Entropy-based stabilizing feedback law under input constraints of a CSTR

N. Ha Hoang^{*,**} Denis Dochain^{**}

* Faculty of Chemical Engineering, University of Technology, VNU-HCM, 268 Ly Thuong Kiet Str., Dist. 10, HCM City, Vietnam ** CESAME, Université Catholique de Louvain, 1348 Louvain-la-Neuve, Belgium (e-mails: {ha.hoang,denis.dochain}@uclouvain.be)

Abstract: The paper deals with nonlinear control under input constraints of a non isothermal Continuous Stirred Tank Reactor (CSTR) using thermodynamic concepts. More precisely, the paper presents an extension of the previous work (Hoang *et al.* (2012)) where the jacket temperature is used as the only control input. Constrained input control strategy is based on the observation that the chemical reactor operates at an unique stationary temperature when the lower or upper bound of the input variable is imposed. This control design results in a global asymptotic stabilizing feedback law that provides a locally exponentially stable behaviour of the overall system.

Keywords: Lyapunov function, thermodynamics, Van Heerden diagram, input constraints.

1. INTRODUCTION

The feedback control design for nonlinear dynamical systems, and in particular for unstable chemical reactors, is typically facing the requirement of both \prec hard constraints \succ (e.g. feasibility and equipment limitations) and \prec soft constraints \succ (such as an optimum tradeoff between conversion and selectivity etc.). In many industrial applications, the hard constraints on the process inputs not only limit the operating condition but can also affect the soft constraints on the dynamical behaviour of the overall system through the influence of the saturation characteristics. As a consequence, the stabilization of such constrained systems may give rise to practical difficulties and theoretical challenging issues (Liu and Michel (1994); Hu and Lin (2001)).

Over the years, a large number of control strategies have been developed to deal with the nonlinear feedback control of chemical reactors. Lyapunov based control (Antonelli and Astolfi (2003); Hoang *et al.* (2013c)), (pseudo) Hamiltonian framework (Hangos *et al.* (2001); Ramírez *et al.* (2013); Dörfler *et al.* (2009); Hoang *et al.* (2011); Alvarez *et al.* (2011), power-shaping control (Favache and Dochain (2010)) and inventory control (Farschman *et al.* (1998)) provide a good overview. The results presented in (Viel *et al.* (1997); Alvarez-Ramírez and Morales (2000); Bayer *et al.* (2011); Balestrino *et al.* (2012)) were dedicated to the design of input/state-constrained control systems for chemical reactors.

This paper presents an extension of the previous works (Hoang *et al.* (2012)) for the stabilization of unstable continuous stirred tank reactors (CSTRs). The key motivation of the present work lies in the fact that the appropriate implementation of the control strategy has to account for the range of operation of the control actuators (like, for instance, the jacket temperature and inlet temperature...) (Bruns and Bailey (1975)). More precisely, the main contribution of this paper with respect to the previous works (Hoang *et al.* (2012)) is the redesign of the asymptotic controller with the presence of physical constraints on the control input in order to maintain a desired reactor operation condition. We shall show that with the proposed controller, the global stabilization is guaranteed with a local exponential behaviour.

The paper is organized as follows. Section 2 represents the CSTR model and thermodynamic foundations required for the present work. The relaxation of the availability into the thermal and material parts as well as its properties usable for the control design are developed in Section 3. This section provides some preliminary results which are instrumental in proving the main results of this work. Section 4 concentrates on the redesign of a global stabilizing feedback control law for the CSTR in presence of input constraints. Numerical simulation results are also included.

2. THE CSTR CASE STUDY

2.1 CSTR model

Let us consider a liquid phase CSTR under isobaric conditions with one first order exothermic chemical reaction

¹ This work is supported by the Vietnam's National Foundation for Science and Technology Development (NAFOSTED) under research proposal number 101.01-2013.23. The authors gratefully acknowledge the support of the FNRS (Belgium). This paper presents research results of the Belgian Network DYSCO (Dynamical Systems, Control and Optimization), funded by the Interuniversity Attraction Poles Programme, initiated by the Belgian State, Science Policy Office. The scientific responsibility rests with its authors.

involving 2 chemical species A and B. The reaction stoichiometry is given as follows :

$$\nu_A A + \nu_B B = 0 \tag{1}$$

where ν_i and ν_j are the suitable signed stoichiometric coefficients : $-\nu_A = \nu_B = 1$ (Hoang and Dochain (2013a)). Let us consider the following assumptions :

(H1) The fluid mixture is ideal and incompressible.

