Partial inventory control of the CSTR via reaction-dependent generalized inventories

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Abstract: Motivated by considering structurally dynamical properties of reaction systems, we develop an approach to deal with the nonlinear control of an unstable CSTR. More precisely, this paper shows that the CSTR dynamics can be split into reaction variant and reaction invariant dynamics modes through the use of linear combinations of system variables (called inventories). Since the reaction invariant dynamics mode is exponentially stable, the control design for an exponential stabilization of the reactor is simply solved together with (partial) inventory control on the basis of controlling the reaction variant dynamics mode. An extension of the approach to multiple chemical reaction systems is briefly outlined. Simulation results for a first order chemical reaction with multiplicity behavior are given to illustrate the theoretical development.

Keywords: Inventory control, Lyapunov function, CSTR, Reaction variants/invariants.

1. INTRODUCTION

Open homogeneous reaction systems and in particular, Continuous Stirred Tank Reactors (CSTRs) belong to a typical class of nonlinear dynamical systems described by Ordinary Differential Equations ODEs (Luyben (1990)). The CSTR is a simple chemical process system but concentrates many intrinsic difficulties and theoretical challenging issues which the system control theory has to overcome: the system dynamics may be involved with possible multiple steady states behavior or non-minimum phase characteristics because of nonlinear constitutive relations (for instance, chemical reaction kinetics and transport phenomena etc.) (Hoang *et al.* (2013b)). The underlying motivation for controlling the CSTRs is that industrial chemical reactors may have to be operated at unstable operating conditions which correspond to some optimal process performances (Bruns & Bailey (1975)). Over the years a number of control strategies have been proposed to deal with the nonlinear feedback control of unstable homogeneous chemical reactors. Generally speaking, these strategies are mainly based on mathematical tools such as Lyapunov methods, differential geometry (Khalil (2002))

and passive techniques (Van Der Schaft (2000)). Besides, the physics-based approach through the application of thermodynamics to the stability analysis and control design of open reaction systems establishes an active research area (Georgakis (1986); Ydstie & Alonso (1997); Srinivasan *et al.* (1998)) and is recently extensively considered in the literature (Ruszkowski *et al.* (2005); Eberard *et al.* (2007); Favache & Dochain (2009); Hoang *et al.* (2011, 2012a,b); Hoang & Dochain (2013a); Hoang *et al.* (2013b); Hoang & Dochain (2013c); Ramírez *et al.* (2013)).

This paper deals with the nonlinear control of an unstable CSTR in the context of thermodynamics on the basis of reaction variant and reaction invariant dynamics of the chemical reactor together with the inventory control (Ydstie & Viswanath (1994); Farschman *et al.* (1998); Hoang *et al.* (2013d)). More precisely, as shown in the pioneering works of (Asbjornsen (1972); Fjeld *et al.* (1974)), the thermodynamic state variables form linear combinations which constitute the reaction variant and reaction invariant dynamics modes. As a consequence, this state transformation allows to reduce the dimension of the state space usable both for the stability analysis and control design of the reaction system since the reaction invariant dynamics mode that belongs to a positive invariant is exponentially stable. On the basis of the reduced state variables, the nonlinear stabilization of the reactor at a desired reference operating point (set-point) is simply solved by adopting an inventory control-related approach. It is shown that the inventory control is based on the idea of passivity and dissipation of high order dynamics which are not controlled and renders

them passive and then dissipative by stabilizing feedback laws on boundary control inputs.

This paper is organized as follows. The inventory control strategy is briefly introduced and the way to obtain the state feedback law is mentioned in section 2. In section 3 the dynamical model of the CSTR is presented and analyzed. This section is devoted to the design of the state feedback law insuring the exponential stability of the entire system. Moreover it is shown that the resulting control is admissible. Finally, numerical simulation results are given in section 4.

2. INVENTORY CONTROL STRATEGY

Throughout the paper, we focus our attention on the CSTRs model which is affine in the control input u and whose dynamics are given by the following set of ODE's by considering the energy and material balance equations :

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

where $x = x(t) \in \mathbb{R}^n$ is the inventory vector [2], $f(x) \in \mathbb{R}^n$ 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 control input.

