Dissipative and conservative structures for thermo-mechanical systems

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Abstract: On this work is shown how to derive a structural representation of a class of thermo-mechanical systems in the Port Hamiltonian framework in order to express explicitly the dissipation along the trajectories of the dynamics. To achieve this goal the entropy is used as the storage function. The dissipation structures are correlated with irreversible processes, while the conservative processes are correlated with reversible or isentropic processes. Finally, three study cases are presented: the first one is an adiabatic gas-piston system, the second is an adiabatic two chambers gas-piston-gas system and the last one is an adiabatic liquid-pendulum system.

Keywords: Port-controlled Hamiltonian systems, Thermodynamics

1. INTRODUCTION

Dissipative and passive systems constitute a very important class of dynamical systems (Willems, 1972a,b) in which the stored energy cannot exceed the energy supplied to them by the environment—the difference being the dissipated energy. In view of this energy-balancing feature, it is clear that dissipativity and passivity are intimately related to the system stability. Furthermore, by invoking the universal principle of energy conservation, it may be argued that all physical systems are dissipative with respect to some suitably variables that couple the system to the environment (Garcia-Canseco et al., 2010). On this direction, 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 some energy dissipates as resources are transformed into products and 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 is not rather easy when it has been applied to chemical processes (Favache and Dochain, 2009). This problem has been addressed by combining irreversible thermodynamics and system 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 criteria in adiabatic stirred flow reactors, and Tarbell (1977) has proposed a Lyapunov function for continuous stirred tank reactor 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

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control design of process systems (see, e.g., Alonso and Ydstie, 2001; Alonso et al., 2002; Alonso and Ydstie, 1996; 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, 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.

On the other hand, in last two decades so-called Port Hamiltonian (PH) systems have attracted attention (Ortega et al., 1999, 2002, 2001), mainly because their Hamiltonian can be seen as a storage function that directly implies passivity properties, that offer a systematic framework for analysis, control and simulation of complex physical systems. Generally speaking, Hamiltonian 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 structure derives from the interconnection of their subsystems. 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 (Dorfler et al., 2009). In this frame, some efforts have been recently done to use physical variables as storage functions in chemical processes (see for instance Hangos et al., 2001; Hoang et al., 2011a,b; Ramirez et al., 2013).

Due to the potential advantages mentioned above, the central objective of this work is to show how to derive a structural representation of a large class of thermomechanical systems in the Port Hamiltonian framework in order to express explicitly the dissipation along the trajectories of the dynamics. However, instead of energy, entropy is used as storage function. In this case, the dissipation structures are correlated with irreversible processes, while the conservative processes have relation with reversible or isentropic processes. The document is organized as follows. In section 2 the PH framework is presented. In section 3 the class of thermo-mechanical systems in study is defined and its thermodynamic properties are analyzed. Then, in section 5 three study cases are presented. The first one is an adiabatic gas-piston system similar to that described by Favache et al. (2010), the second one is an adiabatic two chambers gas-piston-gas system, while the last one is an adiabatic liquid-pendulum system.

2. PORT-CONTROLLED HAMILTONIAN SYSTEMS

Network modeling of lumped-parameter physical systems with independent storage elements leads to models of the form called port-controlled Hamiltonian (PCH) systems (Ortega et al., 2002)

$$\mathscr{H}:\begin{cases} \dot{x} = [J(x) - R(x)] \frac{\partial H}{\partial x}(x) + g(x) u\\ y = g^{\mathsf{T}}(x) \frac{\partial H}{\partial x}(x) \end{cases}$$
(1)

where $x \in \mathbb{R}^n$ are the energy variables, the smooth function $H(x) : \mathbb{R}^n \to \mathbb{R}$ represents the total stored energy and $u, y \in \mathbb{R}^m$ are the port power variables. The port variables u and y are conjugated variables, in the sense that their duality product defines the power flows exchanged with the environment of the system, for instance currents and voltages in electrical circuits or forces and velocities in mechanical systems. The interconnection structure is captured in the $n \times n$ skew-symmetric matrix $J(x) = -J^{\mathsf{T}}(x)$ and the $n \times m$ matrix g(x), while $R(x) = R^{\mathsf{T}}(x) \ge 0$ represents the dissipation, all these matrices depend smoothly on the state x.

Evaluating the rate of change of the total energy we obtain

$$\frac{d}{dt}H = -\left[\frac{\partial H}{\partial x}\left(x\right)\right]^{\mathsf{T}}R\left(x\right)\frac{\partial H}{\partial x}\left(x\right) + u^{\mathsf{T}}y,\qquad(2)$$

where the first term on the right-hand side (which is nonpositive) represents the dissipation due to the resistive (friction) elements in the system.

