Interconnection of Irreversible port Hamiltonian Systems

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Abstract

This paper shows how the interconnection of two controlled Irreversible port Hamiltonian Systems has to be state and co-state modulated in order to ensure the closed-loop Irreversible port Hamiltonian structure, satisfying the first and second laws of Thermodynamics. It proposes a precise parametrization of this modulation from the open-loop systems structures in order to guarantee the consistency of the closed loop energy and entropy balance equations. The results are illustrated by means of the examples of a heat-exchanger, a gas-piston system and a chemical reaction.

Keywords: Port-Hamiltonian systems, irreversible Thermodynamics, thermo-mechanical systems, port-based modeling, state modulated output feedback.

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1. Introduction

Irreversible port-Hamiltonian systems (IPHS) were first introduced in Ramirez et al. (2013a,b) as an extension of port-Hamiltonian systems (PHS) (Maschke and van der Schaft, 1992; Duindam et al., 2009) for irreversible thermo-mechanical systems defined on finite dimensional spaces and later extended to distributed parameter systems defined on one dimensional spatial domains in (Ramirez et al., 2022; Ramirez and Le Gorrec, 2022). One of the main features of the PHS formalism is its modularity, i.e., the capability of modeling complex systems as the interconnection of simpler sub-systems (van der Schaft, 2000; Duindam et al., 2009). This is possible because the output of a PHS is power conjugated with its input defining a passive relation, hence a power-preserving interconnection of two PHS results again in a PHS. This feature has not only been exploited for modeling, but also for Passivity Based Control (PBC) (Ortega et al., 2001, 2002). When dealing with the interconnection of thermodynamic or thermo-mechanic systems (van der Schaft and Maschke, 2018), the interconnected system has to preserve not only the total energy, but also satisfy that the total internal entropy creation is non-negative in order to fulfill the first and second laws of Thermodynamics. This fundamental property is in the core of the different system theoretic formulations of thermodynamic systems which encode the irreversible entropy production in their structure, such as IPHS, pseudo-gradient systems (Favache et al., 2011), metriplectic systems (sum of Hamiltonian and gradient systems) with one or two generating functions (Grmela and Öttinger, 1997; Grmela, 2002) and control Hamiltonian systems defined on contact manifolds (Mrugala et al., 1991; Eberard et al., 2007; Favache et al., 2010; Ramirez et al., 2013a) or their symplectization (van der Schaft and Maschke, 2018). A thermodynamic formulation in which the second law is systematically encoded into the model by means of the interconnection of fundamental elements is found in nonlinearly constrained Lagrangian systems (Gay-Balmaz and Yoshimura, 2020, 2023) which steam from variational principles.

In this work we extend and formalize the preliminary results of (Ramirez and Le Gorrec, 2023) to show that the power preserving interconnection of two thermodynamic systems needs to be modulated such that the interconnected system remains a thermodynamic system. The modulating function depends on the interface, input maps, the conjugated outputs and the temperature of the systems. For the particular case of IPHS, the modulating function is precisely formulated in terms of a pseudo bracket defined by the total entropy and energy functions and the input maps of the subsystems. Moreover, the pseudo bracket precisely defines the thermodynamic driving force of the interconnection. This result reflects a well know property in Thermodynamics that the entropy balance of an open thermodynamic system depends on the entropy generated by the interface/mixing terms. This formalization is a key step in the generalization of control/observer design techniques for IPHS (Ramirez et al., 2016; Maschke et al., 2022; Zenfari et al., 2023) and explains from a thermodynamic system theoretic perspective the fact that preliminary results on control by interconnection of IPHS lead to modulated interconnections between the controller and the plant (Villalobos et al., 2020; Le Gorrec et al., 2022). It is interesting to notice that modulated interconnection can be found in PBC by interconnection approaches which explicitly incorporate the dissipation of the plant into the control design and stability analysis, such as for instance energy shaping (Maschke et al., 2000) or control based on virtual energy tanks (Franken et al., 2011; Ferraguti et al., 2015). In energy shaping the reduction of the dynamics stems from the existence of invariant functions (Casimirs) that relate the states of the controller with those of the plant. However the applicability of energy shapping is restricted by the systems natural dissipation. This restriction has been overcome by explicitly incorporating information on the systems state by means of state modulated power preserving interconnections which allow to shape the closed-loop energy function without the need for Casimir functions (Ortega et al., 2001, 2002). In the approach based on virtual tanks the energy dissipated by the system is stored by the controller in order to later reemploy the system to produce desired behaviors in a passive way. The approach has been further extended by using modulated power preserving interconnections between the energy tanks and the plant to achieve higher flexibility and robustness (Benzi et al., 2022).

The paper is organized as follows. Section 2 motivates this work by commenting on the interconnection of PHS. Section 3 gives the preliminaries on IPHS. Section 4 presents the main results of this work, namely the necessity of a state and co-state modulated interconnection to preserve the entropy production and its precise definition for IPHS. This modulated interconnection is entirely parametrized from the interconnected systems structures and interconnection. Section 5 presents three examples: the ideal heat-exchanger, the gas-piston system and a chemical reaction. Finally in Section 6 the conclusions of the paper are presented.

