Preprints of the 21st IFAC World Congress (Virtual)
Berlin, Germany, July 12-17, 2020

Energy shaping plus Damping injection of Irreversible Port Hamiltonian Systems ⋆

Ignacio Villalobos * **Hector Ramírez** * **Yann Le Gorrec** **

* *Electronics Engineering Department, Universidad Técnica Federico Santa María (UTFSM), Chile.* ignacio.villalobos.a@gmail.com, hector.ramireze@usm.cl
** *Department of Automation and Micro-Mechatronic Systems, FEMTO-ST UMR CNRS 6174, UBFC, 26 chemin de l'épitaphe, F-25030 Besançon, France.* legorrec@femto-st.fr

Abstract: Irreversible port-Hamiltonian systems (IPHS) are an extension of port-Hamiltonian systems (PHS) for irreversible thermodynamics which encompass a large class of thermodynamic systems that may contain reversible and irreversible phenomena. Energy shaping and damping injection are standard structure preserving passivity based control approaches which have proven to be very successful for the stabilization of PHS. However, in the case of irreversible thermodynamics, the non-linear nature of the systems make it non-trivial to apply these approaches for stabilization. In this paper we propose a systematic procedure to perform, in a first control loop, energy shaping by state modulated interconnection with a controller in IPHS form. Then, a second control loop guarantees asymptotic stability by the feedback of a new closed-loop passive output. The approach allows to stabilize IPHS while preserving the IPHS structure in closed-loop, allowing to interpret the closed-loop system as a desired thermodynamic system. The example of the continuous stirred tank reactor is used to illustrate the approach.

Keywords: Port-Hamiltonian systems, Irreversible thermodynamics, Passivity based control, Control by interconnection, Damping injection.

1. INTRODUCTION

The Port Hamiltonian system formulation (PHS) has been used for control and modelling of electrical, mechanical, and in general multiphysics systems (Maschke and van der Schaft, 1992; Duindam et al., 2009; Van Der Schaft, 2004). The framework of the PHS theory formalizes the basic interconnection laws together with the power preserving elements by a geometric structure, using the energy between the elements as the interconnection, and defines the Hamiltonian as the total energy stored in the system. The formalism have been largely used for the control of multiphysical systems (Van Der Schaft, 2004; Duindam et al., 2009) through techniques like control by interconnection and damping injection. The framework of control by interconnection consists in designing a dynamical control system which allows to relate the states of the controller and the process by a set of structural invariants, called Casimir functions (van der Schaft, 2016; Duindam et al., 2009; van der Schaft and Jeltsema, 2014). The Casimir functions are then instrumental to shape the closed-loop Hamiltonian function such that its minimum is at the desired equilibrium. The asymptotic stability is then achieved by the injection of damping.

The PHS formulation express the first principle of thermodynamics, i.e, the conservation of the energy, but fails to express the second principle of the thermodynamics, i.e., the irreversible creation of entropy although there have been extensions of the PHS formulation which encompass systems arising from the Irreversible Thermodynamics (Eberard et al., 2005; Ramirez et al., 2013a). In Ramirez et al. (2013a) a class of quasi PHS, namely irreversible port-Hamiltonian systems (IPHS), has been proposed to encompass a large class of thermodynamic systems. These systems express as a structural property the first and second principles of thermodynamics by adding a non linear real function to the dynamic. By definition IPHS are non-linear systems with a physically meaningful structure and just as PHS systems, they are defined with respect to the total energy of the system. This makes it possible to interconnect them with other reversible or non-reversible systems, or a combination of both (Ramirez et al., 2013b). Some first approaches to control of IPHS have been given in Ramirez et al. (2016) using the framework of an energy based availability function as a candidate for a Lyapunov function, based in the spirit of the works of Alonso and Ydstie (2001); Ydstie (2002).

In this paper we propose a systematic control design method for IPHS, specializing the control by interconnection and damping injection to IPHS. By using a controller in IPHS form and a modulating interconnecting between the process and the controller, a set of matching equations for the generation of Casimir functions are proposed. Using the energy-based availability function as part of the solution, the closed-loop Hamiltonian is designed to have

⋆ This work was supported by the projects FONDECYT 1191544 and BASAL FB0008; and the Dirección de Postgrado y Programas (DPP) of the UTFSM.

a minimum at the desired dynamic equilibrium. Damping with respect to the closed-loop conjugated output is then added to guarantee asymptotic stability. The approach allows to stabilize IPHS while preserving the IPHS structure in closed-loop, allowing to interpret the closed-loop system as a desired thermodynamic system. The paper is organized as follows. Section 2 presents the basics on IPHS. In section 3 we derive an energy shaping plus damping injection IPHS controller for an IPHS system. As illustrative example a non-isothermal RLC circuit is used. In Section 4 the example of the continued stirred tank reactor (CSTR) is presented. Finally in section 5 we present some conclusions and comments on future work.

