

Conservative and dissipative phenomena in thermodynamical systems stability

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Abstract The entropy production of thermodynamical systems with reversible (conservative) and irreversible (dissipative) phenomena is used as a Lyapunov candidate function to address stability properties. First, based on the conjugated variables of the extensive properties, the dissipative and conservative phenomena are identified, then, the dynamic behavior of entropy production is obtained. Based on the properties of the entropy function Hessian, it is found that dissipative phenomena contribute to stability and attraction of the thermodynamical equilibrium. In particular, when only dissipative phenomena are present, the entropy production is a Lyapunov function that guarantees global or local stability, depending on the nonlinearities. Complex behaviors, for instance transitory increments of the entropy production, are due to both conservative phenomena and, far from equilibrium, non linearities of dissipative phenomena. Finally, a case study consisting in a gas-piston system is presented to illustrate these ideas.

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1. INTRODUCTION

Dissipative systems constitute a very important class of dynamical systems of particular interest in engineering and physics (Nicolis, 1986; Willems, 1972). The notion of dissipativity has been widely used to analyze open systems for which it is assumed that the dissipated energy, which is always non-negative, is the difference between the stored energy variation within the system and the amount of energy supplied by the environment or surroundings. Thus, given this energy–balance feature, it is clear that system stability is intimately related to dissipativity. In this context, it has been shown that many physical processes may be dissipative, including those that are constrained by the laws of thermodynamics (Rojas et al., 2008). In particular, these concepts have been successfully applied to mechanical and electrical systems (García-Canseco et al., 2010; Jeltsema and Scherpen, 2007, 2009; Ortega et al., 2001) to address stability properties in terms of energy or power. However, this approach is not easy to apply, and has not been completely successful, when applied to chemical (or thermodynamical) systems, for instances reacting systems (Favache and Dochain, 2009).

Some results in interpreting stability properties for thermodynamical systems based on the irreversibility have been already achieved (Alonso and Ydstie, 2001; Favache, 2009; Favache and Dochain, 2009; Ydstie, 2002; Ydstie and Alonso, 1997). In particular, when a thermodynamical

system is isolated, its total energy and mass remain constant, making impossible to use the energy or power to analyze stability properties, and still, due to irreversibility, the system is able to attain stable equilibrium points. In this context, irreversibility immediately evokes quantities related to the entropy (e.g. the entropy itself, the entropy production, the availability) to be considered as Lyapunov function candidates. For instance, García-Sandoval et al. (2016) presented a procedure to use the entropy production as a Lyapunov (or storage) function for a class of isolated (or open) thermodynamical systems.

In many cases, physical systems are composed of both irreversible and reversible processes, and their interaction may produce more complex behavior. For mechanical systems or fluid dynamics, the reversible processes have been captured in the definition of some differential geometric structures such as Poisson brackets (Arnold, 1989; Olver, 1993), while asymmetric bracket are used to define irreversible processes (Grmela and Öttinger, 1997; Ortega and Planas-Bielsa, 2004). Physical systems, subject simultaneously to reversible and irreversible processes, have been expressed as the sum of gradient and pseudo-Hamiltonian dynamical systems (Dalsmo and van der Schaft, 1998; García-Sandoval et al., 2015; Grmela and Öttinger, 1997; Öttinger and Grmela, 1997).

In this contribution, we combine the results presented in (García-Sandoval et al., 2016) and (García-Sandoval et al., 2015) to include dissipative and conservative processes

in stability analysis. The paper is organized as follows. In section 2 the thermodynamical systems in study and their properties are presented. In section 3, based on the entropy production, the stability analysis is carried out, focusing on the interactions between the dissipative and conservative phenomena. Finally, in section 4, a case study is presented.