The central objective of the inventory control is to control some process inventory such as x to its (constant) set-point x_d by choosing the manipulated input variable u so that the candidate Lyapunov function of the dynamics (1) decreases. A particularly useful candidate for that purpose is the following function (Ydstie & Viswanath (1994); Farschman *et al.* (1998); Hoang *et al.* (2013d)) :

$$\Psi(x) = \frac{1}{2}(x - x_d)^{\mathrm{T}}(x - x_d) \tag{2}$$

One can show that its time derivative is then given by

$$\frac{d\Psi(x)}{dt} = (x - x_d)^{\mathrm{T}} \frac{dx}{dt} \tag{3}$$

From the inventories dynamics $\frac{dx}{dt}$ (1), (3) becomes :

$$\frac{d\Psi(x)}{dt} = (x - x_d)^{\mathrm{T}} \Big(f(x) + g(x)\,u \Big) \tag{4}$$

If the following non linear PF-F (Proportional Feedback-Feedforward) control input u is chosen so that

$$u = g(x)^{\mathrm{T}} \big(g(x)g(x)^{\mathrm{T}}\big)^{-1} \Big(-f(x) - K_c(x)\,(x - x_d) \Big) \tag{5}$$

then,

$$\frac{d\Psi(x)}{dt} = -(x - x_d)^{\mathrm{T}} K_c(x)\,(x - x_d) \tag{6}$$

and

$$\frac{d\Psi(x)}{dt} \leq -2\bar{k}_c \Psi(x) \tag{7}$$

where $K_c(x)$ in (5) is a positive definite gain matrix and $\bar{k}_c$ (7) is its smallest eigenvalue.

It is shown that the candidate Lyapunov function $\Psi(x)$ (2) is positive definite and its time derivative (7) is radially bounded via the feedback law (5). As a consequence, the Lyapunov function $\Psi(x)$ globally exponentially decreases.

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[2] The inventory of a chemical reaction system is a non-negative integral measure that calculates physical properties such as internal energy and total molar number or total mass of each present chemical species (Ydstie & Viswanath (1994); Farschman *et al.* (1998)).

3. THE CSTR CASE STUDY

Let us consider a CSTR with one irreversible reaction involving two chemical species A and B. The stoichiometric relation that represents the (molar) mass conservation of the reaction is given as follows :

$$\nu_A A \rightarrow \nu_B B \tag{8}$$

where the stoichiometric coefficients ν_A and ν_B are signed: $\nu_A < 0$ and $\nu_B > 0$ (Ruszkowski *et al.* (2005); Hoang & Dochain (2013a); Ramírez *et al.* (2013)). The reactor is fed by species A and B and Inert at a fixed inlet temperature T_I. The jacket temperature T_J (assumed to be uniform) together with the inlet molar numbers (N_{AI}, N_{BI}) are considered as the manipulated process inputs.

The following modeling assumptions are considered here :

(**A1**) The reaction mixture is ideal, incompressible and under isobaric conditions.
(**A2**) The heat flow rate $\dot{Q}_J$ coming from the jacket is modelled by the following relation :

$$\dot{Q}_J = \lambda(T_J - T) \tag{9}$$

where $\lambda > 0$ is the heat exchange coefficient and T is the reactor temperature.
(**A3**) The specific heat capacities c_{pA}, c_{pB} and $c_{p\mathrm{Inert}}$ are assumed to be constant.
(**A4**) The molar number of two active species A and B in the reactor and in the inlet molar flow are very low compared to the molar number of the Inert. Hence the reaction volume V can be written as follows :

$$V \simeq v_{\mathrm{Inert}} N_{\mathrm{Inert}} = const \tag{10}$$

where v_{Inert} denotes the (constant) molar volume of species Inert. The volume V is supposed to be constant. As a consequence of the constraint on the constant volume, the inlet and outlet volumetric flow rates are equal (*i.e.* $F_I = F_O = F$).
(**A5**) The reaction rate is described by the mass-action-law :

$$r_{\mathrm{v}} V = k(T) N_A^{|\nu_A|} \tag{11}$$

where the liquid phase reaction kinetics $k(T)$ is assumed to be monotone, non-negative and bounded in accordance to the thermodynamic constraints by (Luyben (1990); Favache & Dochain (2010); Alvarez *et al.* (2011)) :

$$\lim_{T \to 0} k(T) = 0 \quad \text{and} \quad \lim_{T \to +\infty} k(T) = k_{\max} \tag{12}$$

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

$$k(T) = k_0 \exp(\frac{-E_a}{RT}) \tag{13}$$

where E_a and R are the activation energy and the ideal gas constant, respectively. The positive scalar k_0 is the reaction kinetic constant.

