

STABILIZATION OF NON ISOTHERMAL CHEMICAL REACTORS USING TWO THERMODYNAMIC LYAPUNOV FUNCTIONS

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ABSTRACT

The main goal of this paper is to introduce a link between the thermodynamics and control systems theory. More precisely, the paper focuses on Lyapunov based control of process systems, specially the non isothermal Continuous Stirred Tank Reactors in a thermodynamic framework, using either the jacket temperature or the inlet molar flow rate as the only control input. As soon as the constraint on the total mass is considered and the reaction kinetics is a Lipschitz continuous function with respect to the temperature, it shows that the stabilization of thermal solicitations reciprocally entails the one of matter using La Salle's invariance principle. As a consequence, these control problems can be solved if the closed loop Lyapunov functions are chosen to be proportional to the thermal part or material part of the so called thermodynamic availability function. Some numerical simulations for a first order chemical reaction with multiple steady states are given to validate our theoretical developments. The performance of the obtained nonlinear controllers with regard to the conversion rate is also discussed.

Keywords. Thermodynamics, process control, CSTR, Lyapunov function.

1. INTRODUCTION

The paper deals with Lyapunov based stabilization of process systems using the variables directly issued from thermodynamic framework. The most representative example of the process systems chosen in this paper is the non isothermal Continuous Stirred Tank Reactors (CSTRs). In fact, the CSTRs with chemical reaction belong to general thermodynamic systems and exhibit inherently nonlinear dynamical evolutions, for instance, they can be operated under multiplicity and have a highly nonlinear coupling between energy and material balances because of the chemical reaction kinetics. For all these reasons, they are quite difficult to control and monitor. As a consequence, such CSTRs have been considerably studied in literature with respect to stabilization purpose [12, 16, 23, 24]. Numerous methods have been developed to control such nonlinear systems: input/output feedback linearization [20] for control under constraints,

nonlinear PI control [18], classical Lyapunov based control [23, 24], (pseudo) Hamiltonian framework [14, 16, 17, 26, 27], power-shaping control [15] and inventory control [5].

In this paper we only focus on the control design and we assume that molar numbers/concentrations and temperature are measured on-line. The control synthesis is based on thermodynamic concepts defined in [10, 9, 1, 2], specially the thermodynamic availability function A_v . More precisely, we propose a Lyapunov based approach for the stabilization of CSTR about a desired steady state, using either the jacket temperature or the inlet molar flow rate as the only control input. In these two cases, we shall show the convergence property is quite equivalent but it does not lead to the same performance with regard to the conversion rate.

This paper is organized as follows: in section 2 a CSTR case study with one reaction $\nu_A A \rightarrow \nu_B B$ is represented from thermodynamics based view. The *thermodynamic availability* and its decomposition into the thermal and material parts are also reminded. In the section 3, we propose some feedback laws to stabilize the CSTR under consideration around an open loop unstable steady state. More precisely, our control problem is solved by two ways:

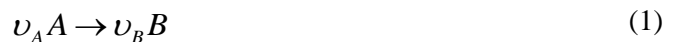
- We first use the thermal part of the availability as a Lyapunov function candidate. The jacket temperature is chosen as the only control input (the inlet molar flow rate is fixed).
- We second consider the material part of the availability as a Lyapunov function candidate. The inlet molar flow rate is then used as the only control input (the jacket temperature is fixed).

The performance of the proposed nonlinear controllers is then discussed with regard to the conversion rate. In this section 3 some numerical simulations are also given to illustrate our theoretical developments. Section 4 ends the paper with concluding remarks and perspectives.

2. A CSTR CASE STUDY $\nu_A A \rightarrow \nu_B B$

2.1. Classical model of CSTR

We consider a jacketed reactor with one reaction schema consisting of two chemical species A and B :



we assume that the reactor is modelled with the so called CSTR model which assumes uniform properties such as temperature, pressure or concentrations inside the reactor see Fig. 1. As a consequence, the reaction mixture is homogeneous.

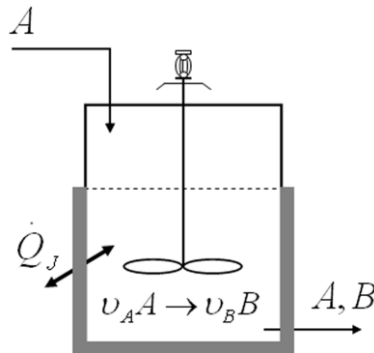


Figure 1. The CSTR model

We consider the following hypotheses:

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

(H2) In the inlet, the reactor is fed by the only species A at a fixed temperature T_I .

(H3) ν_A, ν_B are the stoichiometric coefficients and supposed to be $\nu_A = -1$ and $\nu_B = 1$.

The reaction kinetics is modeled by Arrhenius law¹ $k(T) = k_0 \exp\left(\frac{-E_a}{RT}\right)$ where k_0 is kinetic constant; E_a and R are the activation energy and the gas constant, respectively. As a consequence, the reaction rate is then given by:

$$rV = k(T)N_A \quad (2)$$

(H4) Heat capacities of species c_{pA} and c_{pB} are supposed to be constant.

(H5) The heat flow coming from the jacket \dot{Q}_J

$$\dot{Q}_J = \lambda(T_J - T) \quad (3)$$

(where λ is the heat exchange coefficient) or the inlet molar flow rate F_{AI} is used as the only control input.

