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Hamiltonian formulation and IDA-PBC control of non isothermal continuous stirred tank reactors

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Abstract: This paper proposes a pseudo port Hamiltonian formulation of non isothermal Continuous Stirred Tank Reactor CSTR) model. This structured modeling shows how the opposite of the entropy can be used as Hamiltonian function and how the associated dissipation can be related to the irreversible entropy production due to chemical reaction. The IDA-PBC approach based control is then applied to stabilize the continuous system about an unstable equilibrium point. The chosen control variables are the jacket temperature and the inlet molar flow rate. The chosen hamiltonian storage function of the closed loop system is the thermodynamic availability function. Theoretical developments are illustrated on a first order chemical equilibrated reaction. Some stability properties and analysis of the admissibility of the control variables are given.

Keywords: Hamiltonian formalism, Lyapunov, Thermodynamics, Passivity based control, CSTR.

1. INTRODUCTION

The purpose of this paper is to link thermodynamics to system theory for the modelling and control design of chemical reactors. Chemical reactors belong to thermodynamic systems and exhibit nonlinear dynamics because of reaction kinetics. This class of process is intensively studied in particular through the continuous stirred tank reactor (CSTR) model. Dynamic model of CSTR can be found in any reaction engineering textbooks. In this paper we will use a structured presentation of the CSTR such as given in (Couenne (2006)).

For the representation of mechanical, electrical and electromechanical systems, port Hamiltonian formalism (van der Schaft (2000a)) has been successfully used. The so called Hamiltonian function is the energy of the physical domains under consideration. This Hamiltonian formalism supports some advantages: firstly, it exhibits a geometric structure and the power exchanges within the system. For the reversible system this dissipation does not exist. Dissipation is related to irreversibility. Secondly it allows to apply control strategy such as PBC (van der Schaft (2000b)) and power based control strategies (Ortega (2002)) for instance.

The extension of Hamiltonian formalism for chemical processes is very limited Eberard (2007). Recently, Hamiltonian modelling of CSTRs is proposed in (Otero (2008) or Ramirez (2009)). However, in the case of (Ramirez (2009)), dissipation term does not capture the irreversible nature of the CSTR and the Hamiltonian is not linked to any thermodynamic potentials. In (Otero (2008)), the authors propose an Hamiltonian representation of closed

reaction networks in the isothermal case. In their case the Hamiltonian is not the Gibbs free energy. Its physical interpretation is not obvious.

On the other hand, control design for CSTR has been considered with power-shaping control (Favache (2009)), IDA-PBC approach based control (Ramirez (2009); Dorfler (2009)) and thermodynamical Lyapunov based control (Hoang (2008, 2009)). For IDA-PBC approach, the considered Hamiltonian is in general related to the total mass.

The main contributions of this paper are, firstly to reformulate the dynamics of a CSTR under a thermodynamic Hamiltonian representation and secondly to show that the thermodynamic availability (Ydstie (1997); Ruszkowski (2005); Hoang (2008, 2009)) can be considered as hamiltonian storage function for stabilization objective by using IDA-PBC approach (Ortega (2002)) about a unstable steady state. These results are presented in the case of the equilibrated exothermic reaction $A \rightleftharpoons B$.

For the stabilization objective, we assume that concentrations and temperature are measured and that the chosen control variables are the jacket temperature and feed molar flow rate.

This paper is organized as follows: in section 2, we remind thermodynamical concepts and variables necessary to construct thermodynamic availability as well as Hamiltonian formalism based control. In section 3 the dynamic model of the considered CSTR is presented and analyzed. In this section a pseudo Hamiltonian formalism is proposed and the IDA-PBC approach based control is then used to the design of the state feedback insuring (global) asymptotic

stability at the desired point. The controlled system is again a (pseudo) Hamiltonian system with its storage function linked to the availability. Simulations are given in section 4. It is shown that the resulting control leads to admissible manipulated control variables.

2. SOME OVERVIEWS

2.1 Thermodynamic overview

System in entropy representation In equilibrium thermodynamics, the system variables are divided into extensive and intensive variables, depending on whether their values depend on the "size" of the system or not. The internal energy of a homogeneous system is then expressed in terms of products of pairings of energy conjugate variables such as pressure p/ volume V, temperature T/ entropy S and chemical potential μ_k/ mole number N_k for each species k of the mixture.

