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Modelling and control of multi-energy systems: an irreversible port-Hamiltonian approach

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Abstract

In recent work a class of quasi port Hamiltonian system expressing the first and second principle of thermodynamics as a structural property has been defined: Irreversible port-Hamiltonian system. These systems are very much like port-Hamiltonian systems but differ in that their structure matrices are modulated by a non-linear function that precisely expresses the irreversibility of the system. In a first instance irreversible port-Hamiltonian systems are extended to encompass coupled mechanical and thermodynamical systems, leading to the definition of reversible-irreversible port Hamiltonian systems. In a second instance, the formalism is used to suggest a class of passivity based controllers for thermodynamic systems based on interconnection and Casimir functions. However, the extension of the Casimir method to irreversible port-Hamiltonian systems is not so straightforward due to the "interconnection obstacle". The heat exchanger, a gas-piston system and the non-isothermal CSTR are used to illustrate the formalism.

Keywords: Irreversible thermodynamics, port-Hamiltonian system, control, multi-energy systems

1. Introduction

Port Hamiltonian systems (PHS) [1] have been widely used in modelling and passivity-based control (PBC) of mechanical and electro-mechanical systems [2]. On the state space $\mathbb{R}^n \ni x$, a PHS is defined by the following state equation,

$$\dot{x} = J(x)\frac{\partial U}{\partial x}(x) + g(x)u(t) \tag{1}$$

where $U : \mathbb{R}^n \to \mathbb{R}$ is the Hamiltonian function, $J(x) \in \mathbb{R}^n \times \mathbb{R}^n$ is a skew-symmetric structure matrix, $g(x) \in \mathbb{R}^m \times \mathbb{R}^n$ is the input map and $u(t) \in \mathbb{R}^m$ is a time dependent input. For those systems, the Hamiltonian function represents the total electro-mechanical energy of the system and the skew-symmetric structure matrix represents the energy flows between the different energy domains of the system. Furthermore the structure matrix $J(x)$ relates to symplectic geometry as it defines a Poisson bracket, if it satisfies the Jacobi identities, else it is a pseudo-Poisson bracket (see [3]). If J is constant in some local coordinates then it satisfies the Jacobi identities [4]. In the sequel we will consider only true Poisson brackets (not pseudo-Poisson brackets). The Poisson bracket of two $C^\infty(\mathbb{R}^n)$ functions Z and G is expressed as:

$$\{Z, G\}_J = \frac{\partial Z}{\partial x}^\top(x)J(x)\frac{\partial G}{\partial x}(x). \tag{2}$$

If its structure matrix is not full-rank, then the Poisson bracket a admits a kernel which is characterized by its *Casimir* functions [4], that is $C^\infty(\mathbb{R}^n)$ functions that satisfy $\{C, G\}_J = 0$ for any function G. These Casimir functions are invariants of any Hamiltonian systems defined with respect the Poisson bracket. The PHS dynamics may be expressed in term of the Poisson bracket:

$$\dot{x} = \{x, U\}_J + g(x)u(t). \tag{3}$$

The properties of Poisson brackets such as its skew-symmetry and the existence of Casimir functions correspond to the existence of conservation laws or balance equations for open systems [2]. This is the base of the control using PBC methods [5].

In the case when dissipation is taken into account, Hamiltonian systems have been extended by considering structure matrices which are no more skew-symmetric, defining a so-called Leibniz bracket [6]. A *dissipative* PHS [4] with Hamiltonian function U is defined by a Leibniz bracket which expresses the loss of energy induced by some dissipative phenomenon. However, in this case the Hamiltonian function U is no more invariant, and the dissipative PHS does not represent the conservation of energy. Even due dissipative Hamiltonian systems have reported excellent results in control applications [5], the fact that the Hamiltonian is not an invariant of the system leads to the well known dissipation obstacle [7].

For physical systems representing irreversible phenomena, i.e., transformations that involve irreversible entropy creation, it is not sufficient to express only the conservation of energy (first principle of thermodynamic); it is also necessary to express the irreversible entropy creation (second principle of thermodynamic) as a system theoretic property. The first and second principle express, respectively, the conservation of energy and the irreversible transformation of entropy. It is possible to

represent this by the following equations

$$\frac{dU}{dt} = 0 \qquad \text{and} \qquad \frac{d\mathfrak{S}}{dt} = \sigma\left(x, \tfrac{\partial U}{\partial x}\right) \geq 0 \tag{4}$$

where the Hamiltonian U is the total energy, $\mathfrak{S}$ denotes an entropy like function (that may be equal to the total entropy S) and $\sigma\left(x, \frac{\partial U}{\partial x}\right)$ the irreversible entropy creation which in general depends on the state and the gradient of the total energy. By skew-symmetry of the Poisson bracket the total energy of the system satisfies the energy balance equation

$$\frac{dU}{dt} = \frac{\partial U}{\partial x}^{\top} gu. \tag{5}$$

Indeed, since $g(x)u(t)$ represents the flows through the controlled-ports of the system the only energy variation is due to the interaction with the environment. The entropy variation on the other hand is given by

$$\frac{dS}{dt} = \frac{\partial S}{\partial x}^{\top} J(x)\frac{\partial U}{\partial x} + \frac{\partial S}{\partial x}^{\top} gu.$$

A consequence of the second principle of thermodynamic is that the entropy variation due to internal transformations is always greater than or equal to zero. This actually requires $J(x)$ to explicitly depend on $\frac{\partial U}{\partial x}$,

$$\frac{\partial S}{\partial x}^{\top} J\left(x, \tfrac{\partial U}{\partial x}\right)\frac{\partial U}{\partial x} = \sigma_{int} \geq 0, \tag{6}$$

since this should hold for any generating function $U(x)$. In order to include the second principle an alternative geometric structure has to be considered. This is the reason that for physical systems embedding the internal energy and expressing simultaneously the energy conservation and the irreversible entropy creation as it occurs in chemical engineering for instance, the Hamiltonian formulation has to be questioned.