2. IRREVERSIBLE PORT HAMILTONIAN SYSTEMS

IPHS have been proposed in Ramirez et al. (2013b) as an extension of PHS. These systems represent not only the energy balance but also the entropy balance associated with the irreversible processes. Let us first define a Poisson bracket (Maschke et al., 1992) with respect to a constant skew symmetric matrix $J = -J^\top$ acting on any two smooth functions Z and G as

$$\{Z, G\}_J = \frac{\partial Z^T}{\partial x}(x) J \frac{\partial G}{\partial x}(x). \tag{1}$$

Definition 1. An IPHS is defined by the dynamical equation

$$\dot{x} = J_{ir}\left(x, \tfrac{\partial U}{\partial x}\right)\frac{\partial U}{\partial x} + g\left(x, \tfrac{\partial U}{\partial x}\right)u \tag{2}$$

$$y = g\left(x, \tfrac{\partial U}{\partial x}\right)^\top \frac{\partial U}{\partial x} \tag{3}$$

where $x(t) \in \Re^n$ is the state vector, $u(t) \in \Re^m$ the input, the smooth function $U(x) : \Re^n \to \Re$ is the Hamiltonian and $g \in \Re^{n\times m}$ is the input map. The skew-symmetric structure matrix $J_{ir} \in \Re^{n\times n}$ is defined as

$$J_{ir}\left(x, \tfrac{\partial U}{\partial x}\right) = J_0(x) + R\left(x, \tfrac{\partial U}{\partial x}\right) J \tag{4}$$

with $J = -J^T$, $J_0 = -J_0^T$ and there exists a smooth entropy like function $S(x) : \Re^n \to \Re$ which is a Casimir function of J_0, i.e.,

$$\frac{\partial S}{\partial x}^\top J_0 = 0. \tag{5}$$

The non-linear modulating function R is defined as

$$R\left(x, \tfrac{\partial U}{\partial x}\right) = \gamma\left(x, \tfrac{\partial U}{\partial x}\right)\{S, U\}_J \tag{6}$$

where $\gamma\left(x, \frac{\partial U}{\partial x}\right) : \Re^n \to \Re$, $\gamma \geq 0$, a non linear positive function.

The balance equations of the entropy function $S(x)$ and the energy function $U(x)$ of the IPHS express the first and second principles of thermodynamics: the conservation of the energy and the irreversible creation of entropy. Taking the time derivative of the energy function gives

$$\begin{aligned}\frac{dU}{dt} &= \frac{dU^T}{dx}(J_0 + RJ)\frac{dU}{dx} + \frac{dU^T}{dx}gu \\ &= y^T u\end{aligned}$$

by skew-symmetry of J_{ir}, expressing that the IPHS is a lossless dissipative system with supply rate $y^T u$. If we take the time derivative of the entropy function, and set $u = 0$ for simplicity, it follows that

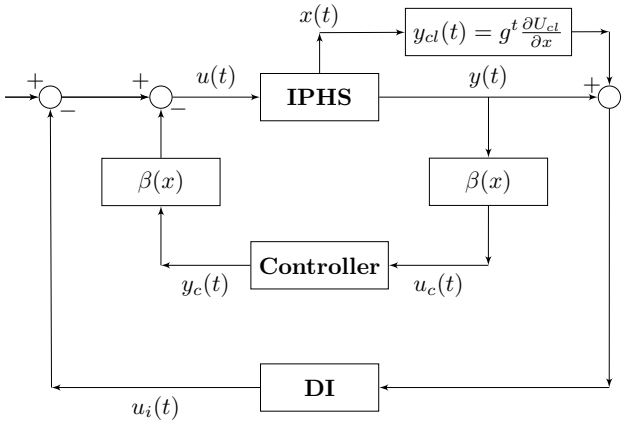

Fig. 1. Energy shaping plus damping injection control of an IPHS.

$$\begin{aligned}\frac{dS}{dt} &= \frac{dS^T}{dx}J_0\frac{dU}{dx} + R\frac{dS^T}{dx}J\frac{dU}{dx} \\ &= \{S, U\}_{J_0} + \gamma\left(x, \tfrac{\partial U}{\partial x}\right)\{S, U\}_J^2 \\ &= \gamma\left(x, \tfrac{\partial U}{\partial x}\right)\{S, U\}_J^2 = \sigma \geq 0\end{aligned}$$

where the term $\{S, U\}_{J_0} = 0$ because of (5) and where σ corresponds to the internal entropy production.