2. THERMODYNAMICAL SYSTEMS

Let us consider a system Π composed of n subsystems (see scheme in Fig. 1) where thermodynamical phenomena take place, for instance gas expansion, heat or mass transfer, convective flow, chemical reactions, etc. Each subsystem is characterized by a set of extensive properties $\{\mathbf{N}_i, U_i, V_i, \mathbf{q}_i, \mathbf{p}_i\}$ as well as its associated intensive properties, for instance $\{-\boldsymbol{\mu}_i, T_i, P_i, \boldsymbol{\phi}_{pot}, \mathbf{v}_i\}$, where $\mathbf{N}_i \in \mathbb{R}^{C_i+}$, $U_i \in \mathbb{R}$, $V_i \in \mathbb{R}^+$, $\mathbf{q}_i \in \mathbb{R}^3$ and $\mathbf{p}_i \in \mathbb{R}^3$ are the moles, internal energy, volume, position and momentum, with C_i is the number of chemical species that interact in subsystem i , and $\boldsymbol{\mu}_i \in \mathbb{R}^{C_i+}$, $T_i \in \mathbb{R}^+$, $P_i \in \mathbb{R}^+$, $\boldsymbol{\phi}_{pot} \in \mathbb{R}^3$ and $\mathbf{v}_i \in \mathbb{R}^3$ are the chemical potentials vector for each compound, temperature, pressure, potential force vector and velocity vector of subsystem i , with $i = 1, 2, \dots, n$, respectively. Finally, the momentum is equal to $\mathbf{p}_i = m_i \mathbf{v}_i$, where

$$m_i = \mathbf{M}_{w,i}^T \mathbf{N}_i, \quad (1)$$

with $\mathbf{M}_{w,i} \in \mathbb{R}^{C_i+}$ as the molar mass vector. By considering that the total energy of each subsystem depends on internal energy, U_i , potential energy, $\Phi_{pot} = \int \boldsymbol{\phi}_{pot} \cdot d\mathbf{q}_i$, and kinetic energy, $K_i = \frac{1}{2} \frac{\mathbf{p}_i \cdot \mathbf{p}_i}{m_i} = \frac{1}{2} m_i (\mathbf{v}_i \cdot \mathbf{v}_i)$, and the total energy is

$$E_i = U_i + \int \boldsymbol{\phi}_{pot} \cdot d\mathbf{q}_i + \frac{1}{2} \frac{\mathbf{p}_i \cdot \mathbf{p}_i}{m_i}. \quad (2)$$

Depending on the particular configuration and characteristics of each subsystem, the state variables that completely define the behavior of each subsystem, $\boldsymbol{\eta}_i \in \mathbb{R}^{\omega_i}$ for $i = 1, 2, \dots, n$, is the set or a subset of extensive properties $\{\mathbf{N}_i, E_i, V_i, \mathbf{q}_i, \mathbf{p}_i\}$, where internal energy has been substituted by total energy using eq. (2). Then, the total mass and energy for system Π are linear functions of $\boldsymbol{\eta}$, i.e.,

$$m = \sum_{i=1}^n m_i = \mathbf{M}^T \boldsymbol{\eta} + m_0 \quad (3)$$

and

$$E = \sum_{i=1}^n E_i = \boldsymbol{\Upsilon}^T \boldsymbol{\eta} + E_0, \quad (4)$$

where \mathbf{M} and $\boldsymbol{\Upsilon}$ are constant matrices and m_0 and E_0 are the mass and total energy of static compounds. For instance, for $\boldsymbol{\eta} = \text{col}\{\mathbf{N}, E\}$, with $\mathbf{N} \in \mathbb{R}^{C+}$, it holds $\mathbf{M} = \text{col}\{\mathbf{M}_w, 0\}$ and $\boldsymbol{\Upsilon} = \text{col}\{\mathbf{0}_{C \times 0}, 1\}$.