Several attempts have been made in order to preserve as much as possible of the PH structure, leading to a class of system called *quasi PHS* [8, 9, 10, 11, 12]. These systems retain as much as possible the port Hamiltonian structure, but differ by their structure matrices and input vector fields which depend explicitly on the gradient of the Hamiltonian. An important remark is that, although the forms of PHS (1) and quasi PHS are very similar and both embed, by skew-symmetry of the structure matrix, the conservation of energy, in the latter the drift dynamic is a *nonlinear function* in the gradient $\frac{\partial U}{\partial x}(x)$. In this sense the symplectic structure of the PHS, given by the Poisson tensor associated with the structure matrix $J(x)$, is destroyed.

In this paper we shall present a class of quasi PHS where the skew-symmetric structure matrix is defined in such a way that both the conservation of the total energy (i.e. the first principle of Thermodynamics) and the irreversible creation of entropy (i.e. the second principle of Thermodynamics) are encoded. These systems have been suggested in [13, chap. 2][14, 15] for models of homogeneous thermodynamic systems and have been called Irreversible Port Hamiltonian Systems (IPHS). In this paper, after having recalled their definition we shall elaborate two main ideas. Firstly, we shall show how these systems may be extended in order to handle systems that couple (reversible) mechanical systems with (irreversible) thermodynamical systems. This actually encompasses the modelling and control of the so called multi-energy systems, also known as multi-physical systems. Secondly we shall show how the notion of Casimir function may easily be extended from the structure matrix J to the modulated matrix RJ as their left kernel are identical, hence the Casimir-based control schemes may also be used for the stabilization of IPHS.

2. Irreversible PHS for homogeneous thermodynamic systems

2.1. Definition of Irreversible Port Hamiltonian Systems

There is a large class of thermodynamic systems that can be expressed as quasi PHS if the Hamiltonian function is selected as a thermodynamic potential such as the internal energy or the entropy [16, 17, 13]. In this paper we shall use the internal energy as generating potential and we shall recall in this section the definition of IPHS according to [13, chap. 2][14, 15] and give some illustrative examples.

Definition 1. [13] *An Irreversible Port Hamiltonian Systems (IPHS) is the nonlinear control system*

$$\dot{x} = R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right) J\frac{\partial U}{\partial x}(x) + W\left(x, \tfrac{\partial U}{\partial x}\right) + g\left(x, \tfrac{\partial U}{\partial x}\right)u, \tag{7}$$

where $x(t) \in \mathbb{R}^n$ is the state vector, $u(t) \in \mathbb{R}^m$ is the control input, and defined by

- *two (smooth) real functions called Hamiltonian function $U(x) : C^\infty(\mathbb{R}^n) \to \mathbb{R}$ and entropy function $S(x) : C^\infty(\mathbb{R}^n) \to \mathbb{R}$,*
- *the structure matrix $J \in \mathbb{R}^n \times \mathbb{R}^n$ which is constant and skew-symmetric,*
- *a real function $R = R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)$ defined as the product of a positive definite function and the Poisson bracket of S and U:*
$$R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right) = \gamma\left(x, \tfrac{\partial U}{\partial x}\right)\{S, U\}_J, \tag{8}$$
with $\gamma(x, \frac{\partial U}{\partial x}) = \hat{\gamma}(x) : C^\infty(\mathbb{R}^n) \to \mathbb{R}$, $\hat{\gamma} \geq 0$, a non-linear positive function of the states and co-states of the system that may be expressed as a function of the states only.
- *two vector fields $W(x, \frac{\partial U}{\partial x}) \in \mathbb{R}^n$ and $g(x, \frac{\partial U}{\partial x})u \in \mathbb{R}^n$ associated with the ports of the system.*

The main difference with the definition of a PHS is that $R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)$ depends on the co-state variables destroying the linearity of any Poisson tensor, considering the mapping $\frac{\partial U}{\partial x}$ to the drift dynamics $R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right) J\frac{\partial U}{\partial x}$ and associated with the matrix RJ. Furthermore, the two vector fields $W\left(x, \frac{\partial U}{\partial x}\right)$ and $g\left(x, \frac{\partial U}{\partial x}\right)u$ may also depend on states and co-states.

Let us comment the Definition 1 for the particular case of thermodynamic systems. The first principle of thermodynamic states that the energy of the system is conserved. This condition is also true for PHS in mechanics. It is then logical that

the Hamiltonian function of IPHS is chosen to be the energy (as for PHS). As for PHS, there is sometimes more than one conserved quantity that may be used as Hamiltonian function. For instance in mass balance systems a conserved quantity frequently used as Hamiltonian function is the total mass of the system [18, 11]. In the case of IPHS there may also exist more than one conserved quantity depending on the constraints of the system. For instance in the case of a continuous stirred tank reactor (CSTR) with constant pressure and volume, the enthalpy is a conserved quantity and may be used as Hamiltonian function.

The second item of Definition 1 states that J is a constant skew-symmetric matrix. As it has been exposed in [1, 19, 20], PHS arise systematically from network models of physical systems. In network models of complex physical systems the overall system is seen as the interconnection of energy-storing elements via basic interconnection (balance) laws as Newton's third law in mechanics or Kirchhoff's laws in electrical circuits, as well as power conserving elements, like transformers together, with energy-dissipating elements. PHS formalize these basic interconnection laws together with the power conserving elements by a geometric structure. In PHS the structure matrix $J(x)$ and the input matrix $g(x)$ are directly associated with the network interconnection structure, while the Hamiltonian is the sum of the energies of all the energy-storing elements. In thermodynamics there is a similar network relation between different domains. The efforts (intensive variables) of one domain generates the flows in other domains (time evolution of the extensive variables). We expect the IPHS to represent this network-like interconnection, thus we also expect J to be constant with coefficients given by the network structure of the system. We will show that for a simple thermodynamic system as the heat exchanger J will just indicate the direction of the flows, thus its elements will be -1, 0, or 1, while for more complex systems such as chemical reactions it is given by the stoichiometry of the chemical network.