2.1 Example: non-isothermal RLC system

Consider a RLC system including the dynamics of the thermal effects of its electrical components. So we can consider that all electrical components are a function of the temperature. The IPHS formulation of the thermodynamic RLC circuit is (Ramirez et al., 2018)

$$\begin{bmatrix}\dot{Q}\\ \dot{\phi}\\ \dot{S}\end{bmatrix} = \left(\begin{bmatrix}0 & 1 & 0\\ -1 & 0 & 0\\ 0 & 0 & 0\end{bmatrix} + \frac{r}{T}\frac{\phi}{L}\begin{bmatrix}0 & 0 & 0\\ 0 & 0 & -1\\ 0 & 1 & 0\end{bmatrix}\right)\begin{bmatrix}\frac{Q}{C}\\ \frac{\phi}{L}\\ T\end{bmatrix} + \begin{bmatrix}0\\ 1\\ 0\end{bmatrix}u \tag{7}$$

with the internal energy $U_e(Q, \phi, S)$ of the system being the sum of the conservative energy plus some thermal related energy function

$$U_e(Q, \phi, S) = \frac{1}{2}\frac{Q^2}{C(S)} + \frac{1}{2}\frac{\phi^2}{L(S)} + U_s(S) \tag{8}$$

where the time variation of the internal energy is

$$\begin{aligned}\frac{dU_e}{dt} &= \frac{\partial U_e}{\partial Q}\dot{Q} + \frac{\partial U_e}{\partial \phi}\dot{\phi} + \frac{\partial U_e}{\partial S}\dot{S} \\ &= -r(S)\left(\tfrac{\phi}{L(S)}\right)^2 + \frac{\partial U_e}{\partial S}\frac{dS}{dt} + y_e^T u_e\end{aligned}$$

From Gibb's relation (Callen, 1985) it is known that $\frac{\partial U_e}{\partial S} = T(S)$. Taking $u_e = 0$ it follows that $\dot{U}_e = 0$ and it goes that

$$\frac{dS}{dt} = \frac{r(S)}{T(S)}\left(\frac{\phi}{L(S)}\right)^2 = \sigma_r. \tag{9}$$

The term σ_r corresponds to the internal entropy production of the system. Note that the RLC system (7) has the structure of the Definition 1 with a structure matrix composed of an irreversible part related to the dissipation and a reversible part related to Kirchhoff's law.

3. PASSIVITY BASED CONTROL

Passivity based control has been used as a model-based non-linear control design method (van der Schaft and

Jeltsema, 2014). PBC techniques such as energy shaping plus damping injection aim at rendering the closed-loop Hamiltonian function with asymptotically stability with respect to some desired energy function. In this section we synthesize an energy shaping plus damping injection controller through a systematic design. Furthermore, we will exploit Definition 1. This definition shows that an IPHS system can be seen as a composition of a conservative part and an irreversible part. The control by interconnection is done following Figure 1. In the first loop the output of the IPHS is interconnected with a control system in IPHS form. This loop is used to shape the closed-loop energy function such that its minimum is at the desired equilibrium. The second loop is in charge of injecting damping to the system to assure the asymptotic stability of the closed-loop system. Notice that the damping injection is performed with respect to the closed-loop output of the system, i.e., the output conjugated to the closed-loop Hamiltonian function. The final control input takes the form $u = u_e + u_i$ where u_e is the input for energy shaping and u_i is the input for damping injection.

3.1 Energy Shaping for IPHS

Energy shaping has been used to modify the natural equilibrium point of a Lyapunov candidate energy function for PHS (van der Schaft, 2016; Ortega et al., 2001) using Casimir functions which are structural invariants of the system. This lead to a set of partial differential equations which characterize the Casimir functions of the system. Let us consider an IPHS controller

$$\begin{aligned}\dot{\xi} &= \bar{R}\left(\xi, \tfrac{\partial U_c}{\partial \xi}\right)(J_c - R_c)\frac{\partial U_c}{\partial \xi}(\xi) + g_c\left(\xi, \tfrac{\partial U_c}{\partial \xi}\right)u_c(t)\\ y_c &= g_c^T\left(\xi, \tfrac{\partial U_c}{\partial \xi}\right)\frac{\partial U_c}{\partial \xi}(\xi)\end{aligned} \tag{10}$$

with $\xi \in \Re^l$ the state space vector; $y_c, u_c \in \Re^m$ with the mapping $g_c(\xi) \in \Re^{l\times m}$ and Hamiltonian function $U_c(\xi)$. Define the state modulated power-preserving interconnection

