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Stability analysis and passivity properties of a class of thermodynamic processes: An internal entropy production approach

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HIGHLIGHTS

- Global stability and passivity are studied for a class of thermodynamical processes.
- Processes may be composed of several spatially homogeneous subsystems.
- Chemical reactions and mass and heat transfer flows among subsystem are considered.
- The overall system may interact with surroundings through convective flows.
- Internal entropy production as Lyapunov/storage function for isolated/open processes.

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ABSTRACT

In this contribution, stability and passivity properties of a class of thermodynamic processes are addressed from a thermodynamical point of view. These thermodynamic processes can be constituted by multiple spatially homogeneous dynamic subsystems modeled by ordinary differential equations. It is shown that the internal entropy production may be used as a Lyapunov function candidate to prove the isolated system stability properties and as a storage function to assess the passivity properties when the system interacts with the surroundings. In addition, it is shown that the stability condition depends on a matrix whose dimension is equal to the number of modeled dynamical phenomena taking place within the system, i.e. the number of phenomena can be smaller than the system dimension. Moreover, a port-controlled Hamiltonian representation of this class of systems based on the internal entropy production is developed. Finally, the theory proposed is applied to three study cases: a heat exchanger, a ideal gas adiabatic chemical reactor and a ideal gas jacketed chemical reactor.

1. Introduction

Dissipative structures are a concept which has been used in physics to discuss the formation of structures organized in space and/or time at the expense of the energy flowing into the system from the outside (Willems, 1972a,b). In fact, by invoking the universal principle of energy conservation, it may be argued that all physical systems are dissipative with respect to some suitable variables that couple the system to the environment (Garcia-Canseco et al., 2010). The space–time structural organization of biological systems starting from the subcellular level up to the level of ecological systems, coherent structures of laser and plasma physics, problems of elastic stability in mechanics, instability of hydrodynamics leading to the development of turbulence, behavior of electrical networks and chemical reactors form a short list of problems treated in this framework (Kubicek and Marek, 1983).

In principle, dissipative structures are maintained at the expense of energy flowing from the outside and hence, one should deal with systems that are generally far from equilibrium with the inherent stability problems that have been addressed by a number of approaches from local stability analysis to system theory. In recent years the stability of dissipative systems has been addressed by combining irreversible thermodynamics and systems theory. For instance, Dammers and Tels (1974), based on the Brussels school of thermodynamics (Glansdorff and Prigogine, 1971), proposed a suitable potential function related to Prigogine's velocity potential to state a stability criterion in adiabatic stirred flow

Abbreviation: CSTR, Continuous stirred tank reactor; PCH, Port-Controlled Hamiltonian

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reactors. Tarbell (1977) has proposed a Lyapunov function for continuous stirred tank reactor (CSTR) with a steady state near the equilibrium point, that resembled the thermodynamical entropy production function, while Georgakis (1986) suggested the use of extensive rather than intensive variables for process control purposes. More recently, Alonso, Ydstie and coworkers have explored this research area, that resulted in very insightful works on the control design of process systems (see e.g. Alonso and Ydstie, 1996, 2001; Alonso et al., 2002; Balaji et al., 2010; Coffey et al., 2000; Ydstie, 2002; Ydstie and Alonso, 1997) to develop stabilizing mass and energy inventory controllers (Farschman et al., 1998) and to derive general structural stability conditions for chemical process networks (Antelo et al., 2007; Baldea et al., 2013; Hangos et al., 1999; Hioe et al., 2013), where, in addition to the concept of inventories, nonlinear extensions of the curvature of the entropy function called availability have been used as it has been proposed within the framework of passivity theory for processes (Ydstie and Alonso, 1997), while in Hangos et al. (2001, 2004), passivity and feedback passivation of chemical processes were considered from a Hamiltonian point of view. In the particular case of reacting systems, continuous stirred tank reactors (CSTRs) have been the subject of a large number of stability and advanced control studies that can be taken into account by system theory: these systems are usually nonlinear and may exhibit multiple steady states and complex dynamic behavior. The features have been also taken into account to address the stability issue by using a number of thermodynamics based approaches usually limited to (local) stability analysis of single unit operation, i.e. chemical reactors (Balaji et al., 2010; Dammers and Tels, 1974; Favache and Dochain, 2009; Hoang et al., 2011, 2012a,b, 2013; Hoang and Dochain, 2013a,b; Ramirez et al., 2013; Tarbell, 1977); however it appears that even for simple reactions, analysis and control issues using thermodynamic properties are still open problems (Hoang et al., 2012a), for instance global stability analysis, reacting systems with multiple complex reactions (van der Schaft et al., 2015) and the effect of the interconnection of several thermodynamic systems. Among the quantities identified in recent research for stability analysis of closed and open processes, internal entropy production offers some flexibility and recently, García-Sandoval et al. (2015) analyzed the stability and passivity properties of a class of ideal gas chemical reactors considering the internal entropy production as a Lyapunov function candidate in order to prove the isolated reactor stability properties and as a storage function to explore the passivity properties when the reactor interacts with the surroundings.