The fact that in the definition of IPHS the structure matrix J is a constant matrix forces the function $R\left(x, \frac{\partial U}{\partial x}\right)$ to capture all the state and co-state dependent behaviour of the internal interconnection of the system. Let us now comment the definition of the modulating function $R\left(x, \frac{\partial U}{\partial x}\right)$ with respect to the energy and entropy balance equations.

Firstly by the skew-symmetry of J, the energy obeys a conservation law. Indeed, computing $\frac{dU}{dt}$ along the trajectories of (7) we obtain

$$\begin{aligned}\frac{dU}{dt} &= \frac{\partial U}{\partial x}^\top \left(RJ\frac{\partial U}{\partial x}\right) + \frac{\partial U}{\partial x}^\top (W + gu)\\ &= R\left(\frac{\partial U}{\partial x}^\top J\frac{\partial U}{\partial x}\right) + \frac{\partial U}{\partial x}^\top (W + gu)\\ &= \frac{\partial U}{\partial x}^\top (W + gu)\end{aligned} \tag{9}$$

due to the skew-symmetry of J. Since the energy of the system is conserved, the only admissible energy variation is through the input and output ports (interaction point with the environment) of the system. In the terminology of PHS [2], the gradient $\frac{\partial U}{\partial x}$ is a vector of efforts, and the vector fields W and gu are vectors of flows. The energy balance equation (9) may then be interpreted as the power product of two port conjugated variables.

The entropy balance of the system is given by

$$\frac{dS}{dt} = R\frac{\partial S}{\partial x}^\top J\frac{\partial U}{\partial x} + \frac{\partial S}{\partial x}^\top (W + gu).$$

If it is assumed that the system is isolated ($W = 0$ and $g = 0$) the balance becomes

$$\frac{dS}{dt} = R\frac{\partial S}{\partial x}^\top J\frac{\partial U}{\partial x}$$

and by definition of the modulating function in (8), it may be written

$$\frac{dS}{dt} = R\frac{\partial S}{\partial x}^\top J\frac{\partial U}{\partial x} = \gamma\left(x, \tfrac{\partial U}{\partial x}\right)\{S, U\}_J^2 = \sigma_{int}, \tag{10}$$

where σ_{int} is called the *internal entropy production*. As the function $\gamma\left(x, \frac{\partial U}{\partial x}\right)$ is defined as positive, the internal irreversible entropy production is always positive according to the second principle of Thermodynamics: $\sigma_{int} \geq 0$. Hence for the open system ($W \neq 0$ and $g \neq 0$) the entropy balance equation is

$$\frac{dS}{dt} = \underbrace{\gamma\left(x, \tfrac{\partial U}{\partial x}\right)\{S, U\}_J^2}_{=\sigma_{int}\geq 0} + \frac{\partial S}{\partial x}^\top (W + gu) \tag{11}$$

Recall that with the choice of the internal energy as Hamiltonian function, the entropy is a state variable and the gradient of the entropy $\frac{\partial S}{\partial x}$ is a vector whose elements are either 1 or 0. Since the Poisson bracket is defined with respect to the constant matrix J, the bracket $\{S, U\}_J$ is a linear combination of the co-energy variables (elements of $\frac{\partial U}{\partial x}$) and it appears that it actually defines the thermodynamic driving force of the irreversible phenomena in the system.

The next two subsections give a brief illustration of this definition through the examples of a heat exchange process and the CSTR.

2.2. Example: the heat exchanger

Consider two simple thermodynamic systems, indexed by 1 and 2 (for instance two ideal gases), which may interact through a conducting wall with compartment 2 interacting with the environment through a heat conducting wall. The dynamics of this system is given by the two entropy balance equations of each compartment

$$\begin{bmatrix}\dot{S}_1\\ \dot{S}_2\end{bmatrix} = \lambda\begin{bmatrix}\frac{T_2(S_2)}{T_1(S_1)} - 1\\ \frac{T_1(S_1)}{T_2(S_2)} - 1\end{bmatrix} + \lambda_e\begin{bmatrix}0\\ \frac{T_e(t)}{T_2(S_2)} - 1\end{bmatrix}$$

where S_1 and S_2 are the entropies of subsystem 1 and 2, $T_e(t)$ a time dependent external heat source and $\lambda > 0$ and $\lambda_e > 0$ denotes Fourier's heat conduction coefficients. The temperatures are modelled as exponential functions of the entropies $T(S_i) = T_0 \exp\left(\frac{S_i}{c_i}\right)$ [21], where T_0 and c_i are constants. This system may be written as a quasi PHS

$$\begin{bmatrix}\dot{x}_1\\ \dot{x}_2\end{bmatrix} = \lambda\left(\frac{1}{\frac{\partial U}{\partial x_2}} - \frac{1}{\frac{\partial U}{\partial x_1}}\right)\begin{bmatrix}0 & -1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\frac{\partial U}{\partial x_1}\\ \frac{\partial U}{\partial x_2}\end{bmatrix} + \lambda_e\begin{bmatrix}0\\ \frac{1}{\frac{\partial U}{\partial x_2}} - \frac{1}{u}\end{bmatrix}u,$$

with state variable $x = [S_1, S_2]^t$, Hamiltonian $U(x_1, x_2) = U_1(x_1) + U_2(x_2)$ being the total internal energy of the overall system composed of the addition of the internal energies of each subsystem, temperatures $T(x) = [T_1(x_1), T_2(x_2)]^t = \left[\frac{\partial U}{\partial x_1}, \frac{\partial U}{\partial x_2}\right]^t$ and $u(t)$, the controlled input that corresponds to the external heat source at temperature $T_e(t)$. This system admits a IPHS formulation (7)

$$\dot{x} = R(x, T)JT(x) + g(T)u(t), \tag{12}$$

with modulating function $R(x, T(x)) = \lambda\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$, constant structure matrix $J = \left[\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right]$ and vector field $gu = \lambda_e \begin{bmatrix} 0 \\ \left(\frac{1}{T_2} - \frac{1}{u}\right) \end{bmatrix} u$. The *total* entropy of the system is given by the sum of the entropies of each compartments $S = S_1 + S_2$. The Poisson bracket $\{S, U\}_J$ is then simply the difference of temperatures between the compartments which is the driving force of the heat conduction

$$\{S, U\}_J = \frac{\partial S}{\partial x}^\top J \frac{\partial U}{\partial x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}^\top \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \end{bmatrix} = T_1 - T_2.$$

