On the relaxing dissipation of dissipative pseudo Hamiltonian models

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Abstract: This paper further explores the link between irreversible thermodynamics and system theory, and its use for port-based modeling for reaction systems. More specifically we show here that a pseudo Hamiltonian representation with R(x) > 0 can be obtained by considering the Brayton-Moser formulation via a unified potential function that verifies a thermodynamic evolution criterion. As a consequence, it gives additional degrees of freedom (i.e. to construct alternate pseudo Hamiltonian models with new passive outputs) usable for further studies on the control design. A representative example of irreversible processes via the non isothermal continuous stirred tank reactor model is used to illustrate the theoretical developments.

Keywords: Port controlled Hamiltonian systems, Brayton-Moser formulation, CSTR.

1. INTRODUCTION

The analysis and design of control algorithms are largely based on system theory tools that refer to energy considerations. These obviously include Lyapunov stability (Khalil (2002)) but also passivity-based approaches (Willems (1970, 1972); Brogliato *et al.* (2007); Van Der Schaft (2000b)). Over the last two decades it has been shown that Port Hamiltonian (PH) framework as well as the Brayton-Moser (BM) formulation can be considered for passivity or power-based control of electromechanical or reaction systems (Van Der Schaft (2000a); Maschke *et al.* (2000); Hudon *et al.* (2008); Favache & Dochain (2010)). Unfortunately for thermodynamical systems such as chemical reactors it is not easy to determine the storage function (Warden *et al.* (1964); Dammers & Tels (1974); Tarbell (1977)).

The chemical reactor models, and in particular the reference case study known as the Continuous Stirred Tank Reactor (CSTR) belongs to nonlinear non-equilibrium thermodynamic systems via the reaction kinetics and irreversibilities of the coupling between matter and temperature. Following the first principle of thermodynamics, the total energy (the energy of the simple system under consideration and its surrounding medium) is conserved. Yet this energy changes of nature moving irreversibly from the material domain to the thermal domain. As a matter of fact the internal energy cannot be considered as an Hamiltonian function because it does not allow to express the inherent irreversibility of the system governed by the second law of thermodynamics. From thermodynamics concepts, some storage functions have been proposed (Ydstie & Alonso (1997); Hangos et al. (2001); Eberard et al. (2007)). More recently pseudo Hamiltonian models have been also proposed for thermodynamical systems such as chemical reactors (Otero-Muras et al. (2008); Dörfler et al. (2009);

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Ramírez et al. (2009); Hoang et al. (2011a)) as well as Brayton-Moser (BM) models (Favache et al. (2011); Hoang et al. (2011b)). In (Dörfler et al. (2009); Ramírez et al. (2009)), the dissipation term does not capture the inherently irreversible nature of the CSTR and the Hamiltonian is not linked to any thermodynamic variable. The use of the physical variables for the Hamiltonian storage function is done in (Otero-Muras et al. (2008)) when considering closed reaction networks in the isothermal case. Nevertheless the (local) Hamiltonian is not the Gibbs free energy (as seen in (Hoang et al. (2011a))) but it is locally linked to the chemical affinity. The use of the irreversible entropy production (due to chemical reaction) as the Hamiltonian potential is proposed in (Favache *et al.* (2011)) with some restrictions on the reaction kinetics. However the derivation of the dissipation term is not straightforward. In (Hoang et al. (2011a)), a thermodynamical pseudo Hamiltonian representation of the CSTRs model using the thermodynamic potentials (Gibbs free energy G (Callen (1985)) and opposite of entropy -S, also called ectropy (Haddad et al. (2005)), for isothermal and non-isothermal cases respectively) as Hamiltonian functions is given. In (Hoang *et al.* (2011b)) it has been shown that a dissipative pseudo Hamiltonian representation for non-isothermal CSTRs can be derived from the BM formulation when a positivity condition (also called thermodynamic stability condition) is satisfied by some chosen potential function. This formulation is based on a structured representation of systems with the variables directly coming from thermodynamical considerations and considers the opposite of entropy -S (extensive variable) and the square of the chemical affinity \mathscr{A} (intensive variable) as Hamiltonian functions. In both cases, the dissipation term can be linked to the natural irreversibility (entropy production) due to chemical reaction.

In this paper, we further explore the link between irreversible thermodynamics and system theory, and its use for dynamical analysis and control design for reaction systems. More specifically contrary to the previous work (Hoang et al. (2011a)) where the damping matrix R(x) is singular, we show here that a pseudo-Hamiltonian representation with R(x) > 0 can be obtained by considering the Brayton-Moser formulation (Brayton & Moser (1964)) via a unified potential function that verifies a thermodynamic evolution criterion. Consequently, it allows to express directly the dissipation of the system dynamics associated to some physical potential function when applied to reaction systems. In addition to this, it gives additional degrees of freedom (i.e. to construct novel pseudo Hamiltonian models with relaxing (generalized) damping elements) usable for further studies on the control design in the sense of $(Ortega \ et \ al. \ (2008)).$

The paper is organized as follows. Section 2 is dedicated to an overview of potential-based modeling (including a general connection to Port Hamiltonian-based modeling on the basis of the Brayton-Moser formulation). Section 3 illustrates the proposed developments for the case study of the non isothermal continuous stirred tank reactor (CSTR) involving one reversible reaction. Section 4 ends the paper with concluding remarks and perspectives.

