



Stability analysis and passivity properties for a class of chemical reactors: Internal entropy production approach

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ABSTRACT

In this contribution, the stability and passivity properties of a class of chemical reactors are addressed from a thermodynamical point of view. For this purpose, a thermodynamical consistent model is derived from a generic gas reactor model whose rate is based on the reaction progress at the mesoscopic scale. It is shown that the internal entropy production may be used as a candidate Lyapunov function to prove the isolated system stability properties and as a storage function to emphasize the passivity properties when the chemical reactor interacts with the surroundings.

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1. Introduction

Dissipative structures is a concept widely used in physics and engineering to address 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 conservative quantities, it may be argued that all physical systems are dissipative with respect to some suitable variables that couple the system to the environment (García-Canseco et al., 2010).

In principle, the term dissipative structures means that the structures are maintained at the expense of energy and/or mass flowing from the outside and hence, one should deal with systems which generally are far from equilibrium with the inherent stability problems that have been addressed by a number of approaches ranging from local stability analysis to system theory. In this regard, it has been shown that many physical processes may be dissipative, including those that obey the laws of thermodynamics (Rojas et al., 2008), since dissipativity, like irreversibility in a thermodynamic system, captures the idea that something dissipates as resources are transformed into products. In addition, in many situations, it is rather easy to describe the Lyapunov theory, a well known tool to address stability properties, in terms of energy for electrical and mechanical systems; however, this approach has not

been applied to reacting systems (Favache and Dochain, 2009), although the link between irreversible thermodynamics and system theory has been an active research area over the years. 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 criteria in adiabatic stirred flow reactors, and 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; Ydstie and Alonso, 1997; Coffey et al., 2000; Alonso et al., 2002; Ydstie, 2002; Balaji et al., 2010) to develop stabilizing mass and energy inventory controllers (Farschman et al., 1998) and to derive general structural stability conditions for chemical process networks (Hangos et al., 1999; Antelo et al., 2007; Baldea et al., 2013; Hioe et al., 2013). In addition to the concept of inventories, they have used a nonlinear extension of the curvature of the entropy function called availability as it has been proposed within the framework of passivity theory for processes. 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. The

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CSTR	continuous stirred tank reactor
Π	thermodynamical system composed of n chemical species
n	total number of chemical species
\mathbf{N}	mole vector
U	internal energy
V	volume
$\boldsymbol{\mu}$	chemical potential vector
T	temperature
P	pressure
$\boldsymbol{\eta}$	vector of state variables of system Π composed of a set or subset of the extensive variables
S	entropy function
$\boldsymbol{\zeta}$	entropy gradient vector
Ω	entropy Hessian matrix
$q(\boldsymbol{\eta})$	component of the entropy function
R	ideal gas constant
\mathbf{u}	internal energy vector per mole of each species
\mathbf{c}_v	heat capacity at constant volume vector
α	stoichiometric coefficient of reactants
β	stoichiometric coefficient of products (or reactants)
$r(\boldsymbol{\zeta})$	specific reaction rate
$\boldsymbol{\Gamma}$	stoichiometric coefficients vector
A	stoichiometric coefficients vector for reactants
B	stoichiometric coefficients vector for products
$\mathbf{c}_{in,i}$	concentrations vectors of the i th surrounding
$F_{in,i}$	inlet volumetric flow rate of the i th surrounding
\mathbf{c}	concentration vector
F_{out}	outlet volumetric flow rate
$h_{in,i}$	specific total enthalpy of the i th surrounding
$\boldsymbol{\zeta}_{s,i}$	entropy gradient vector of the i th surrounding
h	specific total enthalpy of the reactor
u	specific internal energy
σ	total entropy production
$A_s J_s$	entropy flow
Σ	internal entropy production
k_+	kinetic constant for the forward reaction
k_-	kinetic constant for the reverse reaction
c_i	concentration of the i th species
A	reaction affinity
A_d	direct affinity ($\boldsymbol{\mu}^T A$)
A_r	reverse affinity ($\boldsymbol{\mu}^T B$)
γ	reaction path
A_{rxn}	affinity in the reaction path
$c(\gamma)$	probability function
$\Phi(\gamma)$	contribution of the chemical potential related to energy barrier of the chemical reaction
D_r	constant diffusion coefficient
γ_0	transition state
r^+	dimensionless driving force for the forward reaction
r^-	dimensionless driving force for the reverse reaction
ψ	specific rate of reaction “conductivity”
$\varepsilon(\gamma)$	fraction of variation of the reaction path chemical potential
$\boldsymbol{\mu}^0$	standard chemical potential at the temperature of the system
\mathbf{a}	activity vector
$\tau(\gamma)$	dimensionless function associated to the difference of the energy barrier of the chemical reaction and the standard chemical potential in the reaction path
K_{eq}	equilibrium constant