2.2. Thermodynamics based view

2.2.1. Some concepts and balance equations

In thermodynamics based view, the system variables are split into extensive variables (such as the internal energy U , the entropy S , the volume V , the molar number N_i) and intensive variables (such as the temperature T , the pressure P , the chemical potential μ_i). The variation of the internal energy U ² can be derived from the variation of the extensive variables using the Gibbs equation:

$$dH = \sum_{i=A}^B \mu_i dN_i + TdS \quad (4)$$

Since the enthalpy H is an extensive variables, it is a homogeneous function of the degree 1 of (N_A, N_B, S) ([10]). From Euler's theorem we get:

$$H(N_A, N_B, S) = \sum_{i=A}^B \mu_i N_i + TS \quad (5)$$

¹ We can check that it is Lipschitz continuous function with respect to the temperature, i.e. $\|k(T_1) - k(T_2)\| \leq \delta \|T_1 - T_2\|$, $\delta \in \mathfrak{R}^{*+}$

² With isobaric conditions, the pressure P is constant, the enthalpy H can be considered instead of the internal energy U .

As a consequence of eq. (4), we obtain:

$$dS = \sum_{i=A}^B \frac{-\mu_i}{T} dN_i + \frac{1}{T} dH \quad (6)$$

Since the entropy S is also an extensive variable, we get:

$$S(N_A, N_B, H) = \sum_{i=A}^B \frac{-\mu_i}{T} N_i + \frac{1}{T} H \quad (7)$$

The Eq. (6) can be rewritten in a compact form as follows:

$$dS = w^t dZ \Rightarrow w^t = \frac{\partial S(Z)}{\partial Z} = w(Z)^t \quad (8)$$

where³:

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

As a consequence, $w(Z)$ (8) is an homogeneous function of degree 0 of Z .

The system with relation (4) and (5) is called in energy representation $H = H(N_A, N_B, S)$ and with relation (6) and (7) in entropy representation $S = S(N_A, N_B, H)$ [10, 26, 27]. From a mathematical point of view, these representations are equivalent.

In practice, the models are presented in the entropy representation since the energy balance is used (because it is conserved extensive variable) and not entropy one. The dynamics of the system is then given by energy and material balances [23, 24]:

$$\begin{cases} \frac{dN_A}{dt} = F_{A_I} - F_A + \nu_A rV \\ \frac{dN_B}{dt} = -F_A + \nu_B rV \\ \frac{dH}{dt} = \dot{Q}_J + F_{A_I} h_{A_I} - (F_A h_A + F_B h_B) \end{cases} \quad (9)$$

where F_{A_I} , (F_A, F_B) , (ν_A, ν_B) , h_{A_I} and (h_A, h_B) are the inlet molar flow rate, the outlet molar flow rate vector, the stoichiometric vector, the inlet molar enthalpy and the partial molar enthalpy vector, respectively. \dot{Q}_J represents the heat flux coming from the jacket.

Thanks to the local equilibrium hypothesis ([8]), the energy balance $\frac{dH}{dt}$ in (9) can be written in terms of temperature (see [24]):

$$C_p \frac{dT}{dt} = (-\Delta_r H) rV + F_{A_I} (T_I - T) c_{pA} + \dot{Q}_J \quad (10)$$

³ The exponent t holds for the matrix transpose.

where $\Delta_r H = (\nu_A h_A + \nu_B h_B)$ is the enthalpy of reaction and $C_p = (c_{pA} N_A + c_{pB} N_B)$ is the total heat capacity, respectively.

Remark 1. The dynamics of state variables either (N_A, N_B, H) (9) or (N_A, N_B, T) ((9), (10)) completely represent the behavior of the system.

Finally, let us note that the following stoichiometric relation for the reaction (1) is always verified:

$$\nu_A M_A + \nu_B M_B = 0 \quad (11)$$

where M_A and M_B are the molar masses of the species A and B , respectively.

2.2.2. Thermodynamic availability

From the concavity of $S(Z)$ for homogeneous thermodynamic systems (see [10]), it can be shown [9, 1, 2] that the *availability function* A_v :

$$A_v(Z) = S_2 + w_2'(Z - Z_2) - S(Z) \quad (12)$$

is non negative, where Z_2 is some fixed reference point (for example the desired set point for control) and w_2 is intensive variables associated to extensive variables Z_2 .

The availability function (12) can be rewritten (see ([27])):

$$A_v(Z) = -(w - w_2)' Z \quad (13)$$

Remark 2. Because the entropy $S(Z)$ is an homogeneous function of degree 1 with respect to Z ([10]), it is not strictly concave in general case, as a consequence $A_v(Z)$ will not be strictly convex. The strict concavity of the entropy can be obtained if at least one global extensive property (such as volume, total mass, total molar number) is fixed [6]. In the remaining of the paper we suppose that the total mass m_t is constant.

2.2.3. Decomposition of the availability

The availability function $A_v(Z)$ defined by (13) can be explicitly written:

$$A_v(Z) = -\left(\frac{-\mu_A}{T} + \frac{\mu_{A2}}{T_2}\right) N_A - \left(\frac{-\mu_B}{T} + \frac{\mu_{B2}}{T_2}\right) N_B - \left(\frac{1}{T} - \frac{1}{T_2}\right) H \quad (14)$$

The Property 1 represents a separation of the availability $A_v(Z)$ (14) into thermal and material parts denoted by A_{v1} and A_{v2} , respectively.