And one may express the modulating function according to the Definition 1

$$R(x, T) = \lambda\left(\frac{1}{T_2} - \frac{1}{T_1}\right) = \lambda \frac{T_1 - T_2}{T_1 T2} = \gamma(T)\ \{S, U\}_J,$$

with $\gamma(T) = \frac{\lambda}{T_1 T2}$. Since λ, T_1 and T_2 are greater than zero, γ is a positive function. The vector field $g(T_2)u$ defines the entropy flow generated by the interaction of subsystem 2 and the external heat source, hence corresponds to the port of the system. ■

2.3. Example of the CSTR

Consider a continuous stirred tank reactor (CSTR) with a single reaction and the following reaction scheme in gas phase

$$\nu_1 A_1 + \ldots + \nu_l A_l \rightleftharpoons \nu_{l+1} A_{l+1} + \ldots + \nu_m A_m, \qquad m > l \geq 1.$$

The dynamical model consists firstly in the mass balance equations of each species [22]

$$\dot{n}_i = F_{ei} - F_{si} + r_i V \qquad i = 1, \ldots, m \tag{13}$$

where n_i is the number of moles of the species i, F_{ei} and F_{si} are respectively the inlet and outlet molar concentrations, $r_i = \bar{\nu}_i r$, with r being the reaction rate of the reversible reaction $r = (r_f - r_b)$, where r_f and r_b are the rates of the forward and backward reactions respectively. Each reaction rate depends only on the temperature and reaction concentration, and ν_i is the stoichiometric coefficient of the species i: $\bar{\nu}_i = -\nu_i$ if it appears on the left hand side of the reaction scheme, $\bar{\nu}_i = \nu_i$ in the other case (we assume here that each species appears solely either in the educt or product). Following the usual assumptions [22, 23], V the volume in the reactor is assumed to be constant as well as the pressure. The assumptions of constant volume and pressure impose a constraint over the total outlet flow $F_s = \sum_{i=1}^m F_{si}$ rendering the outlet flows F_{si} of each species i, state dependent [21]. Under the previous assumptions the internal energy of the CSTR, derived from Gibbs' equation, is given by

$$U = \sum_{i=1}^m n_i[c_{vi}(T - T_0) + u_{0i}],$$

where c_{vi}, u_{0i} are respectively the heat capacity and reference molar energy.

Secondly, for a non-isothermal CSTR, we shall complete the model with the entropy balance equation

$$\dot{S} = \sum_{i=1}^m (F_{ei} s_{ei} - F_s s_i) + \frac{Q}{T_w} + \sigma, \tag{14}$$

where

$$\sigma = \sum_{i=1}^m \frac{F_{ei}}{T}(h_{ei} - T s_{ei} - \mu_i) + \frac{Q}{T} - \frac{Q}{T_w} - \sum_{i=1}^m \mu_i \nu_i \frac{r}{T}$$

is the entropy creation due to mass transfer, heat transfer and chemical reactions.

The formulation of the dynamics of the CSTR as an IPHS has been presented in detail in [13, chap. 2][15] where its lift to the complete Thermodynamic Phase Space as a control contact system has also been presented. In this paragraph we rapidly recall its formulation as IPHS as an illustration and in order to prepare the control section.

The dynamical equation of the CSTR may be expressed as the IPHS

$$\dot{x} = R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right) J \frac{\partial U}{\partial x}(x) + W(x, F_e) + g\frac{Q}{T} \tag{15}$$

with state vector $x = [n_1, \ldots, n_m, S]^\top$, the internal energy $U(x)$ as Hamiltonian function,

$$J = \begin{bmatrix} 0 & \ldots & 0 & \bar{\nu}_1 \\ 0 & \ldots & 0 & \vdots \\ 0 & \ldots & 0 & \bar{\nu}_m \\ -\bar{\nu}_1 & \ldots & -\bar{\nu}_m & 0 \end{bmatrix}$$

a constant skew-symmetric matrix whose elements are the stoichiometric coefficients of the chemical reaction mapping the network structure of the reaction, and

$$R = \gamma\left(x, \tfrac{\partial U}{\partial x}\right)\{S, U\}_J = \left(\frac{rV}{T\mathcal{A}}\right)\mathcal{A}$$

where $\gamma = \frac{rV}{T\mathcal{A}}$ may be shown to be a strictly positive function [15] and the Poisson bracket $\{S, U\}_J = \mathcal{A}$, which is the chemical affinity of the reaction $\mathcal{A} = -\sum_{i=1}^m \bar{\nu}_i \mu_i$ and indeed corresponds to thermodynamic driving force of the chemical reaction [21, 24]. The port of the IPHS is given by $W + gQ$ and is composed by the extended input and output flow vector and the thermal interaction vector defined respectively as

$$W = \begin{bmatrix} F_{e1} - F_{s2} \\ \vdots \\ F_{em} - F_{sm} \\ \omega \end{bmatrix}, \qquad g = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix} \frac{Q}{T}$$

with $\omega = \frac{1}{T}\sum_{i=1}^m (F_{ei} s_{ei} - F_{si} s_i)$.