3. LUMPED-PARAMETER THERMO-MECHANICAL SYSTEMS

Let us consider a system Π composed of n subsystems where thermodynamical and/or mechanical processes 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 $\{\mathbf{N}_i, U_i, V_i\}$, as well as its associated thermodynamical intensive properties $\{-\boldsymbol{\mu}_i, T_i, P_i\}$, and its mechanical properties $\{z_i, m_i v_i\}$, 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, 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 $i = 1, 2, \ldots, n$. Finally, z_i , v_i and $m_i = \mathbf{M}_i^T \mathbf{N}_i$

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are the subsystems position, velocity and mass, respectively, with $\mathbf{M}_i \in \mathbb{R}^{C_i+}$ as the molecular mass vector. Depending on the particular configuration and characteristics of each subsystem the state variables, $\boldsymbol{\eta}_i \in \mathbb{R}^{\omega_i}$, are selected as a function of the total extensive and motion variables or a subset of them. For instance, if the process is isochoric, then the state variables vector is defined as $\boldsymbol{\eta}_i = \operatorname{col} \{\mathbf{N}_i, U_i\} \in (\mathbb{R}^{C_i+} \times \mathbb{R})$, while for isochoric systems with only one incompressible moving solid, the state variable is defined as $\boldsymbol{\eta}_i = \{U_i, z_i, m_i v_i\} \in \mathbb{R}^3$. In this work it is assumed that each subsystem is homogeneous, i.e. there is no spatial dependence. It is also considered that system II interacts with one or more surroundings systems, therefore the dynamical model under study in term of extensive variables is

$$\Pi : \dot{\boldsymbol{\eta}} = Mf(\boldsymbol{\eta}) + g(\boldsymbol{\eta}, \boldsymbol{\eta}_s) \boldsymbol{F}$$
(3)

where $\boldsymbol{\eta} = \operatorname{col} \{ \boldsymbol{\eta}_i, i = 1, 2, \dots, n \} \in \mathbb{R}^{\omega}, \text{ with } \omega = \sum_{i=1}^n \omega_i, \text{ and } \boldsymbol{\eta}_s \in \mathbb{R}^s$ represent the vectors of extensive and motion properties of the system and the surroundings, respectively, while the vector field $f : \mathbb{R}^{\omega} \to \mathbb{R}^p$ contains the kinetic expressions for reaction, transport and motion phenomena which take place within the system, while matrix $M \in \mathbb{R}^{\omega \times p}$ contains the stoichiometric coefficients for each reaction, transport or motion phenomena. $\boldsymbol{F} \in \mathbb{R}^m$ is the flow vector that takes into account the exchange with the surroundings (it could contain volumetric flows or external forces), while the columns of $g(\boldsymbol{\eta}, \boldsymbol{\eta}_s), g_i : (\mathbb{R}^{\omega} \times \mathbb{R}^s) \to \mathbb{R}^{\omega}$, are correlated with the extensive and motion properties exchanged with the surroundings through the convective flow or external force $F_i, i = 1, 2, \dots, m$.

3.1 Entropy and the conjugated forces

According to the principles of thermodynamics one can introduce for each subsystem of system Π , as for any macroscopic system, a concave real-valued function named entropy $S_i : \mathbb{R}^{\omega_i} \to \mathbb{R}$ at least two times differentiable which depends on the extensive and motion properties, i.e $S_i = S_i(\mathbf{N}_i, U_i, V_i, z_i, v_i)$. The differential behavior of entropy can be defined through the Gibbs relation (Kjelstrup et al., 2010)

$$dS_i = \frac{1}{T_i} dU_i + \frac{P_i}{T_i} dV_i - \frac{\boldsymbol{\mu}_i^{\mathsf{T}}}{T_i} d\mathbf{N}_i \tag{4}$$

Considering that the total energy depends on the internal, potential and kinetic energies, i.e $E_i = U_i + \phi_{pot}(z_i) + \frac{1}{2}m_i v_i^2$, then the aforementioned Gibbs relation is equivalent to

$$dS_i = \frac{1}{T_i} dE_i + \frac{P_i}{T_i} dV_i - \frac{\left(\boldsymbol{\mu}_i - \frac{1}{2}v_i^2 \mathbf{M}_i\right)^{\mathsf{T}}}{T_i} d\mathbf{N}_i$$
$$-\frac{\phi_{pot}^{'}\left(z_i\right)}{T_i} dz_i - \frac{v_i}{T_i} d\left(m_i v_i\right)$$