The Gibbs equation of thermodynamics expresses the variational of the energy U of a single phase system as a function of the variational of the variables $Z = (S, V, N_k)$

$$dU = TdS - pdV + \sum_{k=1}^{n} \mu_k dN_k \qquad (1)$$

with $w(Z) = (T, -p, \mu_k)^T$. Since the energy U is also an extensive variable, it is a homogenous function of degree 1 of Z (Callen (1985)). From Euler's theorem we get:

$$U = TS - pV + \sum_{k=1}^{n} \mu_k N_k. \qquad (2)$$

We will call this representation the *energy representation.*

In a similar way, we can consider the Gibbs equation as

$$dS = \frac{1}{T}dU + \frac{p}{T}dV + \sum_{k=1}^{n} \frac{-\mu_k}{T}dN_k. \qquad (3)$$

S is now considered as a function of the variational of the extensive variables $Z = (U, V, N_k)^T$. (3) can be written in the compact form

$$w(Z) = \frac{\partial S}{\partial Z} \qquad (4)$$

with $w = (\frac{1}{T}, \frac{p}{T}, \frac{-\mu_k}{T})^T$. Since the entropy S is an extensive variable, we get:

$$S(Z) = w^T Z. \qquad (5)$$

As a consequence, $w(Z)$ is a homogenous function of degree 0 of Z. Such a thermodynamic representation is called *the entropy representation.*

Let us note that entropy and energy representations are equivalent. In practice, models are expressed in the entropy representation since energy balance is used and not entropy one.

Thermodynamic availability For homogeneous single phase thermodynamical systems, the entropy function $S(Z)$ is necessarily concave (see Callen (1985)). It is a consequence of the second principle of thermodynamics. This concavity is independent on the dynamic behavior of the system. Inversely the internal energy U is convex with respect to (S, V, N_k).

From the concavity of $S(Z)$, it can be shown (see Ydstie (1997); Ruszkowski (2005); Hoang (2008, 2009)) that the function named *availability* $\mathcal{A}$:

$$\mathcal{A}(Z, Z_2) = S_2 + w_2^T(Z - Z_2) - S(Z) \geq 0 \qquad (6)$$

where Z_2 is some fixed reference point (for example the desired set point for control), is non negative.

Property 1. The availability $\mathcal{A}$ has the following properties:

(1) $\mathcal{A}$ is an homogeneous function of degree 1 with respect to (Z, Z_2). By consequence, one can write:

$$d\mathcal{A} = -(w - w_2)dZ \qquad (7)$$

(2) $\mathcal{A}$ is convex with respect to Z

Property 2. There exists a subspace $\Pi = \left\{ Z \middle| Z = \gamma Z_2, \gamma \in \mathbb{R}_+^\star \right\}$ for which $\forall Z \in \Pi$, $\mathcal{A}(Z, Z_2) = 0$. γ is called the ratio of homogeneity.

Let us notice that if $S(Z)$ is strictly concave, $\mathcal{A}$ is strictly convex and the subspace Π is reduced to the only point Z_2. The strict concavity of entropy can be obtained if at least one extensive property is fixed (Jillson (2007)) which means that the ratio of homogeneity is fixed to 1.

Finally equations (3), (1) and (7) can also be applied in irreversible thermodynamics as soon as the local equilibrium hypothesis is assumed (Groot (1962)): it postulates that the present state of the homogeneous system in any evolution can be characterized by the same variables as at equilibrium and is independent on the rate of evolution. So they can also be applied at any time. In particular we have:

$$\frac{d\mathcal{A}}{dt} = -(w - w_2)\frac{dZ}{dt} \qquad (8)$$

with $\mathcal{A}$ a positive function. In previous papers, we have shown that $\mathcal{A}$ can be used as a Lyapunov candidate to synthesize control law to stabilize the state about the unstable steady state Z_2 Hoang (2008, 2009). In this paper we will use this quantity in order to set the desired closed loop Hamiltonian.