(H2) The reactor is fed by the only species A with the inlet molar flow rate F_{AI} at a fixed temperature T_I .

(H3) The heat flow rate \dot{Q}_J coming from the jacket is modelled by the following relation :

$$\dot{Q}_J = \lambda (T_J - T) \tag{2}$$

where $\lambda > 0$ is the heat exchange coefficient. The jacket temperature T_J is used as the only control input.

 $({\bf H4})$ The reaction rate is described by the mass action law :

$$rV = k(T)N_A \tag{3}$$

where the liquid phase reaction kinetics k(T) is assumed to be monotone, non-negative and bounded in accordance to the thermodynamic principles by (Luyben (1990)) :

$$\lim_{T \to 0} k(T) = 0 \quad \text{and} \quad \lim_{T \to +\infty} k(T) = k_{\max} \tag{4}$$

We can easily check that the above conditions hold for the Arrhenius law

$$k(T) = k_0 \exp\left(\frac{-k_1}{T}\right) \tag{5}$$

where k_0 is the kinetic constant and k_1 is the activation temperature.

2.2 Thermodynamics based view for CSTR modeling

In equilibrium thermodynamics, the system variables are split into extensive variables (such as the internal energy U, the entropy S, the volume V and the molar number N_i) and intensive ones (such as the temperature T, the pressure P and the chemical potential μ_i). When isobaric conditions are considered, the variation of the internal energy U is equal to that of the enthalpy H, given by considering the Gibbs' equation (Callen (1985)) :

$$dH = \mu_A dN_A + \mu_B dN_B + TdS \tag{6}$$

From (6), we equivalently have :

$$dS = \frac{-\mu_A}{T}dN_A + \frac{-\mu_B}{T}dN_B + \frac{1}{T}dH \tag{7}$$

since the absolute temperature T > 0. As the entropy S is also an extensive variable, by using the Euler's theorem (Callen (1985)) we get :

$$S(N_A, N_B, H) = \frac{-\mu_A}{T} N_A + \frac{-\mu_B}{T} N_B + \frac{1}{T} H$$
(8)

 $\left(7\right)$ can then be rewritten in a compact form as follows:

$$dS = w^t dZ \quad \Rightarrow \quad w(Z)^t = \frac{\partial S(Z)}{\partial Z} \tag{9}$$

where

$$w(Z) = \left(\frac{-\mu_A}{T}, \frac{-\mu_B}{T}, \frac{1}{T}\right)^t, \quad Z = \left(N_A, N_B, H\right)^t$$
(10)

The system dynamics is given by considering the energy and material balance equations on the basis of the extensive variables presented in Z (Luyben (1990); Favache and Dochain (2010); Hoang *et al.* (2012)) :

$$\frac{dN_A}{dt} = F_{AI} - F_A - rV \tag{11}$$

$$\frac{dN_B}{dt} = -F_B + rV \tag{12}$$

$$\frac{dH}{dt} = \dot{Q}_J + F_{AI}h_{AI} - (F_Ah_A + F_Bh_B) \qquad (13)$$

where (F_A, F_B) , h_{AI} and (h_A, h_B) are the outlet flow rate vector, the inlet molar enthalpy and the molar enthalpy vector, respectively.