2. Interconnection of port-Hamiltonian systems

On the state space $x \in \mathbb{R}^n$ a PHS (Maschke and van der Schaft, 1992; van der Schaft, 2000) is defined as

$$\begin{aligned} \dot{x} &= (J_0 - D_0)\frac{\partial H_0}{\partial x} + gu \\ y &= g^\top \frac{\partial H_0}{\partial x}, \end{aligned} \tag{1}$$

where the function $H_0(x) : \mathbb{R}^n \to \mathbb{R}$ represents the energy stored in energy storing elements, $J_0(x) = -J_0(x) \in \mathbb{R}^{n\times n}$ is a state-dependent skew-symmetric matrix, $D_0(x) = D_0^\top(x) \in \mathbb{R}^{n\times n} \geq 0$ is a state-dependent positive definite matrix, $g(x) \in \mathbb{R}^{m\times n}$ is the input matrix and $u(t), y(t) \in \mathbb{R}^m$ are the input and the power conjugated output, respectively. The skew-symmetric matrix J_0 characterizes the coupling between energy storing elements and the matrix D_0 characterizes the coupling between energy storing and energy dissipating elements. Furthermore, if J_0 satisfies some integrability conditions, namely the Jacobi identities (Libermann and Marle, 1987), then it is the definition of a *Poisson bracket*. The energy balance of (1) is

$$\dot{H}_0 = -\frac{\partial H_0}{\partial x}^\top D_0 \frac{\partial H_0}{\partial x} + y^\top u, \tag{2}$$

implying that (1) passive if H_0 is bounded from below. It is well known (van der Schaft, 2000) that the power preserving interconnection of two passive system is again a passive system. Take for instance the negative output feedback interconnection between two PHS of state x_1 and x_2

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = k \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \tag{3}$$

where k is a constant. The closed-loop energy is then the sum of the stored energy in each system $H_0 = H_{0_1} + H_{0_2}$ and the total energy balance is

$$\begin{aligned} \dot{H}_0 &= \dot{H}_{0_1} + \dot{H}_{0_2} \\ &= -\frac{\partial H_{0_1}}{\partial x_1}^\top D_{0_1} \frac{\partial H_{0_1}}{\partial x_1} - \frac{\partial H_{0_2}}{\partial x_2}^\top D_{0_2} \frac{\partial H_{0_2}}{\partial x_2} + y_1^\top u_1 + y_2^\top u_2 \\ &= -\frac{\partial H_0}{\partial x}^\top \begin{bmatrix} D_{0_1} & 0 \\ 0 & D_{0_2} \end{bmatrix} \frac{\partial H_0}{\partial x} \leq 0 \end{aligned}$$

with $x = [x_1, x_2]^\top$. The closed-loop dynamics is given by

$$\begin{aligned} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} &= (J_0 - D_0) \begin{bmatrix} \frac{\partial H_{0_1}}{\partial x_1} \\ \frac{\partial H_{0_2}}{\partial x_2} \end{bmatrix} + \begin{bmatrix} g_1 & 0 \\ 0 & g_2 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \\ \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} &= \begin{bmatrix} g_1^\top & 0 \\ 0 & g_2^\top \end{bmatrix} \begin{bmatrix} \frac{\partial H_{0_1}}{\partial x_1} \\ \frac{\partial H_{0_2}}{\partial x_2} \end{bmatrix} \end{aligned} \tag{4}$$

where the closed-loop interconnection and dissipation matrices are

$$J_0 = \begin{bmatrix} J_{0_1} & kg_1g_2^\top \\ kg_2g_1^\top & J_{0_2} \end{bmatrix}, \qquad D_0 = \begin{bmatrix} D_{0_1} & 0 \\ 0 & D_{0_2} \end{bmatrix}$$

and where v_1 and v_2 are a new set of inputs. The power-preserving interconnection (3) leads to a closed-loop PHS with the same passivity properties of the interconnected systems. A practical interpretation of this result is that if two mechanical systems are interconnected, then the resulting system is again a mechanical system.

3. Irreversible port-Hamiltonian systems

Consider the PHS (1), if $D_0 = 0$, then (1) is energy preserving or reversible. On the other hand if $D_0 \neq 0$ the system is dissipative meaning that energy is being transformed into heat by some dissipative phenomena, such as a electrical resistance or mechanical friction. In this case the total energy of the system is the sum of the energy stored in energy storing elements and some thermal energy, which for simplicity we shall assume can be split as

$$H(x, s) = H_0(x) + U(s).$$

where s is the entropy of the system. From the firs law, in the absence of exchange of energy with the surroundings of the system i.e. $u = 0$, the total energy has to be conserved. This implies that

$$\begin{aligned} \dot{H} &= \dot{H}_0 + \dot{U} = 0 \\ &= -\frac{\partial H_0}{\partial x}^\top D_0 \frac{\partial H_0}{\partial x} + \frac{\partial U}{\partial s}\dot{s} = 0 \end{aligned}$$