$$\begin{pmatrix} u_e \\ u_c \end{pmatrix} = \begin{pmatrix} 0 & -\beta(x) \\ \beta(x) & 0 \end{pmatrix}\begin{pmatrix} y \\ y_c \end{pmatrix} \tag{11}$$

where $\beta(x) \in \Re$. The closed-loop system then takes the form

$$\begin{pmatrix} \dot{x} \\ \dot{\xi} \end{pmatrix} = \begin{pmatrix} J_{ir} & -g\beta g_c^T \\ g_c\beta g^T & \bar{R}(J_c - R_c) \end{pmatrix}\begin{pmatrix} \frac{\partial U_{cl}(x,\xi)}{\partial x} \\ \frac{\partial U_{cl}(x,\xi)}{\partial \xi} \end{pmatrix} + \begin{pmatrix} g \\ \mathbf{0} \end{pmatrix} u_i \tag{12}$$

with $\mathbf{0}$ a null matrix of appropriate dimensions and closed-loop Hamiltonian function $U_{cl}(x,\xi) = U(x) + U_c(\xi)$. We look for structural invariant functions of the form $C_i(x,\xi_i) = F_i(x) - \xi_i$, $i = 1,..,l$ with C_i the Casimir function associated to the state ξ_i of the controller and $F(x) = [F_1, ..., F_l] \in \Re^l$ a collection of smooth well defined functions F_i of x. If these invariant functions exist, then on every invariant manifold the relation $\xi - F(x) = \kappa$ with $\kappa = [\kappa_1, ..., \kappa_l] \in \Re^l$ a vector of constants that depend on the initial states of the plant and the controller, holds. The closed-loop Hamiltonian energy function can then be expressed in terms of the states of the plant $U_{cl}(x,\xi) = U(x) + U_c(F(x) + \kappa)$, and the control action as a state feedback

$$u = -\beta(x)y_c\left(F(x) + \kappa\right) \tag{13}$$

The Casimir functions are invariants of the structure of the system, implying that $\frac{\partial C^\top}{\partial x}J_{cl} = 0$, with

$$J_{cl} = \begin{pmatrix} J_{ir} & -g\beta g_c^T \\ g_c\beta g^T & \bar{R}(J_c - R_c) \end{pmatrix}$$

This condition leads to the following set of partial differential equations

$$\begin{aligned}\frac{\partial F^T}{\partial x}(x)J_{ir} &= g_c\beta g^T\\ -\frac{\partial F^T}{\partial x}(x)g\beta g_c^T &= \bar{R}(J_c - R_c)\end{aligned} \tag{14}$$

Following the same procedure as in van der Schaft (2016) we get the set of matching equations

$$\begin{aligned}\frac{\partial F^T}{\partial x}(x)J_{ir} &= g_c\beta g^T\\ R_c &= 0\\ \frac{\partial F^T}{\partial x}J_{ir}\frac{\partial F}{\partial x} &= \bar{R}J_c\end{aligned} \tag{15}$$

These are the matching equations for an IPHS system with a controller in IPHS form, using the state modulated interconnection (11). These matching equations are analogous to the case of control by interconnection of PHS with the difference that J_{ir} depends on the modulating functions R and that the control structure includes a modulating function $\bar{R}$. Assuming that the smooth function $F(x)$ exists, the control law (13) renders the closed-loop Hamiltonian function as $U_{cl}(x) = U(x) + U_c(F(x) + \kappa)$. Furthermore, the energy-input allows to interpret the closed-loop as an IPHS system. In effect, notice that

$$\frac{dx}{dt} = RJ_{ir}\frac{\partial U}{\partial x} - g\underbrace{\beta g_c\frac{\partial (U_c \circ F)}{\partial \xi}}_{u_e} \tag{16}$$

Using the first equation of (15) and the skew-symmetric property of J_{ir}, the relation (16) can be rewritten as

$$\begin{aligned}\frac{dx}{dt} &= RJ_{ir}\frac{\partial U}{\partial x} + J_{ir}\frac{\partial F}{\partial x}\frac{\partial (U_c \circ F)}{\partial \xi}\\ &= RJ_{ir}\frac{\partial U}{\partial x} + J_{ir}\frac{\partial U_c}{\partial x}\end{aligned}$$