2.3 Thermodynamic availability

From the second law of thermodynamics for homogeneous systems, the entropy function S(Z) defined in (8) is necessarily concave with respect to Z (Callen (1985); Hoang and Dochain (2013a)). As a consequence, it can be shown (Ydstie and Alonso (1997); Hoang *et al.* (2012)) that the *availability function* \mathcal{A} defined as :

$$l(Z) = S_d + w_d^t (Z - Z_d) - S(Z) \ge 0$$
 (14)

is non negative. In (14), w_d is the intensive variable vector associated to the fixed extensive variable reference vector Z_d via the relation given in (9). The availability $\mathcal{A}(Z)$ (14) is positive definite and can then be used as a Lyapunov function candidate for control purpose (Alonso and Ydstie (2001); Hoang *et al.* (2011, 2012)). Finally thanks to the homogeneous property of degree one of the entropy S(Z)(8)-(10), the availability function (14) can be simplified as follows (Hoang *et al.* (2011)) :

$$\mathcal{A}(Z) = -S(Z) + w_d^t Z \ge 0 \tag{15}$$

Remark 1. It can be shown in the neighborhood of the reference vector Z_d that the availability \mathcal{A} (15) is viewed as the Legendre transformation of the concave entropy function S with respect to Z (8) (see also (Ruszkowski *et al.* (2005))).

Notation: For the sake of simplicity, let $\mathcal{I} = \{A, B\}$ be the set of chemical species involved in the reaction mixture (1).

3. PRELIMINARIES

3.1 Some properties of the availability A

Theorem 1 proposes a separation of \mathcal{A} (15) into two parts: the thermal part \mathcal{A}_1 and the material part \mathcal{A}_2 .

Theorem 1. (Hoang et al. (2012)) Under (H1), the availability function \mathcal{A} (15) can be expressed as the sum of two functions \mathcal{A}_1 and \mathcal{A}_2 so that :

$$\mathcal{A}_1(N_A, N_B, H) = -\sum_{k \in \mathcal{I}} \Gamma_k(T) N_k - \left(\frac{1}{T} - \frac{1}{T_d}\right) H(16)$$

$$\mathcal{A}_2(N_A, N_B) = -\sum_{k \in \mathcal{I}} \Lambda_k(N_A, N_B) N_k \tag{17}$$

where:

$$\Gamma_{k}(T) = c_{pk} \ln\left(\frac{T}{T_{d}}\right) - \frac{h_{k}}{T} + \frac{h_{kd}}{T_{d}}; \ k \in \mathcal{I}$$

$$\Lambda_{k}(N_{A}, N_{B}) = R \ln\left(\frac{N_{kd} \sum_{i \in \mathcal{I}} N_{i}}{N_{k} \sum_{i \in \mathcal{I}} N_{id}}\right); \ k \in \mathcal{I}$$
(18)

(i) $\mathcal{A}_1(N_A, N_B, H)$ has the following properties :

- $\mathcal{A}_1 \geq 0$
- \mathcal{A}_1 is a homogeneous function of degree one with respect to (N_A, N_B, H) . Consequently,

$$\frac{d\mathcal{A}_1}{dt} = -\sum_{k\in\mathcal{I}}\Gamma_k(T)\frac{dN_k}{dt} - \left(\frac{1}{T} - \frac{1}{T_d}\right)\frac{dH}{dt} \quad (19)$$

(ii) $\mathcal{A}_2(N_A, N_B)$ has the following properties :

- $\mathcal{A}_2 \ge 0$
- \mathcal{A}_2 is a homogeneous function of degree one with respect to (N_A, N_B) . Consequently,

$$\frac{d\mathcal{A}_2}{dt} = -\sum_{k\in\mathcal{I}} \Lambda_k(N_A, N_B) \frac{dN_k}{dt}$$
(20)

Remark 2. The functions \mathcal{A}_1 (16) and \mathcal{A}_2 (17) are strictly convex with respect to Z (10) if one constraint on extensive variables has been fixing (Jillson and Ydstie (2007); Hoang *et al.* (2012)). In what follows, the total molar number

$$N_t = N_A + N_B = const \tag{21}$$

is assumed to be constant 2 . This constraint is guaranteed by adjusting the outlet molar flows of the CSTR (refer to Lemma 1 below).

The availability $\mathcal{A}(Z)$ defined in (15) has been previously used for the passivity based control of reaction systems (Alonso and Ydstie (2001); Hoang *et al.* (2011, 2012, 2013c)). In this paper, we show that the positivity of the thermal part $\mathcal{A}_1(Z)$ (16) will also entail its use as a novel Lyapunov function candidate for the control purpose even when input constraints are imposed.