From Gibbs' fundamental relation, the temperature is a function of the entropy defined as $T = \frac{\partial H}{\partial s}(s) = \frac{\partial U}{\partial s}$, so the internal entropy creation of the system is given by

$$\dot{s} = \frac{1}{T}\frac{\partial H_0}{\partial x}^\top D_0 \frac{\partial H_0}{\partial x} = \sigma \geq 0$$

in accordance with the second law of Thermodynamics. The resulting system is then

$$\begin{aligned} \begin{bmatrix} \dot{x} \\ \dot{s} \end{bmatrix} &= \begin{bmatrix} J_0 & -D_0 \frac{\partial H_0}{\partial x}\frac{1}{T} \\ \frac{1}{T}\frac{\partial H_0}{\partial x}^\top D_0^\top & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H_0}{\partial x} \\ T \end{bmatrix} + \begin{bmatrix} g \\ 0 \end{bmatrix} u, \\ y &= \begin{bmatrix} g & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H_0}{\partial x} \\ \frac{\partial H_0}{\partial s} \end{bmatrix}. \end{aligned} \tag{5}$$

which corresponds to a quasi-Hamiltonian (Ramirez et al., 2013a) since it resembles a PHS but its structure matrix is a function of the gradient of the energy. In this sense the symplectic structure of the PHS, given by the Poisson tensor associated with the structure matrix is destroyed.

IPHS are a particular class of quasi-Hamiltonian systems. The state variables of the IPHS are the $n + 1$ *extensive variables*[1]. The following partition of the state $\mathbf{x} \in \mathbb{R}^{n+1}$ is considered: the first n variables by $x = [q_1, \ldots, q_n]^\top \in \mathbb{R}^n$ and the entropy coordinate by $s \in \mathbb{R}$. The thermodynamic properties of the system are expressed by Gibbs' equation (Callen, 1985), which in its local form with pairs of specific energy-conjugated variables (Duindam et al., 2009, Chapter 3) is

$$dH = Tds + \sum_{i=1}^{n} p_i dq_i \tag{6}$$

where T is the temperature, conjugated to the entropy, and the variables p_i denote the *intensive variables*, which are conjugated to the q_i variables. Gibbs' equation is here understood in a general context in order to account for coupled thermo-electro/magnetic/mechanical systems. Gibbs' equation is equivalent to the existence of a total energy and entropy function, H and s, respectively.

Definition 1. *For any two functions Z and G and for any matrix $\mathcal{G}$ we define the Poisson bracket as*

$$\{Z, G\}_{J_0} = \{Z|\mathcal{G}|G\} = \begin{bmatrix} \frac{\partial Z}{\partial x} \\ \frac{\partial Z}{\partial s} \end{bmatrix} \underbrace{\begin{bmatrix} 0 & \mathcal{G} \\ -\mathcal{G}^\top & 0 \end{bmatrix}}_{J_0} \begin{bmatrix} \frac{\partial G}{\partial x} \\ \frac{\partial G}{\partial s} \end{bmatrix}$$

Definition 2. *An IPHS undergoing j irreversible processes is defined by*

- *a pair of functions: the total energy $H : \mathbb{R}^{n+1} \to \mathbb{R}$ and the total entropy $s \in \mathbb{R}$,*
- *a pair of matrices $J_0 = -J_0^\top \in \mathbb{R}^{n \times n}$ and $G \in \mathbb{R}^{n \times j}$ with $j \leq n$ and the positive real-valued functions $\gamma_i(x, s)$, $i \in \{1, \ldots j\}$,*

and the ODE

$$\begin{aligned} \begin{bmatrix} \dot{x} \\ \dot{s} \end{bmatrix} &= \begin{bmatrix} J_0 & G\mathbf{R} \\ -\mathbf{R}^\top G^\top & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial x} \\ \frac{\partial H}{\partial s} \end{bmatrix} + gu \\ y &= g^\top \begin{bmatrix} \frac{\partial H}{\partial x} \\ \frac{\partial H}{\partial s} \end{bmatrix} \end{aligned} \tag{7}$$

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[1] A variable is qualified as extensive when it characterizes the thermodynamic state of the system and its total value is given by the sum of its constituting parts.

where $u, y \in \mathbb{R}^m$ are respectively the input and power conjugated output, and $g \in \mathbb{R}^{(n+1)\times m}$ the input map. The elements of the vector $\mathbf{R} \in \mathbb{R}^{j\times 1}$ are defined as

$$R_i = \gamma_i \{s|G(:, i)|H\} \tag{8}$$

where the notation $G(:, i)$ indicates the i-th column of the matrix G.

The total energy balance is $\dot{H} = y^\top u$ implying that $\dot{H} = 0$ if $u = 0$ expressing the first law of Thermodynamics. The internal entropy balance is given by the dynamic of the last coordinate with $u = 0$, which can be decomposed using the definition of $\mathbf{R}$ as

$$\begin{aligned}\dot{s} &= -\mathbf{R}^\top G^\top \frac{\partial H}{\partial x} = -\sum_i^j \left(R_i G(:, i)^\top \frac{\partial H}{\partial x}\right)\\ &= \sum_i^j \gamma_i \{s|G(:, i)|H\}^2 = \sum_i^j \sigma_i = \sigma \geq 0,\end{aligned} \tag{9}$$

in accordance with the second law of Thermodynamics. Here $\sigma_i \geq 0$ is the internal entropy production due to the i-th irreversible thermodynamic process and σ is the total internal entropy production. The reader is referred to (Ramirez et al., 2022, 2013a,b) for more details and examples of IPHS.