Property 1. In the case of an ideal mixture, the availability function (14) can be written as the sum of two functions A_{v1} and A_{v2} :

$$\begin{cases} A_{v1}(N_A, N_B, H) = -\Gamma_A(T)N_A - \Gamma_B(T)N_B - \left(\frac{1}{T} - \frac{1}{T_2}\right)H \\ A_{v2}(N_A, N_B) = -\Lambda_A(N_A, N_B)N_A - \Lambda_B(N_A, N_B)N_B \end{cases} \quad (15)$$

where

$$\begin{cases} \Gamma_k(T) = c_{pk} \ln\left(\frac{T}{T_2}\right) - \frac{h_k}{T} + \frac{h_{k2}}{T_2}; k = A, B \\ \Lambda_k(N_A, N_B) = R \ln\left(\frac{N_{k2} \sum_{i=A}^B N_i}{N_k \sum_{i=A}^B N_{i2}}\right); k = A, B \end{cases} \quad (16)$$

and

i. The function $A_{v2}(N_A, N_B)$ has the following properties:

- $A_{v2} = 0$ if $(N_A, N_B) = (N_{A2}, N_{B2})$
- $A_{v2} > 0$ if $\forall (N_A, N_B) \neq (N_{A2}, N_{B2})$
- A_{v2} is an homogeneous function of degree one with respect to (N_A, N_B) . Consequently,

$$\begin{cases} dA_{v2} = -\Lambda_A(N_A, N_B)dN_A - \Lambda_B(N_A, N_B)dN_B \\ \frac{dA_{v2}}{dt} = -\Lambda_A(N_A, N_B)\frac{dN_A}{dt} - \Lambda_B(N_A, N_B)\frac{dN_B}{dt} \end{cases} \quad (17)$$

ii. The function $A_{v1}(N_A, N_B, H)$ has the following properties:

- $A_{v1} = 0$ if $(N_A, N_B, H) = (N_{A2}, N_{B2}, H_2)$
- $A_{v1} > 0$ if $\forall (N_A, N_B, H) \neq (N_{A2}, N_{B2}, H_2)$
- A_{v1} is an homogeneous function of degree one with respect to (N_A, N_B, H) .

Consequently,

$$\begin{cases} dA_{v1} = -\Gamma_A(T)dN_A - \Gamma_B(T)dN_B - \left(\frac{1}{T} - \frac{1}{T_2}\right)dH \\ \frac{dA_{v1}}{dt} = -\Gamma_A(T)\frac{dN_A}{dt} - \Gamma_B(T)\frac{dN_B}{dt} - \left(\frac{1}{T} - \frac{1}{T_2}\right)\frac{dH}{dt} \end{cases} \quad (18)$$

Proof 1. First of all, we recall the definition of the chemical potential for species k ($k = A, B$):

$$\mu_k = h_k - Ts_k \quad (19)$$

where h_k and s_k are the partial molar enthalpy and the partial molar entropy, respectively. In the case of the ideal incompressible mixture (see [7]),

$$s_k = c_{pk} \ln\left(\frac{T}{T_{ref}}\right) + s_{kref} - R \ln\left(\frac{N_k}{\sum_{i=A}^B N_i}\right) \quad (20)$$

where c_{pk} and s_{kref} are the heat capacity and the reference entropy respectively. After some manipulations, we obtain from (19) and (20):

$$\left(\frac{-\mu_k}{T} + \frac{\mu_{k2}}{T_2}\right) = \Gamma_k(T) + \Lambda_k(N_A, N_B) \quad (21)$$

where $\Gamma_k(T)$ and $\Lambda_k(N_A, N_B)$ are given in (16). The availability function $A_v(Z)$ (14) can be rewritten:

$$A_v(N_A, N_B, H) = A_{1v}(N_A, N_B, H) + A_{2v}(N_A, N_B) \quad (22)$$

where $A_{1v}(N_A, N_B, H)$ and $A_{2v}(N_A, N_B)$ are defined in (15). The complete proof can be found in [24, 25].

Remark 3. It can be shown that there exists a positive constant ρ so that (see [25]):

$$0 \leq -\left(1 - \frac{T}{T_2} + \ln\left(\frac{T}{T_2}\right)\right)\rho \leq A_{1v} \quad (23)$$

We can take for ρ , for example:

$$\rho = \min_{N_A, N_B} C_p.$$

Remark 4. Let us note that a positive continuous function $W(x)$ is a Lyapunov candidate for stabilization problem at a desired state \bar{x} of the dynamical evolution:

$$\frac{dx}{dt} = f(x) + g(x)u$$

where $x = (x_1, x_2, \dots, x_n)^t \in \mathfrak{R}^n$ is the state vector, $f(x) \in \mathfrak{R}^n$ represents the smooth nonlinear function with respect to x , $g(x) \in \mathfrak{R}^{n \times m}$ is the input-state map and $u \in \mathfrak{R}^m$ is the input; if and only if it satisfies the three following conditions [11]:

- (a). $W(\bar{x}) = 0$
- (b). $W(x) > 0, \forall x \neq \bar{x}$

$$(c). \frac{dW(x)}{dt} < 0, \forall x \neq \bar{x} \text{ and } \frac{dW(x)}{dt} = 0, \forall x = \bar{x}$$

The same conditions can also be stated for the partial dynamical stability $x_i \in x$ only.