From here it is possible to identify the so called driving or conjugated forces $\left\{\frac{1}{T_i}, \frac{P_i}{T_i}, -\frac{(\mu_i - \frac{1}{2}v_i^2\mathbf{M}_i)}{T_i}, -\frac{\phi'_{pot}(z_i)}{T_i}, -\frac{v_i}{T_i}\right\}$ of the extensive and motion properties, $\{E_i, V_i, \mathbf{N}_i, z_i, m_i v_i\}$. Then, depending of the particular configuration

and characteristics of each subsystem the entropy gradient has the form $^{\rm 1}$

$$\boldsymbol{\zeta}_{i} := \nabla S\left(\boldsymbol{\eta}_{i}\right) \in \mathbb{R}^{\omega_{i}}, \ i = 1, 2, \dots, n$$
(5)

In addition, since Entropy is a concave function, it holds that its Hessian matrix

$$\Omega_i := \nabla^2 S\left(\boldsymbol{\eta}_i\right) \le 0$$

is negative semidefinite. Finally, the total entropy for system Π is the sum of the entropy for each subsystem, i.e.

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

therefore its gradient is

$$\boldsymbol{\zeta} := \nabla S(\boldsymbol{\eta}) = \operatorname{col} \left\{ \nabla S(\boldsymbol{\eta}_i), i = 1, 2, \dots, n \right\}$$
(7)
while its Hessian is the block-diagonal matrix

$$\Omega := \operatorname{diag} \left\{ \Omega_i, i = 1, 2, \dots, n \right\} \le 0$$
(8)

which for construction is also negative definite.

Entropy dynamics The entropy is not a conservative variable, therefore a total entropy balance must have the form

$$\dot{S} = \sigma + AJ_s$$

where $\sigma \geq 0$ is the total entropy production, while AJ_s is the entropy flow. With the entropy gradient (7), the entropy change in system (3.2) is

$$\dot{S} = \boldsymbol{\zeta}^{\mathsf{T}} \dot{\boldsymbol{\eta}} = \boldsymbol{\zeta}^{\mathsf{T}} M f\left(\boldsymbol{\eta}\right) + \boldsymbol{\zeta}^{\mathsf{T}} g\left(\boldsymbol{\eta}, \boldsymbol{\zeta}_{s}\right) \boldsymbol{F}$$

therefore, adding and subtracting $\boldsymbol{\zeta}_{s}^{\mathsf{T}} g\left(\boldsymbol{\eta}, \boldsymbol{\zeta}_{s}\right) \boldsymbol{F}$, the transport and entropy production are respectively

$$AJ_{s} = \boldsymbol{\zeta}_{s}^{\mathsf{T}}g\left(\boldsymbol{\eta},\boldsymbol{\zeta}_{s}\right)\boldsymbol{F}$$

$$\tag{9}$$

$$\sigma = \boldsymbol{\zeta}^{\mathsf{T}} M f(\boldsymbol{\eta}) + \left(\boldsymbol{\zeta}^{\mathsf{T}} - \boldsymbol{\zeta}_{s}^{\mathsf{T}}\right) g(\boldsymbol{\eta}, \boldsymbol{\zeta}_{s}) \boldsymbol{F} \qquad (10)$$

where J_s is the entropy flux across the transversal area A. Note that the entropy production, σ , is composed of a term correlated with the internal entropy production,

$$\Sigma := \boldsymbol{\zeta}^{\mathsf{T}} M f\left(\boldsymbol{\eta}\right) \ge 0,$$

which includes the entropy production from generation, motion and transport phenomena which take place within the system, while the second term, $\left(\boldsymbol{\zeta}^{\mathsf{T}} - \boldsymbol{\zeta}_{s}^{\mathsf{T}}\right)g\left(\boldsymbol{\eta},\boldsymbol{\zeta}_{s}\right)\boldsymbol{F}$, is the entropy due to the interaction with the surroundings, namely the transport and mixing entropy production.

 $3.2\ Reaction,\ transport\ and\ motion\ phenomena\ and\ the\ conjugated\ forces$

In particular, when the system does not interact with the surroundings the entropy change is equal to the internal entropy production

$$\dot{S} = \Sigma \ge 0$$

Therefore, for the non interacting case at equilibrium it holds that $Mf(\boldsymbol{\eta}) = 0$ and $\Sigma = 0$. A feasible solution for both equations is $f(\boldsymbol{\eta}) = 0$. If the driving forces are considered to be $L^{\mathsf{T}}\boldsymbol{\zeta}$, where $L \in \mathbb{R}^{p \times \omega}$, then at equilibrium it also holds that $L^{\mathsf{T}}\boldsymbol{\zeta} = 0$. Therefore, it is not unreasonable to assume that the vector field f, that contains the kinetic expressions for reaction, transport and motion phenomena taking place within the system, depends on the driving forces. Thus, given the matrix $\Psi(\boldsymbol{\zeta}) : \mathbb{R}^{p \times \omega} \longrightarrow \mathbb{R}^{p \times p}$, where $\Psi(\boldsymbol{\zeta})$ is a symmetric positive definite matrix, we assume that f depends only on the conjugated forces as follows

$$f(\boldsymbol{\eta}) = \Psi(\boldsymbol{\zeta}) L^{\mathsf{T}} \boldsymbol{\zeta}$$
(11)