Models in the entropy representation The dynamic behavior of the system is driven by balance equations on $Z = (U, V, N_k)$. It can be written as:

$$\frac{dZ}{dt} = f(Z, t) + g(Z, t)\, u \qquad (9)$$

(9) correspond to the general formulation of models. Thanks to the hypothesis of local equilibrium (Groot (1962)), we complete this formulation by using the time derivative of the entropy S :

$$\frac{dS}{dt} = w^T \frac{dZ}{dt}. \qquad (10)$$

Finally let us notice that the entropy balance of S can directly be written. This balance is not conservative: there is a source term Σ_s which is always positive from the second law of thermodynamics. This term represents the irreversible entropy production: the energy $T\Sigma_s$ associated to this term represents the energy lost from material, space or thermal domains and that will never more contribute to some physical works. So we can write the entropy balance as:

$$\frac{dS}{dt} = \Phi_s + \Sigma_s \text{ and } \Sigma_s \geq 0 \qquad (11)$$

where Φ_s is the entropy exchange flow with environment. From here the entropy balance (11) is identified with (10)

to derive Σ_s. The system with (9) and (11) is called a *thermodynamically consistent model*.

2.2 Hamiltonian formalism based control

Port controlled Hamiltonian systems (PCH) Port controlled Hamiltonian systems with dissipation are given by (van der Schaft (2000a); Maschke (2000)):

$$\begin{cases} \dfrac{dx}{dt} = [J(x) - R(x)]\dfrac{\partial \mathcal{H}(x)}{\partial x} + g(x)u \\ y = g^T(x)\dfrac{\partial \mathcal{H}(x)}{\partial x} \end{cases} \quad (12)$$

where $x \in \mathbb{R}^n$ is the state vector; $u, y \in \mathbb{R}^m$ are the control input and its conjugated power port variable respectively; this means that the unit of the product $u^T y$ is power. The smooth function $\mathcal{H}(x) : \mathbb{R}^n \rightarrow \mathbb{R}$ represents the hamiltonian storage function; the interconnection matrix $J = -J^T$ and the damping matrix $R = R^T \geq 0$ are called structure matrices. J corresponds to energy reversible transfer between the different physical domains of the system, such material one or thermal one, inside the system. R represents the energy irreversible transfer; $g(x)$ is the n × m input-state map.

Remark 1. Port Hamiltonian formulation is related to the existence of a geometric interconnection structure named Dirac structure. This linear structure implies that J may depend on x but not on $\frac{\partial \mathcal{H}(x)}{\partial x}$. Here we don't use this linear property and with an abuse of language will talk about Port Hamiltonian formulation even if J may depends on $\mathcal{H}(x)$. This is due to strong non linearity appearing in thermodynamic and kinetic constitutive relations.

The energy balance immediately follows from (12):

$$\frac{d\mathcal{H}(x)}{dt} = -\left[\frac{\partial \mathcal{H}(x)}{\partial x}\right]^T R \left[\frac{\partial \mathcal{H}(x)}{\partial x}\right] + u^T y \quad (13)$$

The system (12) is passive in the sense that the dissipation

$$d = -\left[\frac{\partial \mathcal{H}(x)}{\partial x}\right]^T R \left[\frac{\partial \mathcal{H}(x)}{\partial x}\right] \quad (14)$$

is always negative and the Hamiltonian $\mathcal{H}$ is bounded from below Brogliato (2007). The term d defined by (14) corresponds to natural dissipation (energy lost due to friction/damping in a mechanical systems or due to resistance in RLC electrical system (van der Schaft (2000a); Maschke (2000)) for example). The following inequality immediately follows from (13) and (14)

$$\frac{d\mathcal{H}(x)}{dt} \leq u^T y \quad (15)$$

From here, a feedback law of the form $u = -Ky$ with $K > 0$ for instance, returns this system to be dissipative.

In this paper the developed controllers are based on these models (12) using IDA-PBC approach (Ortega (2002)). This approach will be briefly reintroduced in the next part.

IDA-PBC Approach The purpose of the control based on IDA-PBC approach is to find a static state-feedback control $u = \beta(x)$ such that the closed loop dynamics is also PCH system with dissipation of the form:

$$\frac{dx}{dt} = [J_d - R_d]\frac{\partial \mathcal{H}_d(x)}{\partial x} \quad (16)$$

where the controlled storage function $\mathcal{H}_d$ has a strict local minimum at the desired equilibrium $x^\star$, and $J_d = -J_d^T$ and $R_d = R_d^T \geq 0$ are some desired interconnection and damping matrices respectively. The state feedback $\beta(x)$ is looked for using $\mathcal{H}_a, J_a$ and R_a such that :

$$\mathcal{H}_d = \mathcal{H} + \mathcal{H}_a, \quad R_d = R + R_a \quad \text{and} \quad J_d = J + J_a \quad (17)$$

and solving the matching equation:

$$\left[J + J_a - (R + R_a)\right]\frac{\partial \mathcal{H}_a(x)}{\partial x} = -[J_a - R_a]\frac{\partial \mathcal{H}(x)}{\partial x} + g(x)\beta(x) \quad (18)$$

obtained from (12) and (16) (with (17)) . In the general case such matching equation can be difficult to solve. We will show that using thermodynamic variables in the case of CSTR, this equation can be trivially solved.