3. Irreversible PHS for coupled mechanical and thermodynamic systems

In this section we shall extend the formulation of Irreversible PHS [13, chap. 2], [14, 15] recalled in the Definition 1, to multi-domain physical systems composed of a mechanical system coupled to a simple thermodynamic system.

3.1. Definition of Reversible-Irreversible Port Hamiltonian Systems

In this case we have to compose the reversible transformation of an ideal lossless mechanical system (port-Hamiltonian system) with the irreversible transformation occurring in a simple thermodynamic system. This leads to define an irreversible port-Hamiltonian system where the skew-symmetric structure matrix is the sum of a structure matrix $J_0(x)$ of a Poisson bracket and the skew-symmetric matrix RJ of the quasi-Poisson bracket.

Definition 2. *A Reversible-Irreversible Port Hamiltonian system (RIPHS) is defined by the dynamical equation*

$$\dot{x} = J_{ir}\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right)\frac{\partial U}{\partial x}(x) + W\left(x, \tfrac{\partial U}{\partial x}\right) + g\left(x, \tfrac{\partial U}{\partial x}\right)u, \qquad (16)$$

where the skew symmetric matrix J_{ir} is defined as the sum :

$$J_{ir}\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right) = J_0(x) + R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right)J \qquad (17)$$

where $J_0(x)$ is the structure matrix of a Poisson bracket and $R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)$ and J are defined according to Definition 1 of an IPHS. Furthermore the entropy function $S(x)$ is a Casimir function of the Poisson structure matrix $J_0(x)$.

This definition may be commented as follows. The RIPHS may be seen as the composition of a PHS and an IPHS with structure matrices being the sum of a Poisson structure matrix and a quasi-Poisson structure matrix in the sense of Definition 1 and with common Hamiltonian function.

Computing the time derivative of the Hamiltonian $U(x)$, by skew-symmetry of $J_{ir}\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)$, the Hamiltonian obeys the same balance equation (9) as for IPHS, depending only on the power product at the port of the system. Now computing the time derivative of the total entropy for an isolated system ($W = 0$ and $g = 0$), one obtains

$$\begin{aligned}
\frac{dS}{dt} &= \frac{\partial S}{\partial x}^{\top} J_{irr}\frac{\partial U}{\partial x} \\
&= \frac{\partial S}{\partial x}^{\top} J_0\frac{\partial U}{\partial x} + R\left(x, \tfrac{\partial U}{\partial x}, \tfrac{\partial S}{\partial x}\right)\left(\frac{\partial S}{\partial x}^{\top} J\frac{\partial U}{\partial x}\right) \\
&= \{S, U\}_{J_0} + \gamma\left(x, \tfrac{\partial U}{\partial x}\right)\{S, U\}_J^2 \\
&= \gamma\left(x, \tfrac{\partial U}{\partial x}\right)\{S, U\}_J^2
\end{aligned}$$

using that $S(x)$ is a Casimir function of the Poisson structure matrix $J_0(x)$, that is it satisfies $\{S, U\}_{J_0} = 0$ for any Hamiltonian $U(x)$. In consequence the entropy balance equation of the RIPHS (16) is identical with the entropy balance equation (10) of the IPHS.

The benefit of the *energy based* formulation of IPHS (Hamiltonian given by the internal energy) is clearly emphasised in this case, since it allows to naturally perform the interconnection with conventional PHS. This is not the case for quasi-Hamiltonian formulations of thermodynamic systems where for instance the entropy (or some function of the entropy) is used as Hamiltonian. As an illustration, let us consider the example of a gas-piston system where a homogeneous simple thermodynamic system (the gas) interacts with a mechanical system, the piston.

3.2. Example of the gas-piston system

Consider a gas contained in a cylinder closed by a piston submitted to gravity. *The thermodynamic properties* of this system may be decomposed into the properties of the piston in the gravitation field and the properties of the perfect gas. The properties of the piston in the gravity field are defined by the sum of the potential and kinetic energies: $H_{mec} = \frac{1}{2m}p^2 + mgz$, where z denotes the altitude of the piston and p its kinetic momentum. The properties of the perfect gas may be defined by its internal energy $U(S, V)$ where S denotes the entropy variable, V the volume variable and the number of moles N is constant as the system is closed (there is no exchange of matter) and hence becomes an index. The total energy of the system is: $E(x) = U((S, V)) + H_{mec}(z, p)$, where $x = [S, V, z, p]^{\top}$ is the vector of state variables. The co-energy variables are defined by the gradient of the total energy

$$\begin{array}{l}
\frac{\partial E}{\partial S} \triangleq T \\
\frac{\partial E}{\partial V} \triangleq -P \\
\frac{\partial E}{\partial z} = mg \triangleq F_g \\
\frac{\partial E}{\partial p} \triangleq v
\end{array} \qquad (18)$$

where T is the temperature, P the pressure, F_g the gravity force, and v the velocity of the piston.

The gas in the cylinder under the piston may undergo a *non-reversible transformation* when the piston moves. We assume that in this case a non-adiabatic transformation due to mechanical friction (and/or viscosity of the gas), and that the dissipated mechanical energy is converted entirely into a heat flow in the gas. The resisting mechanical force due to friction is $F_r = \nu v$. The entropy balance equation is then

$$\frac{dS}{dt} = \frac{1}{T}\nu v^2 = \sigma_{int}$$

which is the irreversible entropy flow at the temperature T, induced by the heat flow νv^2 due to the friction of the piston. As the temperature is positive and the irreversible entropy flow is a quadratic term in the velocity v, it is indeed positive. The coupling between the piston and the gas consists in relating the force F^e and pressure P on the piston and the velocity v of the piston and the variation of volume f_V^e of the gas

$$\begin{bmatrix} f_V^{\mathrm{e}} \\ F^{\mathrm{e}} \end{bmatrix} = \begin{bmatrix} 0 & A \\ -A & 0 \end{bmatrix}\begin{bmatrix} (-P) \\ v \end{bmatrix} \qquad (19)$$

where A denotes the area of the piston.