2. A THEORETICAL OVERVIEW

Let us consider open chemical systems that are affine in the control input u and whose dynamics is given by the following set of ordinary differential equations (ODEs) :

$$\frac{dx}{dt} = f(x) + g(x) \ u, \quad x(t=0) = x_0 \tag{1}$$

where $x \in \mathbb{R}^n$ is the state vector, $f(x) \in \mathbb{R}^n$ represents the smooth nonlinear function with respect to $x, g(x) \in \mathbb{R}^{n \times m}$ is the input-state map and $u \in \mathbb{R}^m$ is the input.

2.1 Brayton-Moser (BM) formulation

The BM formulation (Brayton & Moser (1964); Favache *et al.* (2011)) requires :

• to find a non singular matrix $Q(x) : \mathbb{R}^n \to \mathbb{R}^{n \times n}$ such that its symmetric part is negative definite:

$$Q(x) + Q(x)^{\mathrm{T}} \le 0 \tag{2}$$

where the exponent T stands for the matrix transpose.

• to write the system dynamics (1) into the following equivalent form :

$$Q(x)\frac{dx}{dt} = \nabla_x \mathcal{P}(x) + G(x)u \tag{3}$$

with $\mathcal{P}(x):\mathbb{R}^n\to\mathbb{R}$ a smooth potential function.

From (1)(3) we get the following relations :

$$G(x) = Q(x)g(x) \tag{4}$$

$$\nabla_x \mathcal{P}(x) = Q(x)f(x) \tag{5}$$

The necessary and sufficient condition for the existence of (3) is the symmetry of the Hessian matrix of $\mathcal{P}(x)$:

$$\mathbb{H}(\mathcal{P}) = \mathbb{H}(\mathcal{P})^{\mathrm{T}} \tag{6}$$

The condition (6) can also be viewed as a particular case of the Poincaré Lemma (García-Canseco *et al.* (2010)).

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2.2 Links with the Port controlled Hamiltonian (PCH) systems

Because Q is invertible, the BM form (3) can be rewritten :

$$\frac{dx}{dt} = Q(x)^{-1} \nabla_x \mathcal{P}(x) + g(x)u \tag{7}$$

Since any square matrix can be split into two (symmetric and skew-symmetric) parts, (7) can be transformed into the following form :

$$\frac{dx}{dt} = \left[\frac{Q^{-1} - Q^{-1T}}{2} + \frac{Q^{-1} + Q^{-1T}}{2}\right] \nabla_x \mathcal{P}(x) + g(x)u$$
(8)

Hence (8) can be identified to a general class of PCH systems with dissipation given by (Brogliato *et al.* (2007); Van Der Schaft (2000b)) :

$$\begin{cases} \frac{dx}{dt} = [J(x) - R(x)]\nabla_x \mathcal{H}(x) + g(x)u\\ y = g(x)^{\mathrm{T}}\nabla_x \mathcal{H}(x) \end{cases}$$
(9)

with (Jeltsema (2005)) :

$$\begin{cases} J(x) = \frac{Q(x)^{-1} - Q(x)^{-1\mathrm{T}}}{2} \\ R(x) = -\frac{Q(x)^{-1} + Q(x)^{-1\mathrm{T}}}{2} \ge 0 \end{cases}$$
(10)

The smooth function $\mathcal{H}(x) \equiv \mathcal{P}(x) : \mathbb{R}^n \to \mathbb{R}$ represents the Hamiltonian storage function (or the generalized energy); $J(x) = -J(x)^{\mathrm{T}}$ and $R(x) = R(x)^{\mathrm{T}} \geq 0$ are the structure matrices and correspond to the natural interconnection matrix and the damping matrix, respectively; $u, y \in \mathbb{R}^m$ are the control input and output, respectively, and are power conjugated port variables. The energy balance immediately follows from (9) :

$$\frac{d\mathcal{H}(x)}{dt} = -\nabla_x \mathcal{H}(x)^{\mathrm{T}} R(x) \nabla_x \mathcal{H}(x) + u^{\mathrm{T}} y \qquad (11)$$

The system (9) is passive in the sense that the dissipation

$$d = -\nabla_x \mathcal{H}(x)^{\mathrm{T}} R(x) \nabla_x \mathcal{H}(x) \le 0$$
(12)

is negative semidefinite and the Hamiltonian $\mathcal{H}(x)$ is bounded from below (Brogliato *et al.* (2007); Van Der Schaft (2000b)). The term *d* (12) corresponds to natural dissipation (energy lost due to friction/damping in mechanical systems or resistance in *RLC* electrical systems (Van Der Schaft (2000a); Maschke *et al.* (2000)) or entropy production in the CSTR networks (Hoang *et al.* (2011a)) for example).