The physical variables of the CSTR model are introduced in Table 1.

Table 1. The physical variables of the CSTR

Notation	Unit	
h_{iI}	$Jmol^{-1}$	Inlet molar enthalpy of i ($i = A, B, \text{Inert}$)
h_i	$Jmol^{-1}$	Partial molar enthalpy of i ($i = A, B, \text{Inert}$)
N_{AI}	mol	Inlet mole number of species A
N_{BI}	mol	Inlet mole number of species B
$N_{\text{Inert}I}$	mol	Inlet mole number of species Inert
N_A	mol	Mole number of species A
N_B	mol	Mole number of species B
N_{Inert}	mol	Mole number of species Inert
$d = \frac{F}{V}$	s^{-1}	Dilution rate
$r_{\mathrm{v}}V$	$mols^{-1}$	Reaction rate

Notations: Let $\mathcal{S} = \{A, B\}$ be the set of active chemical species involved in the reaction (8). Let $\mathcal{I} = \mathcal{S} \cup \{\text{Inert}\}$ denote the set composed of all present chemical species.

3.1 The CSTR modeling

The system dynamics are given by considering the energy and material balance equations. When the isobaric conditions are considered (Assumption (**A1**)), the energy balance is written using the enthalpy H instead of internal energy U. The balance equations are then of the following form (Favache & Dochain (2010); Hoang *et al.* (2013e)) :

$$\begin{cases} \dfrac{dH}{dt} = d\left(H_I - H\right) + \dot{Q}_J \\ \dfrac{d\boldsymbol{N}}{dt} = d\left(\boldsymbol{N}_I - \boldsymbol{N}\right) + \boldsymbol{\nu}\, r_{\mathrm{v}}V \end{cases} \quad (14)$$

where $d = \frac{F}{V}$, $\boldsymbol{N}_I = (N_{AI}, N_{BI})^{\mathrm{T}}$ and $\boldsymbol{N} = (N_A, N_B)^{\mathrm{T}}$ are the dilution rate and the vectors composed of inlet and outlet mole numbers, respectively. $\boldsymbol{\nu} = (\nu_A, \nu_B)^{\mathrm{T}}$ is the stoichiometric vector.

Remark 1. Since we suppose the ideality of the reaction mixture, the enthalpy of species i can be expressed as $h_i(T) = c_{pi}(T - T_{ref}) + h_{iref}$, $\forall i \in \mathcal{I}$ where T_{ref} and h_{iref} are the reference temperature and reference molar enthalpy, respectively. The total enthalpy H of the reaction system can then be written as follows :

$$H = \sum_{i \in \mathcal{I}} N_i h_i(T) \quad (15)$$

Thanks to the local equilibrium hypothesis, the energy balance $\frac{dH}{dt}$ given in (14) can also be rewritten in terms of temperature. This is done by using the expression of the enthalpy H (15), we obtain (Favache & Dochain (2010); Hoang *et al.* (2012a, 2013e)) :

$$C_p \frac{dT}{dt} = \left(-\Delta_R H\right) r_{\mathrm{v}}V + d\left(T_I - T\right)C_{pI} + \dot{Q}_J \quad (16)$$

where $\Delta_R H = \sum_{i \in \mathcal{S}} \nu_i h_i(T)$ is the reaction heat [3] and

$C_p = \sum_{i \in \mathcal{I}} c_{pi} N_i$ is the total heat capacity, respectively.

Remark 2. The similar expression of the dynamics of Inert is given as follows :

$$\frac{dN_{\text{Inert}}}{dt} = d\left(N_{\text{Inert}I} - N_{\text{Inert}}\right) \quad (17)$$

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[3] Following usual thermodynamic notations $(-\Delta_R H) > 0$ for exothermic reactions and $(-\Delta_R H) < 0$ for endothermic reactions.