4. Interconnection of IPHS

Before giving our main result we shall comment on the particularity of interconnecting two thermodynamic systems analyzing Gibb's fundamental relation (6).

4.1. The interconnection of thermodynamic systems

Assume for simplicity that a purely thermodynamic reservoir (s_1, T_1) is being interconnected with a purely mechanical system $\left(x_2, \frac{\partial H_2}{\partial x_2}\right)$ through some dissipative port and that the only source of entropy is the interconnection itself. Gibb's relation is then given by

$$\begin{aligned}\dot{H} &= T_1\dot{s}_1 + \sum_{i=1}^n p_i\dot{q}_i\\ &= T_1\dot{s}_1 + \frac{\partial H_2}{\partial x_2}^\top \dot{x}_2\\ &= y_1^\top u_1 + y_2^\top u_2\end{aligned}$$

The power preserving interconnection (3) assures energy conservation since $\dot{H} = 0$. Assuming uniform temperature, i.e. $T_1 = T$ and $s_1 = s$, the second law requires that $\dot{s} \geq 0$, or equivalently that

$$\dot{s} = -\frac{1}{T}\frac{\partial H_2}{\partial x_2}^\top \dot{x}_2 = -\frac{1}{T} y_2^\top u_2 \geq 0 \tag{10}$$

The interconnection law (3) does not guarantee that this inequality holds.

Proposition 3. *The power preserving interconnection of two thermodynamic systems needs to be modulated for the interconnected system to be a thermodynamic system. Furthermore, the modulating function depends on the the interface, input maps, the conjugated outputs (intensive variables) and the temperature of the systems.*

Proof. Consider the modulated power preserving interconnection

$$\begin{bmatrix} u_1\\ u_2\end{bmatrix} = \beta\begin{bmatrix} 0 & 1\\ -1 & 0\end{bmatrix}\begin{bmatrix} y_1\\ y_2\end{bmatrix} \tag{11}$$

with β the modulating function. The entropy production (10) becomes

$$\dot{s} = \beta\frac{1}{T} y_2^\top y_1 \geq 0$$

implying that the modulating function needs to be of the form $\beta = \gamma y_2^\top y_1$, with γ a positive semidefinite function, to satisfy the second law. Similarly, if two thermodynamic reservoirs at different temperatures are interconnected, then Gibb's relation becomes

$$\dot{s} = \dot{s}_1 + \dot{s}_2 = \frac{\dot{H}_1}{T_1} + \frac{\dot{H}_2}{T_2} = \frac{T_2\dot{H}_1 + T_1\dot{H}_2}{T_1T_2}$$

which requires that $T_2\dot{H}_1 + T_1\dot{H}_2 \geq 0$. Since $\dot{H}_i = y_i^\top u_i$, and using (11) this condition becomes

$$\beta(T_2 - T_1) y_2^\top y_1 \geq 0$$

implying that $\beta = \gamma(T_2 - T_1) y_2^\top y_1$. ■

Notice that the modulating function β is precisely defined by the ports of the systems, the temperature and the interface through the positive function γ.

4.2. Main result

Proposition 3 can be stated in a precise manner using the IPHS formulation of two thermodynamic systems.

Proposition 4. *Consider two IPHS, indexed by $i = 1, 2$, defined as*

$$\begin{bmatrix}\dot{x}_i\\ \dot{s}_i\end{bmatrix} = J_i\begin{bmatrix}\frac{\partial H_i}{\partial x_i}\\ \frac{\partial H_i}{\partial s_i}\end{bmatrix} + g_i u_i, \qquad y_i = g_i^\top\begin{bmatrix}\frac{\partial H_i}{\partial x_i}\\ \frac{\partial H_i}{\partial s_i}\end{bmatrix} \tag{12}$$

where

$$J_i = \begin{bmatrix} J_{0i} & G_i\mathbf{R}_i\\ -\mathbf{R}_i^\top G_i^\top & 0\end{bmatrix}$$

with $x_i \in \mathbb{R}^{n_i}$, $s_i \in \mathbb{R}$, $u_i \in \mathbb{R}$, $J_{0_i} \in \mathbb{R}^{n_i\times n_i}$, $g_i \in \mathbb{R}^{(n_i+1)}$. Consider the state modulated interconnection

$$\begin{bmatrix} u_1\\ u_2\end{bmatrix} = R_u\begin{bmatrix} 0 & 1\\ -1 & 0\end{bmatrix}\begin{bmatrix} y_1\\ y_2\end{bmatrix} \tag{13}$$

where the modulating scalar function is defined as

$$R_u = \gamma_u \{s | g_1 g_2^\top | H\} \tag{14}$$

and where $s = s_1 + s_2$ and $H = H_1 + H_2$ are, respectively, the total entropy and the total energy. The interconnection (13) *defines the IPHS*