If we further impose that the symmetric matrix R(x) in (10) is positive definite (i.e. R(x) > 0), R(x) will be full rank, i.e. :

rank
$$R(x) = n$$
 or det $R(x) \neq 0$ (13)

As a consequence, the negative definiteness property of d (12) is guaranteed for $\nabla_x \mathcal{H}(x) \neq 0$. Hence the stationary equilibrium of the unforced system (9) is already asymptotically stable. No feedback control law is then needed since the autonomous system reaches its stationary equilibrium. It follows from (10) that a necessary and sufficient condition for the positive definiteness condition of the symmetric matrix R(x) is :

$$R(x) > 0 \iff Q(x)^{-1} + Q(x)^{-1T} < 0$$
 (14)

The symmetric matrix $Q(x)^{-1} + Q(x)^{-1T}$ is negative definite if and only if $-(Q(x)^{-1} + Q(x)^{-1T})$ is positive

definite. Equivalently it implies that all of the principal minors determinants of $-(Q(x) + Q(x)^{T})$ are positive.

3. THE CSTR CASE STUDY

For the sake of simplicity, let us consider a jacketed reactor with one reversible reaction involving 2 chemical species denoted by A and B (with molar masses M_A and M_B , respectively). Such a chemical reaction is described as follows :

$$|\nu_A|A \stackrel{\mathbf{r}_{\mathbf{f}_{\perp}}}{\underset{\mathbf{r}_{\mathbf{r}}}{\leftarrow}} \nu_B B$$
 (The stoichiometry) (15)

and

 $\nu_A M_A + \nu_B M_B = 0$ (The molar mass conservation) (16) where ν_A and ν_B are the suitable signed stoichiometric coefficients $\nu_A < 0$ and $\nu_B > 0$ (Groot (1962); Antonelli & Astolfi (2003); Hoang *et al.* (2011a); Ramírez *et al.* (2013)). Note that any reversible reaction can be considered as a simple reaction with the net reaction rate :

$$r = r_f - r_r \tag{17}$$

with r_f and r_r the forward and reverse reaction rates, respectively.

The following modeling assumptions are also considered :

(H1) The fluid mixture is ideal, incompressible and under isobaric conditions.

- (H2) In the inlet, the reactor is fed by the species A and B at a given temperature T_I .
- (H3) The heat flow rate \dot{Q}_J coming from the jacket is modelled by the following relation :

$$\dot{Q}_J = \lambda (T_J - T) \tag{18}$$

where $\lambda > 0$ is the heat exchange coefficient. The reactor temperature and jacket temperature are denoted by Tand T_J , respectively.

We assume that the heat flow rate \dot{Q}_J and inlet molar flow rates (F_{AI}, F_{BI}) are the manipulated process inputs.

If we consider energy and mass balances, the non isothermal system dynamics is then given by the following set of ODEs (1) (see also (Hoang & Dochain (2013); Favache *et al.* (2011); Hoang *et al.* (2011b)) for more details) with :

$$x = \begin{pmatrix} N_A \\ N_B \\ H \end{pmatrix}, u = \begin{pmatrix} F_{AI} \\ F_{BI} \\ \dot{Q}_J \end{pmatrix}, f(x) = \begin{pmatrix} \nu_A r V \\ \nu_B r V \\ 0 \end{pmatrix}$$
(19)

$$g(x) = \begin{pmatrix} \left(1 - \frac{N_A M_A}{m_t}\right) & -\frac{N_A M_B}{m_t} & 0\\ -\frac{N_B M_A}{m_t} & \left(1 - \frac{N_B M_B}{m_t}\right) & 0\\ \left[h_{AI} - \frac{M_A H}{m_t}\right] & \left[h_{BI} - \frac{M_B H}{m_t}\right] & 1 \end{pmatrix}$$
(20)

where (N_A, N_B) is the molar numbers vector and (h_{AI}, h_{BI}) is the inlet molar enthalpies vector. The volume and enthalpy are denoted by V and H, respectively.

In the previous works (Hoang *et al.* (2011b); Hoang & Dochain (2013)), it has been shown that there exists a thermodynamic potential function $\mathcal{P}(N_A, N_B, H)$ associated to the reaction mixture (15)(16) and this potential function fulfills :

$$\frac{\partial \mathcal{P}}{\partial N_A} \neq 0, \quad \frac{\partial \mathcal{P}}{\partial N_B} \neq 0, \quad \frac{\partial \mathcal{P}}{\partial H} \neq 0$$
 (21)

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$$\lim_{r \to 0} \frac{\nu_A \frac{\partial \mathcal{P}}{\partial N_A} + \nu_B \frac{\partial \mathcal{P}}{\partial N_B}}{rV} < \infty$$
 (22)

$$\left(-\nu_A \frac{\partial \mathcal{P}}{\partial N_A} - \nu_B \frac{\partial \mathcal{P}}{\partial N_B}\right) r V > 0 \tag{23}$$

Equality holds only when the system reaches its steady state. Inequality (23) that generalizes the positive definiteness of the irreversible entropy production is called the thermodynamic evolution criterion of the mixture with chemical transformations (Hoang & Dochain (2013)).