3.2 Representation of the system dynamics

Lemma 1 proposes a mathematical model of the constrained CSTR.

Lemma 1. The dynamical model of the CSTR defined in (11)-(13) subject to the constraint (21) becomes :

$$\frac{dN_A}{dt} = \left(1 - \frac{N_A}{N_t}\right)F_{AI} - rV \tag{22}$$

$$\frac{dN_B}{dt} = -\frac{N_B}{N_t}F_{AI} + rV \tag{23}$$

$$\frac{dH}{dt} = \left(h_{AI} - \frac{H}{N_t}\right)F_{AI} + \dot{Q}_J \tag{24}$$

where the reaction rate rV is given by (3)(5).

Proof. See (Hoang *et al.* (2012)).
$$\Box$$

Remark 3. Since we assume ideal mixture, the enthalpy of species $i, i \in \mathcal{I}$ can be expressed as follows :

$$h_i(T) = c_{pi}(T - T_{ref}) + h_{iref}$$

$$\tag{25}$$

Hence the energy balance (24) can be rewritten in terms of the temperature T by considering the expression of the total enthalpy as follows :

$$H = \sum_{i \in \mathcal{I}} n_i h_i(T) \tag{26}$$

We therefore obtain :

$$C_p \frac{dT}{dt} = \left(-\Delta H(T)\right) r V - qT + u \tag{27}$$

where $\Delta H(T) = (h_B(T) - h_A(T))$ is the heat of reaction, $C_p = c_{pA}N_A + c_{pB}N_B$ is the total heat capacity, and $q = (F_{AI}c_{pA} + \lambda)$. In (27), we consider that the control input defined by :

$$u = F_{AI}c_{pA}T_I + \lambda T_J \tag{28}$$

is bounded :

$$u_{\min} \le u \le u_{\max} \tag{29}$$

where u_{\min} and u_{\max} are the lower and upper input bounds, respectively.

Remark 4. The dynamics of the CSTR with the chemical transformation (1) are derived by considering the state variable vectors (H, N_A, N_B) or (T, N_A, N_B) .

Proposition 1 shows that the states (N_A, N_B) belong to a positively invariant domain $\begin{bmatrix} 0 & N_t \end{bmatrix}^2$.

Proposition 1. If
$$(N_A(0), N_B(0)) \in [0 \ N_t]^2$$
 then,
 $(N_A(t), N_B(t)) \in [0 \ N_t]^2, \ \forall t$ (30)

Proof. It is straightforward from (22) since $\frac{dN_A}{dt}\Big|_{N_A=0} =$

 $F_{AI} > 0$ and $\frac{dN_A}{dt}\Big|_{N_A = N_t} = -k_0 \exp(-\frac{k_1}{T})N_t < 0$. Hence $N_A(t) \in [0 \quad N_t], \ \forall t$. The rest of the proof automatically follows using (21).

The following corollary presents some properties of the thermal part \mathcal{A}_1 (16).

Corollary 1. There exist positive constants κ_1 and κ_2 such that:

$$\kappa_1 \varphi(T, T_d) \le \mathcal{A}_1 \le \kappa_2 \varphi(T, T_d)$$
 (31)

where the function $\varphi(T, T_d)$

$$\varphi(T, T_d) = -\left[1 - \frac{T}{T_d} + \ln\left(\frac{T}{T_d}\right)\right] \tag{32}$$

is non-negative.

Proof. Under (H1), it can be shown (Hoang *et al.* (2012)) that $\mathcal{A}_1 = -\left[1 - \frac{T}{T_d} + \ln\left(\frac{T}{T_d}\right)\right]C_p$. Let $\psi(T) = \ln(T)$ be a (globally) concave function. Hence the algebraic distance between the function $\psi(T)$ and its tangent passing through the reference temperature T_d is $\ln(T_d) + \frac{1}{T_d}(T - T_d) - \ln(T) \equiv \varphi(T, T_d)$. Thanks to Proposition 1, let us choose $\kappa_1 = \min_{(N_A, N_B) \in [0]} C_p > 0$ and $\kappa_2 =$

 $\max_{(N_A,N_B)\in [0 \ N_t]^2} C_p > 0. \text{ The latter ends the proof.} \qquad \Box$

3.3 Dynamical analysis

In the example considered here, the value of control input u (28) is chosen to be equal to : u = 445 (J.s⁻¹), and the lower and upper bounds are $u_{\min} = 425$ (J.s⁻¹) and

² This is a special variant of the constraint on the constant total mass $m_t = M_A N_A + M_B N_B = const$. Indeed the latter implies that $N_A + N_B = const$ since the molar masses M_A and M_B of the first order reaction (1) are equal with $-\nu_A = \nu_B = 1$.