From (10) it follows that the constraint on the constant volume can only be guaranteed only if $\frac{dN_{\text{Inert}}}{dt} \equiv 0$ or $N_{\text{Inert}} = const$ with respect to time. This condition holds by imposing some appropriate initial condition (*i.e.* $N_{\text{Inert}}(t = 0) = N_{\text{Inert}I}$). Even the species Inert does not participate to the chemical reaction (8), its presence in the reactor should be considered when calculating the total heat capacity C_p as well as the total enthalpy H (15).

3.2 Reaction variant and reaction invariant dynamics

The central core of a decomposition the system dynamics (14) that emphasizes reaction invariant and variant dynamics modes in the sense of (Asbjornsen (1972); Fjeld *et al.* (1974)) is based on a size-preserving transformation of the reaction matrix (Hoang *et al.* (2013e)). It is worth noting that the energy balance $\frac{dH}{dt}$ given in (14) implicitly depends on the reaction rate [4]. In such an instance, it can be considered as an implicit reaction variant. As a consequence for the case we are concerned with here, the reaction matrix reduces to the stoichiometric coefficient vector $\boldsymbol{\nu} = (\nu_A, \nu_B)^{\mathrm{T}}$.

Let $\boldsymbol{\nu}^{\dagger}$ and $\boldsymbol{\nu}^{\perp}$ are the (pseudo) invertible and removal elements of $\boldsymbol{\nu}$, respectively so that :

$$\boldsymbol{\nu}^{\dagger}\boldsymbol{\nu} = 1 \quad \text{and} \quad \boldsymbol{\nu}^{\perp}\boldsymbol{\nu} = 0 \quad (18)$$

It follows that :

$$\boldsymbol{\nu}^{\dagger} = \left(\frac{1}{2\nu_A}, \frac{1}{2\nu_B}\right)^{\mathrm{T}} \quad \text{and} \quad \boldsymbol{\nu}^{\perp} = \left(-\frac{1}{\nu_A}, \frac{1}{\nu_B}\right)^{\mathrm{T}} \quad (19)$$

Let us now define a state transformation :

$$\boldsymbol{\mathcal{M}} = \mathcal{T}\boldsymbol{N} \quad (20)$$

where $\boldsymbol{\mathcal{M}} = (\overline{\mathcal{M}}, \underline{\mathcal{M}})^{\mathrm{T}}$ and the transformation matrix $\mathcal{T}$ is defined as follows :

$$\mathcal{T} = \begin{pmatrix} \boldsymbol{\nu}^{\dagger} \\ \boldsymbol{\nu}^{\perp} \end{pmatrix} \equiv \begin{pmatrix} \dfrac{1}{2\nu_A} & \dfrac{1}{2\nu_B} \\ -\dfrac{1}{\nu_A} & \dfrac{1}{\nu_B} \end{pmatrix} \quad (21)$$

Remark 3. Since the vectors $\boldsymbol{\nu}^{\dagger}$ and $\boldsymbol{\nu}^{\perp}$ (18)(19) are linearly independent, it is straightforward to show the square matrix $\mathcal{T}$ (21) is non singular. As a consequence of (20), we have :

$$\boldsymbol{N} = \mathcal{T}^{-1}\boldsymbol{\mathcal{M}} \quad (22)$$

where :

$$\mathcal{T}^{-1} = \begin{pmatrix} \nu_A & -\dfrac{\nu_A}{2} \\ \nu_B & \dfrac{\nu_B}{2} \end{pmatrix} \quad (23)$$

Remark 4. Thanks to the thermodynamic relation (15) and since $N_{\text{Inert}} = const$, the temperature T can be derived as a (nonlinear) function of $(H, \overline{\mathcal{M}}, \underline{\mathcal{M}})$, *i.e.* $T = \hat{T}(H, \overline{\mathcal{M}}, \underline{\mathcal{M}})$ (see Hoang & Dochain (2013a)) through the use of the (inverse) state transformation (22)(23) :

$$T = \frac{H - \boldsymbol{h}_{ref}^{\mathrm{T}}\mathcal{T}^{-1}\boldsymbol{\mathcal{M}} - h_{\text{Inert}ref}N_{\text{Inert}}}{\boldsymbol{c}_p^{\mathrm{T}}\mathcal{T}^{-1}\boldsymbol{\mathcal{M}} + c_{p\text{Inert}}N_{\text{Inert}}} + T_{ref} \quad (24)$$

Let us state the following proposition.