3. CASE STUDY: NON ISOTHERMAL CSTR

3.1 Assumptions of the model

We consider a jacketed homogeneous CSTR with the first-order equilibrated chemical reaction: $A \rightleftharpoons B$. The temperature of the jacket T_w (supposed to be uniform) and the inlet molar flow rate F_{Ae} are used as control inputs. The following assumptions are made:

- The reaction mixture is ideal and incompressible.
- The pressure p is constant.
- The pure component A is fed with molar flow rate F_{Ae} at a fixed temperature T_e.
- The total molar number N_T is constant.
- The heat flow exchanged with the jacket is represented by $\dot{Q} = \lambda(T_w - T)$.
- The forward and reserve kinetics of the liquid phase reaction is modelled thanks to the Arrhenius law:

$$k_f(T) = k_{0f}\exp(\frac{-k_{1f}}{T}) \text{ and } k_r(T) = k_{0r}\exp(\frac{-k_{1r}}{T}) \quad (19)$$

The total reaction rate $r_v V$ is then given by:

$$r_v V = k_f(T)N_A - k_r(T)N_B \quad (20)$$

Let us notice that it is necessary to fix one global extensive variable in order to insure strict convexity of availability. We choose that N_T is constant.

Under these assumptions, we obtain:

$$Z = (H, N_A, N_B) \quad \text{and} \quad w = (\frac{1}{T}, \frac{-\mu_A}{T}, \frac{-\mu_B}{T}) \quad (21)$$

where H is the enthalpy of the system. Finally table 1 gives notation of the model.

Notation	Units	
F_{Ae}	mol/s	Inlet molar flow rate of A
F_i	mol/s	Outlet molar flow rate of i ($i = A, B$)
F	mol/s	Total outlet molar flow rate
h_{Ae}	J/mol	Inlet molar enthalpy of A
h_i	J/mol	Molar enthalpy of species i ($i = A, B$)
H	J	Total enthalpy of the mixture
N_i	mol	Mole number of species i ($i = A, B$)
T	K	Temperature in the CSTR
N_T	mol	Total mole number
r_v	$mol/m^3/s$	Reduced reaction rate
U	J	Internal energy
μ_i	J/mol	chemical potential os species i, $i = A, B$

Table 1. Notation of the variables of the model.

3.2 Thermodynamically consistent CSTR modelling

The material balances are given by:

$$\begin{cases} \dfrac{dN_A}{dt} = F_{Ae} - F_A - r_{\mathrm{v}}V \\ \dfrac{dN_B}{dt} = -F_B + r_{\mathrm{v}}V \end{cases} \tag{22}$$

where $r_{\mathrm{v}}V$ is given in (20) and subject to the previous assumptions the energy balance can be written as:

$$\frac{dH}{dt} = \dot{Q} + F_{Ae}h_{Ae} - (F_A h_A + F_B h_B) \tag{23}$$

From the total mole number constraint ($\frac{dN_T}{dt} = 0$), it follows that the outlet molar flow rate $F = F_{Ae}$ and then $F_A = \frac{N_A}{N_T}\,F_{Ae}$ and $F_B = \frac{N_B}{N_T}\,F_{Ae}$.

Finally in order to complete this *thermodynamic consistent model* we give Φ_s and Σ_s of the entropy balance (11) (see Couenne (2006)):

$$\Phi_s = F_{Ae}s_{Ae} - \left(F_A s_A + F_B s_B\right) + \frac{\dot{Q}}{T_w} \tag{24}$$

$$\Sigma_s = \overbrace{\frac{F_{Ae}}{T}(h_{Ae} - Ts_{Ae} - \mu_A)}^{\Sigma_s^{\mathrm{mix.}} \geq 0} + \overbrace{\left(\frac{\dot{Q}}{T} - \frac{\dot{Q}}{T_w}\right)}^{\Sigma_s^{\mathrm{ex.}} \geq 0} + \overbrace{\left(\frac{\mu_A}{T} - \frac{\mu_B}{T}\right)r_{\mathrm{v}}V}^{\Sigma_s^{\mathrm{reac.}} \geq 0} \tag{25}$$

$\Sigma_s^{\mathrm{mix.}}$, $\Sigma_s^{\mathrm{ex.}}$ and $\Sigma_s^{\mathrm{reac.}}$ are irreversible entropy productions due to mixing, to exchange and to reaction respectively.

