Cascade control of a class of chemical reactors based on entropy production shaping [*]

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Abstract: On this contribution a cascade control for a class of continuous chemical reactors is presented. Given that the internal entropy production of the reacting systems under study can be considered as a storage function, the inner loop is designed to shape the entropy production using the outflow rate as the control variable. The tracking reference for the entropy production of the inner loop is computed by an outer loop that regulates a typical process variable such as temperature or pressure inside the reactor. In the resulting cascade control structure, the inner loop guarantees the stability of the reacting system, while the outer loop can be used to fulfil safety or operational conditions.

Keywords: Port-controlled Hamiltonian systems, Thermodynamics, Cascade control, Chemical reactor

1. INTRODUCTION

The concept of dissipation proposed by Willems (1972) has been useful to model dynamical systems that represent open physical processes where the energy plays a central role. Its main statement is that the energy consumed by an open system should be less or equal than the input. Numerous examples of dissipative systems have been analyzed and their thermodynamic properties have been used for process control purposes and stability analysis with continuous reacting systems as the main challenge (Bao and Lee, 2007; Dammers and Tels, 1974; Favache and Dochain, 2009, 2010; Hoang et al., 2011; Otero-Muras et al., 2008; Ramírez et al., 2013). In particular, the interest on analyzing this class of reacting systems with emphasis on the reaction rates has grown, thus leading to several approaches (García-Sandoval et al., 2016; Hoang et al., 2014; Hudon et al., 2015). In this regard, it has been shown that the internal entropy production of a class of thermodynamically consistent models of continuous chemical reactors can be used as a storage function to analyze its stability and passivity properties (García-Sandoval et al., 2015).

It is well known that passive systems have a relative degree equal to one with respect to the storage function and output ports, and if the passive system is also zero-state detectable, then it is easy to find reduced order passivity-based controllers (PBC) to stabilize a given equilibrium point. Two common PBC approaches are energy shaping and power shaping. There are several ways to achieve energy shaping, the most physically appealing is the so-called energy-balancing PBC (or control by interconnection) method (Ortega et al., 2002; van der Schaft, 2000). However this method cannot be applied when the system has persistent dissipation and in this case it has been proposed an alternative methodology called power shaping where, as suggested by its name, stabilization is achieved shaping a function similar to power instead of the energy function (Ortega et al., 2003).

These two PBC approaches have been successfully applied to mechanical and electrical systems, because the interconnection ports are easily correlated with forces, currents and voltages. However, for thermodynamical systems with mass flows the energy and power shaping methodologies cannot be directly applied because the interconnection ports may not be correlated with energetic or power variables. To solve this problem, based on the formalism of an extension to nonequilibrium thermodynamics (Kjelstrup et al., 2010), it has been suggested a methodology called *entropy production shaping* (García-Sandoval et al., 2016), analogue to power shaping (but with units of power/temperature), which is the natural extension to include momentum, energy (electrical, kinetic and internal) and mass flows in the interconnection ports.

On the other hand, cascade control schemes have been used for more than 60 years to improve the performance of closed loop systems (Franks, 1956), mainly because these schemes are able to compensate the effect of strong disturbances and time delays (Zhang et al., 2015), and nowadays are commonly used to regulate typical process variables, such as flow, pressure or temperature (Kaya et al., 2007; Ramírez-Castelán et al., 2016). Although there are many configurations, the basic cascade control structure consists on two control loops: an inner (or secondary) loop embed-
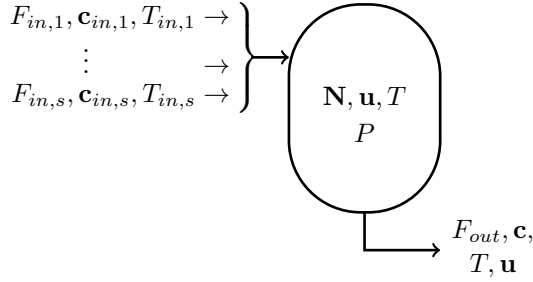
Fig. 1. Reaction system.

ded into an outer (or primary) loop. In many cases, the inner loop focuses on guaranteeing the process stability by regulating key process variables around a reference signal provided by the outer loop, that is designed to fulfill some predetermined performance index. Several approaches have been used to design cascade control schemes, mainly based on classical control techniques for linear systems with PI and/or PID controllers, for both, the inner and outer loop (see, e.g. Hua et al., 2004; Jeng, 2012; Lee et al., 2002, 1998; Leva and Donida, 2009; Nandong and Zang, 2014).