Remark 1. As a consequence of the second law of thermodynamics (Groot (1962); Ydstie & Alonso (1997); Hoang *et al.* (2012); Callen (1985)), both the square of the chemical affinity and the ectropy (defined as the opposite of the entropy (Haddad *et al.* (2005))) satisfy (21)-(23) (Hoang *et al.* (2011b); Hoang & Dochain (2013)). In addition, if the reaction kinetics is such that $\nu_A \frac{\partial rV}{\partial N_A} + \nu_B \frac{\partial rV}{\partial N_B} \leq 0$ (e.g. Eq. (4.2) and Assumption 2 in (Favache *et al.* (2011))) the irreversible entropy production is decreasing along the system trajectories and meets (23).

In what follows, we shall see that the thermodynamic evolution criterion (23) gives some guidelines to derive a dissipative PCH representation on the basis of the BM formulation of the system dynamics (1)(17)(19)(20). Consequently, the dissipation term is linked to the natural irreversibility defined by (23).

3.1 On the Hamiltonian formulations of the CSTR

A pseudo Hamiltonian representation with singular damping element Let us first apply the method proposed in (Hoang et al. (2011a)) to the system (1)(17)(19)(20) in order to derive a PCH representation where its Hamiltonian storage function is :

$$\mathcal{H} = \mathcal{P} \tag{24}$$

(an)

with \mathcal{P} given in (21)-(23). Indeed the non isothermal system dynamics given by (1)(17)(19)(20) is rewritten as follows :

$$\frac{dx}{dt} = g(x)u + \begin{pmatrix} \nu_A r_f V - \nu_A r_r V \\ \nu_B r_f V - \nu_B r_r V \\ 0 \end{pmatrix}$$
(25)

Since (21) holds for any evolution, (25) becomes :

$$\frac{d}{dt} \begin{pmatrix} H\\ N_A\\ N_B \end{pmatrix} = g(x)u + \mathcal{M} \begin{pmatrix} \frac{\partial \mathcal{P}}{\partial N_A}\\ \frac{\partial \mathcal{P}}{\partial N_B}\\ \frac{\partial \mathcal{P}}{\partial H} \end{pmatrix}$$
(26)
where $\mathcal{M} = \begin{pmatrix} \nu_A r_f V \frac{1}{\frac{\partial \mathcal{P}}{\partial N_A}} & -\nu_A r_r V \frac{1}{\frac{\partial \mathcal{P}}{\partial N_B}} & 0\\ \nu_B r_f V \frac{1}{\frac{\partial \mathcal{P}}{\partial N_A}} & -\nu_B r_r V \frac{1}{\frac{\partial \mathcal{P}}{\partial N_B}} & 0\\ 0 & 0 & 0 \end{pmatrix}.$

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This matrix \mathcal{M} can be decomposed into symmetric and skew symmetric parts as follows : $\mathcal{M} = J - R$ with $J = \frac{\mathcal{M} - \mathcal{M}^{\mathrm{T}}}{2}$ and $R = -\frac{\mathcal{M} + \mathcal{M}^{\mathrm{T}}}{2}$. Consequently, we have :

$$J = \frac{1}{2} \begin{pmatrix} 0 & -\nu_A \omega_B - \nu_B \omega_A & 0 \\ \nu_A \omega_B + \nu_B \omega_A & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$
(27)

and

$$R = -\frac{1}{2} \begin{pmatrix} 2\nu_A \omega_A & -\nu_A \omega_B + \nu_B \omega_A & 0\\ -\nu_A \omega_B + \nu_B \omega_A & -2\nu_B \omega_B & 0\\ 0 & 0 & 0 \end{pmatrix}$$
(28)

where : $\omega_A = r_f V \frac{1}{\frac{\partial P}{\partial N_A}}$ and $\omega_B = r_r V \frac{1}{\frac{\partial P}{\partial N_B}}$. The control input u and the input-state map g are given in (19) and (20), respectively. The conjugate output y is then given as follows :

$$y = \begin{pmatrix} \left(1 - \frac{N_A M_A}{m_t}\right) \frac{\partial \mathcal{P}}{\partial N_A} - \frac{N_B M_A}{m_t} \frac{\partial \mathcal{P}}{\partial N_B} \\ + \left[h_{AI} - \frac{M_A H}{m_t}\right] \frac{\partial \mathcal{P}}{\partial H} \\ - \frac{N_A M_B}{m_t} \frac{\partial \mathcal{P}}{\partial N_A} + \left(1 - \frac{N_B M_B}{m_t}\right) \frac{\partial \mathcal{P}}{\partial N_B} \\ + \left[h_{BI} - \frac{M_B H}{m_t}\right] \frac{\partial \mathcal{P}}{\partial H} \\ \frac{\partial \mathcal{P}}{\partial H} \end{pmatrix}$$
(29)

Finally it is easy to check from the definition (12) that the dissipation term d equals $\left(\nu_A \frac{\partial \mathcal{P}}{\partial N_A} + \nu_B \frac{\partial \mathcal{P}}{\partial N_B}\right) r V$ which is negative due to the property (23).