Finally let us notice that $\Sigma_s^{\mathrm{mix.}}$ and $\Sigma_s^{\mathrm{ex.}}$ depend on the control inputs and that $\Sigma_s^{\mathrm{reac.}}$ depends only on the system states.

3.3 Port Hamiltonian representation

The very natural approach consists in considering internal energy of the system as Hamiltonian. Then it is natural to consider the energy representation $H = H(S, N_k)$ (2) with material balances (22) and entropy balance (11) with (24) and (25):

$$\frac{d}{dt}\underbrace{\begin{pmatrix} S \\ N_A \\ N_B \end{pmatrix}}_{x} = \begin{pmatrix} F_S \\ F_{Ae} - F_A \\ -F_B \end{pmatrix} + \frac{r_{\mathrm{v}}V}{T}\begin{pmatrix} 0 & 1 & -1 \\ -1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}\underbrace{\begin{pmatrix} T \\ \mu_A \\ \mu_B \end{pmatrix}}_{\nabla_x H} \tag{26}$$

with $F_S = F_{Ae}s_{Ae} - (F_A s_A + F_B s_B) + \frac{\dot{Q}}{T_w} + \Sigma_s^{\mathrm{mix.}} + \Sigma_s^{\mathrm{ex.}}$. We remark that the interconnection matrix linking $\nabla_x H$ and $\frac{dx}{dt}$ is skew-symmetric. The system is naturally under Hamiltonian form without dissipation which seems to be natural since the internal energy is conserved. In fact the energy is only transformed (from material domain to thermal one as an example) and the previous formulation doesn't express the irreversibility of the reaction. To overcome this drawback,, we propose to use the entropy representation for the CSTR model. In proposition 1 a passive Hamiltonian representation of the CSTR model is given.

Proposition 1. The non isothermal system given by (22) and (23) is a thermodynamic Port Controlled Hamiltonian system (12) with $x = [\,H\ N_A\ N_B\,]^T$ and furthermore:

- The Hamiltonian is

$$\mathcal{H} = -S \tag{27}$$

where S is the entropy concave function w.r.t. x

- Structure matrices are

$$J = \frac{T}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & k_r\dfrac{N_B}{\mu_B} - k_f\dfrac{N_A}{\mu_A} \\ 0 & k_f\dfrac{N_A}{\mu_A} - k_r\dfrac{N_B}{\mu_B} & 0 \end{pmatrix} \tag{28}$$

and

$$R = \frac{T}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 2k_f\dfrac{N_A}{\mu_A} & -(k_f\dfrac{N_A}{\mu_A} + k_r\dfrac{N_B}{\mu_B}) \\ 0 & -(k_f\dfrac{N_A}{\mu_A} + k_r\dfrac{N_B}{\mu_B}) & 2k_r\dfrac{N_B}{\mu_B} \end{pmatrix} \tag{29}$$

- The input-state map is

$$g^T = \begin{pmatrix} 1 & 0 & 0 \\ h_{Ae} - \dfrac{H}{N_T} & 1 - \dfrac{N_A}{N_T} & -\dfrac{N_B}{N_T} \end{pmatrix} \tag{30}$$

- The control input and the output y are respectively:

$$u^T = \begin{pmatrix} \dot{Q} & F_{Ae} \end{pmatrix} \tag{31}$$

and

$$y = \begin{pmatrix} -\dfrac{1}{T} \\ -(h_{Ae} - \dfrac{H}{N_T})\dfrac{1}{T} + (1 - \dfrac{N_A}{N_T})\dfrac{\mu_A}{T} - \dfrac{N_B}{N_T}\dfrac{\mu_B}{T} \end{pmatrix} \tag{32}$$

