



# Generalized Hamiltonian representation of thermo-mechanical systems based on an entropic formulation

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## ABSTRACT

In this work, we present an approach to construct generalized Hamiltonian representations for thermo-mechanical systems. Using entropic formulation of thermodynamic systems, the construction is applied to a class of thermo-mechanical systems. The proposed approach leads to an explicit expression of the dissipation along the trajectories of the dynamics. The considered thermo-mechanical systems are, in a thermodynamical sense, systems for which the dynamics of the extensive variables are functions of the intensive variables with respect to an entropic formulation. Using the entropy as the storage function, the dissipative structures of an analogue to a port-controlled Hamiltonian (PCH) representation are identified with irreversible phenomena, while the conservative structures are identified with reversible or isentropic phenomena. Examples are presented to illustrate the application of the proposed methodology, including a reacting system.

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## 1. Introduction

Dissipative and passive systems constitute a very important class of dynamical systems [1] for which the dissipated energy, been the difference between the stored energy variation with the system and the amount of energy supplied by the environment, is always non-negative. In view of this energy–dissipation feature, it is clear that dissipativity and passivity are intimately related to system stability. In this context, it has been shown that many physical processes may be dissipative, including those that obey the laws of thermodynamics [2], since dissipativity, like irreversibility in a thermodynamic system, captures the idea that some mechanical, electrical or chemical energy is dissipated as heat.

Using dissipativity and passivity properties to develop stability conditions and feedback stabilization design techniques for electrical and mechanical systems is well-established [3]. However, this development has shortcomings when applied to chemical systems [4], particularly when chemical reactions occur. Indeed, chemical processes models are written in such a way that dissipative and conservative structures are not explicit and depend on intensive variables and although in some cases the total mass and energy remain constant, the system still has, in some sense, dissipative

phenomena that lead to a certain steady state and one interesting question is what does it dissipate? Hence, one has to find decomposition approaches to identify those dissipative and conservative structures. A solution adopted by many consists in considering extensive variables rather than intensive variables for chemical process systems analysis purposes, an approach related to multidomain modelling reviewed in [5] adapted to thermodynamic systems. This approach, based on the Legendre transformation with respect to a known potential (the energy or the entropy), was considered within the framework of passivity theory in [6,7]. More recently, the idea of representing the dynamics of a system using both intensive and extensive variables was considered in [8].

Alternatively, the port Hamiltonian (PH) approach, as described in [9] and successfully adopted for electrical and mechanical systems, was also considered for the analysis of thermodynamical systems [10]. Generally speaking, the Hamiltonian function refers to any energy function, while Hamiltonian systems are dynamical systems governed by Hamilton's equations. Thus, PH systems are open dynamical systems that interact with their surroundings through ports, and whose geometric structures are derived from the interconnection of their sub-systems. In addition PH systems provide a framework for the geometric description of network models of physical systems, where the dissipative and conservative structures can be explicitly expressed in the interconnection matrix [11]. Based on this general framework, some efforts have

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been recently done to use physical variables as storage functions for chemical processes analysis [see for instance [4,8,10,12]].

Due to the potential advantages mentioned above, the central objective of this work is to show how to derive a structural representation for a large class of thermo-mechanical systems in the port Hamiltonian systems in order to express explicitly the dissipation along the trajectories of the dynamics. In the present paper, entropy is used as the storage function instead of energy. As a result, dissipative structures directly outline irreversible phenomena, while conservative structures identify reversible (isentropic) phenomena within the process. If we compare our proposed approach to those given in the literature, it is noted that identifying dissipative and conservative structures reduces computations for chemical systems analysis. For example, computations of stability conditions in [10], where a thermodynamic potential is considered for stability, and in [8], where a particular thermodynamic geometric framework is considered for design, are cumbersome because the balance equations are not written with identified conservative and dissipative structures.

The paper is organized as follows. In Section 2, the class of thermo-mechanical systems under study is defined and its thermodynamic properties are analyzed. The representation of thermo-mechanical systems as port Hamiltonian systems using entropy is presented in Section 3. The adiabatic gas–piston system studied in [13] is used throughout to illustrate the different elements of the proposed methodology. The study of this system shows that the approach is developed in a general form, and can be apply directly to any system that can be arbitrarily decomposed as interconnected subsystems. Then, in Section 4, two complete case studies of thermo-mechanical systems are developed: an adiabatic liquid pendulum system, and an adiabatic gas–piston system with chemical reactions.