In addition, matrix M can be split in two terms M = R+J, that, together with matrices L and Ψ , are such that

$$R\Psi\left(\boldsymbol{\zeta}\right)L^{\mathsf{T}} = L\Psi^{\mathsf{T}}\left(\boldsymbol{\zeta}\right)R^{\mathsf{T}} \ge 0 \\ J\Psi\left(\boldsymbol{\zeta}\right)L^{\mathsf{T}} = -L\Psi^{\mathsf{T}}\left(\boldsymbol{\zeta}\right)J^{\mathsf{T}}$$
 (12)

Here, we presume that if system is thermodynamical consistent the structural properties of $f(\eta)$ and M described in equations (11) and (12) hold. These equations are instrumental to obtain an entropic analogue representation of PCH systems described in equations (1) and (2) as shown in the following section.

4. ENTROPY BASED PCH REPRESENTATION

Considering equations (11) and (12) system Π is equivalent to

$$\dot{\boldsymbol{\eta}} = (R+J) \Psi \left(\boldsymbol{\zeta} \right) L^{\mathsf{T}} \boldsymbol{\zeta} + g \left(\boldsymbol{\eta}, \boldsymbol{\eta}_{s} \right) \boldsymbol{F}$$
(13)

while the internal entropy production becomes

$$\Sigma = \boldsymbol{\zeta}^{\mathsf{T}} \left(R + J \right) \Psi \left(\boldsymbol{\zeta} \right) L^{\mathsf{T}} \boldsymbol{\zeta}$$

however, using equations (12) the internal entropy production reduces to

$$\Sigma = \boldsymbol{\zeta}^{\mathsf{T}} R \Psi \left(\boldsymbol{\zeta} \right) L^{\mathsf{T}} \boldsymbol{\zeta} \ge 0$$

therefore matrix R can be associated to processes that produce entropy, while matrix J is associated with reversible or isentropic processes.

Now, given the entropy gradient definition (7) and equation (13), it is possible to represent system Π as

$$\mathscr{E}: \begin{cases} \dot{\boldsymbol{\eta}} = (R+J) \Psi(\boldsymbol{\zeta}) L^{\mathsf{T}} \nabla S(\boldsymbol{\eta}) + g(\boldsymbol{\eta}, \boldsymbol{\eta}_s) \boldsymbol{F} \\ \mathbf{y} = g^{\mathsf{T}}(\boldsymbol{\eta}, \boldsymbol{\eta}_s) \nabla S(\boldsymbol{\eta}) \end{cases}$$
(14)

which is an entropic analogue version of the PCH system (1). In addition, the entropy dynamics can be rewritten as

$$\frac{d}{dt}S = \left[\nabla S\left(\boldsymbol{\eta}\right)\right]^{\mathsf{T}}R\Psi\left(\boldsymbol{\zeta}\right)L^{\mathsf{T}}\nabla S\left(\boldsymbol{\eta}\right) + \boldsymbol{F}^{\mathsf{T}}\mathbf{y}$$

which is analogue to equation (2), however in this case $[\nabla S(\boldsymbol{\eta})]^{\mathsf{T}} R\Psi(\boldsymbol{\zeta}) L^{\mathsf{T}} \nabla S(\boldsymbol{\eta}) \geq 0$. Note that for a thermomechanical system that does not interact with the surroundings, i.e $g(\boldsymbol{\eta}, \boldsymbol{\eta}_s) = 0$, and that initially is out of equilibrium, its total energy remains constant, therefore a PCH representation based on total energy may fail to identify the dissipative structures. However, in this case the entropy will be increasing until the system attains the equilibrium. Thus, the negative of the entropy may be used as a storage function as Hoang et al. (2011b) have suggested.

5. STUDY CASES

5.1 Adiabatic gas-piston system

Let consider an adiabatic gas-piston system similar to the described by Favache et al. (2010) and shown in Figure 1. For simplicity in the analysis and the nomenclature the gas is considered ideal and named subsystem 1, while the piston is named subsystem 2.