Finally, the system is passive with dissipation (14),

$$d = -\Sigma_s^{\mathrm{reac.}} \leq 0 \tag{33}$$

Proof. The balance equations (22)) and ((23) can be written with the help of (19), (20) and $H = \sum_k N_k h_k$ as :

$$\frac{d}{dt}\begin{pmatrix} H \\ N_A \\ N_B \end{pmatrix} = \begin{pmatrix} \dot{Q} + F_{Ae}\left(h_{Ae} - \dfrac{H}{N_T}\right) \\ F_{Ae} - \dfrac{N_A}{N_T}F_{Ae} \\ -\dfrac{N_B}{N_T}F_{Ae} \end{pmatrix} + \begin{pmatrix} 0 \\ -r_{\mathrm{v}}V \\ r_{\mathrm{v}}V \end{pmatrix} \tag{34}$$

(34) is then written in the form as below

$$\frac{d}{dt}\begin{pmatrix} H \\ N_A \\ N_B \end{pmatrix} = g\,u + T\underbrace{\begin{pmatrix} 0 & 0 & 0 \\ 0 & -k_f\dfrac{N_A}{\mu_A} & k_r\dfrac{N_B}{\mu_B} \\ 0 & k_f\dfrac{N_A}{\mu_A} & -k_r\dfrac{N_B}{\mu_B} \end{pmatrix}}_{=\,\Xi}\begin{pmatrix} \dfrac{-1}{T} \\ \dfrac{\mu_A}{T} \\ \dfrac{\mu_B}{T} \end{pmatrix} \tag{35}$$

The matrix Ξ can be decomposed as $\Xi = J - R = \frac{\Xi - \Xi^T}{2} - \left(-\frac{\Xi + \Xi^T}{2}\right)$. J and R are given in (28) and (29) respectively. The Hamiltonian (27) immediately follows because $\left(\frac{\partial S}{\partial H} = \frac{1}{T}, \frac{\partial S}{\partial N_A} = -\frac{\mu_A}{T}, \frac{\partial S}{\partial N_B} = -\frac{\mu_B}{T}\right)$. The control input and the output are then given as in (31) and (32). Finally, it is easy to show that $d = -\left[\frac{\partial\mathcal{H}(x)}{\partial x}\right]^T R\left[\frac{\partial\mathcal{H}(x)}{\partial x}\right] = -(\frac{\mu_A}{T} - \frac{\mu_B}{T})r_{\mathrm{v}}V$ is equal to $-\Sigma_s^{\mathrm{reac.}} < 0$ (see (25)).

Remark 1. As previously stated, the proposed formulation is called pseudo hamiltonian formulation with regard to (12) because in this case, structure matrices J and R depend not only on the state variables x but also on $\partial_x\mathcal{H}$. This is due to nonlinear expressions of chemical potentials and kinetics constant. This is not the case in electric or mechanic domain where linear constitutive relations are often used.

3.4 IDA-PBC synthesis

In this section we propose the IDA-PBC synthesis of the stabilizing control.

Proposition 2. The system ((22), (23)) with the Hamiltonian representation given in Proposition 1 is stabilized at desired point $P_2 = (w_2, Z_2)$ with the following feedback

$$\begin{cases} T_w = \dfrac{1}{\lambda}\left\{ -C_r\alpha\dfrac{\partial \mathcal{H}_d}{\partial H} - F_{Ae}\left(h_{Ae} - \dfrac{H}{N_T}\right)\right\} + T \\ F_{Ae} = \left(\alpha\left[-\dfrac{\partial \mathcal{H}_d}{\partial N_A} + \dfrac{\partial \mathcal{H}_d}{\partial N_B}\right] + k_f N_A - k_r N_B\right)\left(1 - \dfrac{N_A}{N_T}\right)^{-1} \end{cases}$$
(36)

Furthermore, the closed loop system is chosen purely dissipative as:

$$\frac{dx}{dt} = \left[-R_d \right] \partial_x \mathcal{H}_d \tag{37}$$

where: $x = \left[H \ N_A \ N_B \right]^T$. The shaped Hamiltonian is

$$\mathcal{H}_d = C_d \mathcal{A} \tag{38}$$

with $C_d > 0$ and $\mathcal{A}$ is the availability (6). The shaped structure matrice is chosen as

$$R_d = \alpha \begin{pmatrix} C_r & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix} \tag{39}$$

with $C_r > 0$ and $\alpha > 0$.

Proof. The proof of the proposition immediately follows by solving the equation (18). On one side the structure matrices of the open loop system H, J and R are defined in (27). On the other side the closed loop matrices are chosen as follows :

- H_d is chosen proportional to the availability (38).
- J_d is chosen equal to zero.
- R_d is chosen definite positive and such it guarantees the structural invariant $N_T = cte$ (39). We recall that this constraint implies the strict convexity of the availability.