 $u_{\text{max}} = 475 \text{ (J.s}^{-1}\text{)}$. Numerical values and thermodynamic parameters of the CSTR are given in (Hoang *et al.* (2012)).

Let $(\bar{N}_A, \bar{N}_B, \bar{T})$ be the steady states of the system dynamics defined in (3)(5)(22)-(24). We derive the following relations after some elementary calculations :

$$\bar{N}_A = \frac{F_{AI}}{\frac{F_{AI}}{N_t} + k(\bar{T})} , \quad \bar{N}_B = k(\bar{T}) \frac{N_t}{\frac{F_{AI}}{N_t} + k(\bar{T})}$$
(33)

and

$$\left(-\Delta H(\bar{T})\right)k(\bar{T})\frac{F_{AI}}{\left(\frac{F_{AI}}{N_t}+k(\bar{T})\right)} = q\bar{T}-u \tag{34}$$

It is shown (Van Heerden (1953)) that the left side of (34) is strongly related to the energy produced E_p during the reaction course,

$$E_p(\bar{T}) = \left(-\Delta H(\bar{T})\right) k(\bar{T}) \frac{F_{AI}}{\left(\frac{F_{AI}}{N_t} + k(\bar{T})\right)}$$
(35)

and the right side is the energy consumed E_c due to exchanges with the surrounding environment

$$E_c(\bar{T}, u) = q\bar{T} - u \tag{36}$$

The geometric representation of $E_p(\bar{T})$ (35) and $E_c(\bar{T}, u)$ defined in (36) with respect to \bar{T} provides the Van Heerden diagram as seen in Figure 1. The intersection of these curves that presents a (stationary) heat balance between the heat production and the heat consumption gives possible steady states of the CSTR. This diagram shows that a steady state is said to be (locally) stable if and only if the tangent of the heat production lies below the heat consumption (Van Heerden (1953)). Hence when the input



Fig. 1. Van Heerden diagram of the CSTR

control u = 445 is chosen, Figure 1 shows that there exist three steady states P_1 , P_2 and P_3 . Steady states P_1 and P_3 are (locally) stable, whereas the intermediate steady state P_2 is unstable. The stable steady state P'_1 resulting from $u_{\min} = 425$ or P'_3 calculated at $u_{\max} = 475$ is unique.

To end this part, we state the following proposition which plays a central role for the control design of the reaction system on the basis of the thermal part \mathcal{A}_1 defined in (16) of the availability function.

Proposition 2. The isothermal dynamics $(T \equiv \overline{T})$ of the system defined in (3)(5)(22)-(24) is globally asymptotically stable (e.g. $\overline{N}_A \to \overline{N}_A$ and $N_B \to \overline{N}_B$).

Proof. When the isothermal condition $(T \equiv \overline{T})$ is considered, the system dynamics (3)(5)(22)-(24) reduces to :

$$\frac{dN_A}{dt} = \left(1 - \frac{N_A}{N_t}\right) F_{AI} - k(\bar{T}) N_A \tag{37}$$
$$\frac{dN_B}{dN_B} = \frac{N_B}{N_B} F_{AI} + k(\bar{T}) N_A \tag{39}$$

$$\frac{N_B}{dt} = -\frac{N_B}{N_t} F_{AI} + k(\bar{T}) N_A \tag{38}$$

It is shown that (37) is globally stable at \bar{N}_A (33) with a Lyapunov function candidate given by $\mathcal{W}(N_A) = \frac{1}{2}(N_A - \bar{N}_A)^2$. The same argument can be used for the dynamics N_B (38).

Let us finally state the control problem.