¹ We use the notation $\nabla_x := \partial/\partial x$, $\nabla_x^2 := \partial^2/\partial x^2$ —when clear from the context the argument will be omitted. Also, all vectors, including the gradient, are column vectors



Fig. 1. Adiabatic piston from (Favache et al., 2010)

Model Under the assumption of ideal gas the adiabatic piston model presented in (Favache et al., 2010) takes the form

• Subsystem 1: Balances for the gas (Internal energy, U_1 , and volume, V_1)

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

• Subsystem 2: Balance for the piston (Internal energy, U_2 , position, z_2 , and velocity, v_2)

$$\dot{U}_2 = -\kappa (T_2 - T_1) + \alpha v_2^2$$
$$\dot{z}_2 = v_2$$
$$m_2 \dot{v}_2 = AP_1 - F_{ext} - m_2 g - \alpha v_2$$

where T_1 and T_2 are the gas and piston temperatures, respectively, $P_1 = N_1 R T_1 / V_1$ is the gas pressure, with N_1 and R as the moles of gas and the ideal gas constant, F_{ext} is the external force applied to the piston, A is the transverse chamber area, m_2 is the piston mass, α is the friction coefficient, κ is a heat exchange constant and gis the gravitational acceleration constant. In addition, the volume of the chamber can be correlated with the piston position as

$$V_1 = Az_2 + c$$

where c is a constant, which without loss of generality will be considered equal to zero in the following analysis; thus, the gas volume depends on the piston position, reducing to 4 the systems' state variables, for instance one could choose (U_1, U_2, z_2, v_2) . In addition, the relation between internal energies and temperatures are

$$U_1 = N_1 \left(u_{1,0} + \int_{T_0}^{T_1} c_{v,1} dT \right)$$
(15)

$$U_2 = m_2 \left(u_{2,0} + \int_{T_0}^{T_2} c_{v,2} dT \right)$$
(16)

where c_{v1} , c_{v2} , $u_{1,0}$ and $u_{2,0}$ are the molar and mass heat capacities and reference internal energy at temperature T_0 , respectively.

On the other hand, the total energy of the piston is the sum of the internal, kinetic and potential energy, i.e $E_2 = U_2 + \frac{1}{2}mv_2^2 + mgz_2$, therefore, the dynamic behavior of this energy is $\dot{E}_2 = -\kappa (T_2 - T_1) + (AP_1 - F_{ext}) v_2$, that depends on the gas-piston heat exchange rate, and the

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force equilibrium between the gas and the external force. In addition, the dynamic of the total gas-piston system energy, $E = U_1 + E_2$, is $\dot{E} = -v_2 F_{ext}$. Therefore, the system gains or losses energy depending on the value of the product between the piston velocity and the external force.

Entropy dynamics The total gas-piston system entropy change is

$$dS = \frac{dU_1 + P_1 dV_1}{T_1} + \frac{dU_2}{T_2} \tag{17}$$

Therefore the entropy dynamics is

$$\dot{S} = \frac{\dot{U}_1 + P_1 \dot{V}_1}{T_1} + \frac{\dot{E}_2 - m_2 v_2 \dot{v}_2 - m_2 g \dot{z}_2}{T_2}$$
$$= \kappa \left(T_2 - T_1\right) \left(\frac{1}{T_1} - \frac{1}{T_2}\right) + \alpha \frac{v_2^2}{T_2} \tag{18}$$

which is correlated with the irreversibility of the heat exchange and the momentum dissipation due to the pistonchamber friction.

Driving forces Note that, considering the work as $dW = P_1 dV_1$, equation (17) is equivalent to

$$dS = \frac{dU_1 + dW}{T_1} + \frac{dE_2 - dW}{T_2} + \frac{(P_1A - m_2g)dz_2}{T_2} - \frac{m_2v_2dv_2}{T_2}$$
(19)

Now let define the following variables change: $\eta =$ col $\{U_1 + W, E_2 - W, z_2, v_2\}$. Thus, the dynamics of the gas-piston system can be expressed in compact form as system Π (Eq. (3.2)), with

$$f(\boldsymbol{\eta}) = \begin{pmatrix} \kappa (T_2 - T_1) \\ v_2 \\ AP_1 - m_2 g \end{pmatrix}, \ M = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{\alpha}{m_2} & \frac{1}{m_2} \end{pmatrix}$$

 $\mathbf{F} = F_{ext}$ and

$$\varphi\left(\boldsymbol{\eta},\boldsymbol{\zeta}_{s}\right) = \left(0 \ -v_{2} \ 0 \ -\frac{1}{m_{2}}\right)^{\mathsf{T}}.$$
 (20)

Note that the driving forces and the external forces are clarified, i.e the driving forces are three: the difference of temperature $(T_2 - T_1)$ (correlated with the thermal equilibrium), the velocity v_2 (correlated to the momentum equilibrium), and the difference between the force which applies the gas to the piston through pressure and the gravitational force, $AP_1 - m_2g$ (correlated to mechanical or force equilibrium), while the external force is F_{ext} , respectively.