Remark 2. Another pseudo Hamiltonian representation with singular damping element can also be obtained by using the same procedures as the previous case. Indeed (25) with (17) can be rewritten :

$$\frac{dx}{dt} = g(x)u + \begin{pmatrix} \nu_A rV\\ \nu_B rV\\ 0 \end{pmatrix}$$
(30)

(30) is equivalent to :

$$\frac{d}{dt} \begin{pmatrix} H\\ N_A\\ N_B \end{pmatrix} = g(x)u + \mathcal{M} \begin{pmatrix} \frac{\partial \mathcal{P}}{\partial N_A}\\ \frac{\partial \mathcal{P}}{\partial N_B}\\ \frac{\partial \mathcal{P}}{\partial H} \end{pmatrix}$$
(31)
where $\mathcal{M} = \begin{pmatrix} \nu_A r V \frac{1}{\frac{\partial \mathcal{P}}{\partial N_A}} & 0 & 0\\ 0 & \nu_B r V \frac{1}{\frac{\partial \mathcal{P}}{\partial N_B}} & 0\\ 0 & 0 & 0 \end{pmatrix}$.

We can easily check in this case that J = 0 and $R = -\mathcal{M}$. *Remark 3.* The obtained structural representations are suitable to the definition (9), in this case some structure matrices depend not only on the state variables x but also the co-state variables $\nabla \mathcal{H}$ (i.e. $J = J(x, \nabla \mathcal{H})$ and $R = R(x, \nabla \mathcal{H})$). The resulting representation together with this property define the so-called pseudo Hamiltonian models. Furthermore, it is worth noting that the symmetric damping matrix R is singular since its determinant is equal to 0. In other words, this matrix violates the rank condition given in (13).

It will now be shown that the evolution criterion (21)-(23)provides some guidelines to obtain a pseudo Hamiltonian representation with (strict) dissipation on the basis of the Brayton-Moser formulation.

A structure preserving pseudo Hamiltonian representation In this section we show that the proposed criteria (21)-(23)can be helpful to obtain a Port Hamiltonian representation with dissipation using the Brayton-Moser formulation for the non-isothermal system dynamics (1)(17)(19)(20).

Proposition 1. The dynamics (1)(17)(19)(20) can be represented as a Port (pseudo) Hamiltonian system (9) with $x = (N_A, N_B, H)^{\mathrm{T}}$. Its Hamiltonian storage function is given by $\mathcal{H} = \mathcal{P}$ and the structure matrices are written as follows :

$$J = \frac{1}{2\Delta} \begin{pmatrix} 0 & \frac{(-\gamma - 2c)\beta e^2}{4(1-\alpha)b} & -\gamma e\left(\frac{\nu_A}{\nu_B}\right) \\ \frac{-(-\gamma - 2c)\beta e^2}{4(1-\alpha)b} & 0 & ec \\ \gamma e\left(\frac{\nu_A}{\nu_B}\right) & -ec & 0 \end{pmatrix}$$

$$R = -\frac{1}{2\Delta} \begin{pmatrix} \frac{2\alpha\beta e^2\left(\frac{\nu_A}{\nu_B}\right)^2}{(1-\alpha)} & \frac{\alpha\beta e^2\frac{\nu_A}{\nu_B}}{(1-\alpha)} & \gamma e\left(\frac{\nu_A}{\nu_B}\right) \\ \frac{\alpha\beta e^2\frac{\nu_A}{\nu_B}}{(1-\alpha)} & \frac{\beta e^2}{2(1-\alpha)} & -ec \\ \gamma e\left(\frac{\nu_A}{\nu_B}\right) & -ec & 2\left[\gamma\left(b\left(\frac{\nu_A}{\nu_B}\right) + c\right) + c^2\right] \end{pmatrix}$$
with $0 < \alpha < 1, \beta > 1$, and

V

$$\begin{split} \gamma &= 4\alpha b \frac{\nu_A}{\nu_B}, \ b = \frac{1}{\nu_A} \left(\frac{\nu_B}{\nu_A} \frac{\partial \mathcal{P}}{\partial N_B} + \frac{\partial \mathcal{P}}{\partial N_A} \right) \frac{1}{rV} \\ c &= -\frac{1}{\nu_A} \frac{\partial \mathcal{P}}{\partial N_B} \frac{1}{rV}, \ e = -\frac{1}{\nu_A} \left(\frac{\partial \mathcal{P}}{\partial H} \frac{1}{rV} \right) \\ \Delta &= \frac{\alpha \beta e^2}{(1-\alpha)} \left(b \left(\frac{\nu_A}{\nu_B} \right)^2 + c \frac{\nu_A}{\nu_B} \right) + \frac{\beta e^2 c^2}{4(1-\alpha)b} \neq 0 \end{split}$$