Finally, by simple factorization and adding an input u_i to the closed-loop system, we get

$$\dot{x} = J_{ir}\frac{\partial U_{cl}}{\partial x} + gu_i \tag{17}$$

$$y_{cl} = g^\top\frac{\partial U_{cl}}{\partial x} \tag{18}$$

where y_{cl} is the passive output defined with respect to $U_{cl}(x)$. This approach allows to see the closed-loop system as an IPHS; i.e, without destroying the structure of IPHS, and therefore can be interconnected with others IPHS systems and interpreted in the framework of the energy-Casimir plus damping design for control purposes. Next, we calculate the time derivative of the entropy in the closed-loop system

$$\begin{aligned}\frac{dS}{dt} &= \frac{dS^\top}{dx}J_0\frac{dU_{cl}}{dx} + R\frac{dS^\top}{dx}J\frac{dU_{cl}}{dx}\\ &= \underbrace{R\frac{dS^\top}{dx}J\frac{dU}{dx}}_{\sigma(t)} + \underbrace{R\frac{dS^\top}{dx}J\frac{dU_c}{dx}}_{\sigma_c(t)}\end{aligned}$$

where $\sigma \geq 0$ is the internal entropy variation of the system and σ_c is the external entropy variation due to the inputs of the system. As the control objective is to set a desired entropy, the rate $\sigma_c = -\sigma$ in the stationary state.

The time variation of the closed-loop energy function is now given by

$$\dot{U}_{cl} = y_{cl}^{\top} u_i \tag{19}$$

Since the internal energy of irreversible thermodynamic systems does not have a strict minimum, a now standard candidate Lyapunov function for control is the availability function (Alonso and Ydstie, 2001; Ydstie, 2002; Jillson and Ydstie, 2007). The availability function uses the convexity of the internal energy or the negativity of the entropy, together with the assumption that one of the extensive variables is fixed, to construct a strictly convex extension which serves as Lyapunov function for a desired dynamical equilibrium. This approach has been widely used in the control of thermodynamic systems in the last decade (Hoang et al., 2011, 2012; Ramirez et al., 2016). We shall use the availability function as the target closed-loop function for the *irreversible part* of the IPHS in the energy-shaping design. Next we give one definition for this function.

Definition 2. (Ramirez et al., 2016) The energy based availability function is defined as

$$A(x, x^*) = U(x) + U_a(x, x^*) \tag{20}$$

Where $U_a(x, x^*) = -U(x^*) - \frac{\partial U}{\partial x}(x^*)^T(x - x^*)$, with $U(x)$ being the internal energy of the system and x^* the desire equilibrium point of an irreversible variable x.

3.2 Damping Injection for IPHS

The energy shaping input shapes the Hamiltonian of the system and guarantees the closed-loop stability of the system, but one have yet to guarantee the asymptotic stability at the equilibrium point. Suppose that the closed-loop IPHS (17) has a minimum at x^*. Set u_i as

$$u_i = -Kg^{\top} y_{cl} = -Kg^{\top} \frac{\partial U_{cl}}{\partial x} \tag{21}$$

with $K = K^{\top} > 0$. The closed-loop system is then given by

$$\dot{x}(t) = (J_{ir} - gKg^T)\frac{\partial U_{cl}}{\partial x}. \tag{22}$$

The time derivative of the closed-loop energy function is

$$\begin{aligned} \frac{dU_{cl}}{dt} &= \frac{dU_{cl}^T}{dx}(J_{ir} - gKg^T)\frac{\partial U_{cl}}{\partial x} \\ &= \{U_{cl}, U_{cl}\}_{J_{ir}} - \{U_{cl}, U_{cl}\}_M \\ &= -\{U_{cl}, U_{cl}\}_M < 0 \end{aligned}$$

since $\{U_{cl}, U_{cl}\}_{J_{ir}} = 0$ and where $M = gKg^T \geq 0$. By Lasalle's invariance theorem it is then showed that the closed-loop system converges asymptotically to x^*.

3.3 Example: non-isothermal RLC system (continued)

We apply the results of the subsections 3.1 and 3.2 to get an energy-shaping plus damping injection control. We look for Casimir functions for the system (7) with $F(x) = F(Q, \phi, S)$. Applying the third equation of (15) we get $J_c = 0$ and $g_c = 1$. The first equation of (15) results in the following relations

$$-\frac{\partial F}{\partial \phi} = 0, \qquad \frac{\partial F}{\partial Q} + \frac{r\phi}{TL}\frac{\partial F}{\partial S} = \beta, \qquad -\frac{r\phi}{TL}\frac{\partial F}{\partial \phi} = 0$$

which have multiple solution. Taking

$$\frac{\partial F}{\partial Q} = \alpha_1 \qquad \frac{\partial F}{\partial \phi} = 0 \qquad \frac{\partial F}{\partial S} = \alpha_2$$