## 2. Lumped-parameter thermo-mechanical systems

Let us consider a system  $\Pi$  composed of  $n$  subsystems where thermodynamical and/or mechanical phenomena are taking place, for instance gas expansion, heat transfer, displacement and movement of mechanical components, etc. Each subsystem is characterized by a set of thermodynamical extensive properties, for instance  $\{\mathbf{N}_i, U_i, V_i\}$ , its associated thermodynamical intensive properties, for instance  $\{-\mu_i, T_i, P_i\}$  [14], and its mechanical properties, for instance  $\{z_i, m_i p_i\}$ , where  $\mathbf{N}_i \in \mathbb{R}^{C_i+}$ ,  $U_i \in \mathbb{R}$  and  $V_i \in \mathbb{R}^+$  are the moles, energy and volume inventories, with  $C_i$  as the number of chemical species interacting in the subsystem, and  $\mu_i \in \mathbb{R}^{C_i}$ ,  $T_i \in \mathbb{R}^+$  and  $P_i \in \mathbb{R}^+$  are the chemical potential, and the absolute temperature and pressure of subsystem  $i$ , with  $i = 1, 2, \dots, n$ , respectively. Finally  $z_i$ ,

$$p_i = m_i v_i \quad (1)$$

and

$$m_i = \mathbf{M}_{w,i}^T \mathbf{N}_i \quad (2)$$

are the subsystems position, momentum and mass, respectively, with  $\mathbf{M}_{w,i} \in \mathbb{R}^{C_i+}$  the molar mass vector, and  $v_i$  as the velocity. Depending on the particular configuration and characteristics of each subsystem, the state variables,  $\eta_i \in \mathbb{R}^{\beta_i}$ , are selected within the set of the extensive and motion variables. For instance, if the process is isochoric, then the state variables vector may be defined as  $\eta = \text{col}\{\mathbf{N}, U\} \in (\mathbb{R}^{C^+} \times \mathbb{R})$ , while for isochoric systems with only one incompressible moving solid, the state variable may be defined as  $\eta = \{U, z, mv\} \in \mathbb{R}^3$ . In this work it is assumed that each subsystem is homogeneous, i.e., there is no spatial dependence in the considered thermo-mechanical systems. It is also considered that

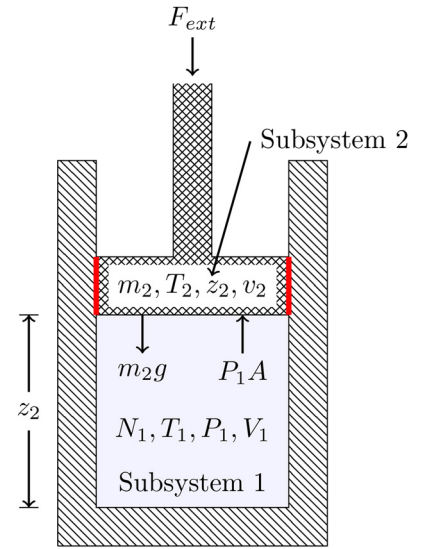


Fig. 1. Adiabatic piston from [13].

system  $\Pi$  may interact with one or more surrounding systems, therefore the dynamical model under study is expressed as

$$\Pi : \dot{\eta} = Mf(\eta) + g(\eta, \eta_s)\mathbf{F}, \quad (3)$$

where  $\eta = \text{col}\{\eta_i, i = 1, 2, \dots, n\} \in \mathbb{R}^{\beta}$ , with dimension  $\beta = \sum_{i=1}^n \beta_i$ , and  $\eta_s \in \mathbb{R}^s$  represent the vectors of extensive and motion properties of the system and its surroundings, respectively. The vector field  $f : \mathbb{R}^{\beta} \rightarrow \mathbb{R}^{\beta}$  contains the kinetic expressions for reaction, transport, motion or mechanical phenomenon that take place within the system, while matrix  $M \in \mathbb{R}^{\beta \times \beta}$  contains the stoichiometric coefficients for each reaction, transport, motion and mechanical phenomena. The flow vector  $\mathbf{F} \in \mathbb{R}^m$  takes into account the exchange with the surroundings (it could contain volumetric, molar or mass flows and/or external forces), while the columns of  $g(\eta, \eta_s)$ ,  $g_i : (\mathbb{R}^{\beta} \times \mathbb{R}^s) \rightarrow \mathbb{R}^{\beta}$ , are associated with the extensive and motion properties exchanged with the surroundings through the flow or external force  $F_i, i = 1, 2, \dots, m$ .

For instance, let us consider an adiabatic gas–piston system similar to the one described in [13] and shown in Fig. 1. For simplicity, the gas is assumed ideal and denoted subsystem 1, while the piston is denoted subsystem 2.

Under the ideal gas assumption, the adiabatic piston model takes the form

- **Subsystem 1:** Balances equations for the internal energy,  $U_1$ , and volume,  $V_1$ , of the gas

$$\dot{U}_1 = \kappa(T_2 - T_1) - Av_2 P_1,$$

$$\dot{V}_1 = Av_2.$$

- **Subsystem 2:** Balance equations for the internal energy,  $U_2$ , position,  $z_2$ , and velocity,  $v_2$ , of the piston

$$\dot{U}_2 = -\kappa(T_2 - T_1) + \alpha v_2^2,$$

$$\dot{z}_2 = v_2,$$

$$m_2 \dot{v}_2 = AP_1 - F_{ext} - m_2 g - \alpha v_2,$$

where  $T_1$  and  $T_2$  are the gas and piston temperatures, respectively,  $P_1 = N_1 R_g T_1 / V_1$  is the gas pressure, with  $N_1$  and  $R_g$  denotes the mole number in the chamber and the ideal gas constant, respectively.

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