Control Problem: we propose to operate the reactor at the temperature T = 330.1997 (K) which corresponds to the unstable intermediate steady state P_2 using the control input u (28). Furthermore the control variable u has the input constraints (29).

4. CONTROLLER SYNTHESIS

4.1 Thermodynamics based nonlinear controllers

For the sake of simplicity, let us first consider the case without input constraints and restate some results presented in (Hoang *et al.* (2012)).

Proposition 3. (Hoang et al. (2012)) The reaction system dynamics (3)(5)(22)-(24) is globally asymptotically stable and admits $(N_{Ad}, N_{Bd}, H_d)^t \equiv P_2$ as a desired operating point with the following state feedback law for u (28) :

$$u = \lambda T - \left[-c_{pA}T_{ref} + h_{Aref} - \frac{H}{N_t} \right] F_{AI} + K \left(\frac{1}{T} - \frac{1}{T_d} \right)$$

$$- \left(\frac{1}{T} - \frac{1}{T_d} \right)^{-1} \left(\Gamma_A(T) \frac{dN_A}{dt} + \Gamma_B(T) \frac{dN_B}{dt} \right)$$
(39)

where the tuning parameter K is positive. $\Gamma_A(T)$ and $\Gamma_B(T)$ are given in (18).

Proof. Let us consider the thermal part A_1 and the control input *u* defined in (16) and (28), respectively. From (2)(24)(39) and (19), we obtain :

$$\frac{d\mathcal{A}_1}{dt} = -K\left(\frac{1}{T} - \frac{1}{T_d}\right)^2 < 0 \tag{40}$$

Hence \mathcal{A}_1 decreases and reaches 0 when $T = T_d$. Finally, Proposition 2 completes the proof.

Remark 5. In the neighborhood of the desired temperature T_d , there exists a positive constant δ (e.g. $\delta = \frac{T_d^2}{2}$) so that we obtain from (32): $\varphi(T, T_d) \approx \delta \left(\frac{1}{T} - \frac{1}{T_d}\right)^2$. Using Corollary 1 and (40), we therefore have :

$$\frac{d\mathcal{A}_1}{dt} \le -\gamma \mathcal{A}_1 \quad \text{with} \quad \gamma = \frac{K}{\kappa_2 \delta} \tag{41}$$

Thus the positive definite function \mathcal{A}_1 is bounded above by itself. The stabilization is then globally asymptotic and locally exponential. For the sake of simulation, we assume that the CSTR is initialized in open loop at the stable high and low temperature steady states given by P_1 with $(T = 320.67 \text{ (K)}, N_A =$ $1.64 \text{ (mol)}, N_B = 0.36 \text{ (mol)})$ and P_3 with (T = $377.88 \text{ (K)}, N_A = 0.14 \text{ (mol)}, N_B = 1.86 \text{ (mol)})$. The following value of controller gain in (39) is consdered : $K = 10^5$. Figure 2 shows that the closed loop responses converge to the desired opertating state P_2 from the initial conditions P_1 and P_3 . Furthermore the control input is smooth as seen in Figure 3.



Fig. 2. Some closed loop responses in phase plane



Fig. 3. Control input u without constraints

4.2 Control with input constraints

An additional assumption (Viel *et al.* (1997); Alvarez-Ramírez and Morales (2000)) is considered. This assumption corresponds to the so-called feasibility condition.

(H5) The input constraints u_{\min} and u_{\max} are imposed so that the feedback law defined in (39) fulfills,

$$u_{\min} < u(T_d, N_A, N_B) < u_{\max}, \ \forall (N_A, N_B) \in [0 \quad N_t]^2$$
(42)

Assumption (H5) implies that there exists a temperature interval $\begin{bmatrix} T_1 & T_2 \end{bmatrix}$ such that $T_1 < T_d < T_2$ and the following inequality

$$u_{\min} < u(T, N_A, N_B) < u_{\max} \tag{43}$$

holds for all $(T, N_A, N_B) \in [T_1 \quad T_2] \times [0 \quad N_t]^2$. We can check for the CSTR example that $T_1 = 297.5$ (K) and $T_2 = 331$ (K).