The input-state map is g(x) given by (20), and the input u by (19). The output y is $y = g(x)^{\mathrm{T}} \nabla_x \mathcal{H}(x)$. Finally, the system is passive with dissipation (12):

$$d = \left(\nu_A \frac{\partial \mathcal{P}}{\partial N_A} + \nu_B \frac{\partial \mathcal{P}}{\partial N_B}\right) r V < 0 \tag{32}$$

Proof. The proof is done by using the Brayton-Moser formulation (see Section 2). Let us consider Q on the form :

$$Q = \begin{pmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{pmatrix}$$
(33)

The key requirement is that the solution Q of the Brayton-Moser formulation is such that its symmetric part is negative definite (see (2)). Equivalently it implies that all of the

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principal minors determinants of $-(Q(x)+Q(x)^{T})$ are positive. See (Favache *et al.* (2011); Hoang *et al.* (2011b)) for a complete version of the proof.

Remark 4. Contrary to the previous singular cases (e.g. (28)), the positive definiteness property (or the consequent rank condition (13)) of the damping matrix R of Proposition 1 holds thanks to the BM formulation and since the negative definite symmetric part of the matrix Q (14) is mathematically guaranteed by the two scalars α and β .

As a consequence of the positive definiteness property (or the consequent rank condition (13)) of the damping matrix R, we state the following proposition which is central to derive an alternate PCH model of the results of Proposition 1. For the sake of simplicity, the explicit expansions will not be given here.

Proposition 2. (New output with relaxing damping). The PCH system defined by

$$\begin{cases} \frac{dx}{dt} = (J - R)\nabla_x \mathcal{H} + g \ u \\ y_{new} = \left[g + 2\mathcal{T}\right]^{\mathrm{T}} \nabla_x \mathcal{H} \end{cases}$$
(34)

where $\mathcal{T} = \mathcal{T}_{n \times m}$ and :

or
$$\mathcal{T} = R^{-1} \nabla_x \mathcal{H} u^{\mathrm{T}}$$
, or $T = R \nabla_x \mathcal{H} u^{\mathrm{T}}$, (35)

or
$$\mathcal{T} = -(J-R)^{-1} \nabla_x \mathcal{H} u^{\mathrm{T}}$$
, or $T = -(J-R) \nabla_x \mathcal{H} u^{\mathrm{T}}$
(36)

are such that the (generalized) damping matrix $\mathscr{R} = \begin{bmatrix} R & \mathcal{T} \\ \mathcal{T}^T & 0 \end{bmatrix} = \mathscr{R}^T$ satisfies the following relaxing damping condition¹:

$$\begin{bmatrix} \nabla_x \mathcal{H}^{\mathrm{T}} & u^{\mathrm{T}} \end{bmatrix} \mathscr{R} \begin{pmatrix} \nabla_x \mathcal{H} \\ u \end{pmatrix} \ge 0$$
(37)

is passive with storage function $\mathcal{H},$ i.e. :

$$\frac{d\mathcal{H}}{dt} \le u^{\mathrm{T}} y_{new} \tag{38}$$

Proof. Let us first rewrite (11) as follows :

$$\frac{d\mathcal{H}}{dt} = \nabla_x \mathcal{H}^{\mathrm{T}}(-R)\nabla_x \mathcal{H} + \nabla_x \mathcal{H}^{\mathrm{T}}gu \qquad (39)$$

where $y = g^{\mathrm{T}} \nabla_x \mathcal{H}$ has been used. From this we have :

$$\frac{d\mathcal{H}}{dt} = \nabla_x \mathcal{H}^{\mathrm{T}}(-R) \nabla_x \mathcal{H}
+ \nabla_x \mathcal{H}^{\mathrm{T}}(-\mathcal{T})u + \nabla_x \mathcal{H}^{\mathrm{T}} \mathcal{T} u
+ u^{\mathrm{T}}(-\mathcal{T})^{\mathrm{T}} \nabla_x \mathcal{H} + u^{\mathrm{T}} \mathcal{T}^{\mathrm{T}} \nabla_x \mathcal{H}
+ \nabla_x \mathcal{H}^{\mathrm{T}} g u$$
(40)

(40) is equivalent to :

$$\frac{d\mathcal{H}}{dt} = -\left[\nabla_{x}\mathcal{H}^{\mathrm{T}} \quad u^{\mathrm{T}}\right] \begin{pmatrix} R & \mathcal{T} \\ \mathcal{T}^{\mathrm{T}} & 0 \end{pmatrix} \begin{pmatrix} \nabla_{x}\mathcal{H} \\ u \end{pmatrix} \\
+ \underbrace{\nabla_{x}\mathcal{H}^{\mathrm{T}}\mathcal{T}u + u^{\mathrm{T}}\mathcal{T}^{\mathrm{T}}\nabla_{x}\mathcal{H}}_{=\nabla_{x}\mathcal{H}^{\mathrm{T}}(2\mathcal{T})u} + \nabla_{x}\mathcal{H}^{\mathrm{T}}gu \quad (41)$$

