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Irreversible port-Hamiltonian systems: A general formulation of irreversible processes with application to the CSTR

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HIGHLIGHTS

- Hamiltonian systems (IPHS) are adapted to irreversible thermodynamic systems.
- IPHS express the first and second principle as a structural property.
- IPHS define control contact systems on the complete Thermodynamic Phase Space.
- The balance equations of a CSTR are expressed as IPHS and as control contact system.

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ABSTRACT

In this paper we suggest a class of quasi-port-Hamiltonian systems called Irreversible port-Hamiltonian Systems, that expresses simultaneously the first and second principle of thermodynamics as a structural property. These quasi-port-Hamiltonian systems are defined with respect to a structure matrix and a modulating function which depends on the thermodynamic relation between state and co-state variables of the system. This modulating function itself is the product of some positive function γ and the Poisson bracket of the entropy and the energy function. This construction guarantees that the Hamiltonian function is a conserved quantity and simultaneously that the entropy function satisfies a balance equation containing an irreversible entropy creation term. In the second part of the paper, we suggest a lift of the Irreversible Port-Hamiltonian Systems to control contact systems defined on the Thermodynamic Phase Space which is canonically endowed with a contact structure associated with Gibbs' relation. For this class of systems we have suggested a lift which avoids any singularity of the contact Hamiltonian function and defines a control contact system on the complete Thermodynamic Phase Space, in contrast to the previously suggested lifts of such systems. Finally we derive the formulation of the balance equations of a CSTR model as an Irreversible Port-Hamiltonian System and give two alternative lifts of the CSTR model to a control contact system defined on the complete Thermodynamic Phase Space.

1. Introduction

The use of physical invariants such as the total energy, momentum or mass, has lead to a huge variety of efficient methods for the modelling, simulation and control of physical systems. These invariants structure the dynamical models of physical systems. For mechanical systems, arising from variational formulations, Lagrangian and *Hamiltonian systems* are derived (Arnold, 1989) and have been extended to control systems representing open physical systems called controlled Hamiltonian or Lagrangian systems or input–output Hamiltonian systems (Brockett, 1977; van der Schaft, 1986), (Marsden, 1992, Chapter 7). For the Hamiltonian systems, the Hamiltonian function is a dynamical invariant (other invariants may arise from its symmetries) and is often equal to the (free) energy of the mechanical system. The other fundamental invariant of these systems is its geometric structure, the *symplectic structure* which is defined by a canonical skew-symmetric tensor on the co-state variables of the system and defined in practice, by some skew-symmetric matrix, called *structure matrix*. For physical systems, it represents the canonical reversible coupling between two physical domains (e.g. the elastic and the kinetic energy exchange in a perfect oscillator).

These Hamiltonian formulations may be extended to electrical systems and networks by considering Hamiltonian systems defined with respect to a generalization of symplectic structure, i.e., *Poisson*

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structures (Arnold, 1989) which may be associated with the topology of the system such as graphs of electrical circuits or the kinematic relations of a mechanism for instance (Maschke et al., 1995; van der Schaft and Maschke, 2009) and whose extension to open or controlled physical systems is called *port-Hamiltonian Systems* (Maschke and van der Schaft, 1992; van der Schaft and Maschke, 1995; Duindam et al., 2009).

However when irreversible phenomena have to be described then this Hamiltonian frame is not adapted anymore. The Hamiltonian systems have to be completed with an additional term representing the dissipation leading to a system composed of the sum of a Hamiltonian and a gradient system (van der Schaft, 2004) which is defined by a Riemannian metric which is defined in practice by some symmetric positive matrix. For electro-mechanical systems which are assumed to be in isothermal conditions and for which it is not necessary to represent the thermal domain, these systems are *dissipative Hamiltonian systems* with a well defined geometric structure generalizing the Poisson structure (Ortega and Planas-Bielsa, 2004).

When, as it is the case in chemical engineering, furthermore the energy (or equivalently the entropy) balance equation have to be included in the model, then the preceding models cannot be used anymore. And a variety of models have been suggested; their main characteristics is to represent all balance equations of the models, including the total energy and entropy balance equations. Two main classes of systems have been suggested, *quasi-gradient systems* (Favache and Dochain, 2010; Favache et al., 2011) and *quasi-Hamiltonian systems* (Grmela and Öttinger, 1997; Öttinger and Grmela, 1997; Mushik et al., 2000; Hoang et al., 2011, 2012; Ramirez et al., 2009; Johnsen et al., 2008), the latter being the subject of this paper.