The dynamics of the gas-piston system is then given by

$$\begin{aligned}\frac{dS}{dt} &= \frac{1}{T}\nu v^2 \triangleq \sigma_{int}\\ \frac{dV}{dt} &= Av\\ \frac{dz}{dt} &= v\\ \frac{dp}{dt} &= -F_g + AP - F_r = -mg + AP - \nu v\end{aligned}$$

The first equation is the entropy balance accounting for the irreversible creation of entropy due to mechanical friction. The second equation indicates that the motion of the piston induces a variation of the volume of the gas. The third equation defines the velocity of the piston. The last equation is simply Newton' law applied to the piston. This control system may be written in state space representation form as follows

$$\frac{d}{dt}\begin{bmatrix} S\\ V\\ z\\ p\end{bmatrix} = \underbrace{\begin{bmatrix} 0 & 0 & 0 & \frac{\nu v}{T}\\ 0 & 0 & 0 & A\\ 0 & 0 & 0 & 1\\ -\frac{\nu v}{T} & -A & -1 & 0\end{bmatrix}}_{J_{irr}(T,v)}\begin{bmatrix} T\\ -P\\ F\\ v\end{bmatrix} \tag{20}$$

This system is a quasi-Hamiltonian system as its skew-symmetric structure matrix depends on two co-energy variables, the velocity v and the temperature T. However it may be written in RIPHS form according to Definition 2 by decomposing further its structure matrix as the sum

$$J_{irr}(T,v) = J_0 + R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right) J$$

with the constant *Poisson* structure matrix

$$J_0 = \begin{bmatrix} 0 & 0 & 0 & 0\\ 0 & 0 & 0 & A\\ 0 & 0 & 0 & 1\\ 0 & -A & -1 & 0\end{bmatrix}$$

and the structure matrix associated with the dissipative phenomenon, the friction of the piston

$$J = \begin{bmatrix} 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ -1 & 0 & 0 & 0\end{bmatrix}$$

The Poisson structure matrix J_0 is indeed associated with the reversible coupling composed of the symplectic coupling $\left(\begin{smallmatrix} 0 & 1\\ -1 & 0\end{smallmatrix}\right)$ between the kinetic and potential energies of the mechanical system and the coupling through the piston area A. The modulating function for the irreversible phenomenon is $R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right) = \gamma\left(x, \frac{\partial U}{\partial x}\right)\{S, U\}_J$ with the Poisson bracket

$$\{S, U\}_J = \begin{bmatrix} 1 & 0 & 0 & 0\end{bmatrix} J \begin{bmatrix} T\\ -P\\ F\\ v\end{bmatrix} = v$$

which is the velocity of the piston and indeed the driving force of the friction and function

$$\gamma\left(x, \frac{\partial U}{\partial x}\right) = \gamma(T) = \frac{\nu}{T}$$

which is strictly positive as the temperature and the friction coefficient are strictly positive. It may be easily checked that the entropy is a Casimir function of J_0 as its first row (and column) is zero.

Assuming now that there is an external force F_{mot} acting on the piston and that the gas is subject to an exchange of heat with a thermostat at temperature T_e through a wall with Fourier's heat conduction coefficient $\lambda_e > 0$, the system may be completed to the control system (16) with input vector $[u_1, u_2] = [T_e, F_{mot}]$ and the vector field associated with the port:

$$gu = \begin{bmatrix} \lambda_e\left(\frac{1}{T} - \frac{1}{u_1}\right) & 0\\ 0 & 0\\ 0 & 0\\ 0 & 1\end{bmatrix} u \tag{21}$$

4. Passivity-based control of IPHS

The Port Hamiltonian formulation may be used in a straightforward way for passivity-based control methods [25, 4] by using the associated energy balance equation (5). Moreover, the port-Hamiltonian structure and the Poisson structure matrix $J(x)$ in (1) allow to use other invariants and their associated balance equations, defined by the Casimir functions for synthesis methods based on the interconnection-reduction method or in the Interconnection and Damping Assignment Passivity-based methods (IDA-PBC) [7, 5, 26, 27, 2].

IPHS share a similar structure with PHS with the precise difference that the Poisson structure matrix J is multiplied by the modulating function $R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)$ depending on the gradient $\frac{\partial U}{\partial x}$. Obviously the energy balance equation (9) may also be used for passivity-based control. Moreover the notion of Casimir function may easily be extended from the structure matrix J to the modulated matrix RJ as their left kernel are identical, hence the Casimir-based control schemes may also be used. On the other side the entropy balance equation (11) clearly shows the controllability problems which may arise due to the irreversible entropy creation.

In this section, we shall elaborate on the control by embedding and reduction by Casimir functions, also called *control by interconnection* [7, 5].

4.1. Control by interconnection of IPHS

Let us first recall the method of stabilization by modulated interconnection and adapt it to the IPHS. Consider first an IPHS (7), where we assume the vector field $W = 0$; this might be for instance obtained by a change of the control variable.

The first step is to embed the IPHS into a higher dimensional system by interconnecting it with a PHS through a feedback interconnection. In this paper we shall consider the most simple

Hamiltonian system namely a simple integrator with controller state $x_c \in \mathbb{R}^m$ with Hamiltonian and dynamical model

$$\Sigma_c \left\{ \begin{array}{rcl} \dot{x_c} & = & u_c \\ y_c & = & \frac{\partial H_c}{\partial x_c}(x_c) \end{array} \right.$$

This is indeed a Hamiltonian system with structure matrix $J_c = 0$ and Hamiltonian $H_c(x_c)$.