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[4] Indeed the alternative expression of the energy balance in terms of temperature (16) is strongly related to the reaction kinetics. This is of course due to the thermodynamic relation (15). However, (16) is not considered in this work since the temperature T is not an inventory (or an extensive quantity).

Proposition 1. The state transformation defined in (20)(21) transforms the system dynamics (14) into reaction variant and reaction invariant dynamics modes. Their explicit forms are given as follows :

$$\begin{cases} \dfrac{dH}{dt} = d\,(H_I - H) + \dot{Q}_J \\ \dfrac{d\overline{\mathcal{M}}}{dt} = d\,(\overline{\mathcal{M}}_I - \overline{\mathcal{M}}) + r_{\mathrm{v}}V \\ \dfrac{d\underline{\mathcal{M}}}{dt} = d\,(\underline{\mathcal{M}}_I - \underline{\mathcal{M}}) \end{cases} \tag{25}$$

where the reaction rate $r_{\mathrm{v}}V$ is a nonlinear function of $(H, \overline{\mathcal{M}}, \underline{\mathcal{M}})$.

Proof. The proof immediately follows. Indeed, one obtains from (20)(21) :

$$\frac{d\boldsymbol{\mathcal{M}}}{dt} = d\,(\boldsymbol{\mathcal{M}}_I - \boldsymbol{\mathcal{M}}) + \begin{pmatrix} 1 \\ 0 \end{pmatrix} r_{\mathrm{v}}V$$

where the dynamics $\frac{d\boldsymbol{N}}{dt}$ in (14) have been used. Finally, we conclude the proof by considering the reaction rate $r_{\mathrm{v}}V$ (11)(13) with (22)-(24). □

In what follows, let (H_d, N_{Ad}, N_{Bd}) be the desired stationary state of the dynamics (14) corresponding to nominal operating conditions :

$$T_J = T_J^{no}, \quad N_{AI} = N_{AI}^{no} \quad \text{and} \quad N_{BI} = N_{BI}^{no} \tag{26}$$

Equivalently, the dynamics (25) has its desired set-point $(H_d, \overline{\mathcal{M}}_d, \underline{\mathcal{M}}_d)$ calculated by considering the state transformation (20)(21) at $\boldsymbol{N} = \boldsymbol{N}_d$:

$$\begin{cases} \overline{\mathcal{M}}_d = \dfrac{1}{2\nu_A}N_{Ad} + \dfrac{1}{2\nu_B}N_{Bd} \\ \underline{\mathcal{M}}_d = -\dfrac{1}{\nu_A}N_{Ad} + \dfrac{1}{\nu_B}N_{Bd} \end{cases} \tag{27}$$

In particular, let us also note from (25) that

$$\underline{\mathcal{M}}_d = \underline{\mathcal{M}}_I \tag{28}$$

where :

$$\underline{\mathcal{M}}_I = -\frac{1}{\nu_A}N_{AI}^{no} + \frac{1}{\nu_B}N_{BI}^{no} \tag{29}$$

Remark 5. Since $\nu_A < 0$ and $\boldsymbol{N} > 0$, from (20)(21) it follows that $\underline{\mathcal{M}}$ is positive. The dynamics of $\underline{\mathcal{M}}$ in (25) represents a simple form of the (molar) mass conservation in the reactor. Since $d > 0$, it is shown that $\underline{\mathcal{M}}$ exponentially converges to $\underline{\mathcal{M}}_d = \underline{\mathcal{M}}_I$. Futhuremore, the domain $\Omega = \left\{ \underline{\mathcal{M}}(t) \middle| 0 \le \underline{\mathcal{M}}(t=0) \le \underline{\mathcal{M}}_I \right\}$ is positively invariant.

The central objective of this work is to design state feedback control laws for the variable process inputs T_J, N_{AI} and N_{BI} in order to stabilize the reactor dynamics (14) at the desired operating point (set-point) (H_d, N_{Ad}, N_{Bd}). In the following, we show that the control design can simply be solved by using the equivalent dynamics (25) through the elimination of the reaction invariant dynamics (*i.e.* model reduction).

3.3 Controller synthesis

Let us state the following proposition that allows to reduce the dimension of the dynamics (25).