In this contribution, we extend the results presented in García-Sandoval et al. (2015) to a general case where several interconnected thermodynamic subsystems or units, modeled by spatially homogeneous dynamics that may include internal processes like chemical reactions, interact among them through mass and heat transfer flows and with the surroundings through convective flows. Then, exploiting the fact that the entropy production is (semi)-positive definite and the Hessian of the entropy is (semi)-negative definite, the stability and passivity properties of this class of systems are addressed by using the internal entropy production as a Lyapunov-candidate function when the system is isolated and as a storage function when the system interacts with the surroundings. Then, based on the passivity results, the (quasi-)Port-Hamiltonian representation for the thermodynamical systems in study is obtained a posteriori and is not required to investigate stability. The paper in study is organized as follows. We shall first introduce in Section 2 the fundamental thermodynamical basis related to the intensive and extensive properties of systems as well as their entropy and entropy production. Then in Section 3 the core of the paper is presented; it is shown that the internal entropy production can be considered as a Lyapunov function candidate for the isolated system and conditions to guarantee asymptotic stability are established. Then, the same internal entropy production is used as a storage function when the system interacts with the surroundings in order to show its dissipative or passivity properties depending on the variables that couple the system to the surroundings and the system's quasi-port-controlled Hamiltonian representation is presented. Finally, the theory proposed is applied to three study cases: a heat exchanger, a ideal gas adiabatic chemical reactor and a ideal gas jacketed chemical reactor.

2. Fundamentals of thermodynamics

2.1. Extensive and intensive properties

Let us consider a system Π composed of n subsystems as depicted in Fig. 1. The state of each subsystem is described by a primary vector of non-negative variables called inventories (Farschman et al., 1998) which is a set or subset of extensive properties $\{\mathbf{N}_i, U_i, V_i\}$, and each subsystem also has its associated intensive properties $\{-\boldsymbol{\mu}_i, T_i, P_i\}$ that are dual to inventories, where $\mathbf{N}_i \in \mathbb{R}_+^{C_i}$, $U_i \in \mathbb{R}$ and $V_i \in \mathbb{R}_+$ are the molar, energy and volume inventories, respectively, with C_i being the number of chemical species interacting in the subsystem i, while $\boldsymbol{\mu}_i \in \mathbb{R}_+^{C_i}$, $T_i \in \mathbb{R}_+$ and $P_i \in \mathbb{R}_+$ are the chemical potential, and the absolute temperature and pressure of subsystem i, with $i = 1, 2, \ldots, n$, respectively. Depending on the particular configuration and characteristics of each subsystem, the state variables, $\boldsymbol{\eta}_i \in \mathbb{R}^{\omega_i}$, with $\omega_i \le C_i + 2$, are selected as the total extensive variables ($\omega_i = C_i + 2$) or a subset of them ($\omega_i < C_i + 2$). For instance, if the process is isochoric, then the state variable vector is defined as $\boldsymbol{\eta}_i = \mathrm{col}\{\mathbf{N}_i, U_i\} \in (\mathbb{R}_+^{C_i} \times \mathbb{R})$, while for isochoric systems with only one incompressible fluid or closed isobaric gas systems with variable volume, the state variable is defined as $\eta_i = U_i \in \mathbb{R}$, the only difference in both cases is the state equation used to describe the relation between the pressure, the volume and the moles. In this work it is assumed that each subsystem is spatially homogeneous. It is also considered that system Π interacts with one or more environments. Therefore the dynamical model under study in terms of extensive variables is given by

$$\Pi: \dot{\boldsymbol{\eta}} = Mf(\boldsymbol{\eta}) + g(\boldsymbol{\eta}, \boldsymbol{\eta}_s)\mathbf{F} \tag{1}$$

where $\boldsymbol{\eta} = \mathrm{col}\{\boldsymbol{\eta}_i, i = 1, 2, \ldots, n\} \in \mathbb{R}^{\omega}$, with $\omega = \sum_{i=1}^{n} \omega_i$, and $\boldsymbol{\eta}_s \in \mathbb{R}^s$ representing the vectors of extensive properties of system Π and the surroundings, respectively, while the vector field $f: \mathbb{R}^{\omega} \to \mathbb{R}^p$ is the

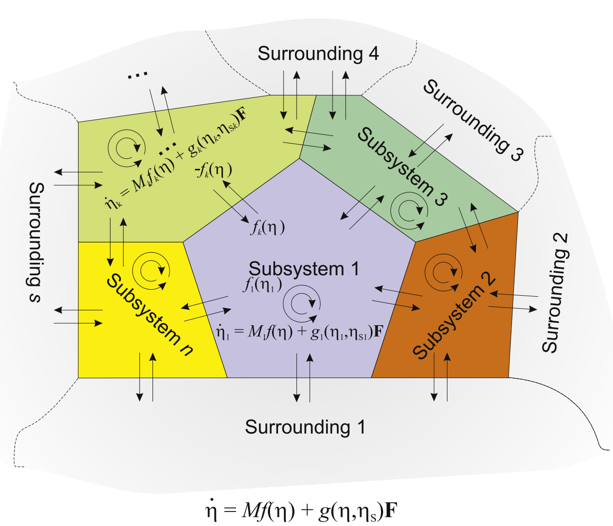

Fig. 1. System Π: Schematic subsystems interconnections and exchange with the surroundings.