On this contribution, based on the approach proposed in (García-Sandoval et al., 2015), a cascade control for a class of continuous chemical reactors based on passivity techniques is presented. The proposed cascade algorithm uses the internal entropy production as a storage function that is regulated in the inner loop, while the outer loop regulates a typical process variable such as temperature, or pressure inside the reactor. This document is organized as follows: The reactor model and its passivity properties are presented in Section 2, then in Section 3 the cascade control scheme is proposed and, finally, this control scheme is tested via numerical simulations in Section 4.

2. REACTING SYSTEM

2.1 System description

Consider a single phase, adiabatic, perfectly mixed, continuous chemical reactor with constant volume, V, as depicted in Figure 1. The reacting system contains n chemical species, where $k + l$ of these species participate in the reversible chemical reaction

$$\boldsymbol{A}^{\mathrm{T}}\mathbf{E} \rightleftharpoons \boldsymbol{B}^{\mathrm{T}}\mathbf{E} \qquad (1)$$

where $\mathbf{E} = \mathrm{col}\{E_1, \ldots, E_n\}$ is the vector of chemical species, while $\boldsymbol{A} = \mathrm{col}\{\alpha_1, \ldots, \alpha_k, \mathbf{0}\}$ and $\boldsymbol{B} = \mathrm{col}\{\mathbf{0}, \beta_1, \ldots, \beta_l\}$ are the stoichiometric coefficients for the k reactants and l products, respectively.

Since the process is isochoric, the state of reacting system can be described by the extensive properties $\boldsymbol{\eta} = \mathrm{col}\{\mathbf{N}, U\}$, where $\mathbf{N} \in \mathbb{R}^n_{\geq 0}$ is the mole vector and $U = \mathbf{u}^{\mathrm{T}}\mathbf{N} \in \mathbb{R}$ is the total internal energy, with $\mathbf{u}$ as the vector of molar internal energies of each species. In order to derive simpler expressions and without any loss of generality, in this work it is considered that all species are ideal gases that obey the state equation $PV = \mathbf{1}^{\mathrm{T}}\mathbf{N}RT$, where $\mathbf{1} \in \mathbb{R}^n$ is a vector of ones and P and T are the pressure and temperature inside the reactor, respectively.

2.2 Mass, energy and entropy balances

Due to the perfectly mixed assumption, the chemical reactor does not have spatial gradients. Then, the mass balance is given by

$$\dot{\mathbf{N}} = \boldsymbol{\Gamma}Vr + \sum_{i=1}^{s}\mathbf{c}_{in,i}F_{in,i} - \mathbf{c}F_{out}, \qquad (2)$$

where $\boldsymbol{\Gamma} = \boldsymbol{B} - \boldsymbol{A}$ is the stoichiometric vector, $r : \mathbb{R}^{n+1} \to \mathbb{R}$ is the rate of reaction per unit of volume, $\mathbf{c}_{in,i} \in \mathbb{R}^n_{\geq 0}$ is the concentration vector of the ith surrounding entering at $F_{in,i} \in \mathbb{R}_{\geq 0}$ volumetric flow, while $\mathbf{c} = \mathbf{N}/V$ is the reactor concentration vector and $F_{out} \in \mathbb{R}_{\geq 0}$ is the total volumetric outflow rate. On the other hand, the internal energy balance under the adiabatic assumption is

$$\dot{U} = \sum_{i=1}^{s}h_{in,i}F_{in,i} - hF_{out}, \qquad (3)$$

where $h_{in,i}$ is the specific total enthalpy of the ith surrounding, while $h = u + P$ is the total enthalpy per unit of volume and $u = U/V = \mathbf{u}^{\mathrm{T}}\mathbf{c}$. Then, the dynamic behavior of the state variables, $\boldsymbol{\eta} = \mathrm{col}\{\mathbf{N}, U\}$, is