Remark 5. A_{1v} and A_{2v} are also strictly convex functions with respect to $Z = (N_A, N_B, H)$ if one constraint on extensive variable has been fixing (see Remark 2). We recall that the total mass m_t is assumed to be constant.

The availability $A_v(Z)$ has been successfully used for Lyapunov based control or closed loop Hamiltonian function of transport reaction systems [3, 4, 23, 24, 26, 27]. As we saw in Property 1, A_{1v} and A_{2v} have the same properties as $A_v(Z)$ that will entail their use as close loop Lyapunov functions for control design.

Up to this point, we just remind some existent results and nothing is substantially new.

3. MAIN RESULTS

In this paper, we consider the total mass $m_t = M_A N_A + M_B N_B$ is constant. As a consequence, the outlet molar flow rates F_A and F_B can be directly expressed from the inlet molar flow rate F_{AI} (see [27]):

$$\begin{cases} F_A = \frac{N_A M_A}{m_t} F_{AI} \\ F_B = \frac{N_B M_A}{m_t} F_{AI} \end{cases} \quad (24)$$

Using (24), the non isothermal balance equations given in (9) are rewritten (25):

$$\frac{d}{dt} \underbrace{\begin{pmatrix} N_A \\ N_B \\ H \end{pmatrix}}_x = \underbrace{\begin{pmatrix} \left(1 - \frac{N_A M_A}{m_t}\right) & 0 \\ -\frac{N_B M_A}{m_t} & 0 \\ \left(h_{AI} - \frac{M_A H}{m_t}\right) & 1 \end{pmatrix}}_{g(x)} \underbrace{\begin{pmatrix} F_{AI} \\ \dot{Q}_J \end{pmatrix}}_u + \underbrace{\begin{pmatrix} \nu_A r V \\ \nu_B r V \\ 0 \end{pmatrix}}_{f(x)}. \quad (25)$$

All numerical parameters can be found in [23, 24].

3.1. Open loop

Manipulated variables are chosen as:

$$F_{AI} = 0.0183(\text{mol}/s), T_I = 310(K), T_J = 300(K) \quad (26)$$

with this operating conditions, the system has three steady states P_1 , P_2 and P_3 . The states P_1 and P_3 are locally stable. Otherwise, the state P_2 is unstable. A mathematical analysis and numerical value of these stationary states can be found in [23, 24].

For simulation, we use the two following initial conditions: (IC₁) with

$$(T_0 = T(t=0) = 325(K), N_{A0} = N_A(t=0) = 1.8(mol), N_{B0} = N_B(t=0) = 0.2(mol))$$

and (IC₂) with

$$(T_0 = T(t=0) = 300(K), N_{A0} = N_A(t=0) = 1.6(mol), N_{B0} = N_B(t=0) = 0.4(mol)).$$

The open loop simulations from these two initial conditions are given in Fig. 2. It shows that the dynamical trajectory converges to state P_1 (or P_3) and not P_2 .

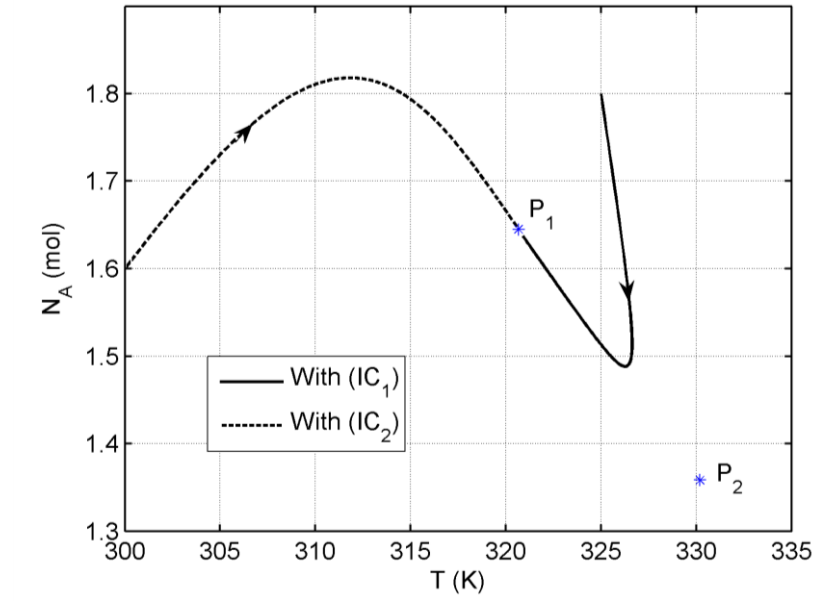


Figure 2. Some trajectories in the phase plane

Let us notice that at steady states $(\bar{N}_A, \bar{N}_B, \bar{T})$, one can get the following relation from (25) using the hypothesis (H3):

$$\bar{N}_A = \frac{F_{A1}}{\frac{M_A}{m_t} F_{A1} + k_0 \exp\left(\frac{-E_a}{RT}\right)}. \quad (27)$$

Hence the relation between \bar{N}_A and \bar{T} is bijective. It means that if we can regulate the temperature inside the reactor, consequently the concentrations immediately follow, or vice versa. This statement leads to the **Control Problem**.