with $\beta = \alpha_1 + \alpha_2 \frac{r\phi}{TL}$ where $\alpha_1, \alpha_2 \in \Re$, we obtain

$$F = \alpha_1 Q + \alpha_2 S$$

The corresponding Casimir function allows to shape the coordinate of the capacitor and the entropy of the system. We set as desired closed-loop Hamiltonian

$$U_{cl}(Q, \phi, S) = \frac{1}{2}\frac{(Q - Q^*)^2}{C} + \frac{1}{2}\frac{\phi^2}{L} + A(S, S^*)$$

where $A(S, S^*) = U_s(S) - [U_s(S^*) + T^*(S - S^*)]$ is the availability function (20) for the irreversible part of the system. The closed-loop energy function is given by

$$U_{cl}(Q, \phi, S) = U + U_c$$

where U_c is the energy provided by the controller and U is the internal energy of the system. The simplest choice for U_c is

$$U_c = -\frac{QQ^*}{C} + \frac{1}{2}\frac{(Q^*)^2}{C} - U_s(S^*) - T(S^*)(S - S^*)$$

Taking $\alpha_1 = \frac{-Q^*}{C}$ and $\alpha_2 = -T^*$ with $\kappa = \frac{1}{2}\frac{(Q^*)^2}{C} - U_s(S^*) + T^*S^*$ it follows that $\beta = \frac{-Q^*}{C} - T^*\frac{r\phi}{TL}$. The control input is then given by

$$u_e = -\beta\frac{\partial U_c}{\partial \xi} = -\beta = \frac{Q^*}{C} + T^*\frac{r\phi}{TL}$$

We have the energy shaping control input so we have yet to design the damping injection input in order for the closed-loop system to converge to x^*. Following the result presents in the subsection 3.2 we select $u_i(t) = -K\frac{\phi}{L}$. The control law for the system then takes the form

$$u(t) = \frac{Q^*}{C} + T^*\frac{r\phi}{TL} - K\frac{\phi}{L}$$

which is a classic proportional plus integration control law.

4. EXAMPLE: THE CSTR SYSTEM

In this section we design an energy shaping plus damping injection controller for a continuous stirred tank reactor (CSTR). The IPHS model is presented in subsection 4.1 and a particular case of a reaction of two species is considered. In subsection 4.2 the controller is designed.

4.1 IPHS Model

Let us consider a CSTR system with the following reversible reaction scheme:

$$\sum_{i=1}^{m} \xi_i A_i \overset{r}{\rightleftharpoons} \sum_{i=1}^{m} \eta_i A_i \tag{23}$$

with ξ_i, η_i being the constant stoichiometric coefficients for species A_i in the reaction. We will consider the following assumptions for the standard operation of the reactor (Aris, 1989; Favache and Dochain, 2009):

Assumption 3. The following holds

1. The reactor operates in liquid phase.
2. The molar volume of each species are identical and the total volume V in the reactor is constant through the reaction.
3. The initial number of moles of the species in the reactor is equal to the number of moles of the inlet of the sames species.
4. For a given steady state temperature T and steady state input, there is only one possible steady state for the mass. This mean that each steady state temperature is associated with a one unique steady state temperature.

The IPHS model of the CSTR is (Ramirez et al., 2016).

$$\dot{x}(t) = RJ\frac{\partial U}{\partial x}(x) + gu(t)$$

with the state vector $x = [\mathbf{n}\ S]^T$, where $\mathbf{n} = (n_1, ..., n_m)^T$ with n_i the number of moles of the species i inside the reactor; S the total entropy of the system and $U(x)$ the internal energy function, and

$$J = \begin{bmatrix} 0 & \cdots & 0 & \bar{\nu}_1 \\ & & & \vdots \\ 0 & \cdots & 0 & \bar{\nu}_m \\ -\bar{\nu}_1 & \cdots & -\bar{\nu}_m & 0 \end{bmatrix}, \frac{\partial U}{\partial x} = \begin{bmatrix} \mu_1 \\ \vdots \\ \mu_m \\ T \end{bmatrix}, R = \frac{rV}{T}$$

where J is a constant skew-symmetric matrix whose elements are the signed stoichiometric coefficients of the chemical reaction $\bar{\nu}_i = \xi_i - \eta_i$, a number which is positive or negative depending on whether the species i is a product or a reactant; $\frac{\partial U}{\partial x}$ corresponds to the intensive variables with T being the temperature in the reactor and μ_i the chemical potential of the species i; R is the modulating function, where $r = r(\mathbf{n}, T)$ is the reaction rate which depends on the temperature and on the reactant mole numbers vector $\mathbf{n}$. The input vector is $u = [u_1, u_2]^T$ with $u_1 = F/V$ the dilution rate, where F is the volumetric flow rate, and $u_2 = Q$ the heat flux from the cooling jacket; the input map g is given by