Proposition 4 proposes a stabilizing feedback law under input constraints (29) for the controller defined in (39). It is the major contribution of this paper. *Proposition 4.* A bounded stabilizing feedback law given by

$$u^{new} = \begin{cases} u_{\min} \text{ if } (T > T_d) \text{ and } u \notin (u_{\min} \quad u_{\max}) \\ u \text{ if } u \in (u_{\min} \quad u_{\max}) \\ u_{\max} \text{ if } (T < T_d) \text{ and } u \notin (u_{\min} \quad u_{\max}) \end{cases}$$
(44)

globally stabilizes the reactor at the desired operating point $(N_{Ad}, N_{Bd}, H_d)^t \equiv P_2$.

Proof. The following two scenarios are considered when the input control u lies outside its desired interval $[u_{\min} \quad u_{\max}]$:

• If $T > T_2$ then from the definition (44) we have $u = u_{\min}$. In this case, the dynamics of the temperature defined in (27) is :

$$C_p \frac{dT}{dt} = \underbrace{\left(-\Delta H(T)\right) rV}_{E_p(T)} - \underbrace{\left(qT - u_{\min}\right)}_{E_c(T, u_{\min})}$$

Thanks to the Van Heerden diagram (Figure 1), we obtain $E_p(T) < E_c(T, u_{\min})$ and consequently, $\frac{dT}{dt} < 0$ since $C_p > 0$. We conclude that T decreases to T_2 . If $T < T_1$ then the definition (44) gives $u = u_{\max}$.

• If $T < T_1$ then the definition (44) gives $u = u_{\text{max}}$ The dynamics of the temperature (27) becomes :

C

$$\int_{D} \frac{dI}{dt} = \underbrace{\left(-\Delta H(T)\right)rV}_{E_{p}(T)} - \underbrace{\left(qT - u_{\max}\right)}_{E_{c}(T,u_{\max})}$$

Same arguments as the previous case can be considered. Consequently, T increases to T_1 .

The temperature trajectory is trapped within its positively invariant interval $[T_1 \ T_2]$ even when $u(t = 0) = u_{\min}$ or $u(t = 0) = u_{\max}$. Under (H5), the feedback law u defined in (39) then plays its role for the stabilization. The latter ends the proof.

Remark 6. If the heat consummation curve $E_c(\bar{T}, u)$ corresponding to $u = u_{\min}$ or $u = u_{\max}$ has more than two intersections with the heat production curve $E_p(\bar{T})$ on the Van Heerden diagram (Figure 1) then an additional control input (for instance the inlet molar flow rate of the supplied species F_{AI}) should be considered for further developments. Such a situation has been previously studied in (Viel *et al.* (1997)) based on feedback linearization.

Only the initial condition P_3 is considered for numerical simulations since the control input u of the unconstrained reactor initialized at P_3 is out of its bounds $\begin{bmatrix} u_{\min} & u_{\max} \end{bmatrix}$ (refer to Figure 3). Figures 4 and 5 present the closed loop time response and the control variable with the input constraints, respectively.

5. CONCLUSION

In this work, we have shown how to stabilize an unstable CSTR at any desired operating point (including unstable open loop stationary point) by means of the Lyapunovbased method under input constraints using physical insights. More precisely, the closed loop Lyapunov function candidate is the thermal part of the availability function directly derived from some concepts and foundations of thermodynamics. Besides, the strategy adopted for the input-constrained control problem is intrinsically based



Fig. 4. Closed loop time response



Fig. 5. Control with input constraints

on energetic transformations of the reaction system on the basis of the analysis of the Van Heerden diagram. The global asymptotic stabilization of the reactor is theoretically guaranteed with a local exponential behavior. The numerical simulation results showed that convergence objective is satisfied and that the state feedback law is implementable. It remains now to evaluate performances and robustness of the proposed results in terms of perturbations and parameters uncertainty; extend to the multiple chemical reaction system and the infinite dimensional thermodynamic systems. First results of the research perspective can be found in (Hoang and Dochain (2013a,b)).