Control Problem: we are interested to operate the reactor at the unstable operating point P_2 (corresponding to $T = 330.1997 (K)$, $N_A = 1.3585 (mol)$) using the feedback law either on the only T_J (with fixed F_{A1}) or the only F_{A1} (with fixed T_J).

3.2. Nonlinear controllers synthesis

This subsection proposes nonlinear controllers to solve the *Control Problem*.

Proposition 1 (The jacket temperature as the only control input): The system (25) is stable and asymptotically converges to the desired operating point $\bar{x} = Z_2 \equiv P_2$ with the nonlinear feedback law (where T_1 and F_{A1} are fixed as their open loop values (26)):

$$T_J = \frac{1}{\lambda} \left[K_1 \left(\frac{1}{T} - \frac{1}{T_2} \right) - \left(h_{A1} - \frac{M_A H}{m_t} \right) F_{A1} + \left(\frac{1}{T} - \frac{1}{T_2} \right)^{-1} \left(-\Gamma_A(T) \frac{dN_A}{dt} - \Gamma_B(T) \frac{dN_B}{dt} \right) \right] + T \quad (28)$$

and $K_1 > 0$ is tuning parameter.

Proof 1. Using the thermal part of the availability A_{v1} (18), we can write:

$$\frac{dA_{v1}}{dt} = -\Gamma_A(T) \frac{dN_A}{dt} - \Gamma_B(T) \frac{dN_B}{dt} - \left(\frac{1}{T} - \frac{1}{T_2} \right) \frac{dH}{dt}.$$

By introducing the $\frac{dH}{dt}$ (given in (25) with Q_J (3) using the feedback law T_J (28)) into the above equation, we obtain:

$$\frac{dA_{v1}}{dt} = -K_1 \left(\frac{1}{T} - \frac{1}{T_2} \right)^2 \leq 0.$$

Because $A_{v1} \geq 0$, it is a Lyapunov function for stabilization of thermal oscillations inside the reactor. As a consequence from (23), the temperature T radically decreases and converges to its desired value T_2 after finite time Δt . Once T reaches T_2 at $\forall t > \Delta t$, from (17) A_{v2} qualifies as a Lyapunov function for stabilization of the state variables (N_A, N_B) at (N_{A2}, N_{B2}) . In fact, using the law of conservation of mass (11), the hypothesis (H3) and the constraint on $m_t = const$, we can write from (17):

$$\frac{dA_{v2}}{dt} = \left(-\Lambda_A - \frac{\nu_B}{\nu_A} \Lambda_B \right) \frac{dN_A}{dt}$$

and it is (or becomes) negative: $\frac{dA_{v2}}{dt} < 0$ (at $\forall t > \Delta t$), see ([24]) for more details. The largest

invariant set contained in $\left\{ (N_A, N_B) \mid \frac{dA_{v2}}{dt} = 0 \right\}$ equals $\{(N_{A2}, N_{B2})\}$. Asymptotic stability immediately follows invoking La Salle's invariance principle [11]. The latter ends the proof.

Remark 6. Let us note that (see [24])

$$\lim_{T \rightarrow T_2} \left(\frac{1}{T} - \frac{1}{T_2} \right)^{-1} \Gamma_A(T) < \infty$$

and

$$\lim_{T \rightarrow T_2} \left(\frac{1}{T} - \frac{1}{T_2} \right)^{-1} \Gamma_B(T) < \infty$$

The feedback law control (28) is well-defined.

The stabilizing feedback control law similar to (28) has been obtained by [24, 25]. By this way, we have already used the thermal part of availability to stabilize the temperature inside the reactor. Consequently the concentrations immediately follow.

In what follows, we shall show the use of the material part of the availability to stabilize the concentrations and as a matter of fact, the temperature is then accomplished (see the relation (27)). It is completely given in the Proposition 2. The following developments are main contributions of the paper.

Proposition 2. (The inlet molar flow rate as the only control input): The system (25) is stable and asymptotically converges to the desired operating point $\bar{x} = Z_2 \equiv P_2$ with the nonlinear feedback law (where T_I and T_J are fixed as their open loop values (26)):

$$F_{AI} = \frac{\nu_A \Lambda_A + \nu_B \Lambda_B}{\Theta} - K_2 \Theta \quad (29)$$

where

$$\Theta = -\Lambda_A \left(1 - \frac{N_A M_A}{m_t} \right) + \Lambda_B \frac{N_B M_A}{m_t} \quad (30)$$

and $K_2 > 0$ is tuning parameter.

Proof 2. Using the material part of the availability A_{v2} (17), we can write:

$$\frac{dA_{v2}}{dt} = -\Lambda_A(N_A, N_B) \frac{dN_A}{dt} - \Lambda_B(N_A, N_B) \frac{dN_B}{dt}$$

By introducing the expressions of $\frac{dN_A}{dt}$ and $\frac{dN_B}{dt}$ ((25)) into the above equation, we have:

$$\frac{dA_{v2}}{dt} = \Theta F_{AI} - (\nu_A \Lambda_A + \nu_B \Lambda_B) rV \quad (31)$$

where Θ is given in (30). Using F_{AI} (29), we obtain:

$$\frac{dA_{v2}}{dt} = -K_2 \Theta^2 \leq 0$$

because $A_{v2} \geq 0$, it is a Lyapunov function for asymptotic stabilization of the state variables (N_A, N_B) at (N_{A2}, N_{B2}) . The later and the relation (27) end the proof.