$$g = \begin{bmatrix} \bar{\mathbf{n}} & \mathbf{0} \\ \phi(x) & 1/T \end{bmatrix}$$

with $\bar{\mathbf{n}} = \mathbf{n}_e - \mathbf{n}$, where $\mathbf{n}_e = (n_{e1}, ..., n_{em})^T$ is the vector containing the numbers of moles of species i at the inlet and $\phi(x) = \sum_{i=1}^{m}(n_{ei}s_{ei} - n_i s_i) + \frac{n_{ei}}{T}(h_{ei} - Ts_{ei} - \mu_i)$, where s_{ei} is the inlet molar entropy,s_i is the molar entropy and h_{ei} is the inlet specific molar ethalpy of species i. As a particular case, in order to control the system, we take $m = 2$ and the reaction is

$$\xi_1 A_1 + \xi_2 A_2 \overset{r}{\rightleftharpoons} \eta_1 A_1 + \eta_2 A_2 \tag{24}$$

This reaction is then characterized by the IPHS with

$$J = \begin{bmatrix} 0 & 0 & \bar{\nu}_1 \\ 0 & 0 & \bar{\nu}_2 \\ -\bar{\nu}_1 & -\bar{\nu}_2 & 0 \end{bmatrix} \quad \frac{\partial U}{\partial x} = \begin{bmatrix} \mu_1 \\ \mu_2 \\ T \end{bmatrix} \quad g = \begin{bmatrix} \bar{n}_1 & 0 \\ \bar{n}_2 & 0 \\ \phi(x) & 1/T \end{bmatrix}$$

with $\phi(x) = \sum_{i=1}^{2}(n_{ei}s_{ei} - n_i s_i) + \frac{n_{ei}}{T}(h_{ei} - Ts_{ei} - \mu_i)$ and with state space vector $x(t) = [n_1\ n_2\ S]^T$; the input of the system is $u = (u_1, u_2)^T$.

4.2 Passivity based control of the CSTR

The system has by states n_1, n_2, S so we will parametrize the design and look for Casimir functions of the form $C_1(n_1, \xi_1) = F_1(n_1) - \xi_1$, $C_2(n_2, \xi_2) = F_2(n_2) - \xi_2$ and $C_3(S, \xi_3) = F_3(S) - \xi_3$ such that $\xi_1 = F_1(n_1) + \kappa_1$, $\xi_2 = F_2(n_2) + \kappa_2$ and $\xi_3 = F_3(S) + \kappa_3$ with $F(n_1, n_2, S) = [F_1\ F_2\ F_3]$. Define the IPHS controller by $x_c = [\xi_1\ \xi_2\ \xi_3]^T$, $J_c \in \Re^{3\times 3}$, β a scalar function and

$$g_c = \begin{bmatrix} g_{11} & g_{21} & g_{31} \\ g_{12} & g_{22} & g_{32} \end{bmatrix}^\top$$

Since there is no reversible part, we set as desired closed-loop Hamiltonian the availability function (20) $U_{cl} = U(x) - [U(x^*) + \frac{\partial U}{\partial x}(x^*)^T(x - x^*)]$, hence the energy of the controller is chosen as

$$\begin{aligned} U_c &= -[U(x^*) + \frac{\partial U}{\partial x}(x^*)^T(x - x^*)] \\ &= (-\mu_1^* n_1 + \mu_1^* n_1^*) + (-\mu_2^* n_2 + \mu_2^* n_2^*) + \\ &\quad (-T^* S + T^* S^*) - U(n_1^*, n_2^*, S^*) \end{aligned}$$

The choice of Casimir functions and controller Hamiltonian leads to following condition on F

$$\frac{\partial F}{\partial x} = \begin{bmatrix} -\mu_1^* & 0 & 0 \\ 0 & -\mu_2^* & 0 \\ 0 & 0 & -T^* \end{bmatrix}$$

Applying the matching equations, from the first equation of (15) we get

$$\begin{aligned} &g_{11} = 0 && g_{21} = 0 && g_{31} = \frac{T^*\bar{\nu}_2}{\bar{n}_2} \\ &g_{12} = -\mu_1^*\bar{\nu}_1 T^* && g_{22} = -\mu_2^*\bar{\nu}_2 T^* && g_{31} = \frac{T^*\bar{\nu}_1}{\bar{n}_1} \\ &g_{32} = -g_{31}\phi T^* && \beta = R \end{aligned}$$