s_0	specific entropy vector at the reference state
u_0	specific internal energy vector at the reference state
P_0	reference pressure
T_0	reference temperature
Π_r	reacting system
Π_0	isolated system
\mathbf{v}	inputs of the open system
\mathbf{y}	outputs vector of the open system
w	supply rate of the open system
\mathbf{F}	flows vector
\mathbf{y}_{in}	outputs associated to the inlet flow
\mathbf{y}_{out}	outputs associated to the outlet flow
E_a	activation energy

features have been also taken into account to address the stability issue by using a number of thermodynamics based approaches (Dammers and Tels, 1974; Tarbell, 1977; Favache and Dochain, 2009; Balaji et al., 2010; Hoang et al., 2011b, 2012, 2012, 2013; Ramirez et al., 2013; Hoang and Dochain, 2013, 2013); however, it appears that even for simple reactions, analysis and control issues using thermodynamic properties are still open problems (Hoang et al., 2012).

In this contribution, the stability and passivity properties of a class of chemical reactors are addressed by using the internal entropy production as a Lyapunov-candidate function when the reactor is isolated and as a storage function when the reactor interacts with the surroundings. The paper 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. The moles, internal energy and entropy balances of the considered reactor system are developed in Section 3 and, for the sake of consistency with thermodynamics, a chemical reaction rate based on the progress of the reaction at mesoscopic scale is formulated. Based on this thermodynamically consistent reaction rate, it is shown that the internal entropy production of the reactor is a positive definite function and as a consequence, may be considered as a Lyapunov function candidate. Thereafter, in Section 4 the core of the paper is presented; it is shown that the internal entropy production fulfills all the requirements of a Lyapunov function for the isolated reactor guaranteeing the asymptotic stability and the same internal entropy production is used as a storage function when the reactor interacts with the surroundings in order to show its dissipative or passivity properties depending on the variables that couple the system to the surroundings.

2. Fundamentals of thermodynamics

2.1. Extensive and intensive properties

Let us consider a single phase lumped parameter thermodynamical system Π composed of n chemical species which interact with one or more surroundings systems as depicted in Fig. 1. The state of system Π is described by a primary vector of variables called inventories (Farschman et al., 1998) which is a set or subset of extensive properties $\{\mathbf{N}, U, V\}$ and its associated intensive properties $\{-\boldsymbol{\mu}, T, P\}$ that are dual to inventories, where $\mathbf{N} \in \mathbb{R}_{\geq 0}^n$, $U \in \mathbb{R}$ and $V \in \mathbb{R}_+$ are the mole, internal energy and volume inventories, while $\boldsymbol{\mu} \in \mathbb{R}^n$, $T \in \mathbb{R}_+$ and $P \in \mathbb{R}_+$ are the chemical potentials vector, the absolute temperature and pressure of system Π . Depending on the particular configuration and characteristics of system Π the state variables, $\boldsymbol{\eta} \in \mathbb{R}^\omega$, $\omega \leq n+2$, are selected as

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