Then H_a, J_a and R_a are deduced from (17). Especially,

$$\mathcal{H}_a = \mathcal{H}_d + S \Rightarrow \begin{cases} \dfrac{\partial \mathcal{H}_a}{\partial H} = \dfrac{\partial \mathcal{H}_d}{\partial H} + \dfrac{1}{T} \\ \dfrac{\partial \mathcal{H}_a}{\partial N_A} = \dfrac{\partial \mathcal{H}_d}{\partial N_A} - \dfrac{\mu_A}{T} \\ \dfrac{\partial \mathcal{H}_a}{\partial N_B} = \dfrac{\partial \mathcal{H}_d}{\partial N_B} - \dfrac{\mu_B}{T} \end{cases}$$

Finally, the global asymptotic stability is insured because $\mathcal{H}_d$ can be considered as Lyapunov function of the closed loop system Hoang (2008). In fact, from (37) we obtain:

$$\frac{d\mathcal{H}_d}{dt} = -\alpha\left(C_r\left(\frac{\partial \mathcal{H}_d}{\partial H}\right)^2 + \left(\frac{\partial \mathcal{H}_d}{\partial N_A} - \frac{\partial \mathcal{H}_d}{\partial N_B}\right)^2\right) < 0$$

4. SIMULATIONS

In this section we present simulations results of the open and closed loop system with $\alpha = 1$. Numerical values that are used are given in table 2.

Simulations are performed from four initial conditions (see table 3)

(C_1)	$T_0 = 350$	$N_{A0} = 1$	$N_{B0} = 1$
(C_2)	$T_0 = 335$	$N_{A0} = 1.4$	$N_{B0} = 0.6$
(C_3)	$T_0 = 325$	$N_{A0} = 1.4$	$N_{B0} = 0.6$
(C_4)	$T_0 = 320$	$N_{A0} = 0.7$	$N_{B0} = 1.3$

Table 3. Four initial conditions for simulations

Notation	Numerical value (units)	
c_{pA}	75.24 $(J/K/mol)$	Heat capacity of species A
c_{pB}	60 $(J/K/mol)$	Heat capacity of species B
h_{Aref}	0 (J/mol)	Reference enthalpy of A
h_{Bref}	-4575 (J/mol)	Reference enthalpy of B
k_{0f}	$0.12 \ 10^{10}$ $(1/s)$	Forward kinetic constant
k_{1f}	$8.7 \ 10^3$ (K)	Param. of forward reaction
k_{0r}	$1.33 \ 10^8$ $(1/s)$	Reverse kinetic constant
k_{1r}	$9 \ 10^3$ (K)	Param. of reverse reaction
p	10^5 (Pa)	Pressure
T_{ref}	300 (K)	Reference temperature
$v_A = v_B$	0.0005 (m^3/mol)	Molar volume
V	0.001 (m^3)	Reaction volume
λ	0.05808 (W/K)	Heat transfer coefficient
s_{Aref}	50.6 $(J/K/mol)$	Reference entropy of A
s_{Bref}	180.2 $(J/K/mol)$	Reference entropy of B

Table 2. Parameters of the CSTR.

Open loop   Manipulated variables are chosen as:

$F_{Ae} = 0.0183 \ (mol/s), \ T_e = 310 \ (K) \ T_w = 300 \ (K)$ (40)

With this operating conditions, the system has three steady states (Hoang (2008)). We choose to stabilize the system about the unstable steady state that we call $P2$ corresponding to $N_{A2} = 1.3083$ and $T_2 = 331.9204$.

The open loop simulations from the four initial conditions are given in Fig. 1. The system in open loop is a passive pseudo Hamiltonian system. The dissipation term d (14,33) is linked to irreversible entropy production due to reaction. So it is negative as shown in Fig. 2.
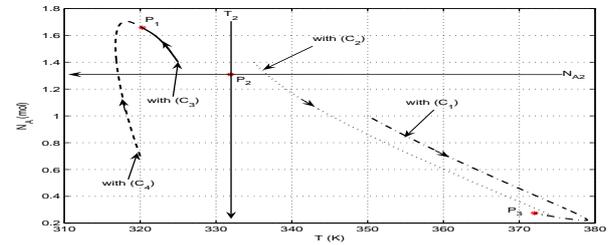
Fig. 1. Some trajectories in the phase plane
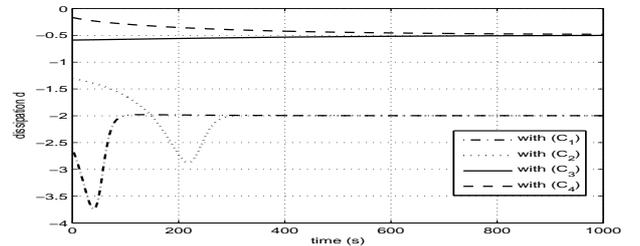
Fig. 2. The dissipation term in function of time