In the first part of the paper, we shall elaborate on the definition of these quasi-Hamiltonian systems. Indeed in order to represent simultaneously the total energy and entropy balance, a simple example of heat transfer phenomena will be used to show that these formulations are not dissipative Hamiltonian as the matrices defining the symmetric and skew-symmetric tensors are functions of the co-state variables which destroys the linearity associated with tensors (Eberard et al., 2007).[1] But we shall characterize this nonlinearity of the structure matrices in a more precise way, as a function depending on the co-state variables. We suggest a quasi-Hamiltonian system called *Irreversible Port-Hamiltonian System* (IPHS) defined with respect to a skew-symmetric structure matrix composed of the product of a constant skew-symmetric matrix with this modulating function and give a physical interpretation.

In the second part of the paper, we use an alternative formulation based on an intrinsic geometric structure associated with Gibbs' relations, characterized as the set of tangent planes and defined as *contact structure* (Hermann, 1973, 1974; Arnold, 1989). This geometric structure is intrinsic to the Thermodynamic Phase Space (TPS) composed of all extensive and intensive variables of a thermodynamic system in the same way as the symplectic structure is intrinsic to the configuration-momentum space of a mechanical system and is actually closely related to it. Following earlier work on the formulation of reversible (Mrugała, 1993) and irreversible transformations (Grmela and Öttinger, 1997; Grmela, 2001) for closed and its extensions to open thermodynamic systems (Eberard et al., 2005, 2007; Favache et al., 2009, 2010), we shall express the Irreversible Port-Hamiltonian Systems as *control contact systems* on the complete Thermodynamic Phase Space.

In the third part, we consider a Continuous Stirred Tank Reactor (CSTR) model and firstly remind different dissipative Hamiltonian formulations of the balance equations, showing precisely the dependence of the structure matrices on the co-state variables. Secondly we derive the formulation of the CSTR as an Irreversible Port-Hamiltonian System and give physical interpretation of the Poisson structure matrix in terms of the stoichiometry of the reaction and the modulating function and in its relation with the irreversible entropy creation. Finally the lift of this system to the complete Thermodynamic Phase Space is performed and an alternative is discussed.

[1] Note that this is also the case with the quasi-gradient formulations in Favache and Dochain (2010) and Favache et al. (2011).

2. Port-Hamiltonian formulation of open thermodynamic systems

2.1. Reminder on port-Hamiltonian systems

Port-Hamiltonian systems (PHS) (Maschke and van der Schaft, 1992) have been widely used in modelling and passivity-based control (PBC) of mechanical and electro-mechanical system (Duindam et al., 2009; Ortega et al., 2008). 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 state-dependent skew-symmetric matrix, $g(x) \in \mathbb{R}^m \times \mathbb{R}^n$ is the input matrix and $u(t) \in \mathbb{R}^m$ is a time dependent input. If it satisfies some integrability conditions, the Jacobi identities (Libermann and Marle, 1987), the skew-symmetric matrix $J(x)$ is the definition in coordinates of a *Poisson bracket*, that is a map from the pairs of $C^\infty(\mathbb{R}^n)$ functions Z and G to a $C^\infty(\mathbb{R}^n)$ function denoted by $\{Z,G\}_J$ and defined as

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

From (2), it is seen that the structure matrix $J(x)$ also defines a 2-contravariant tensor on the co-states. As a consequence, the variation of any function Z along the PHS dynamics (1) may be expressed in term of the Poisson bracket:

$$\dot{Z} = \{Z,U\}_J + \sum_{i=1}^{m} L_{g_i}Z(x)u_i(t)$$

where $L_{g_i}Z$ denotes the Lie derivative of Z with respect to the vector fields defined by the columns $g_i(x)$ of the input matrix $g(x)$ and is expressed in coordinates as $L_{g_i}Z(x) = (\partial Z/\partial x)^T g_i(x)$. By the skew-symmetry of the matrix $J(x)$ (and its Poisson bracket), the Hamiltonian function obeys the following balance equation:

$$\dot{U} = \sum_{i=1}^{m} L_{g_i}U(x)u_i(t)$$

which implies that it is conserved when the input is identically 0 and also leads to the definition of outputs conjugated to the inputs: $y_i = L_{g_i}Z(x)$. For (isothermal) electro-mechanical systems, the Hamiltonian function is often chosen to be the total (free) energy.

The port-Hamiltonian system (1) is an extension of Hamiltonian systems with an input term defined by input vector fields g_i which are not necessarily Hamiltonian (Maschke and van der Schaft, 1992; van der Schaft and Maschke, 1995) and hence also an extension of control Hamiltonian systems (Brockett, 1977; van der Schaft, 1989). Notice that when the structure matrix is constant then the Jacobi identities are satisfied. This case encompasses the structure of standard Hamiltonian systems with external forces where $J = \left[\begin{smallmatrix} 0_m & I_m \\ -I_m & 0_m \end{smallmatrix}\right]$ (0_m denoting the square null matrix and I_m the identity matrix of dimension m). In general the structure matrices $J(x)$ and $g(x)$ are defined by the *topology* of the system, that is the interconnection relations in the system such as Kirchhoff's laws of circuits (Maschke et al., 1995), the kinematic