It follows that
$$R^{-1} = (R^{-1})^{\mathrm{T}} > 0$$
 since $R = R^{\mathrm{T}} > 0$ and note also that

$$\nabla_x \mathcal{H}^{\mathrm{T}} \mathcal{T} u > 0$$

with \mathcal{T} given in (35) or (36) for $\nabla_x \mathcal{H} \neq 0$ and $u \neq 0$. The latter concludes the proof.

Remark 5. It is important to note that the different values of the damping matrix R of a given dynamics (e.g. R defined in (28), Propositions 1 and 2) may change the dissipation nature and therefore affect the control design for the stabilization purpose (e.g. the dissipation obstacle problem when the conditions for Casimir generation are considered using energy shaping via control by interconnection). The infinite dissipation obstacle for energy balancing passivitybased control may be overcome by a suitable choice of Hamiltonian models. In other words, this eliminates the possibility of infinite dissipation. Further discussions on this issue are given in (Ortega *et al.* (2008)).

4. CONCLUSION

In this work, the pseudo Hamiltonian formulations of the CSTR dynamics are considered in order to express the irreversibility along the trajectories. The first one is realized on the basis of the functional separation thanks to the support of constitutive equations of thermodynamics as shown in (Hoang *et al.* (2011a)), a pseudo Hamiltonian representation with singular damping matrix is then obtained. The second representation allows to circumvent this inherent difficulty through the use of the BM formulation. In both cases, although the amount of the dissipation is explicitly derived, the latter gives more degrees of freedom usable for further studies on the control design.

It remains now to further explore the properties of the matrix Q (see e.g. the dissipation obstacle (Ortega *et al.* (2003))) when the positive definiteness condition of the damping matrix R (14) is met through the support of an expansion given by (Xu *et al.* (1993)). In this context, the adaptation of the Interconnection and Damping Assignment Passivity-Based Control (IDA-PBC) method, control by interconnection, energy balancing passivity based control or the power-based control (Ortega *et al.* (2002, 2008); García-Canseco *et al.* (2010); Favache & Dochain (2010)) to the potential-based representations for the stabilization purpose of the reaction system at any desired operating point has to be studied. First results of such an approach are given in (Hoang *et al.* (2014)).

ACKNOWLEDGEMENTS

The Viet Nam National Foundation for Science and Technology Development (NAFOSTED) is acknowledged for financial support through project code 104.99-2014.74. Part of this work was carried out while the first author was working as a research associate at CESAME, Université catholique de Louvain, Belgium. The hospitality of this institution is gratefully acknowledged. The scientific responsibility rests with its authors.

REFERENCES

Antonelli R., & Astolfi A. (2003). Continuous stirred tank reactors: Easy to stabilise? *Automatica*. 39:1817-1827.

¹ A (generalized) damping element \mathscr{R} is relaxed if its quadratic form restricted on the basis of the co-state variables $\nabla_x H(x)$ and the input u only is positive semidefinite, and not $\mathscr{R} \geq 0$.