Remark 7. In the case under consideration (hypothesis (H3)), (31) becomes:

$$\frac{dA_{v2}}{dt} = \Theta F_{AI} - (-\Lambda_A + \Lambda_B)rV \quad (32)$$

and the equation (30) is (using (11) with $M_A = M_B$)

$$\Theta = (-\Lambda_A + \Lambda_B) \left(1 - \frac{N_A}{N_t} \right) \quad (33)$$

where $N_t = N_A + N_B$ is the total molar number.

We derive from (32) and (33):

$$\frac{dA_{v2}}{dt} = (-\Lambda_A + \Lambda_B) \left[\left(1 - \frac{N_A}{N_t} \right) F_{AI} - rV \right]. \quad (34)$$

The feedback law (29) is then simplified to:

$$F_{AI} = \frac{rV - K_2(-\Lambda_A + \Lambda_B)}{\left(1 - \frac{N_A}{N_t} \right)} \quad (35)$$

with (35), the eq. (34) becomes $\frac{dA_{v2}}{dt} = -K_2(-\Lambda_A + \Lambda_B)^2 \leq 0$. As a consequence, A_{v2} is a Lyapunov function for the stabilization of the state variables (N_A, N_B) . Finally, the feedback law (35) is also well-defined because $\left(1 - \frac{N_A}{N_t} \right) > 0$.

Remark 8. The stabilization of the system (25) at the unstable operation point P_2 (via the state variables (N_A, N_B) using the feedback law (35) is related to the inventories control (see [5], Case I, page 3557). But our result is quite interesting because we have shown that the material part A_{v2} of the thermodynamic availability can be used as Lyapunov function candidate for inventories.

Remark 9. The convergence speed of the controlled system goes faster by increasing the parameters $K_1 > 0$ and $K_2 > 0$.

3.3. Simulation for controlled dynamics

1) *Simulation:* For the continuity of control variables (see [24]), the tuning parameters $K_1 > 0$ and $K_2 > 0$ are calculated from the following conditions:

$$2) \quad T_J(t=0) = T_0, \quad F_{AI}(t=0) = 0 \quad (36)$$

where T_0 is the initial temperature inside the reactor. The Figures Fig. 3 and Fig. 4 present the time responses of the state variables. Their evolutions converge to the unstable point P_2 ($T = 330.1997(K)$, $N_A = 1.3583$ (mol)).

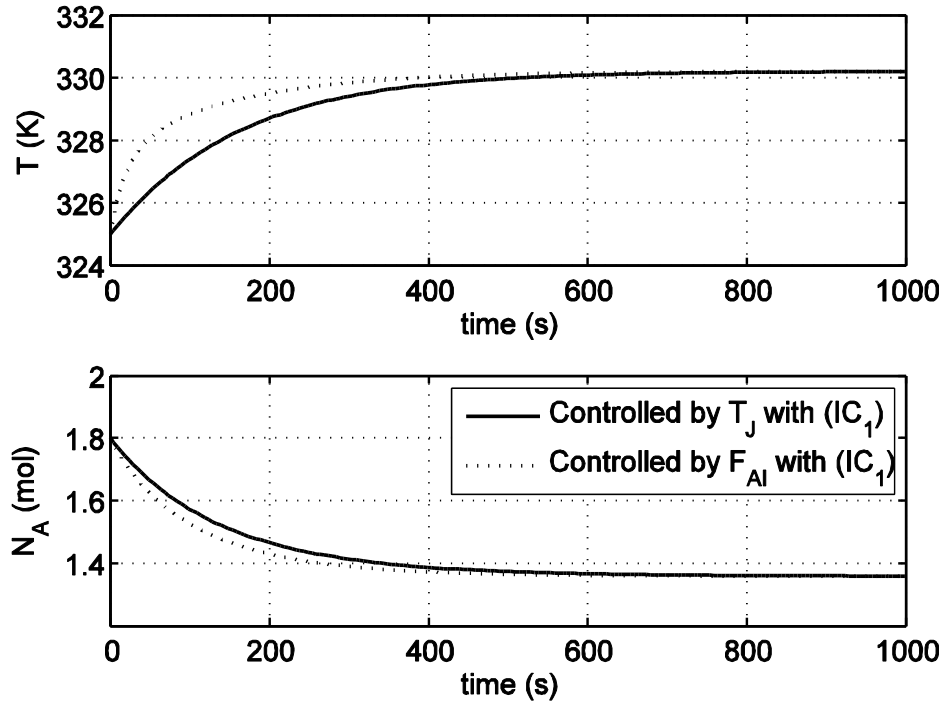


Figure 3. Time response of the controlled non isothermal system with (IC_1)