The system has a solution if

$$\frac{\bar{n}_1}{\bar{\nu}_1} = \frac{\bar{n}_2}{\bar{\nu}_2} \tag{25}$$

In Prigogine and Defay. (1954) for batch reactors the equality (25) is the expression of De Donder's extent of reaction

$$\frac{n_{0i} - n_i}{\bar{\nu}_i} = \xi$$

where this property can be extended to the CSTR under Assumption 3. This result is a particular case of the one obtained in Ramirez et al. (2016) where an IDA-PBC like approach is used to design a controller for a class of CSTR. The third equation of (15) gives

$$J_c = T^* \begin{bmatrix} 0 & 0 & \mu_1^*\bar{\nu}_1 \\ 0 & 0 & \mu_2^*\bar{\nu}_2 \\ -\mu_1^*\bar{\nu}_1 & -\mu_2^*\bar{\nu}_2 & 0 \end{bmatrix}$$

with $\bar{R} = T^*$ a real constant. The controller is then given by

$$\begin{aligned} x_c &= T^* \begin{bmatrix} 0 & 0 & \mu_1^*\bar{\nu}_1 \\ 0 & 0 & \mu_2^*\bar{\nu}_2 \\ -\mu_1^*\bar{\nu}_1 & -\mu_2^*\bar{\nu}_2 & 0 \end{bmatrix} \begin{bmatrix} -\mu_1^* \\ -\mu_2^* \\ -T^* \end{bmatrix} \\ &\quad + \begin{bmatrix} 0 & -\mu_1^*\bar{\nu}_1 T^* \\ 0 & -\mu_2^*\bar{\nu}_2 T^* \\ T^*\xi & -(T^*)^2\xi\phi \end{bmatrix} u_c \\ y_c &= g_c^T \begin{bmatrix} -\mu_1^* \\ -\mu_2^* \\ -T^* \end{bmatrix} \end{aligned}$$

The energy shaping control law is then given by

$$u_e = -\frac{rV}{T}\begin{bmatrix} -(T^*)^2\xi \\ -(\mu_1^*)^2\bar{\nu}_1 T^* - (\mu_2^*)^2\bar{\nu}_2 T^* - (T^*)^3\xi\phi \end{bmatrix}$$

For the damping injection we chose a $K \in \Re^{2\times 2}$ such that $M = gKg^T \geq 0$. The simplest choice is $K = \alpha\ \mathrm{diag}(0, T^2)$ which gives $M = diag(0, 0, \alpha)$, for some tuning parameter $\alpha > 0$. The damping injection input takes the form

$$u_i = -\alpha \begin{bmatrix} 0 \\ T(T - T^*) \end{bmatrix}$$

The closed-loop system is finally given by

$$\dot{x} = (-gKg^T + RJ)\frac{\partial U_{cl}}{\partial x}$$

with $\frac{\partial U_{cl}}{\partial x} = [\mu_1 - \mu_1^*\ \mu_2 - \mu_2^*\ T - T^*]^T$. The asymptotic stability follows from the time derivative of the closed-loop energy function (subsection 3.2)

$$\frac{dU_{cl}}{dt} = -\frac{\partial U_{cl}^T}{\partial x} M \frac{\partial U_{cl}}{\partial x} = -\alpha(T - T^*)^2 \leq 0$$

by applying La Salle's invariance principle in a sufficient small region of $T = T^*$, under the conditions of Assumption 3.

5. CONCLUSION

A systematic procedure to perform energy shaping and damping injection, while preserving the IPHS structure has been proposed. In a first control loop, energy shaping is achieved by a stated modulated interconnection with a controller in IPHS form. To this end, the existence of Casimir functions are instrumental to relate the states of the plant and the controller. Using the Casimir functions a dynamic controller which shapes the closed-loop Hamiltonian into an energy based availability function with minimum at the desired dynamic equilibrium is designed. A second control loop is used to guarantee asymptotic stability by the feedback of a closed-loop passive output defined with respect the closed-loop Hamiltonian. The approach allows to stabilize IPHS while preserving the IPHS structure in closed-loop, allowing to interpret the closed-loop system as a desired thermodynamic system which can be connected with others IPHS systems, and which can be interpreted in the framework of the energy-Casimir method for control purposes. A non-isothermal RLC circuit has been developed along the paper and the non-trivial example of the continuous stirred tank reactor has been used to illustrate the approach. Future work will deal with the numerical implementation of the controller and the study of non-trivial coupled mechanical-thermodynamic systems.

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