$$\begin{aligned} \begin{bmatrix} \dot{x}_1 \\ \dot{s}_1 \\ \dot{x}_2 \\ \dot{s}_2 \end{bmatrix} &= J \begin{bmatrix} \frac{\partial H}{\partial x_1} \\ \frac{\partial H}{\partial s_1} \\ \frac{\partial H}{\partial x_2} \\ \frac{\partial H}{\partial s_2} \end{bmatrix} + \begin{bmatrix} g_1 & 0 \\ 0 & g_2 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \\ \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} &= \begin{bmatrix} g_1^\top & 0 \\ 0 & g_2^\top \end{bmatrix} \begin{bmatrix} \frac{\partial H}{\partial x_1} \\ \frac{\partial H}{\partial s_1} \\ \frac{\partial H}{\partial x_2} \\ \frac{\partial H}{\partial s_2} \end{bmatrix} \end{aligned} \tag{15}$$

where

$$J = \begin{bmatrix} J_1 & R_u g_1 g_2^\top \\ -R_u g_2 g_1^\top & J_2 \end{bmatrix}$$

and where v_1 and v_2 are a new set of inputs.

Corollary 5. *The internal entropy production of* (15) *is $\sigma = \sigma_1 + \sigma_2 + \sigma_u \geq 0$, where σ_1 and σ_2 are respectively the internal entropy production of system 1 and 2, and*

$$\sigma_u = \gamma_u \{s | g_1 g_2^\top | H\}^2 \geq 0$$

is the entropy produced by the interconnection of the systems.

Proof. System (15) is directly obtained using the state modulated interconnection (13). Assume for simplicity and without loss of generality that $v_1 = v_2 = 0$. The structure matrix of the interconnected system J is skew-symmetric, hence $\dot{H} = 0$ and conservation of the total Hamiltonian function is obtained. On the other hand, the time derivative of the total entropy function is, define $z = [x_1^\top, s_1, x_2^\top, s_2]^\top$,

$$\begin{aligned} \dot{s} &= \dot{s}_1 + \dot{s}_2 \\ &= \frac{\partial s}{\partial z}^\top \dot{z} = \frac{\partial s}{\partial z}^\top J \frac{\partial H}{\partial z} = \frac{\partial s}{\partial z}^\top (J' + J_u) \frac{\partial H}{\partial z} \\ &= \{s, H\}_{J'} + \{s, H\}_{J_u} \end{aligned}$$

where

$$J' = \begin{bmatrix} J_1 & 0 \\ 0 & J_2 \end{bmatrix}, \quad \text{and} \quad J_u = \begin{bmatrix} 0 & R_u g_1 g_2^\top \\ -R_u g_2 g_1^\top & 0 \end{bmatrix}.$$

Developing the first bracket we obtain

$$\begin{aligned} \{s, H\}_{J'} &= \begin{bmatrix} \frac{\partial s}{\partial x_1} \\ \frac{\partial s}{\partial s_1} \end{bmatrix}^\top J_1 \begin{bmatrix} \frac{\partial H}{\partial x_1} \\ \frac{\partial H}{\partial s_1} \end{bmatrix} + \begin{bmatrix} \frac{\partial s}{\partial x_2} \\ \frac{\partial s}{\partial s_2} \end{bmatrix}^\top J_2 \begin{bmatrix} \frac{\partial H}{\partial x_2} \\ \frac{\partial H}{\partial s_2} \end{bmatrix} \\ &= -\mathbf{R_1}^\top G_1^\top \frac{\partial H_1}{\partial x_1} + -\mathbf{R_2}^\top G_2^\top \frac{\partial H_2}{\partial x_2} \\ &= \sigma_1 + \sigma_2 \geq 0 \end{aligned}$$

Developing the second bracket we obtain

$$\{s, H\}_{J_u} = R_u \{s | g_1 g_2^\top | H\} = \gamma_u \{s | g_1 g_2^\top | H\}^2 = \sigma_u \geq 0$$

where σ_u is the entropy produced by the interconnection of the systems. Hence, the entropy balance is

$$\dot{s} = \sigma_1 + \sigma_2 + \sigma_u \geq 0$$

in accordance with the second law. ■

Notice that if in Proposition 4 the IPHS systems (12) reduce to PHS, i.e., $T_1 = T_2$ and $\dot{s}_1 = 0$ and $\dot{s}_2 = 0$, then the modulated function of the interconnection can be set to $\beta = k$ and the power-preserving interconnection (3) is obtained.

5. Examples

The interconnection law proposed in Propositions 3 and 4 are illustrated in this section by means of three examples, the heat-exchanger, the gas-piston system and a chemical reaction.