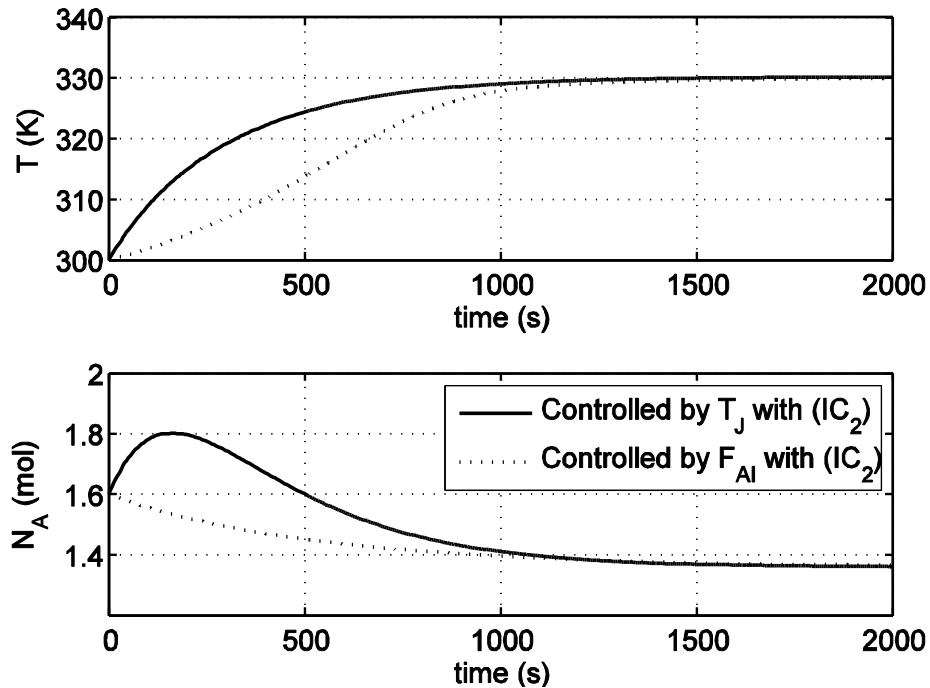


Figure 4. Time response of the controlled non isothermal system with (IC_2)

The controlled inputs T_J (28) and F_{AI} (29) are given in Fig. 5. Their dynamics are smooth and acceptable.

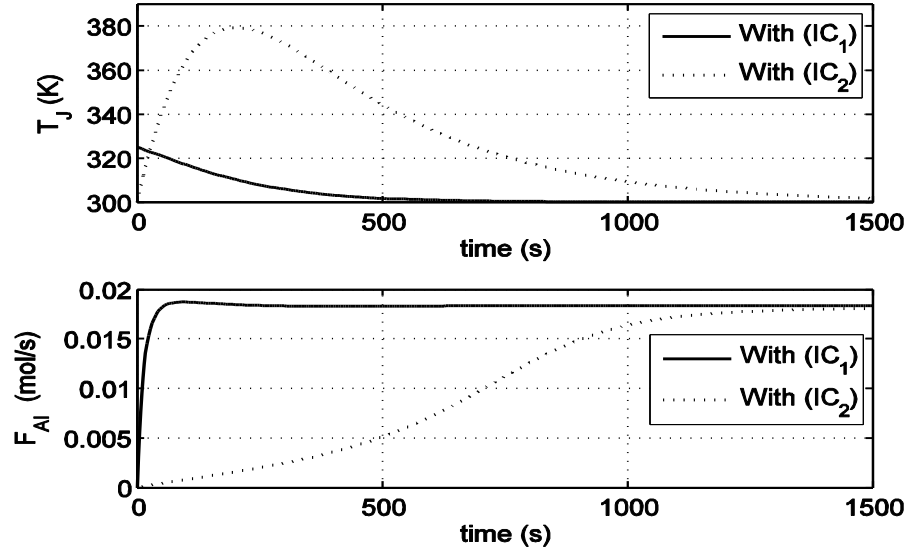


Figure 5. The controlled inputs T_J and F_{AI}

Finally, Fig.6 shows that A_{v1} (for the jacket temperature T_J used as the only control input) and A_{v2} (for the inlet molar flow rate F_{AI} used as the only control input) are Lyapunov functions for the initial conditions (IC₁) and (IC₂).

