for process control in recent decades. The MPC objective function serves naturally as a closed-loop Lyapunov function (Mayne, Rawlings, Rao, & Scokaert, 2000). However, it is not linked to physical phenomena and it does not give information about the unforced system. As we shall see in our study case, the potential function of the Brayton–Moser formulation is a Lyapunov function candidate for the unforced system. This potential function has been given a physical interpretation in the case of electro-mechanical systems.

This paper is concerned with the design of power-shaping control for reaction systems. The main obstacle for using the power-shaping approach is to write the dynamics in the required form because it needs the solution of a partial differential equation (PDE) system submitted to sign constraints. We shall propose an approach for circumventing this difficulty and illustrate it on our particular study case. First we shall briefly introduce the concepts of the power-shaping approach in Section 2. Then in Section 3 we present the dynamics of our study case. We shall then present our approach for obtaining the Brayton–Moser form of the CSTR, which consists in finding a solution to the Brayton–Moser partial differential equation system, starting from the mathematical dynamical model (Section 4). The obtained Brayton–Moser form shall then be used to design a control system for the CSTR using the power-shaping approach.

2. Power-shaping control[1]

2.1. The Brayton–Moser formulation

Let us consider a dynamic 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 $u_c \in \mathbb{R}^m$. The power-shaping control theory is based on the Brayton–Moser formulation of the system dynamics (Brayton & Moser, 1964). In this formulation the system dynamics are of following form:

$$\mathbf{Q}(x)\frac{\mathrm{d}x}{\mathrm{d}t} = \nabla\mathscr{P}(x) + G(x)u_c \tag{1}$$

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

$$\mathbf{Q}(x) + \mathbf{Q}^t(x) \preceq 0. \tag{2}$$

The function $\mathscr{P}(x)$ is called the potential function. In electrical and mechanical systems, it has the units of power and is related to the dissipated power in the system. In the first one it is related to the so-called content and co-content of the resistances (Jeltsema & Scherpen, 2007; Ortega et al., 2003); in the latter it is related to the Rayleigh dissipation function (Jeltsema &, 2003).

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

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x) + g(x)u_c \tag{3}$$

where $f(x) : \mathbb{R}^N \to \mathbb{R}^N$ and $g(x) : \mathbb{R}^N \to \mathbb{R}^N \times \mathbb{R}^m$. The system (3) can be written in the form (1) if there exists a non-singular matrix $\mathbf{Q}(x)$ fulfilling (2) and that solves the following PDE system[2]:

$$\nabla(\mathbf{Q}(x)f(x)) = \nabla^t(\mathbf{Q}(x)f(x)). \tag{4}$$

$\mathscr{P}(x)$ is then the solution of the following PDE system:

$$\nabla\mathscr{P}(x) = \mathbf{Q}(x)f(x) \tag{5}$$

and the function $G(x)$ is given by $G(x) = \mathbf{Q}(x)g(x)$.

2.2. Power-shaping control

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

$$\mathbf{Q}(x)\frac{\mathrm{d}x}{\mathrm{d}t} = \nabla\mathscr{P}_d(x) \tag{6}$$

where $\mathscr{P}_d(x) : \mathbb{R}^N \to \mathbb{R}$ is the re-shaped potential function. The desired equilibrium x^* must be a local minimum of the potential function $\mathscr{P}_d(x)$ in order to be locally asymptotically stable. The function $\mathscr{P}_d(x)$ can be used as a Lyapunov function for the closed-loop system.

The function $\mathscr{P}_d(x)$ cannot be chosen arbitrarily since the following relation must be fulfilled:

$$g^{\perp}(x)\mathbf{Q}^{-1}(x)\nabla\mathscr{P}_a(x) = 0 \tag{7}$$

where $\mathscr{P}_a(x) = \mathscr{P}_d(x) - \mathscr{P}(x)$ and $g^{\perp}(x)$ is a full-rank left annihilator of $g(x)$.[3] Under these conditions, the control input $u_c(x)$ that re-shapes $\mathscr{P}(x)$ into $\mathscr{P}_d(x)$ is the following one:

$$u_c(x) = (g^t(x)\mathbf{Q}^t(x)\mathbf{Q}(x)g(x))^{-1}g^t(x)\mathbf{Q}^t(x)\nabla\mathscr{P}_a(x). \tag{8}$$

Remark 1. One may note that the above proposed control law is not defined if $g^t(x)\mathbf{Q}^t(x)\mathbf{Q}(x)g(x) = 0$. Due to the non-singularity of the matrix $\mathbf{Q}(x)$, this is the case if and only if $g(x) = 0$. Hence this implies that whatever the value of $u_c(x)$ it does not influence the state dynamics (3). One can therefore choose any value for $u_c(x)$.

3. The CSTR case study

Contrary to previous work which focused mostly on electro-mechanical systems, we have chosen to illustrate the power-shaping approach on an example from chemical engineering, namely the non-isothermal CSTR. This study case is a benchmark example both in chemical engineering and in dynamical system theory due to its highly nonlinear dynamics. In this section we shall introduce our dynamical model. Unlike the model version commonly used in control theory, it is built directly from thermodynamic considerations, and is the most exact one from a thermodynamic point of view. However, in some cases, it shall be necessary to turn to a simplified version of it, which corresponds to the more usual CSTR model used in system theory.

Let us consider a liquid-phase CSTR with constant volume V containing N_c species and in which N_r reactions take place. The reactor is cooled/heated by a surrounding jacket. As has been shown in Favache and Dochain (2009c) the dynamics of such a system are given by the following relations:

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \frac{F}{V}(C_i^{in}V - n_i) + \sum_{l=1}^{N_r}\Gamma_{il}r_l(T, n) \tag{9a}$$

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \frac{F}{V}(h^{in}V - H) + \dot{Q} \tag{9b}$$

[1] The statements in this section are given without any proof. For more details, the reader can refer to García-Canseco et al. (2010), Jeltsema and Scherpen (2007), Ortega et al. (2003) and Scherpen (2003).

[2] This condition is equivalent to the existence of $\mathscr{P}(x)$.

[3] i.e. $g^{\perp}(x) : \mathbb{R}^N \to \mathbb{R}^{N-m} \times \mathbb{R}^N$ such that $g^{\perp}(x)g(x) = 0$ with $\mathrm{rank}(g^{\perp}(x)) = N - m$.