5.1. The heat-exchanger

Consider two simple thermodynamic systems, indexed by 1 and 2, which may interact only through a conducting wall. Assuming that the two compartments contain pure ideal gases and that they undergo no deformation, and are closed, the temperatures may be modeled as functions of the entropy (Couenne et al., 2006). The IPHS formulation of each system is

$$\dot{s}_i = u_i, \qquad y_i = \tfrac{\partial U_i}{\partial s_i} = T_i$$

where s_1 and s_2 (resp. T_1 and T_2) are the entropies (resp. the temperatures) and U_1 and U_2 the internal energies of system 1 and 2. The inputs u_1 and u_2 correspond to the entropy flow that the systems exchange and y_1 and y_2 are the energy conjugated outputs. According to Fourier's law the entropy flows into each subsystem are driven by its corresponding thermodynamic driving force (Kondepudi and Prigogine, 1998), which is the temperature difference between the compartments $u_1 = \frac{\lambda}{T_1}(T_2 - T_1)$ and $u_2 = \frac{\lambda}{T_2}(T_1 - T_2)$, where $\lambda > 0$ denotes Fourier's heat conduction coefficient of the heat conducting wall between the two compartments. According to Proposition 3 the previous relation can be equivalently written as

$$\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \beta \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \end{bmatrix}$$

where $\beta = \frac{\lambda}{T_1 T_2}(T_2 - T_1)$. The interconnected system is then

$$\begin{aligned}\begin{bmatrix}\dot{s}_1\\ \dot{s}_2\end{bmatrix} &= \frac{\lambda}{T_1 T_2}(T_2 - T_1)\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}\begin{bmatrix}T_1\\ T_2\end{bmatrix}\\ \begin{bmatrix}y_1\\ y_2\end{bmatrix} &= \begin{bmatrix}T_1\\ T_2\end{bmatrix}\end{aligned} \tag{16}$$

which is the IPHS model of the heat exchanger (Ramirez et al., 2013a,b). Consider now Proposition 4. Defining the total internal energy and the total entropy of the interconnected system as $U = U_1 + U_2$ and $s = s_1 + s_2$, respectively, we obtain

$$\begin{aligned}\{s|1|U\} &= \frac{\partial s}{\partial x}^{\top}\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}\frac{\partial U}{\partial x} = \begin{bmatrix}1\\ 1\end{bmatrix}^{\top}\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}\begin{bmatrix}T_1\\ T_2\end{bmatrix}\\ &= T_2 - T_1.\end{aligned}$$

which is the driving force of the entropy flow between the compartments. Consequently $\gamma = \frac{\lambda}{T_1 T_2}$ and $R = \beta$.

Consider in a second instance that the inputs are the heat flows rather than the entropy flows. The dynamical model of the heat exchanger is then

$$\dot{s}_i = \frac{1}{T_i}u_i, \qquad y_i = \frac{1}{T_i}\frac{\partial U_i}{\partial s_i} = 1$$

In this case the energy conjugated outputs are physically meaningless. The heat flow between the compartments are in this case $u_1 = \lambda(T_2 - T_1)$ and $u_2 = \lambda(T_1 - T_2)$, which can be equivalently written as

$$\begin{bmatrix}u_1\\ u_2\end{bmatrix} = \beta\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}\begin{bmatrix}1\\ 1\end{bmatrix}$$

with $\beta = \lambda(T_2 - T_1)$ in accordance with Proposition 3. From Proposition 4 we have that

$$\begin{aligned}\{s|(T_1T_2)^{-1}|U\} &= \begin{bmatrix}1\\ 1\end{bmatrix}^{\top}\frac{1}{T_1 T_2}\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}\begin{bmatrix}T_1\\ T_2\end{bmatrix}\\ &= \frac{1}{T_1} - \frac{1}{T_2}.\end{aligned}$$

which is the thermodynamic force that drives the heat flow (Kondepudi and Prigogine, 1998). Consequently $\gamma = \lambda T_1 T_2$ and $R = \frac{\beta}{T_1 T_2}$.

5.2. *The gas-piston system*

Consider an ideal gas contained in a cylinder with no exchange of matter enclosed by a moving piston which is attached to a spring (Ramirez et al., 2013b). For simplicity consider that the cylinder is not subject to external forces and does not exchange heat with the environment. The system is characterized by the mechanical properties of the piston and the thermodynamic properties of the gas. The dynamic equations of the moving piston are $\dot{q} = v$ and $\dot{p} = F_g - F_r - F$, where q is the relative position of the spring, p is the momentum, $v = \frac{p}{m}$ is the velocity of the piston, $F = Kq$ is the force applied by the spring, F_g is the force applied on the piston by the gas pressure and F_r represents the mechanical friction with m the mass of the piston and K Hooke's constant. The mechanical energy of the piston is $H_0(q, p) = \frac{1}{2m}p^2 + \frac{1}{2}Kq^2$ and its PHS formulation

$$\begin{aligned}\begin{bmatrix}\dot{q}\\ \dot{p}\end{bmatrix} &= J_0\frac{\partial H_0}{\partial x} + \begin{bmatrix}g_{p_1} & g_{p_2}\end{bmatrix}\begin{bmatrix}u_{p_1}\\ u_{p_2}\end{bmatrix}\\ \begin{bmatrix}y_{p_1}\\ y_{p_2}\end{bmatrix} &= \begin{bmatrix}g_{p_1}^{\top}\\ g_{p_2}^{\top}\end{bmatrix}\frac{\partial H_0}{\partial x} = \begin{bmatrix}-v\\ v\end{bmatrix}\end{aligned}$$