$$\dot{\boldsymbol{\eta}} = MVr + \boldsymbol{g}\mathbf{F}_{in} + \Psi\boldsymbol{\eta}F_{out} \qquad (4)$$

where $\boldsymbol{g} = (\varphi_{in,1} \cdots \varphi_{in,s})$, with $\varphi_{in,i} = \mathrm{col}\{\mathbf{c}_{in,i}, h_{in,i}\}$, $\mathbf{F}_{in} = \mathrm{col}\{F_{in,1}, \ldots, F_{in,s}\} \in \mathbb{R}^s_{\geq 0}$ is the vector of volumetric inflow rates, $M^{\mathrm{T}} = (\Gamma^{\mathrm{T}} \ 0)$ and

$$\Psi = \frac{1}{V}\begin{pmatrix} \mathbf{I}_n & \mathbf{0} \\ RT\mathbf{1}^{\mathrm{T}} & 1 \end{pmatrix},$$

where $\mathbf{I}_n$ is a $n \times n$ identity matrix and $\mathbf{0}$ is a null vector.

According to the postulates of thermodynamics, the entropy $S(\boldsymbol{\eta})$ is a scalar function at least two times differentiable and, assuming local equilibrium (Demirel, 2014), the differential behavior of the entropy can be computed through the Gibbs relation, that for isochoric systems reads

$$dS = \frac{1}{T}dU - \frac{\boldsymbol{\mu}^{\mathrm{T}}}{T}d\mathbf{N}, \qquad (5)$$

where $T \in \mathbb{R}_+$ is the absolute temperature, $\boldsymbol{\mu} \in \mathbb{R}^n$ is the vector of the chemical potentials defined as $\boldsymbol{\mu} = \boldsymbol{\mu}^{\mathrm{o}} + \ln(\mathbf{a})$, with $\boldsymbol{\mu}^{\mathrm{o}}$ as the vector of standard chemical potentials and $\ln(\mathbf{a})$ as the vector of the logarithm of the activities.

The entropy gradient is defined as

$$\boldsymbol{\zeta} := \left[\frac{\partial S(\boldsymbol{\eta})}{\partial \boldsymbol{\eta}}\right]^{\mathrm{T}} \in \mathbb{R}^{n+1}, \qquad (6)$$

so Equation (5) can be rewritten as $dS = \boldsymbol{\zeta}^{\mathrm{T}}d\boldsymbol{\eta}$, where the entropy gradient has been identified as $\boldsymbol{\zeta} = \mathrm{col}\{-\boldsymbol{\mu}/T, 1/T\}$, which is the intensive properties vector, conjugate to $\boldsymbol{\eta}$. In particular, for isochoric ideal gas systems their thermodynamic properties can be easily computed: $\boldsymbol{\mu}^{\mathrm{o}} = \mathbf{u} - T\left(\mathbf{s}_{ref} - \mathbf{1}R + \int_{T_{ref}}^{T}\frac{\mathbf{c}_v}{T}dT\right)$, $\ln(\mathbf{a}) = \ln(\mathbf{N}/N_{ref})$, and $\mathbf{u} = \mathbf{u}_{ref} + \int_{T_{ref}}^{T}\mathbf{c}_v dT$. Also, the Hessian of the entropy, $\Omega := \partial\boldsymbol{\zeta}/\partial\boldsymbol{\eta}$, is

$$\Omega = \begin{pmatrix} -\left(\frac{\mathbf{u}\mathbf{u}^{\mathrm{T}}}{\mathbf{N}^{\mathrm{T}}\mathbf{c}_v T^2} + R\left[\mathrm{diag}\left(\mathbf{N}\right)\right]^{-1}\right) & \frac{\mathbf{u}}{\mathbf{N}^{\mathrm{T}}\mathbf{c}_v T^2} \\ \frac{\mathbf{u}^{\mathrm{T}}}{\mathbf{N}^{\mathrm{T}}\mathbf{c}_v T^2} & -\frac{1}{\mathbf{N}^{\mathrm{T}}\mathbf{c}_v T^2} \end{pmatrix} < 0,$$