From equation (19) it is easy to see that the conjugated variable of η must be

$$\boldsymbol{\zeta}^{\mathsf{T}} = \frac{\partial S}{\partial \boldsymbol{\eta}} = \left(\frac{1}{T_1} \ \frac{1}{T_2} \ \frac{P_1 A - m_2 g}{T_2} \ -\frac{m_2 v_2}{T_2}\right).$$

Note that defining matrices

$$\Psi\left(\boldsymbol{\zeta}\right) = \begin{pmatrix} \kappa T_1 T_2 & 0 & 0\\ 0 & T_2 & 0\\ 0 & 0 & T_2 \end{pmatrix} \text{ and } L = \begin{pmatrix} 1 & 0 & 0\\ -1 & 0 & 0\\ 0 & 0 & 1\\ 0 & -\frac{1}{m_2} & 0 \end{pmatrix}$$



Fig. 2. Adiabatic gas-piston-gas system.

the driving force vector, $f(\eta)$, for this particular model is similar to equation (11), while with matrices

$$R = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & -\frac{\alpha}{m_2} & 0 \end{pmatrix} \text{ and } J = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{1}{m_2} \end{pmatrix}$$

it holds that M = R + J, and conditions (12) are satisfied with

Note that the eigenvalues of $R\Psi(\boldsymbol{\zeta}) L^{\mathsf{T}}$ are $\left\{0, 0, 2\kappa T_1 T_2, \frac{\alpha T_2}{m_2^2}\right\}$ the same structure of system Π (Eq. (3.2)), with while the eigenvalues of $J\Psi\left(\boldsymbol{\zeta}\right)L^{\mathsf{T}}$ are $\left\{0,0,\pm\frac{T_{2}}{m_{2}}i\right\}$. Thus, using matrices (21) and (22) and vector (20), the gaspiston model has an equivalent representation to system (14). Finally, it is straightforward to verify that equations (12) are fulfilled.

5.2 Adiabatic two chambers gas-piston-gas system

Now let us consider an adiabatic gas-piston-gas system composed of two chambers as depicted in figure 2.

The proposed model is composed of three subsys-Model tems:

• Subsystem 1: Balances for the gas in chamber 1 (Internal energy, U_1 , and volume, V_1)

$$\frac{dU_1}{dt} = \kappa_1 \left(T_3 - T_1\right) - Av_3 P_1$$
$$\frac{dV_1}{dt} = Av_3$$

• Subsystem 2: Balances for the gas in chamber 2 (Internal energy, U_2 , and volume, V_2)

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$$\frac{dU_2}{dt} = -\kappa_2 \left(T_2 - T_3\right) + Av_3 P_2$$
$$\frac{dV_2}{dt} = -Av_3$$

• Subsystem 3: Balance for the piston (Internal energy, U_3 , position, z_3 , and velocity, v_3)

$$\frac{dU_3}{dt} = -\kappa_1 (T_3 - T_1) + \kappa_2 (T_2 - T_3) + \alpha v_3^2$$
$$\frac{dz_3}{dt} = v_3$$
$$m_3 \frac{dv_3}{dt} = AP_1 - AP_2 - \alpha v_3 - F_{ext}$$

In addition, the total energy of the piston is $E_3 =$ $U_3 + \frac{1}{2}m_3v_3^2$, therefore its dynamic is

$$\dot{E}_3 = -\kappa_1 (T_3 - T_1) + \kappa_2 (T_2 - T_3) + Av_3 (P_1 - P_2) - v_3 F_{ext}$$

On the other hand, the total volume of the system, V = $V_1 + V_3 + V_2$, is constant; thus, the system can be defined by 5 state variables, for instance $(U_1, U_2, U_3, z_3, v_3)$.

Entropy dynamics The total entropy change is the sum of the gases and piston entropy changes, dS_1 , dS_2 and dS_3 , i.e

$$dS = \frac{dU_1 + P_1 dV_1}{T_1} + \frac{dU_2 + P_2 dV_2}{T_2} + \frac{dU_3}{T_3}$$

where the piston's internal energy is $dU_3 = d\left(E_3 - \frac{1}{2}mv_3^2\right)$, therefore the entropy dynamic is

$$\dot{S} = \kappa_1 \frac{\left(T_3 - T_1\right)^2}{T_1 T_3} + \kappa_2 \frac{\left(T_2 - T_3\right)^2}{T_2 T_3} + \frac{\alpha v_3^2}{T_3}$$

Similarly to the previous example, it is Driving forces possible to use the work done by the gases $dW_1 = P_1 dV_1$, $dW_2 = P_2 dV_2$, to define the new state vector $\boldsymbol{\eta} = \operatorname{col} \{U_1 +$

$$f(\boldsymbol{\eta}) = \begin{pmatrix} \kappa_1 (T_3 - T_1) \\ \kappa_2 (T_2 - T_3) \\ v_3 \\ A (P_1 - P_2) \end{pmatrix}, \ M = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -\frac{\alpha}{m_3} & \frac{1}{m_3} \end{pmatrix}$$