with $u_{p_1} = F_r$, $u_{p_2} = F_p$, $\frac{\partial H_0}{\partial x} = \begin{bmatrix}Kq & \frac{p}{m}\end{bmatrix}^{\top} = \begin{bmatrix}F & v\end{bmatrix}^{\top}$, $J_0 = \begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}$, $g_{p_1} = \begin{bmatrix}0 & -1\end{bmatrix}^{\top}$ and $g_{p_2} = \begin{bmatrix}0 & 1\end{bmatrix}^{\top}$. Notice that for ease of presentation the input map has been split into two vectors, one associated to the irreversible phenomena and other to the reversible phenomena, respectively g_{p_1} and g_{p_2}.

On the other hand the dynamic equations of the gas in the piston are given by $\dot{V} = q_v$ and $\dot{s} = \sigma$, where V is the volume and s is the entropy of the gas, q_v is the gas flow due to the displacement of gas by the moving piston and σ is the irreversible creation of entropy due to the non-reversible transformation of mechanical friction into heat when the piston moves. The internal energy of the perfect gas, $U(s, V)$, is a function of the entropy and the volume. The intensive variables of the gas are the temperature $T = \frac{\partial U}{\partial s}$ and the pressure $-P = \frac{\partial U}{\partial V}$. Furthermore, the temperature, the volume and the pressure of the gas are related by the law of the ideal gases. The IPHS formulation of the gas is

$$\begin{aligned}\begin{bmatrix}\dot{V}\\ \dot{s}\end{bmatrix} &= \begin{bmatrix}g_1 & g_2\end{bmatrix}\begin{bmatrix}u_1\\ u_2\end{bmatrix}\\ \begin{bmatrix}y_1\\ y_2\end{bmatrix} &= \begin{bmatrix}g_1^{\top}\\ g_2^{\top}\end{bmatrix}\frac{\partial U}{\partial x} = \begin{bmatrix}-P\\ T\end{bmatrix}\end{aligned}$$

with $u_1 = q_v$, $u_2 = \sigma$, $g_1 = \begin{bmatrix}1 & 0\end{bmatrix}^{\top}$ and $g_2 = \begin{bmatrix}0 & 1\end{bmatrix}^{\top}$.

The piston and the gas are interconnected through a reversible and an irreversible relation. The reversible interconnection relates the gas flow and the velocity of the piston and the pressure of the gas with the force applied on the piston. This interconnection can be formulated as the power preserving interconnection (3),

$$\begin{bmatrix}u_1\\ u_{p_2}\end{bmatrix} = A\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}\begin{bmatrix}y_1\\ y_{p_2}\end{bmatrix}$$

where A is the transversal area of the piston.

The irreversible interconnection relates the temperature of the gas with the mechanical friction force and the entropy creation with the velocity of the piston. The mechanical friction can be modeled as $F_r = bv$, and consequently the entropy creation is $\sigma = \frac{1}{T}bv^2$, with $b > 0$ the friction constant. The interconnection is formulated according to Proposition 3 as

$$\begin{bmatrix} u_{p_1} \\ u_2 \end{bmatrix} = \beta \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} y_{p_1} \\ y_2 \end{bmatrix}$$

with $\beta = \frac{b}{T}v$. Using these interconnections the gas-piston system is formulated as the IPHS

$$\begin{bmatrix} \dot{q} \\ \dot{p} \\ \dot{V} \\ \dot{s} \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & A & -R \\ 0 & -A & 0 & 0 \\ 0 & R & 0 & 0 \end{bmatrix} \begin{bmatrix} F \\ v \\ (-P) \\ T \end{bmatrix}$$

The total energy of the system is the sum of the mechanical energy and the internal energy

$$H = H_0 + U = \frac{1}{2m}p^2 + \frac{1}{2}Kq^2 + U(s, V)$$

and from Proposition 4 we have

$$\left\{ s \middle| \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix} \middle| H \right\} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}^\top \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} F \\ v \\ (-P) \\ T \end{bmatrix} = v$$

i.e., the velocity of the moving piston, which induces the heating of the gas and corresponds to the thermodynamic driving force of the interconnection. Consequently $\gamma = \frac{b}{T}$ and $R = \beta$.