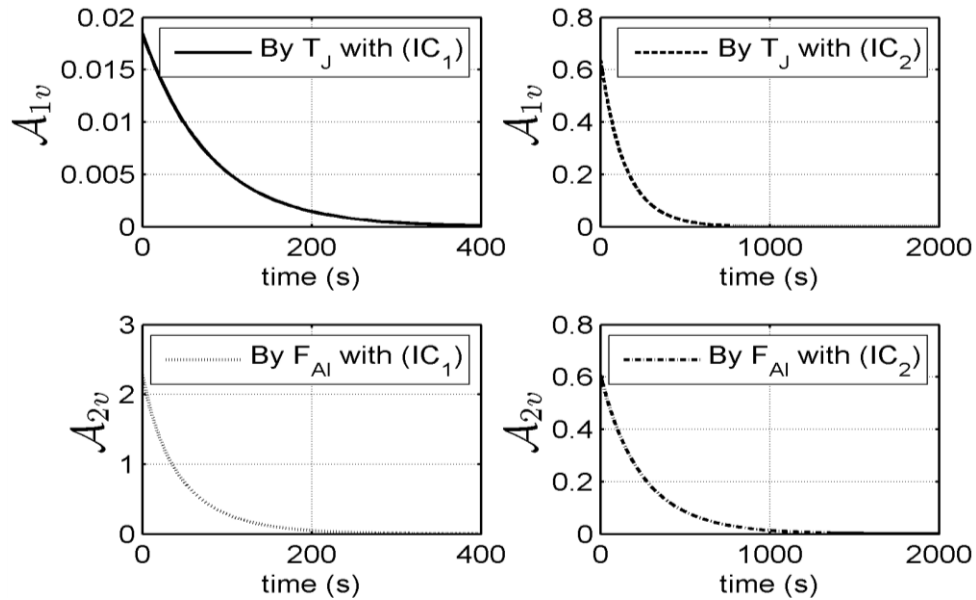


Figure 6. Lyapunov functions: A_{v1} and A_{v2}

3) *Performance of nonlinear controllers:* In this part, we shall discuss about the performance of synthesized nonlinear controllers with regard to the conversion rate. Let us recall the expression of the conversion rate defined for the reactant A [22, 13],

$$X_A(t) = \frac{\frac{dN_A}{dt}\Big|_{t=0} - \frac{dN_A}{dt}\Big|_t}{\frac{dN_A}{dt}\Big|_{t=0}}.$$

Let us note that $X_A(t=0) = 0$ and $X_A(t=\infty) = 1$. The Figures 7 and 8 present the conversion rate $X_A(t)$ with T_J or F_{A1} used as the only control input, respectively.

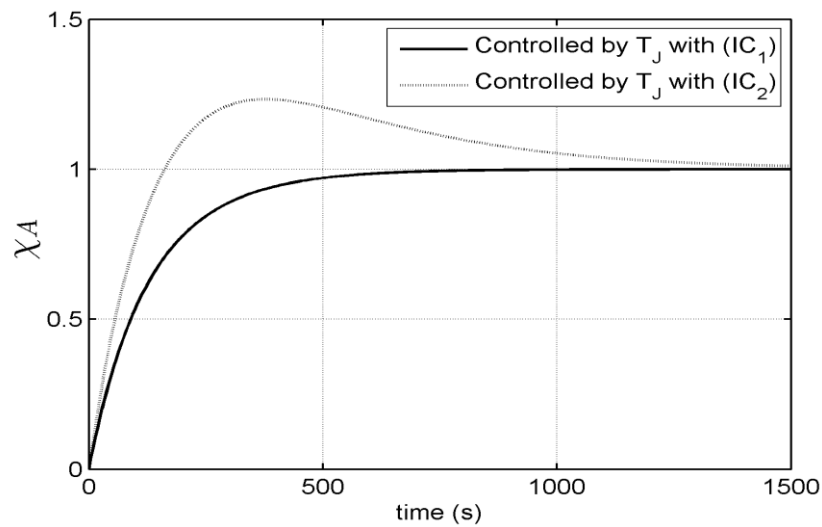


Figure 7. Conversion rate curve by using T_J as the only control input

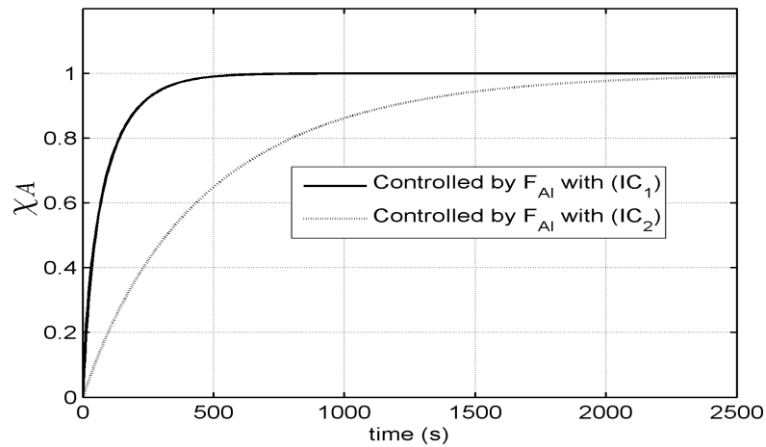


Figure 8. Conversion rate curve by using F_{A1} as the only control input

Depending on the operating conditions, the conversion rate curve may present an overshoot, see Fig. 7. However, the conversion ratio controlled by the jacket temperature T_j generally reaches faster its final value. This result matches with the one obtained in [21] using simple extensive variables for the control design by regulating the fast mode.

4. CONCLUSION

In this work, we have presented an interesting link between the thermodynamic insight and systems theory for process control. In fact, we have shown by means of Lyapunov based method how to stabilize the CSTR system at a desired operating point (an unstable middle steady state for instance) using thermal and material parts of the thermodynamic availability. The numerical simulation results showed that convergence objective is satisfied and that the state feedback laws are physically implementable. Moreover, it also showed that the conversion rate controlled by the thermal part goes faster to its final value. It remains now to generalize the proposed approach to complex reaction networks. Furthermore the irreversible nature of the chemical reaction systems is an inherently natural property. A perspective of the work is the use of the thermodynamic passive (pseudo) Hamiltonian representation to capture the irreversibility. The most recent result of such an approach is given in [28].

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