Remark 3. *In the case where this system is a constant source, the Hamiltonian is chosen as $H_c(x_c) = -u^* x_c$.*

Consider the following feedback interconnection of the two systems modulated by the $m \times m$ matrix $\beta(x)$

$$\begin{pmatrix} u \\ u_c \end{pmatrix} = \begin{pmatrix} 0 & \beta(x) \\ -\beta(x) & 0 \end{pmatrix} \begin{pmatrix} y \\ y_c \end{pmatrix}$$

The total system, embedding the IPHS, may then be expressed as follows

$$\begin{array}{rcl} \frac{d}{dt}\begin{pmatrix} x \\ x_c \end{pmatrix} & = & \begin{pmatrix} R\,J & g(x)\beta(x) \\ -\beta^t(x)\,g^t(x) & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial H_{cl}}{\partial x} \\ \frac{\partial H_{cl}}{\partial x_c} \end{pmatrix} \\ y & = & \left(g(x)^t,\, 0\right) \begin{pmatrix} \frac{\partial H_{cl}}{\partial x} \\ \frac{\partial H_{cl}}{\partial x_c} \end{pmatrix} \end{array}$$

where $H_{cl}(x,\, x_c) = U(x) + H_c(x_c)$ with structure matrix

$$J_{cl}(x,\, x_c) = \begin{pmatrix} R\,J & g(x)\beta(x) \\ -\beta^t(x)\,g^t(x) & 0 \end{pmatrix}.$$

This again defines a quasi-Poisson bracket as the modulating function is $R = \gamma\left(x, \frac{\partial U}{\partial x}\right)\{S, U\}_J$ and depends on the co-energy variables as $\frac{\partial U}{\partial x} = \frac{\partial H_{cl}}{\partial x}$.

The second step is to prepare the reduction of the embedding system by analysing the condition for the existence of m Casimir functions $C(x,\, x_c)$ of the structure matrix $J_{cl}(x,\, x_c)$. Therefore we look for Casimir functions $C(x,\, x_c)$ of the type

$$C(x,\, x_c) = F(x) - x_c.$$

Then the function $F(x)$ should satisfy

$$\left(\frac{\partial F}{\partial x}^t,\, -I_m\right) \begin{pmatrix} R\,J & g(x)\beta(x) \\ -\beta^t(x)\,g^t(x) & 0 \end{pmatrix} = 0$$

which is equivalent to

$$\begin{array}{rcl} -R\,J\,\frac{\partial F}{\partial x} + \beta(x)\,g(x) & = & 0 \\ \frac{\partial F}{\partial x}^t\,g(x)\beta(x) & = & 0 \end{array} \tag{22}$$

If the system (22) has a solution $F(x)$ then the interconnected system is again IPHS with structure matrix

$$\begin{pmatrix} R\,J & g(x)\beta(x) \\ -\beta^t(x)\,g^t(x) & 0 \end{pmatrix} = R \begin{pmatrix} J & J\,\frac{\partial F}{\partial x} \\ -\left(J\,\frac{\partial F}{\partial x}\right)^T & 0 \end{pmatrix}.$$

Indeed denoting

$$J_e(x) = \begin{pmatrix} J & J\,\frac{\partial F}{\partial x} \\ -\left(J\,\frac{\partial F}{\partial x}\right)^T & 0 \end{pmatrix}$$

the entropy function $S(x)$ does not depend on the control state variables x_c hence $\{S, U\}_J = \{S,\, H_{cl}\}_{J_e}$ and one may express the modulating function

$$R = \gamma\left(x, \frac{\partial H_{cl}}{\partial x}\right)\{S, U\}_{J_e}.$$

The third step consists, assuming that (22) has a solution $F(x)$, to reduce the embedding system by restriction to the invariant manifold $C(x,\, x_c) = F(x) - x_c = 0$. In a similar way as for PHS, it may be shown that this manifold admits as coordinates x and its dynamics may be written

$$\begin{array}{rcl} \frac{dx}{dt} & = & R\,J\frac{\partial H_0}{\partial x} + g(x)\beta(x)\,\frac{\partial H_c}{\partial x_c}(F(x)) \\ & = & R\,J\frac{\partial H_0}{\partial x} + \left(R\,J\,\frac{\partial F}{\partial x}\right)\frac{\partial H_c}{\partial x_c} \circ F(x) \end{array}$$

Hence the reduced system is the following IPHS with identical structure matrix and modified Hamiltonian

$$\frac{dx}{dt} = R\,J\,\frac{\partial}{\partial x}\left(H_0 + H_c \circ F\right). \tag{23}$$

It is equivalent to the IPHS with the state feedback $u(x) = \beta(x)\,\frac{\partial H_c}{\partial x_c} \circ F(x)$ which may be interpreted as *shaping the Hamiltonian* to $H_{cl}(x) = (U + H_c \circ F)(x)$.

Remark 4. *In the case where the control is a constant source u^*, then the control is $u(x) = \beta(x)\,u^*$ and the shaped Hamiltonian is $(U - u^* F(x))(x)$.*

The fourth step is the stabilizing control synthesis. Now assume that (x^*, u^*) defines some equilibrium of the IPHS. And assume that there exists a solution $F(x)$ of (22) such that the shaped Hamiltonian is a Lyapunov function for the closed-loop system (23). Then, by Lasalle's theorem, the control $u(x) = \beta(x)\left(\frac{\partial H_c}{\partial x_c} \circ F\right)(x) + v$ with $v = -k\,g^t(x)\,\frac{\partial H_{cl}}{\partial x}$ stabilizes the system to the largest invariant set included in the set $\left\{x \in \mathbb{R}^n \;s.t.\; g^t(x)\,\frac{\partial H_{cl}}{\partial x} = 0\right\}$.