Proposition 2. Since the reaction invariant dynamics are (exponentially) stable, the dynamics (25) reduce to a lower dimensional ones described by (1) with :

$$x = \begin{pmatrix} H \\ \overline{\mathcal{M}} \end{pmatrix}, \; u = \begin{pmatrix} \dot{Q}_J \\ \overline{\mathcal{M}}_I \end{pmatrix}, \; f(x) = \begin{pmatrix} d(H_I - H) \\ -d\overline{\mathcal{M}} + r_{\mathrm{v}}V \end{pmatrix} \tag{30}$$

$$g(x) = \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix} \tag{31}$$

Furthermore, $g(x)$ is invertible.

Proof. The proof immediately follows. □

In what follows, the control design is realized through the application of the inventory control strategy to derive a feedback control law for u (30) that allows to stabilize the reduced dynamics (1)(30)(31) at $x_d = (H_d, \overline{\mathcal{M}}_d)$. Let us state the following proposition.

Proposition 3. The following state feedbacks :

$$\begin{cases} \dot{Q}_J = -K_1(H - H_d) - d\,(H_I - H) \\ \overline{\mathcal{M}}_I = \dfrac{1}{d}\Big(-K_2(\overline{\mathcal{M}} - \overline{\mathcal{M}}_d) - r_{\mathrm{v}}V \Big) + \overline{\mathcal{M}} \end{cases} \tag{32}$$

with the tuning parameters $K_1 > 0$ and $K_2 > 0$, exponentially globally stabilize the reduced dynamics (1)(30)(31) at the desired state $x_d = (H_d, \overline{\mathcal{M}}_d)$.

Proof. The proof immediately follows by using (2)(5) of the inventory control with $K_c(x) = \mathrm{diag}(K_1, K_2)$. □

Remark 6. As a consequence of Proposition 3, the nonlinear state feedback laws considered for the physical inputs of the process (*i.e.* the jacket temperature T_J and the inlet molar number vector $\boldsymbol{N}_I = (N_{AI}, N_{BI})^{\mathrm{T}}$) are of the following expressions through the use of the (inverse) state transformation (22)(23) and (9) :

$$\begin{cases} T_J = T + \dfrac{1}{\lambda}\dot{Q}_J \\ \boldsymbol{N}_I = \mathcal{T}^{-1}\boldsymbol{\mathcal{M}}_I \end{cases} \tag{33}$$

where $\boldsymbol{\mathcal{M}}_I = (\overline{\mathcal{M}}_I, \underline{\mathcal{M}}_I)^{\mathrm{T}}$ and $\dot{Q}_J$ are given in (29)(32).

Remark 7. Let us consider a CSTR involving n_r independent chemical reactions with n_c (active) chemical species S_j ($j = 1 \ldots n_c$). The stoichiometric representation of such a reactions network is expressed as follows (Ruszkowski *et al.* (2005); Hoang & Dochain (2013a)) :

$$\sum_{j=1}^{n_c} \nu_{ij}S_j = 0, \quad i = 1 \ldots n_r \tag{34}$$

Let us note that the following condition,

$$n_r + 1 \le n_c \tag{35}$$

holds for industrial chemical reaction networks.

As previously shown, the reaction matrix $\boldsymbol{\nu}$ is completely formed by stoichiometric coefficients. We therefore have :

$$\boldsymbol{\nu} = \Big(\nu_{ij} \Big)_{n_c \times n_r} \tag{36}$$

Since $n_r < n_c$ (35), it follows that $\mathrm{rank}(\boldsymbol{\nu}) = n_r$. In other words, there exists a non singular square matrix $\mathcal{T}$ so that (Hoang *et al.* (2013e)) :

$$\mathcal{T}\boldsymbol{\nu} = \begin{pmatrix} \mathbb{I}_{n_r \times n_r} \\ \mathbf{0}_{(n_c - n_r) \times n_r} \end{pmatrix}_{n_c \times n_c} \tag{37}$$

where $\mathbb{I}_{n_r \times n_r}$ and $\mathbf{0}_{(n_c - n_r) \times n_r}$ are the identity and the zero matrices, respectively. The state transformation defined by $\boldsymbol{\mathcal{M}} = \mathcal{T}\boldsymbol{N}$ (20) therefore gives :

$$\boldsymbol{\mathcal{M}} = \begin{pmatrix} \overline{\boldsymbol{\mathcal{M}}}_{n_r \times 1} \\ \underline{\boldsymbol{\mathcal{M}}}_{(n_c - n_r) \times 1} \end{pmatrix}_{n_c \times 1} \tag{38}$$

where the dynamics of the (generalized) inventories $\overline{\mathcal{M}}$ and $\underline{\mathcal{M}}$ allow to emphasize the reaction variant and reaction invariant dynamics modes of the original system dynamics, respectively. Finally, the control design of the non isothermal reaction network is then solved on the basis of the lower dimensional dynamics associated to $x = (H, \overline{\mathcal{M}})_{(n_r+1)\times 1}$ by using the inventory control strategy.