 $\mathbf{F} = F_{ext}$ and

$$\varphi\left(\boldsymbol{\eta},\boldsymbol{\zeta}_{s}\right) = \left(0 \ 0 \ -v_{3} \ 0 \ -\frac{1}{m_{3}}\right)^{\mathsf{T}}.$$
 (23)

In this case the driving forces are four: the differences of temperature $(T_3 - T_1)$ and $(T_2 - T_3)$ (correlated with the thermal equilibrium), the velocity v_2 (correlated to the momentum equilibrium), and the difference between the forces that apply the gases to the piston through pressure, $P_1 - P_2$ (correlated to mechanical or force equilibrium), while the external force is F_{ext} , respectively. Also note that, as in the previous example, the driving force correlated with the mechanical equilibrium, $P_1 - P_2$ for this case, does not appear in the entropy production

$$\Sigma := \kappa_1 \frac{(T_3 - T_1)^2}{T_1 T_3} + \kappa_2 \frac{(T_2 - T_3)^2}{T_2 T_3} + \frac{\alpha v_3^2}{T_3}$$

where the conjugated variable of η must be

$$\boldsymbol{\zeta}^{\mathsf{T}} = \frac{\partial S}{\partial \boldsymbol{\eta}} = \left(\frac{1}{T_1} \ \frac{1}{T_2} \ \frac{1}{T_3} \ \frac{(P_1 - P_2) A}{T_3} \ -\frac{m_3 v_3}{T_3}\right).$$

In addition, the driving force vector is equivalent to equation (11) with matrices

$$\Psi(\boldsymbol{\zeta}) = \begin{pmatrix} \kappa_1 T_1 T_3 & 0 & 0 & 0 \\ 0 & \kappa_2 T_2 T_3 & 0 & 0 \\ 0 & 0 & T_3 & 0 \\ 0 & 0 & 0 & T_3 \end{pmatrix}$$

and

$$L^{\mathsf{T}} = \begin{pmatrix} -1 & 0 & 1 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{m_3} \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

respectively. While defining matrices

it holds that M = R + J, and conditions (12) are satisfied

 $\left(\begin{array}{ccc} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{array}\right)$ Note that the eigenvalues of $R\Psi(\boldsymbol{\zeta}) L^{\mathsf{T}}$ are $\left\{0, 0, \left(\kappa_1 T_1\right)\right\}$

$$+\kappa_{2}T_{2}\pm\sqrt{\left(\kappa_{1}T_{1}\right)^{2}+\left(\kappa_{2}T_{2}\right)^{2}-\kappa_{1}\kappa_{2}T_{1}T_{2}}\right), \frac{\alpha T_{3}}{m_{3}^{2}}\right\}, \text{ while}$$

the eigenvalues of $J\Psi\left(\boldsymbol{\zeta}\right)L^{\mathsf{T}}$ are $\left\{0,0,0,\pm\frac{T_{3}}{m_{3}}i\right\}$. Thus,

using matrices (24) and (25) and vector (23), the adiabatic gas-piston-gas system can be expressed as system (14). Finally, it is straightforward to verify that equations (12) are fulfilled.

5.3 Adiabatic liquid-pendulum system

Let us now consider a pendulum immersed in an incompressible liquid bath as shown in Figure 3.

Under the assumption of incompressible liquid, Model the system can be split in two subsystems:

• Subsystem 1: Balances for the liquid (Internal energy, U_1)

$$\dot{U}_1 = \kappa \left(T_2 - T_1 \right)$$

• Subsystem 2: Balance for the pendulum (Internal energy, U_2 , angle position, θ_2 , and angular velocity, $\omega_2)$

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Fig. 3. Adiabatic liquid-pendulum system scheme.

$$\dot{U}_2 = -\kappa (T_2 - T_1) + \alpha (l\omega_2)^2$$
$$\dot{\theta}_2 = \omega_2$$
$$m_2 l\dot{\omega}_2 = -m_2 g \sin(\theta_2) - \alpha l\omega_2 + \frac{\tau}{l}$$

while the total energy of the pendulum is $E_2 = U_2 +$ $\frac{1}{2}m_2l^2\omega_2^2 + m_2gl(1-\cos{(\theta_2)})$, therefore its dynamical behavior is $\dot{E}_2 = -\kappa (T_2 - T_1) + \omega_2 \tau$.

The total energy of the system is $E = U_1 + E_2$, with dynamics $\dot{E} = \omega_2 \tau$, where τ is the torque.