Control Problem: we are interested to operate the reactor at $T = 331.9204 \ (K)$ corresponding to the unstable steady state operating point P_2 and at fixed T_e. As a consequence, control feedback laws on T_w and F_{Ae} are necessary.

Closed loop-controlled dynamic   The continuity of the control inputs (36) is considered as in Hoang (2009). The values of design coefficients C_d and C_r are then calculated (Table 4) by imposing: $F_{Ae}\big|_{t=0} = \dfrac{F_{Ae}^{ol}}{3}$ and $T_w\big|_{t=0} = T_0$.

(C_1)	$C_d = -0.0025 < 0$	$C_r = -53.6 \ 10^5 < 0$
(C_2)	$C_d = 0.0043 > 0$	$C_r = 180.47 \ 10^5 > 0$
(C_3)	$C_d = 0.0010 > 0$	$C_r = 340.95 \ 10^5 > 0$
(C_4)	$C_d = 0.2800e - 3 > 0$	$C_r = 4704.5 \ 10^5 > 0$

Table 4. C_d and C_r

From Table 4, it can be seen that the system is stabilized with (C_2), (C_3) and (C_4). Fig. 3 gives closed loop simulations.
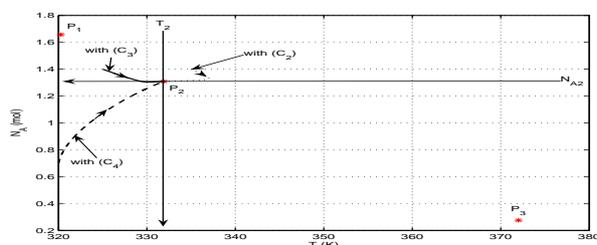
Fig. 3. Phase plane of the controlled non isothermal system

The controlled inputs are given in Fig. 4. Their dynamics are slow enough and admissible.
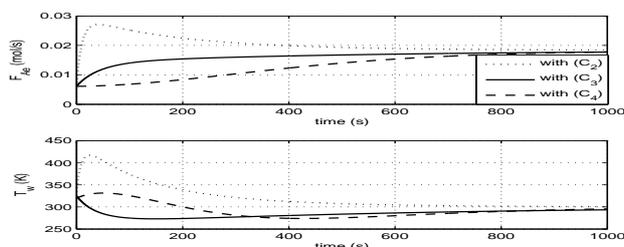
Fig. 4. The control inputs

Finally, Fig. 5 shows that $\mathcal{H}_d$ is a Lyapunov function for the three considered initial conditions (C_2) (C_3) and (C_4).
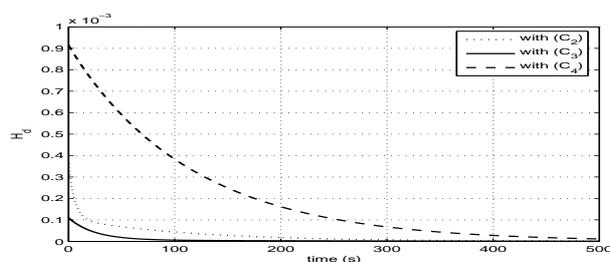
Fig. 5. The Hamiltonian as a Lyapunov function

5. CONCLUSION

In this paper, we have proposed a pseudo Hamiltonian representation of a non isothermal CSTR model. The proposed Hamiltonian is the opposite of entropy and the dissipation term is linked to the irreversible entropy production due to the reaction. This representation can be easily generalized to any reactions.

The IDA-PBC approach permits to control the system about the desired operating point using the availibrity function as closed loop Hamiltonian. The simulation results showed that convergence objectives are satisfied and that the state feedback laws are physically implementable.

It is moreover very easy to synthesize. The generalization of IDA-PBC approach to more complex reactions has to be studied.

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