- Brayton R.K., & Moser J.K. (1964). A theory of nonlinear networks I. Quaterly of Applied Mathematics, 22, 1-33.
- Brogliato B., Lozano R., Maschke B., & Egeland O. (2007). Dissipative systems analysis and control. Springer, London, 2nd edition.
- Callen H.B. (1985). Thermodynamics and an introduction to thermostatics. John Wiley & Sons, New York, 2nd edition.
- Dammers W.R., & Tels M. (1974). Thermodynamic stability and entropy production in adiabatic stirred flow reactors. *Chem. Eng. Sci.*, 29(1), 83-90.
- De Groot S.R., & Mazur P. (1962). Non-Equilibrium Thermodynamics. Dover Pub. Inc., Amsterdam, 1st edition.
- Dörfler F., Johnsen J.K., & Allgöwer F. (2009). An introduction to interconnection and damping assignment passivity-based control in process engineering. J. Proc. Control, 19(9), 1413-1426.
- Eberard D., Maschke B., & Van Der Schaft A. (2007). An extension of pseudo-Hamiltonian systems to the thermodynamic space: Towards a geometry of nonequilibrium thermodynamics. *Reports on Mathematical Physics*, 60(2), 175-198.
- Favache A., & Dochain D. (2010). Power-shaping of reaction systems : The CSTR case study. Automatica, 46(11), 1877-1883.
- Favache A., Dochain D., & Winkin J. (2011). Powershaping control: Writing the system dynamics into the Brayton-Moser form. Systems & Control Letters, 60(8), 618-624.
- García-Canseco E., Jeltsema D., Ortega R., & Scherpen J.M.A. (2010). Power-based control of physical systems. *Automatica*, 46, 127-132.
- Haddad W.M., Chellaboina V., & Nersesov S.G. (2005). *Thermodynamics: A dynamical systems approach*. Princeton, NJ:Princeton Univ. Press, Princeton Series in Applied Mathematics.
- Hangos K.M., Bokor J., & Szederkényi G. (2001). Hamiltonian view on process systems. AIChE J., 47(8), 1819-1831.
- Hoang H., Couenne F., Jallut C., & Le Gorrec Y. (2011a). The Port Hamiltonian approach to modeling and control of Continuous Stirred Tank Reactors. J. Proc. Control, 21(10), 1449-1458.
- Hoang H., Couenne F., Le Gorrec Y., & Dochain D. (2011b). From Brayton-Moser formulation to Port Hamiltonian representation: The CSTR case study. *Proc.* 18th IFAC World Congress, Milano, Italy, 1628-1633.
- Hoang H., Couenne F., Jallut C., & Le Gorrec Y. (2012). Lyapunov-based control of non isothermal continuous stirred tank reactors using irreversible thermodynamics. J. Proc. Control, 22(2), 412-422.
- Hoang H., & Dochain D. (2013). On an evolution criterion of homogeneous multi-component mixtures with chemical transformation. *Systems & Control Letters*, 62(2), 170-177.
- Hoang H., Dochain D., Couenne F., & Le Gorrec Y. (2014). Dissipative pseudo Hamiltonian realization of irreversible processes: The CSTR case study revisited. In revision for publication in Systems & Control Letters.
- Hudon N., Höffner K., & Guay M. (2008). Equivalence to dissipative Hamiltonian realization, Proc. 47th IEEE CDC, 3163-3168.

- Jeltsema D. (2005). Modeling and control of nonlinear networks - A power-based perspective. PhD thesis, The Delft University of Technology, 2005. ISBN: 90-8559-048-5.
- Khalil H.K. (2002). Nonlinear systems. Prentice Hall, 3rd edition.
- Maschke B., Ortega R., & Van Der Schaft A. (2000). Energy based Lyapunov functions for forced Hamiltonian systems with dissipation. *IEEE Trans.on Autom. Control*, 45(8), 1498-1502.
- Ortega R., Van Der Schaft A., Maschke B., & Escobar G. (2002). Interconnection and damping assignment passivity-based control of port-controlled Hamiltonian Systems. *Automatica*, 38, 585-596.
- Ortega R., Jeltsema D., & Scherpen J.M.A. (2003). Power shaping: A new paradigm for stabilization of nonlinear *RLC* circuits. *IEEE Trans. Autom. Control*, 48(10), 1762-1767.
- Ortega R., Van Der Schaft A., Castaños F., & Astolfi A. (2008). Control by interconnection and standard passivity-based control of Port Hamiltonian systems. *IEEE Trans.on Autom. Control*, 53(11), 2527-2542.
- Otero-Muras I., Szederkényi G., Alonso A.A., & Hangos K.M. (2008). Local dissipative Hamiltonian description of reversible reaction networks. Systems & Control Letters, 57(7), 554-560.
- Ramírez H., Maschke B., & Sbarbaro D. (2013). Irreversible port-Hamiltonian systems: A general formulation of irreversible processes with application to the CSTR. *Chem. Eng. Sci.* 89:223-234.
- Ramírez H., Sbarbaro D., & Ortega R. (2009). On the control of non-linear processes: An IDA-PBC approach. J. Proc. Control, 19, 405-414.
- Tarbell J.M. (1977). A thermodynamic Lyapunov function for the near equilibrium CSTR. Chem. Eng. Sci., 32(12), 1471-1476.
- Van Der Schaft A. (2000a). Port-controlled Hamiltonian systems: Towards a theory for control and design of nonlinear physical systems. J. Soc. Instr. Control Eng. Japan, 39(2), 91-98.
- Van Der Schaft A. (2000b). L_2 -gain and passivity techniques in nonlinear control. Springer-Verlag, London, 2^{nd} edition.
- Warden R.B., Aris R., & Amundson N.R. (1964). An analysis of chemical reactor stability and control - VIII. The direct method of Lyapunov. Introduction and applications to simple reactions in stirred vessels. *Chem. Eng. Sci.*, 19(3), 149-172.
- Willems J.L. (1970). Stability theory of dynamical systems, Nelson, London.
- Willems J.C. (1972). Dissipative dynamical systems. Part I: General theory. Arch. Rat. Mech. and Analysis, 45(5), 321-351.
- Xu S. J., Darouach M., & Schaefers J. (1993). Expansion of det(A+B) and robustness analysis of uncertain state space systems. *IEEE Trans. Autom. Control*, 38(11), 1671-1675.
- Ydstie B.E., & Alonso A.A. (1997). Process systems and passivity via the Clausius-Planck inequality. Systems & Control Letters, 30(5), 253-264.