Entropy dynamics The total entropy change is the sum of the liquid and pendulum entropy changes

$$dS = \frac{dU_1}{T_1} + \frac{dE_2 - m_2 l^2 \omega_2 d\omega_2}{T_2} - \frac{m_2 g l \sin(\theta_2) d\theta_2}{T_2}$$
(26)

therefore the entropy dynamic is

$$\dot{S} = \kappa \frac{(T_2 - T_1)^2}{T_1 T_2} + \frac{\alpha (l\omega_2)^2}{T_2}$$

Let define the state vector $\boldsymbol{\eta} = \operatorname{col} \{U_1, V_2\}$ Driving forces E_2, θ_2, ω_2 , whose dynamic is similar to system Π (Eq. (3.2)) with

$$f(\boldsymbol{\eta}) = \begin{pmatrix} \kappa (T_2 - T_1) \\ \omega_2 \\ m_2 g \sin(\theta_2) \end{pmatrix}, \ M = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\frac{\alpha}{m_2} & -\frac{1}{m_2 l} \end{pmatrix}$$

 $\mathbf{F} = \tau$ and

$$\varphi\left(\boldsymbol{\eta},\boldsymbol{\zeta}_{s}\right) = \left(0 \ \omega_{2} \ 0 \ \frac{1}{m_{2}l^{2}}\right)^{\mathsf{T}}.$$
 (27)

For this case the driving forces are three: the difference of temperature $(T_2 - T_1)$ (correlated with the thermal equilibrium), the angular velocity ω_2 (correlated to the momentum equilibrium), and the position of the pendulum $\sin(\theta_2)$ (correlated to mechanical or force equilibrium), while the external force is τ , respectively. In addition,

from equation (26) it is easy to see that the conjugated variable of η must be

$$\boldsymbol{\zeta}^{\mathsf{T}} = \frac{\partial S}{\partial \boldsymbol{\eta}} = \left(\frac{1}{T_1} \ \frac{1}{T_2} \ -\frac{m_2 g l \sin\left(\theta_2\right)}{T_2} \ -\frac{m_2 l^2 \omega_2}{T_2}\right)$$

Note that the driving force vector is equivalent to equation (11) with

$$\Psi\left(\boldsymbol{\zeta}\right) = \begin{pmatrix} \kappa T_1 T_2 & 0 & 0\\ 0 & T_2 & 0\\ 0 & 0 & T_2 \end{pmatrix} \text{ and } L = \begin{pmatrix} 1 & 0 & 0\\ -1 & 0 & 0\\ 0 & 0 & \frac{1}{l}\\ 0 & -\frac{1}{m_2 l^2} & 0 \end{pmatrix}$$

respectively. While defining matrices

$$R = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & -\frac{\alpha}{m_2} & 0 \end{pmatrix} \text{ and } J = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -\frac{1}{m_2 l} \end{pmatrix}$$

it holds that M = R + J, and conditions (12) are satisfied

Note that the eigenvalues of $R\Psi(\boldsymbol{\zeta}) L^{\mathsf{T}}$ are $\{0, 0, 2\kappa T_1 T_2, \alpha T_2/m_2^2 l^2\}$, while the eigenvalues of $J\Psi(\boldsymbol{\zeta}) L^{\mathsf{T}}$ are $\{0, 0, \pm i(T_2/m_2 l^2)\}$. Thus, using matrices (28) and 28 and vector 27, the adiabatic liquid-pendulum system can be expressed as system (14). Finally, it is straightforward to verify that equations (12) are fulfilled.

CONCLUDING REMARKS

On this work the entropy is used as a storage function in order to derive a structural representation of a class of thermo-mechanical systems in the Port Hamiltonian framework. The dissipation structures are correlated with irreversible processes and in our nomenclature the matrix $R\Psi(\boldsymbol{\zeta})L^{\mathsf{T}}$ is the analogue to the damping matrix for the PH systems and shows the dissipation, or the damping present in the network. In addition, it is remarkable that in the three study cases the number of non zero eigenvalues of this matrix is equal to the number of terms (phenomena) included in the internal entropy production and, as a matter of fact, $\boldsymbol{\zeta}^{\mathsf{T}} R \Psi(\boldsymbol{\zeta}) L^{\mathsf{T}} \boldsymbol{\zeta}$ is precisely the internal entropy production. On the other hand, the skew-symmetric matrix $J\Psi(\boldsymbol{\zeta}) L^{\mathsf{T}}$ is the analogue to the PH energy interconnection matrix, that in this case can be correlated with the reversible processes, since $\boldsymbol{\zeta}^{\mathsf{T}} J \Psi(\boldsymbol{\zeta}) L^{\mathsf{T}} \boldsymbol{\zeta} = 0$. In addition, the non zero eigenvalues of matrix $J\Psi(\boldsymbol{\zeta}) L^{\mathsf{T}}$ are purely imaginary. Finally, it is also important to remark that in general the dissipative structures in PH systems based on the energy for electric and mechanic systems

are correlated with the losses of energy (mechanical or electrical) due to friction, which are directly correlated with entropy production, therefore the proposed analysis in an extension that allows to include the thermal effects.

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