4. SIMULATION

In this section, the exothermic chemical reaction (8) is considered for simulation with $\nu_A = -1$ and $\nu_B = 1$ (*i.e.* a first order reaction (Viel *et al.* (1997); Favache & Dochain (2010))). The numerical values of the CSTR model can be found in (Hoang *et al.* (2013e)). The objective of this section is to illustrate the application of the proposed control laws (33) for the stabilization of the CSTR at a desired operating point.

The open and closed loop simulations are carried out with two different initial condition scenarios, IC_1 with $\left(T_0 = 335\ (K), N_{A0} = 0.04\ (mol), N_{B0} = 0.001\ (mol)\right)$ and IC_2 with $\left(T_0 = 300\ (K), N_{A0} = 0.14\ (mol), N_{B0} = 0.03\ (mol)\right)$.

4.1 Open loop simulation

First of all let us consider open loop simulation with the nominal operating conditions (26) defined by (39) :

$$T_J^{no} = 298\ (K), N_{AI}^{no} = 0.18\ (mol), N_{BI}^{no} = 0\ (mol) \quad (39)$$

We assume that the additional process inputs

$$T_I = 298\ (K) \quad \text{and} \quad N_{\text{Inert}I} = 3.57\ (mol) \quad (40)$$

are fixed during the reaction course. Details on analysis of the steady states can be found in (Hoang & Dochain (2013c)). As shown with the Van Heerden diagram at a stationary regime (Figure 1), the reaction system exhibits three steady states denoted by P_1, P_2 and P_3, respectively. The states P_1 and P_3 are (locally) stable whereas the middle steady state P_2 is unstable. In the next section,
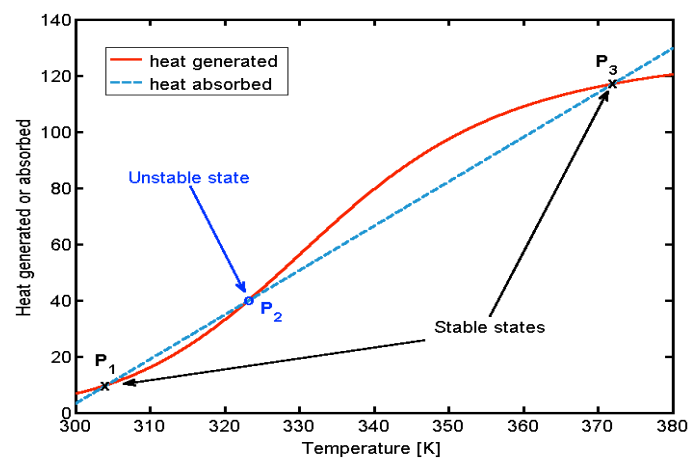

Fig. 1. The Van Heerden diagram of the CSTR

we propose to operate the reaction system at the unstable middle steady state P_2 using the state feedback laws proposed in (33).

4.2 Closed loop simulation

Let us assume that the system variables are completely measured. The reaction system is then closed using the state feedback laws (33) with $K_1 = 0.008$ and $K_2 = 0.005$.

In Figure 2 the closed loop phase plane is represented. It is shown that the system dynamics converge to the desired operating point P_2. Furthermore, the dynamics of the manipulated process inputs (33) are physically admissible in terms of amplitude and dynamics as seen in Figure 3.