REFERENCES

- Alonso A.A. and Ydstie B.E. (2001). Stabilization of distributed systems using irreversible thermodynamics, *Automatica*. 37:1739-1755.
- Alvarez-Ramírez J. and Morales A. (2000). PI control of continuously stirred tank reactors: stability and performance. *Chem. Eng. Sci.* 55(22):5497-5507.
- Alvarez J., Alvarez-Ramírez, J., Espinosa-Perez G. and Schaum A. (2011). Energy shaping plus damping injection control for a class of chemical reactors. *Chem. Eng. Sci.* 66(23):6280-6286.
- Antonelli R. and Astolfi A. (2003). Continuous stirred tank reactors: easy to stabilise? *Automatica*. 39:1817-1827.
- Bayer F., Bürger M., Guay M. and Allgöwer F. (2011). On State-Constrained Control of a CSTR. *IFAC World Congress*, Milano, Italia. 6079-6084.
- Balestrino A., Caiti A. and Grammatico S. (2012). Multivariable constrained process control via Lyapunov Rfunctions. J. Proc. Control. 22:1762-1772.

- Bruns D.D. and Bailey J.E. (1975). Process operation near an unstable steady state using nonlinear feedback control. *Chem. Eng. Sci.*, Vol. 30, pp. 755-762.
- Callen H.B. (1985). Thermodynamics and an introduction to thermostatics. John Wiley & Sons, New York, 2nd ed.
- Dörfler F., Johnsen J.K. and Allgöwer F. (2009). An introduction to interconnection and damping assignment passivity-based control in process engineering. J. Proc. Control. 19:1413-1426.
- Favache A. and Dochain D. (2010). Power-shaping of reaction systems : the CSTR case study. Automatica. 46(11):1877-1883.
- Farschman C.A., Viswanath K.P. and Ydstie B.E. (1998). Process systems and inventory control. AIChE journal. 44(8):1841-1857.
- Hangos K.M., Bokor J. and Szederkényi G. (2001). Hamiltonian view on process systems. AIChE journal. 47(8):1819-1831.
- Hoang H., Couenne F., Jallut C. and Le Gorrec Y. (2011). The Port Hamiltonian approach to modeling and control of Continuous Stirred Tank Reactors. J. Proc. Control. 21(10):1449-1458.
- Hoang H., Couenne F., Jallut C. and 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. and Dochain D. (2013a). On an evolution criterion of homogeneous multi-component mixtures with chemical transformation. *Syst. & Contr. Let.* 62(2):170-177.
- Hoang H. and Dochain D. (2013b). A thermodynamic approach to the passive boundary control of tubular reactors. *Proc. 9th IFAC-NOLCOS*. Toulouse, France.
- Hoang H., Couenne F., Jallut C. and Le Gorrec Y. (2013c). Thermodynamics based stability analysis and its use for nonlinear stabilization of CSTR. *Computers & Chemical Engineering.* 58(11):156-177.
- Hu T. and Lin Z. (2001). Control systems with actuator saturation: analysis and design. Boston: Birkhäuser.
- Liu D. and Michel A.N. (1994). Dynamical systems with saturation nonlinearities. New York: Springer-Verlag.
- Luyben W.L. (1990). Process modeling, simulation, and control for chemical engineers. McGraw-Hill, Singapore.
- Jillson K.R. and Ydstie B.E. (2007). Process networks with decentralized inventory and flow control. J. Proc. Control. 17:399-413.
- Ramírez H., Maschke B. and Sbarbaro D. (2013). Irreversible port-Hamiltonian systems: A general formulation of irreversible processes with application to the CSTR. *Chem. Eng. Sci.* 89:223-234.
- Ruszkowski M., Garcia-Osorio V. and Ydstie B.E. (2005). Passivity based control of transport reaction systems. *AIChE Journal.* 51:3147-3166.
- Van Heerden C. (1953). Autothermic processes. Ind. Eng. Chem. 45(6):1242-1247.
- Viel F., Jadot F. and Bastin G. (1997). Global stabilization of exothermic chemical reactors under input constraints. *Automatica*. 33(8):1437-1448.
- Ydstie B.E. and Alonso A.A. (1997). Process systems and passivity via the Clausius-Planck inequality. Syst. & Contr. Let. 30(5):253-264.