4.2. Application to the heat exchanger system

Consider now the IPHS representation of the heat exchanger as presented in the Section 2.2. Let us first perform the following change of input variable $u' = \left(\frac{u}{T_2} - 1\right)$ which is regular as the temperature is positive: $T_2 > 0$. Then the heat exchanger is written as IPHS with input vector field $g' = \lambda_e \begin{pmatrix} 0 \\ -1 \end{pmatrix}$. It may be noticed that g' is Hamiltonian with respect to J and generated by $(-\lambda_e\, S_1)$

$$\begin{array}{rcl} g' = \lambda_e \begin{pmatrix} 0 \\ 1 \end{pmatrix} & = & \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \frac{\partial}{\partial S}(-\lambda_e S_1) \\ & = & J\,\frac{\partial}{\partial S}(-\lambda_e S_1). \end{array}$$

Secondly, let us characterize the equilibria (x^*, u^*) of the control system. As the matrix J is symplectic, the equilibrium point

(x^*, u^*) is given by the equivalent conditions

$$\begin{array}{ll} & R\,J\,\frac{\partial U}{\partial x}(x^*) + g' u'^* = 0 \\ \Leftrightarrow & R\,\frac{\partial U}{\partial x}(x^*) + u'^* \frac{\partial}{\partial S}(-\lambda_e S_1) = 0 \\ \Leftrightarrow & \begin{cases} R(x^*)\ \frac{\partial U}{\partial x_1}(x^*) - \lambda_e u'^* = 0 \\ R(x^*)\ \frac{\partial U}{\partial x_1}(x^*) = 0 \end{cases} \\ \Leftrightarrow & \begin{cases} R(x^*) & = 0 \\ u^* & = T_2^* \end{cases} \\ \Leftrightarrow & \begin{cases} T_1^* - T_2^* & = 0 \\ u^* & = T_2^* \end{cases} \end{array}$$

Let us now check the existence of a Casimir function. The condition (22) is equivalent to

$$\begin{aligned} -R\,\frac{\partial F}{\partial x} + \beta(x)\,\lambda_e \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= 0 \\ \frac{\partial F}{\partial x}^t \lambda_e \begin{pmatrix} 0 \\ -1 \end{pmatrix} \beta(x) &= 0 \end{aligned}$$

which is equivalent to $\frac{\partial F}{\partial x_2} = 0$ and

$$\beta(x) = \frac{1}{\lambda_e} R\,\frac{\partial F}{\partial S_1}(S_1)$$

where $F(x_1)$ is freely chosen as the transversality condition is always satisfied

$$\frac{\partial F}{\partial x}^t \lambda_e \begin{pmatrix} 0 \\ -1 \end{pmatrix} \beta(x) = \left(\frac{\partial F}{\partial x_1}, 0\right) \lambda_e \begin{pmatrix} 0 \\ -1 \end{pmatrix} \beta(x) = 0.$$

Choosing the control system Hamiltonian to be $H_c(x_c) = -u^*$, the feedback is $u'(x) = u^* \beta(x)$ which may be interpreted as *shaping the Hamiltonian* to $H_{cl}(S) = (U(S) - u^* F(S_1))(x) = U_1(S_1) - u^* F(S_1) + U_2(S_2)$.

Let us now choose $u^* F(S_1) = A\left(S_1, S_1^*\right)$ as the *energy based availability function* of compartment 1 [1]

$$A(S_1, S_1^*) = U_1(S_1) - \left[U_1(S_1^*) + \frac{\partial U_1}{\partial S_1}^\top (S_1^*)(S_1 - S_1^*)\right] \geq 0. \tag{24}$$

For simple homogeneous thermodynamic systems, the energy based availability function $A(S_1, S_1^*)$ is a strictly convex function with an unique minimum at S_1^*, where S_1^* is the desired equilibrium. This follows from the second law of thermodynamics, where the internal energy is a convex function [28, 29].

Then by the properties of IPHS one has the energy balance equation $\frac{d\mathcal{H}_{cl}}{dt} = 0$. However this cannot lead to stability of the desired equilibrium point as the Hamiltonian $H_{cl}(S) = A(S_1, S_1^*) + U_2(S_2)$ has a strict minimum in its first component by energy shaping but the second component is invariant and has no strict minimum. Although discouraging, this "interconnection obstacle", is not entirely unexpected, since it may be interpreted in terms of the well known dissipation obstacle for dissipative PHS [30].

This implies that for this system one has to use not only energy shaping methods by interconnection but needs also some IDA-PBC synthesis methods which are beyond the scope of this paper.

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5. Conclusion

A class of quasi port-Hamiltonian systems (PHS) that encompasses a large set of thermodynamic systems, including heat exchangers and continuous stirred tank reactors (CSTR) has been defined: Irreversible port-Hamiltonian Systems (IPHS). It includes as a structural property the conservation of energy and the irreversible production of entropy, expressed by a Poisson bracket evaluated on these two quantities. The structure of the IPHS resembles classical PHS since the constant structure matrix represents the network structure of the system (direction of flows for the heat exchanger and stoichiometric chemical network for the CSTR). The modelling of coupled mechanical-thermodynamical systems has also been studied and an extension of IPHS have been proposed: Reversible-IPHS (RIPHS). These systems are composed by the interconnection of a PHS and an IPHS, being the total Hamiltonian the sum of the individual Hamiltonians of the systems. Additionally, the skew-symmetric structure matrix of RIPHS is the sum of a structure matrix of a Poisson bracket (with Casimir function the total entropy) and a skew-symmetric matrix of a quasi-Poisson bracket.

The stabilization by interconnection of IPHS has been addressed. Since IPHS share a similar structure with PHS, with the precise difference that the Poisson structure matrix J is multiplied by the modulating function $R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)$, it may seem that the Casimir method could be extended to this kind of systems in a rather straightforward manner. However the irreversible entropy creation, related to $R\left(x, \frac{\partial U}{\partial x}, \frac{\partial S}{\partial x}\right)$, limits the Casimir method and makes it not possible to shape the closed-loop Hamiltonian in all its components. This "interconnection obstacle", although discouraging, is not entirely unexpected, since it may be interpreted in terms of the well known dissipation obstacle for dissipative PHS [30].

Future work will study the IPHS for complex chemical reaction networks and how to overcome the interconnection obstacle and specialize these results for the stabilization of complex thermodynamic systems, such as the CSTR.

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