2.1 Entropy and conjugated forces

According to the second principle of thermodynamics, it is possible to introduce for each subsystem Π , as for any macroscopic system, a concave real-valued function

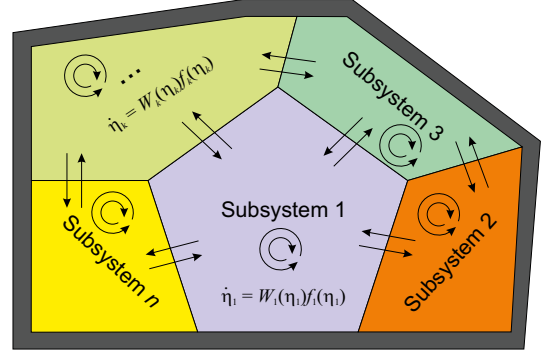


Figure 1. Scheme of system Π .

called entropy $S_i : \mathbb{R}^{\omega_i} \rightarrow \mathbb{R}$ at least twice differentiable that depends on the extensive properties, i.e., $S_i = S_i(\mathbf{N}_i, E_i, V_i, \mathbf{q}_i, \mathbf{p}_i)$. Under the assumption of local equilibrium, the derivative of the entropy can be obtained by the Gibbs relation (Kjelstrup et al., 2010): $dG_i = \boldsymbol{\mu}_i^T d\mathbf{N}_i = dU_i + P_i dV_i - T_i dS_i$. By considering eqs. (1) and (2), dS_i is equivalently written as

$$dS_i = \frac{1}{T_i} dE_i + \frac{P_i}{T_i} dV_i - \frac{\left(\boldsymbol{\mu}_i - \frac{1}{2}(\mathbf{p}_i \cdot \mathbf{p}_i) \mathbf{M}_{w,i}\right)^T}{T_i} d\mathbf{N}_i - \frac{\boldsymbol{\phi}_{pot} \cdot d\mathbf{q}_i}{T_i} - \frac{\mathbf{v}_i \cdot d\mathbf{p}_i}{T_i}. \quad (5)$$

From this expression, it is possible to identify the so-called conjugated variables $\left\{ -\frac{\left(\boldsymbol{\mu}_i - \frac{1}{2}(\mathbf{p}_i \cdot \mathbf{p}_i) \mathbf{M}_{w,i}\right)^T}{T_i}, \frac{1}{T_i}, \frac{P_i}{T_i}, -\frac{\boldsymbol{\phi}_{pot}}{T_i}, -\frac{\mathbf{v}_i}{T_i} \right\}$ of the extensive properties, $\{\mathbf{N}_i, E_i, V_i, \mathbf{p}_i\}$. Then, depending on the particular configuration and characteristics of each subsystem, the entropy gradient has the form $\boldsymbol{\zeta}_i := \left(\frac{\partial S_i}{\partial \boldsymbol{\eta}_i}\right)^T \in \mathbb{R}^{\omega_i}$, $i = 1, 2, \dots, n$.

In addition, since the entropy is a concave function (Öttinger, 2005), its Hessian matrix, $\Omega_i := \frac{\partial \boldsymbol{\zeta}_i}{\partial \boldsymbol{\eta}_i} \leq 0$, is negative (semi-)definite. Finally, the total entropy of system Π is the sum of the entropy of each subsystem

$$S(\boldsymbol{\eta}) = \sum_{i=1}^n S_i(\boldsymbol{\eta}_i), \quad (6)$$

therefore, its gradient is

$$\boldsymbol{\zeta} := \left(\frac{\partial S}{\partial \boldsymbol{\eta}}\right)^T = \text{col} \left\{ \left(\frac{\partial S_i}{\partial \boldsymbol{\eta}_i}\right)^T, i = 1, 2, \dots, n \right\}, \quad (7)$$

while its Hessian is a block-diagonal matrix, $\Omega := \text{diag}\{\Omega_i, i = 1, 2, \dots, n\} \leq 0$, that by construction is negative (semi-)definite.

2.2 Dynamical behavior

In this work, we consider that each subsystem is homogeneous or perfectly mixed, i.e., there is no spatial dependency, while the total system is isolated from the surroundings. Therefore, the dynamical model that describes the behavior of the extensive variables from molar, energy and momentum balances and state equations has the general form

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