Remark 8. The convergence speed goes faster when increasing the tuning parameters K_1 and K_2.
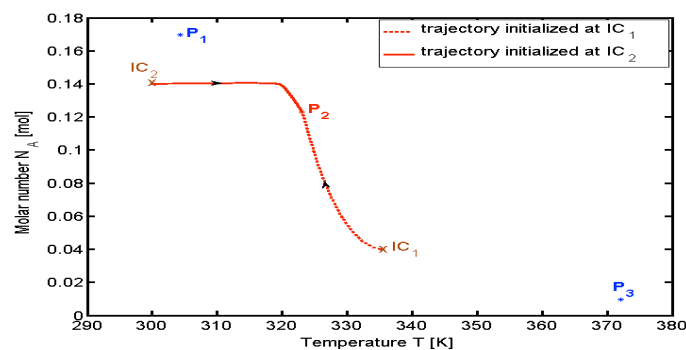

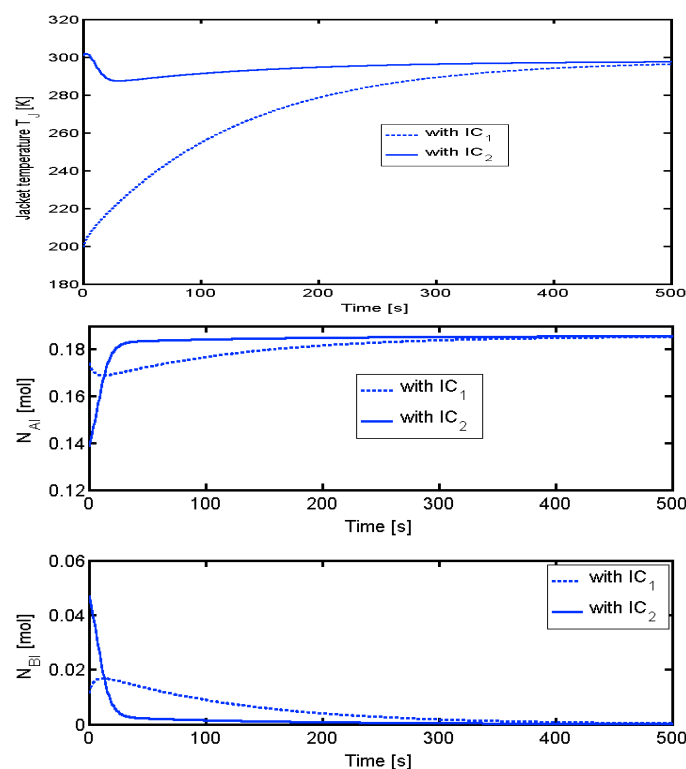Fig. 2. The representation of the close loop phase plane

Fig. 3. The dynamics of the manipulated process inputs

As previously shown, the storage function $\Psi(x)$ (2) plays the role of Lyapunov function. Furthermore, its dynamics converge to 0 with an exponentially decay (Figure 4).

5. CONCLUSION

In this work, we have shown that the dynamics of a homogeneous reaction network can be split into reaction
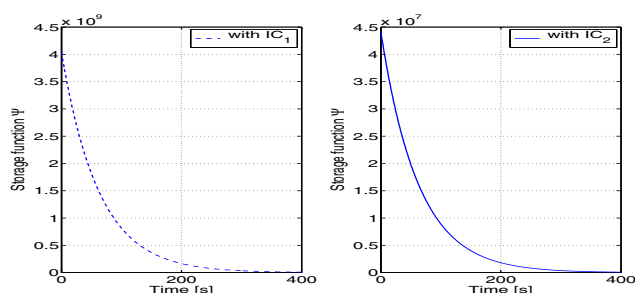
Fig. 4. The dynamics of $\Psi(x)$

variant and reaction invariant dynamics modes through a size-preserving transformation of the reaction matrix. This matrix is composed of stoichiometric coefficients. Since the reaction invariant dynamics which represent the (molar) mass conservations of each reaction in such a network are exponentially stable, the control design of the reaction system is then treated via reaction variant dynamics. In other words, when a subset of (generalized) inventories reaches its desired values, the dynamical convergence of the overall system to its set-point is guaranteed. Consequently, it allows to reduce considerably the dimension of the original system dynamics, in particular for chemical reactors involving a large number of chemical species and reactions. On the basis of the reduced dynamics, the (partial) inventory control is implemented to design the state feedback laws for an exponential stabilization of the reaction system. The simulation results showed that convergence objective is satisfied and that the state feedback laws are admissible. It remains now to evaluate performances and robustness of the proposed results in terms of perturbations and parameters uncertainty and extend to the infinite dimensional thermodynamic systems.

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