5.3. A chemical reaction

Let us consider for simplicity a single reaction occurring at a reactor with constant volume under adiabatic conditions, i.e., there is no exchange of matter or heat with the surroundings, with the following reversible reaction scheme (Horn and Jackson, 1972; Feinberg, 1987)

$$\sum_{i=1}^{m} \zeta_i B_i \overset{r}{\rightleftharpoons} \sum_{i=1}^{m} \eta_i B_i$$

with ζ_i, η_i being the constant stoichiometric coefficients for species B_i in the reaction and r is the reaction velocity (Kondepudi and Prigogine, 1998). Before the reaction takes place the total energy and entropy balance are zero and the mole balance of each species can be written as the IPHS

$$\dot{\mathbf{n}} = g u_n, \qquad y_n = g^\top \frac{\partial U_n}{\partial \mathbf{n}} \tag{17}$$

where $\mathbf{n} = [n_1, \ldots, n_m]^\top$ with n_i the number of moles of the species i, $g = \boldsymbol{\nu} = [\bar{\nu}_1, \ldots, \bar{\nu}_m]^\top$ is the stoichiometric vector whose elements are the signed stoichiometric coefficients of the chemical reaction $\bar{\nu}_i = \zeta_i - \eta_i$, U_n is the internal energy of the species, $\frac{\partial U_n}{\partial \mathbf{n}} = \boldsymbol{\mu} = [\mu_1, \ldots, \mu_m]^\top$ with μ_i the chemical potential of the species i, the input u_n is the net conversion of the reactants to products, the output $y_n = \boldsymbol{\nu}^\top \boldsymbol{\mu} = \sum_{i=1}^{m} \bar{\nu}_i \mu_i = -\mathcal{A}$ is the negative of the chemical affinity of the reaction and s the total entropy. The entropy balance is given by the IPHS

$$\dot{s} = u_s \qquad y_s = \frac{\partial U_s}{\partial s}, \tag{18}$$

where u_s is entropy flow, U_s the internal energy in the reactor and $\frac{\partial U_s}{\partial s} = T$ the temperature in the reactor. Before the species are mixed in the reactor there is no reaction so $u_n = 0$ and $u_s = 0$. The moment the species mix they are interconnected according to Proposition 4

$$\begin{bmatrix} u_n \\ u_s \end{bmatrix} = R \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} y_n \\ y_s \end{bmatrix}.$$

Let us compute the modulating function $R = \gamma\{s|\boldsymbol{\nu}|U\}$ with respect to the total internal energy $U = U_n + U_s$. The bracket is given by

$$\begin{aligned} \{s|\boldsymbol{\nu}|U\} &= \begin{bmatrix} 0_{m\times 1} \\ 1 \end{bmatrix}^\top \begin{bmatrix} 0_{m\times m} & \boldsymbol{\nu} \\ \boldsymbol{\nu}^\top & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\mu} \\ T \end{bmatrix} \\ &= -\sum_{i=1}^{m} \bar{\nu}_i \mu_i = \mathcal{A} \end{aligned}$$

which corresponds to the affinity of reaction which is the thermodynamic driving force of the chemical reaction. Consequently, and according to De Donder's fundamental relation (Aris, 1989; Kondepudi and Prigogine, 1998), $\gamma = \frac{r}{T\mathcal{A}} \geq 0$ and the inputs of each subsystem are

$$\begin{aligned} u_n &= R y_s = r \\ u_s - R y_n &= -\frac{r}{T}\mathcal{A} = -\frac{r}{T} \sum_{i=1}^{m} \bar{\nu}_i \mu_i = \sigma \geq 0 \end{aligned}$$

respectively the reaction velocity and the entropy production due to the chemical reaction σ. The closed-loop system corresponds to the dynamic of the chemical reaction and is given by

$$\dot{\mathbf{n}} = r\boldsymbol{\nu} \qquad \dot{s} = -\frac{r}{T} \sum_{i=1}^{m} \bar{\nu}_i \mu_i \tag{19}$$

which can equivalently be written as the IPHS

$$\begin{bmatrix} \dot{\mathbf{n}} \\ \dot{s} \end{bmatrix} = \frac{r}{T} \begin{bmatrix} 0_{m\times m} & \boldsymbol{\nu} \\ \boldsymbol{\nu}^\top & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\mu} \\ T \end{bmatrix} \tag{20}$$

where the structure matrix is a constant skew-symmetric matrix modulated by the reaction velocity and the temperature whose elements are the signed stoichiometric coefficients of the chemical reaction.

Notice that interconnection procedure encompasses the IPHS formulation of the continuous stirred tank reactor (CSTR) (Ramirez et al., 2013a, 2016) as well as quasi Hamiltonian formulations of chemical reaction networks and the CSTR (Hoang et al., 2011; Tefera et al., 2022; van der Schaft, 2023).

6. Conclusion

This paper shows that the traditional power preserving interconnection of two irreversible port Hamiltonian systems does not systematically lead to an irreversible port Hamiltonian system. It is mainly due to the fact that in case of irreversible Thermodynamic systems the interface between two systems plays an important role and has to be taken into account in the overall entropy balance equation. To overcome this issue and preserve the closed loop irreversible port Hamiltonian structure during the interconnection, a precise parametrization of a modulated interconnection is proposed. The state and co-state modulated interconnection is entirely defined from the original systems IPHS structure and from the interconnection relations. The main perspective of this work is the study of the impact of this modulation function on control design and how the well-known control by interconnection and energy shaping methods can be generalized to IPHS formulations. This approach should help in overcoming the traditional limitations associated with the dissipation obstacle. Another perspective is to compare the features of interconnected IPHS in terms of system-theroretic properties for control with the one of alternative approaches such as GENERIC (or metriplectic) systems or port-Lagrange systems.

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